Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 01:55 PM EDT

PDB ID	:	1YAJ / pdb_00001yaj
Title	:	Crystal Structure of Human Liver Carboxylesterase in complex with benzil
Authors	:	Fleming, C.D.; Bencharit, S.; Edwards, C.C.; Hyatt, J.L.; Morton, C.M.; Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.
Deposited on	:	2004-12-17
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

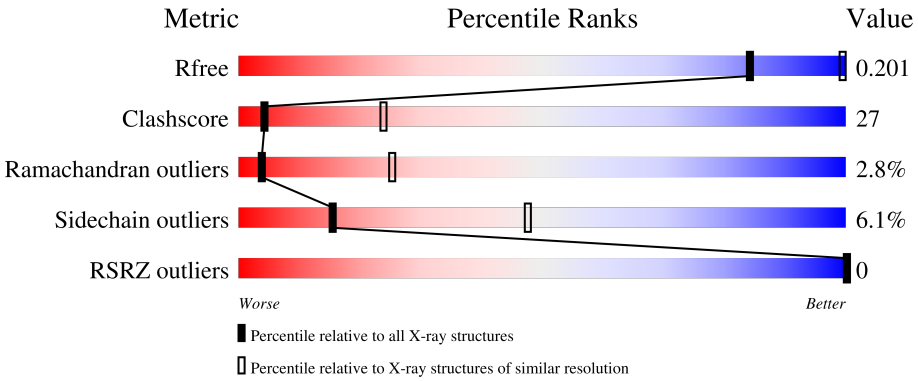
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	532	50% 45% 6%
1	B	532	54% 41% 5%
1	C	532	54% 41% 5%
1	D	532	49% 44% 6%
1	E	532	51% 45%

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Mol	Chain	Length	Quality of chain
1	F	532	53% 43%
1	G	532	52% 43% 5%
1	H	532	51% 43% 5%
1	I	532	46% 46% 7%
1	J	532	51% 44% 5%
1	K	532	51% 42% 7%
1	L	532	49% 43% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1279	X	-	-	-
2	NAG	F	2379	X	-	-	-
2	NAG	G	3179	X	-	-	-
2	NAG	J	4179	X	-	-	-
2	NAG	K	4279	X	-	-	-
3	SIA	A	1181	-	-	X	-
5	BEZ	A	11	-	X	-	-
5	BEZ	B	12	-	X	X	-
5	BEZ	D	2385	-	X	-	-
5	BEZ	G	3386	-	X	-	-
5	BEZ	H	3387	-	X	-	-

2 Entry composition (i)

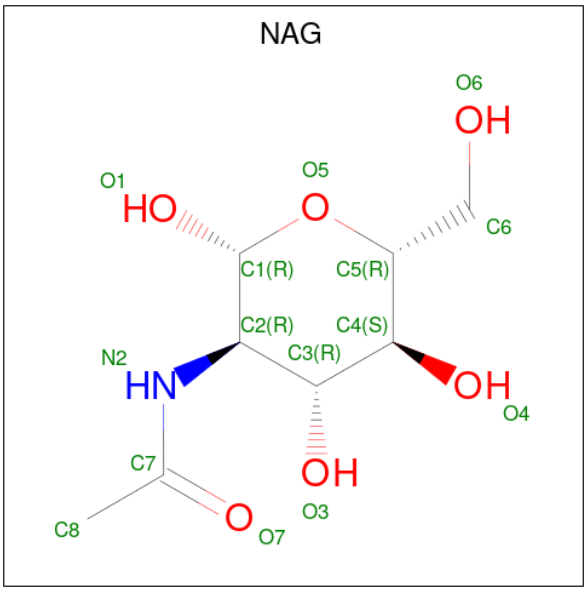
There are 6 unique types of molecules in this entry. The entry contains 50793 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CES1 protein.

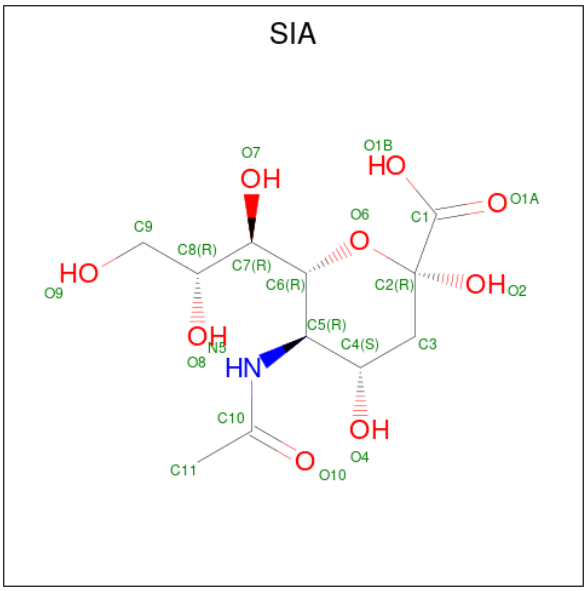
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	C	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	F	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	532	Total	C	N	O	S	0	0	0
			4129	2662	685	762	20			
1	I	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	J	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			
1	K	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	L	532	Total	C	N	O	S	0	0	0
			4131	2662	685	764	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



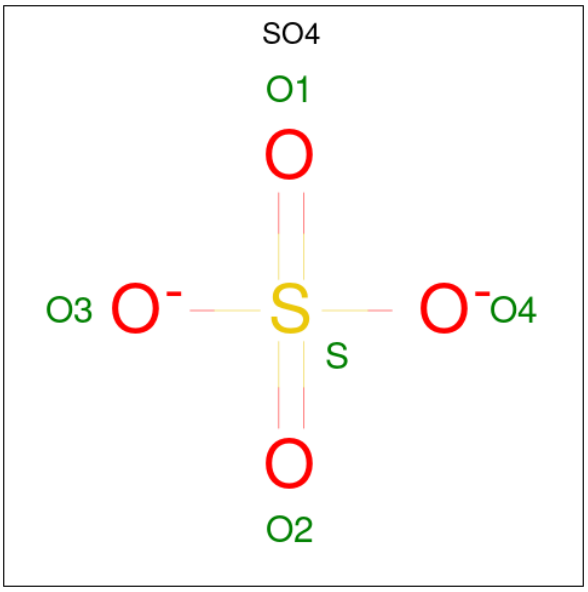
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	E	1	Total C N O 14 8 1 5	0	0
2	F	1	Total C N O 14 8 1 5	0	0
2	G	1	Total C N O 14 8 1 5	0	0
2	H	1	Total C N O 14 8 1 5	0	0
2	I	1	Total C N O 14 8 1 5	0	0
2	J	1	Total C N O 14 8 1 5	0	0
2	K	1	Total C N O 14 8 1 5	0	0
2	L	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 21 11 1 9	0	0
3	A	1	Total C N O 21 11 1 9	0	0
3	B	1	Total C N O 21 11 1 9	0	0
3	D	1	Total C N O 21 11 1 9	0	0
3	E	1	Total C N O 21 11 1 9	0	0
3	F	1	Total C N O 21 11 1 9	0	0
3	G	1	Total C N O 21 11 1 9	0	0
3	H	1	Total C N O 21 11 1 9	0	0
3	I	1	Total C N O 21 11 1 9	0	0
3	J	1	Total C N O 21 11 1 9	0	0
3	K	1	Total C N O 21 11 1 9	0	0
3	L	1	Total C N O 21 11 1 9	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0

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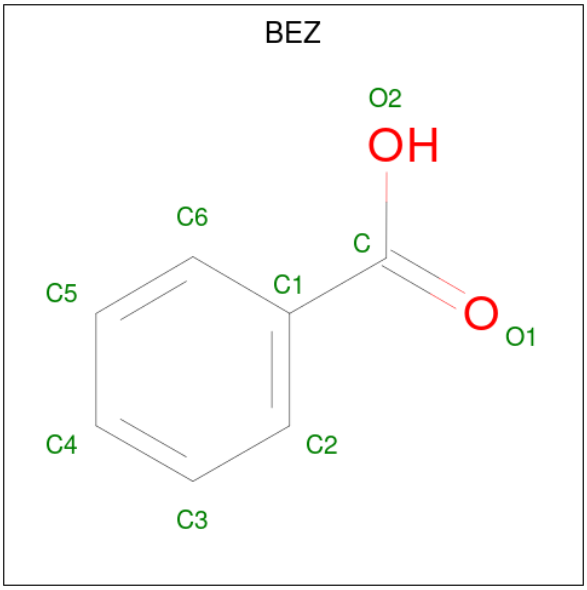
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

- Molecule 5 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	C	1	Total	C	O	0	0
			8	7	1		
5	C	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	F	1	Total	C	O	0	0
			8	7	1		
5	F	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	H	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	I	1	Total	C	O	0	0
			9	7	2		
5	J	1	Total	C	O	0	0
			8	7	1		
5	J	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		
5	K	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 9 7 2	0	0
5	L	1	Total C O 9 7 2	0	0

- Molecule 6 is water.

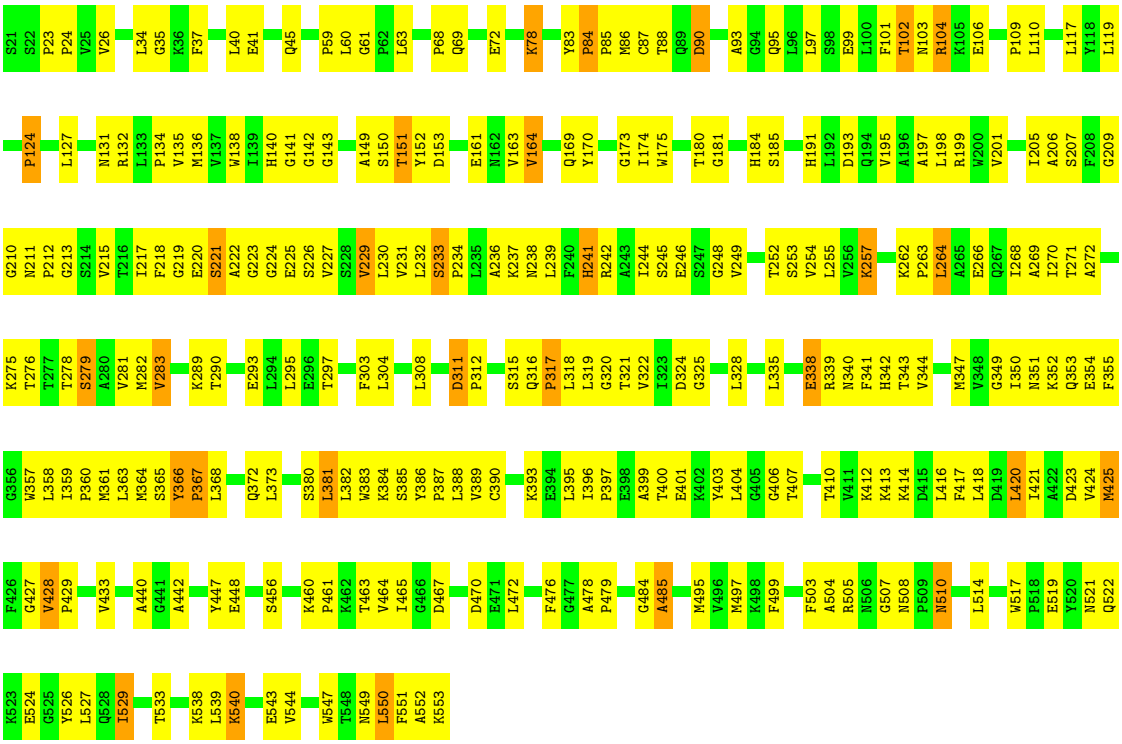
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	30	Total O 30 30	0	0
6	C	33	Total O 33 33	0	0
6	D	49	Total O 49 49	0	0
6	E	38	Total O 38 38	0	0
6	F	42	Total O 42 42	0	0
6	G	41	Total O 41 41	0	0
6	H	37	Total O 37 37	0	0
6	I	34	Total O 34 34	0	0
6	J	38	Total O 38 38	0	0
6	K	50	Total O 50 50	0	0
6	L	39	Total O 39 39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

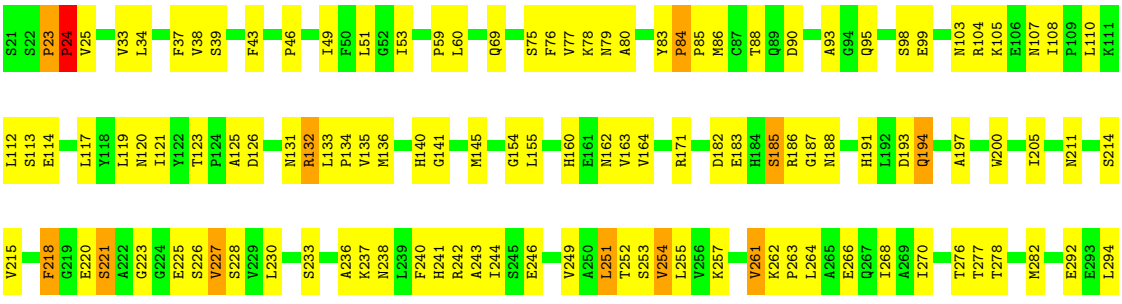
• Molecule 1: CES1 protein

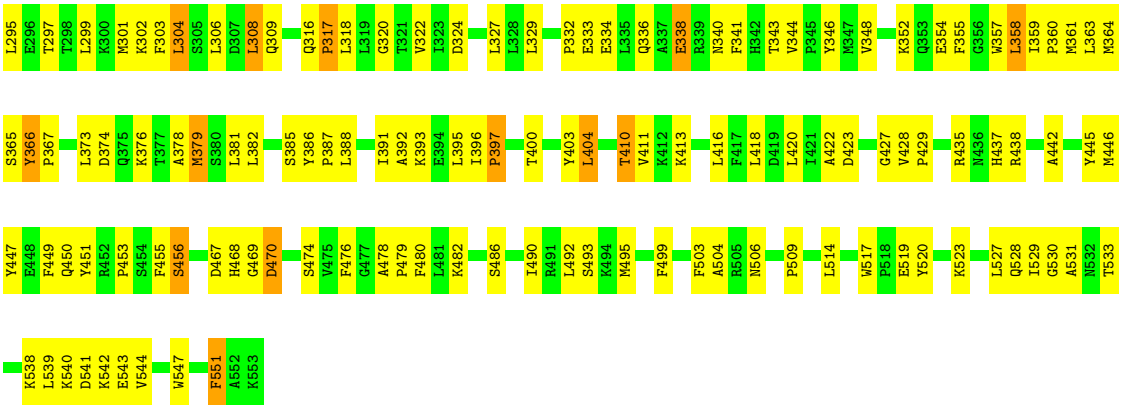
Chain A:



• Molecule 1: CES1 protein

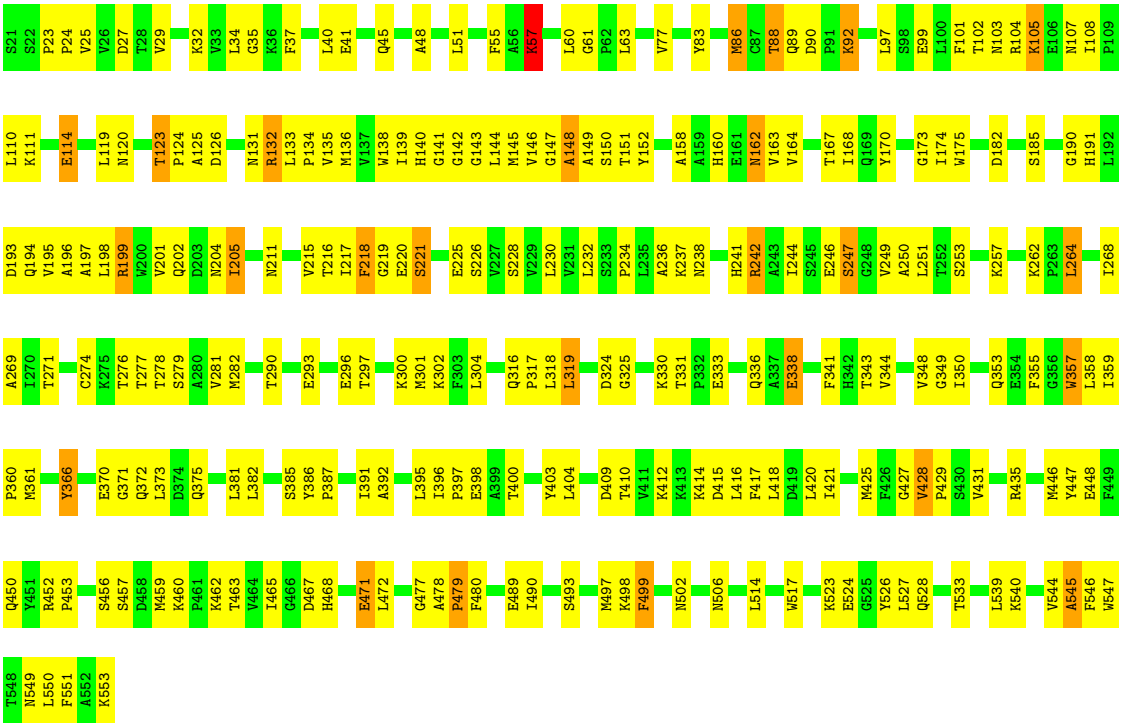
Chain B:





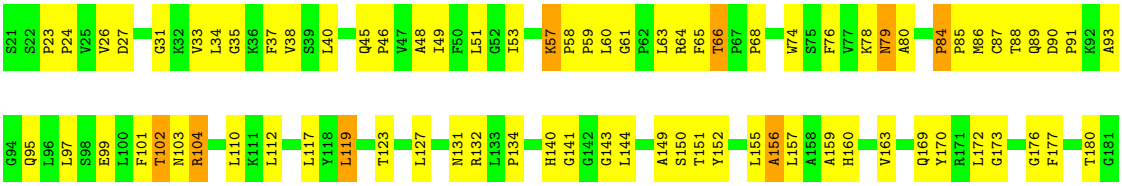
• Molecule 1: CES1 protein

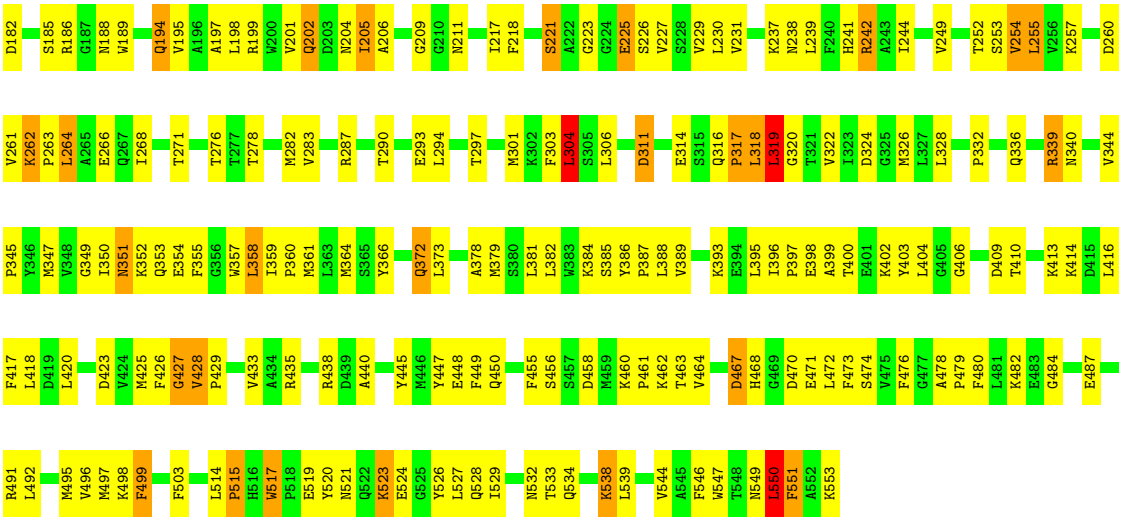
Chain C:



• Molecule 1: CES1 protein

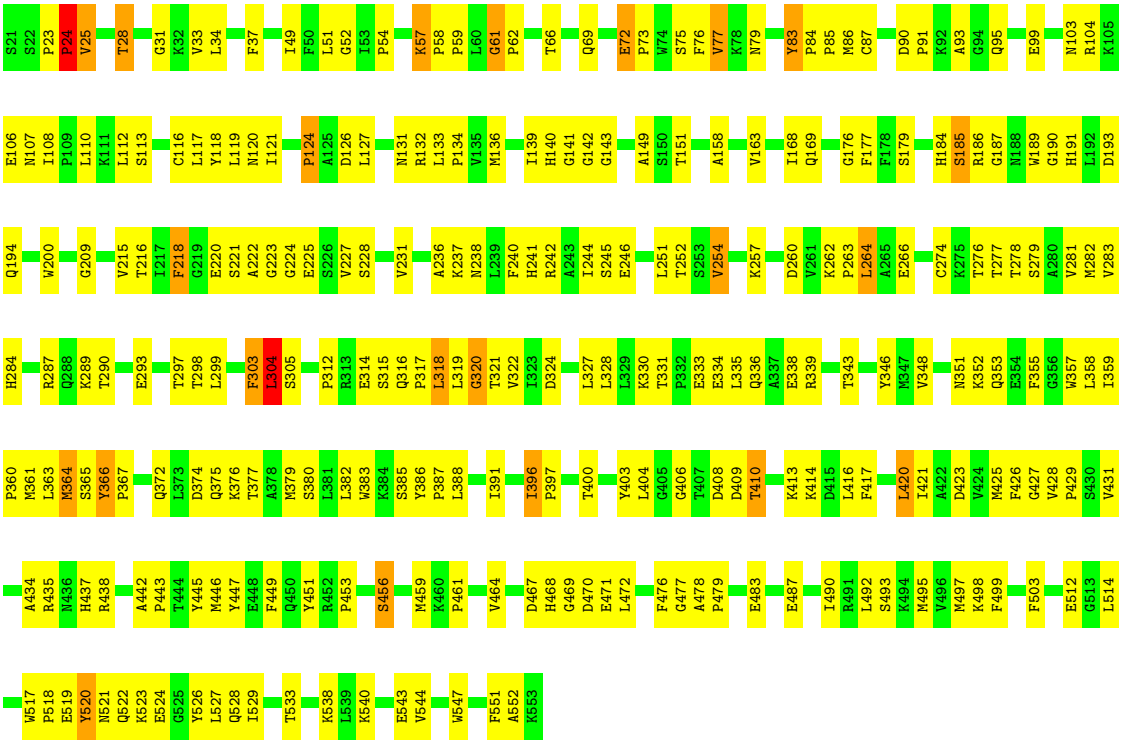
Chain D:





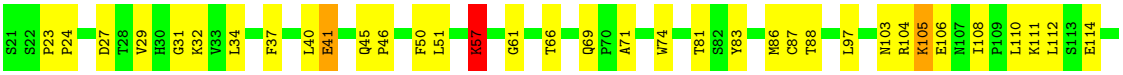
• Molecule 1: CES1 protein

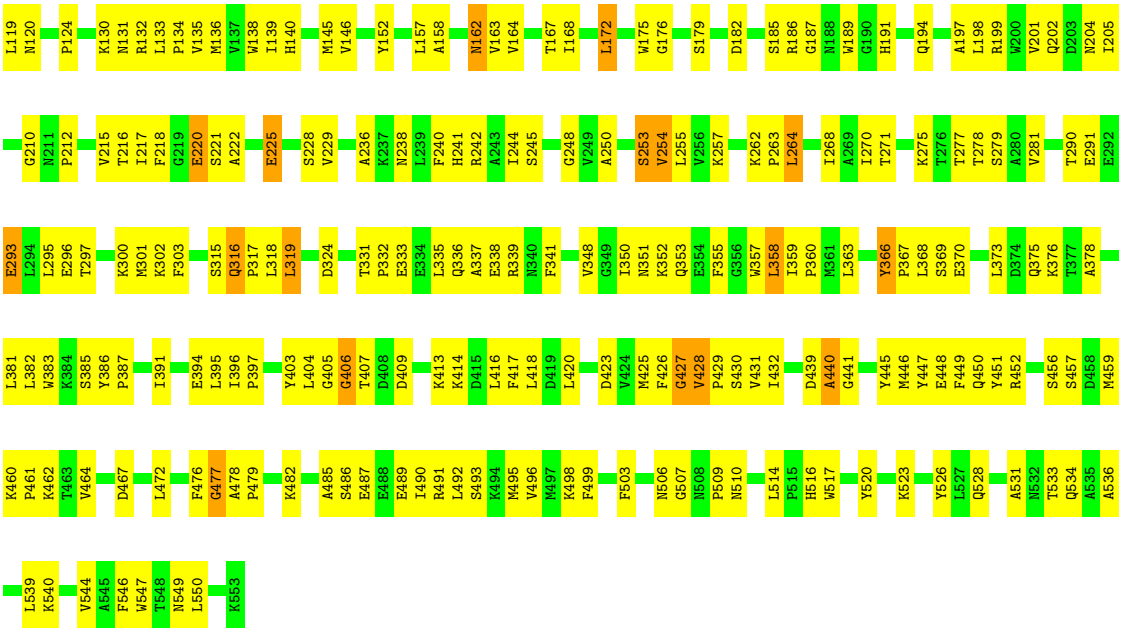
Chain E:



• Molecule 1: CES1 protein

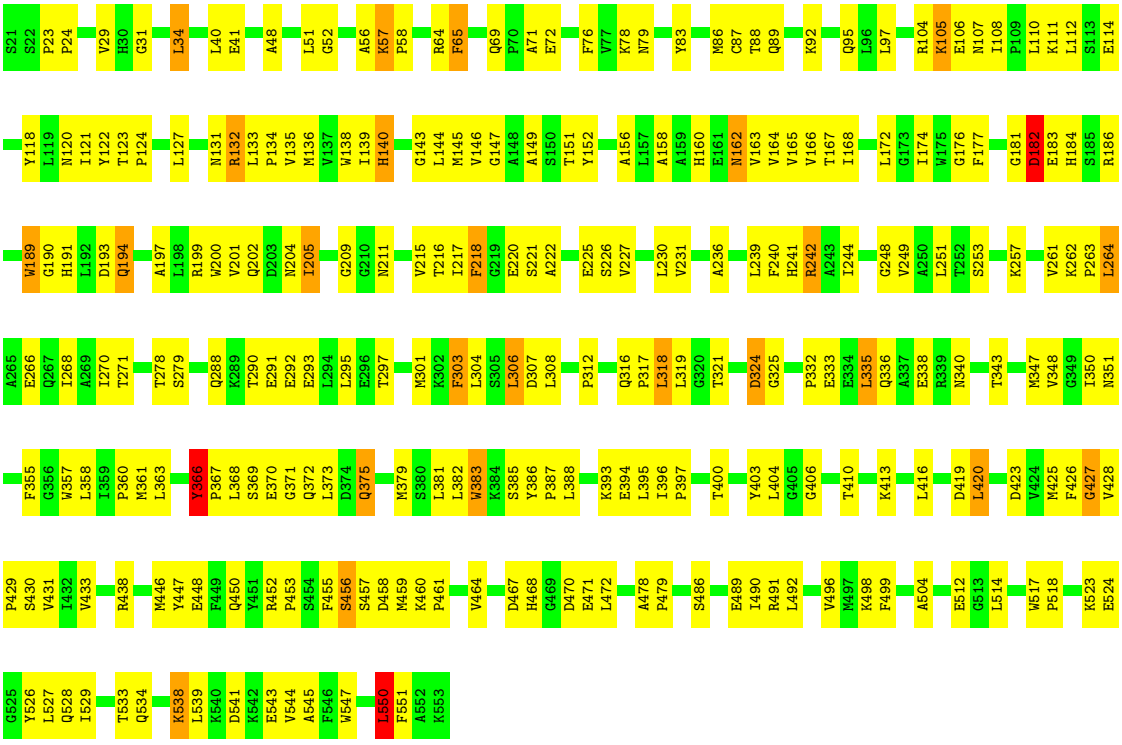
Chain F:





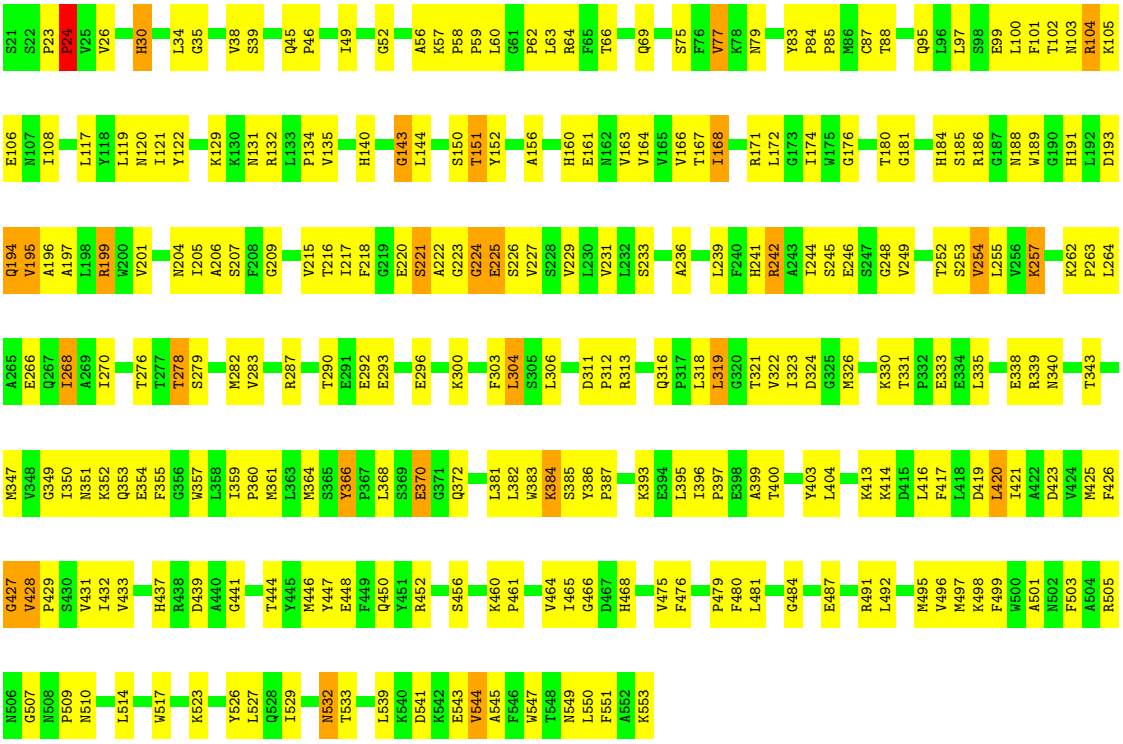
• Molecule 1: CES1 protein

Chain G:



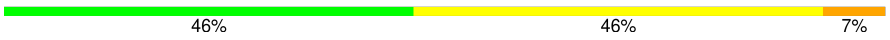
• Molecule 1: CES1 protein

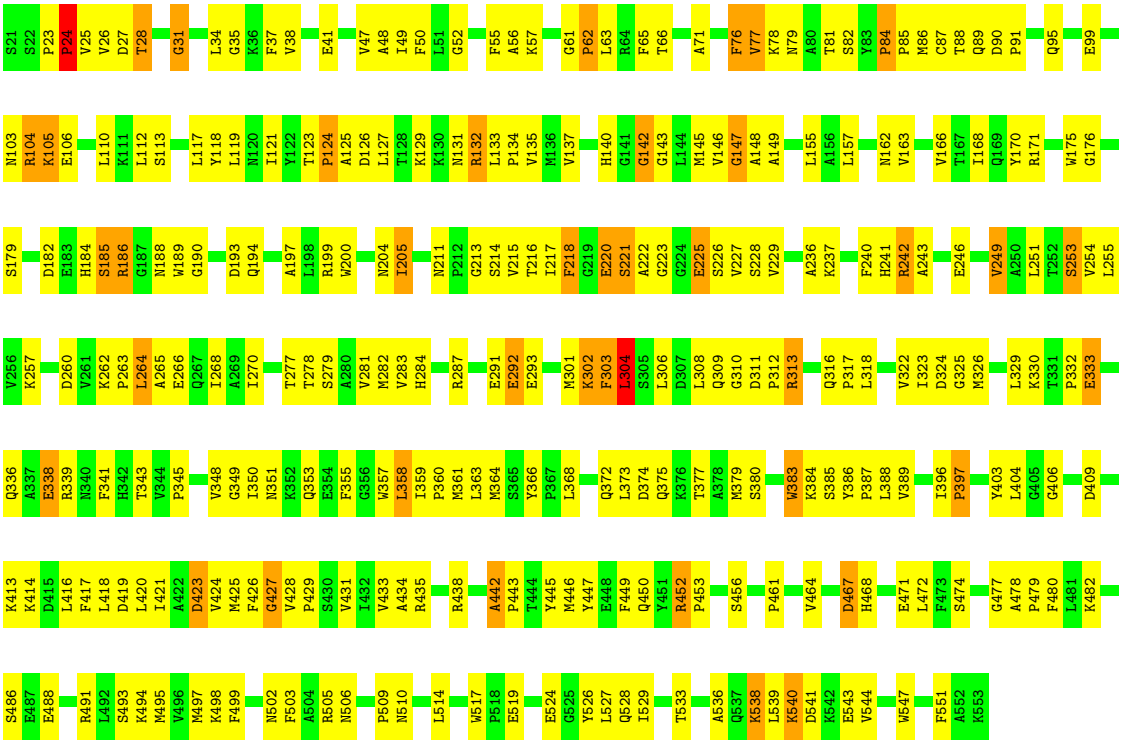
Chain H:



• Molecule 1: CES1 protein

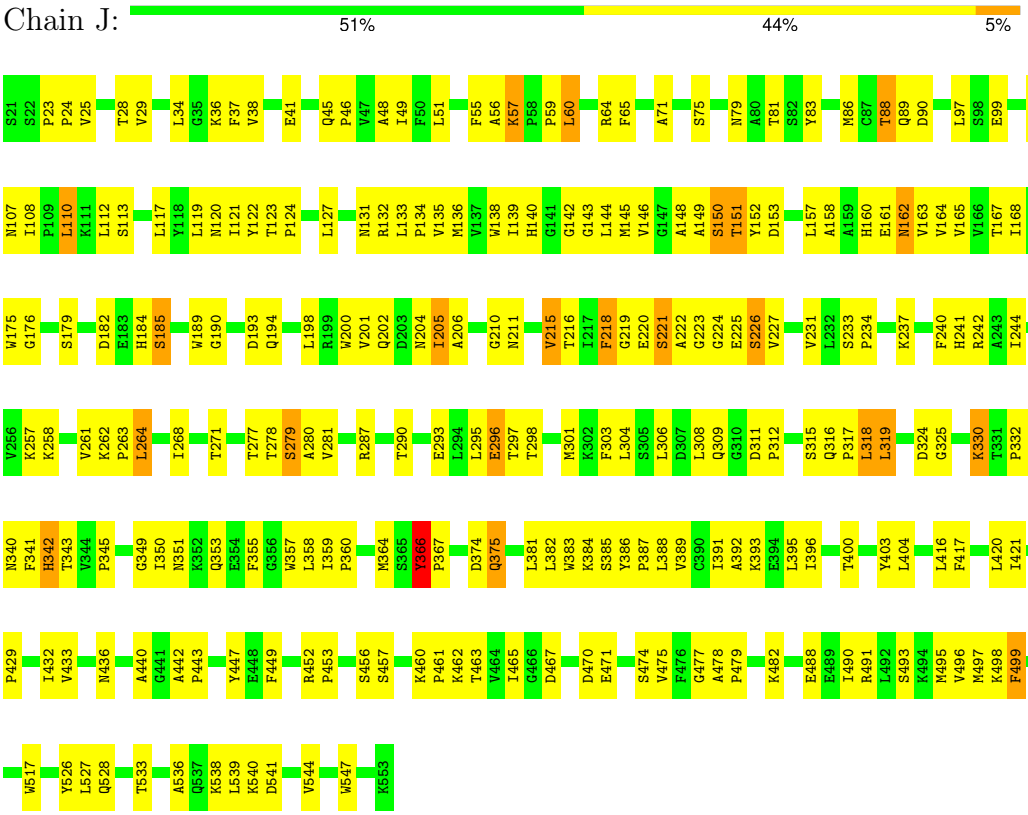
Chain I:





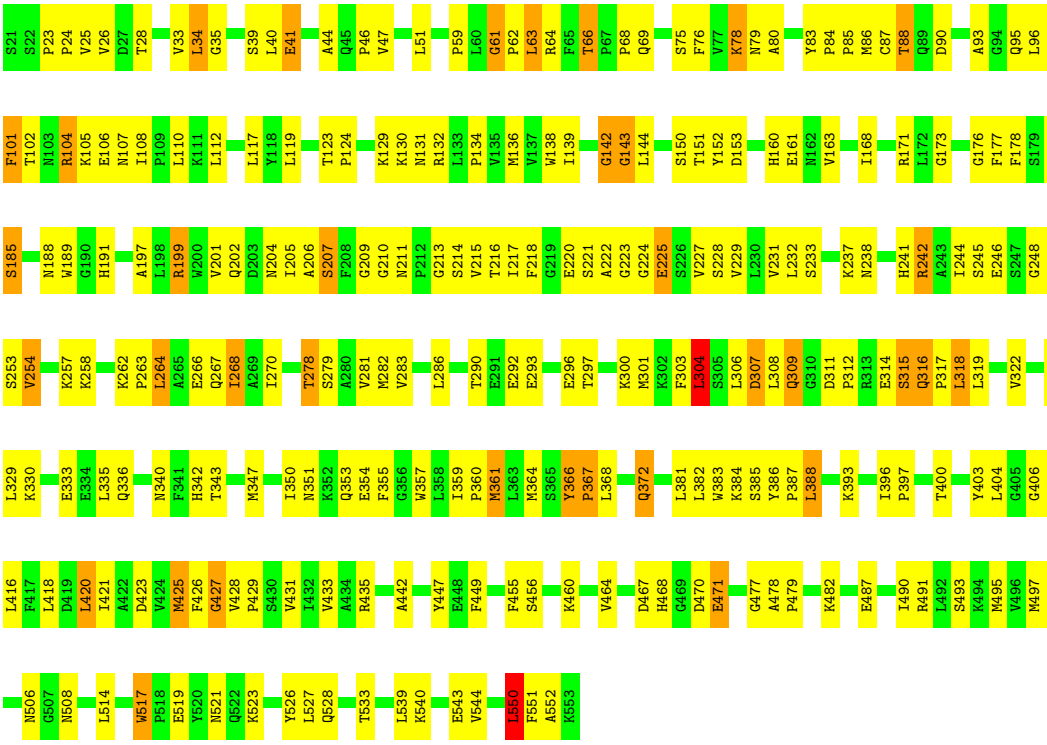
• Molecule 1: CES1 protein

Chain J:



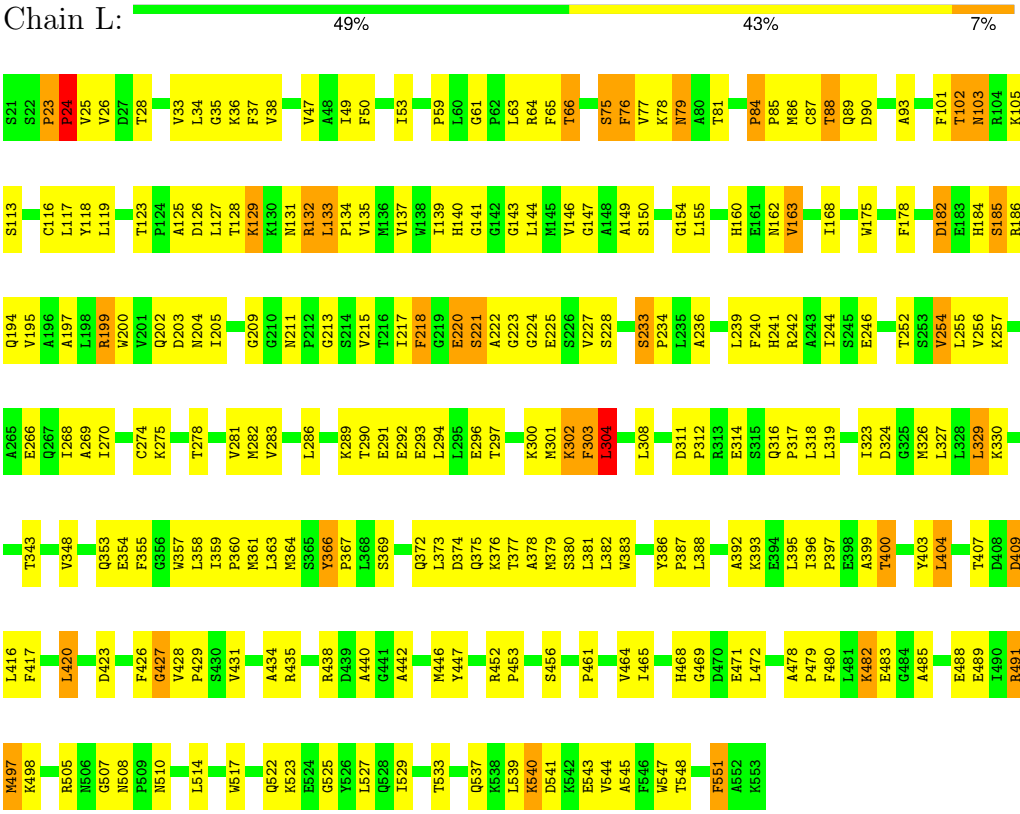
• Molecule 1: CES1 protein

Chain K:



• Molecule 1: CES1 protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.56Å 181.49Å 202.71Å 90.12° 89.93° 89.72°	Depositor
Resolution (Å)	54.56 – 3.20 54.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.56-3.20) 95.8 (54.56-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.287 0.198 , 0.201	Depositor DCC
R_{free} test set	6249 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-l 0.377 for -h,k,-l 0.389 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	50793	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BEZ, SO4, SIA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	3/4236 (0.1%)	1.09	21/5754 (0.4%)
1	B	0.76	2/4237 (0.0%)	1.02	19/5754 (0.3%)
1	C	0.75	3/4237 (0.1%)	1.01	13/5754 (0.2%)
1	D	0.73	1/4236 (0.0%)	1.04	19/5754 (0.3%)
1	E	0.86	6/4237 (0.1%)	1.09	27/5754 (0.5%)
1	F	0.78	5/4237 (0.1%)	1.01	10/5754 (0.2%)
1	G	0.99	12/4236 (0.3%)	1.15	20/5754 (0.3%)
1	H	0.80	4/4235 (0.1%)	1.06	24/5752 (0.4%)
1	I	0.97	15/4237 (0.4%)	1.10	33/5754 (0.6%)
1	J	0.76	3/4237 (0.1%)	0.99	11/5754 (0.2%)
1	K	0.76	3/4236 (0.1%)	1.04	25/5754 (0.4%)
1	L	0.74	4/4237 (0.1%)	1.02	13/5754 (0.2%)
All	All	0.81	61/50838 (0.1%)	1.05	235/69046 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	2
1	K	0	1
All	All	0	4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	550	LEU	CA-C	26.19	1.87	1.52
1	G	550	LEU	C-N	-25.11	1.00	1.33
1	E	24	PRO	CA-C	21.23	1.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	24	PRO	CA-C	20.29	1.77	1.52
1	B	24	PRO	CA-C	18.73	1.76	1.52
1	E	77	VAL	CA-CB	-17.40	1.32	1.53
1	A	550	LEU	CA-C	16.76	1.75	1.52
1	H	23	PRO	C-N	16.05	1.54	1.33
1	I	383	TRP	CD2-CE2	15.21	1.67	1.41
1	I	383	TRP	CE2-CZ2	13.71	1.68	1.39
1	I	383	TRP	CD2-CE3	12.91	1.60	1.40
1	I	383	TRP	NE1-CE2	12.88	1.51	1.37
1	A	550	LEU	C-O	-12.76	1.08	1.24
1	H	77	VAL	CB-CG1	12.57	1.94	1.52
1	K	550	LEU	C-N	12.47	1.51	1.33
1	E	23	PRO	C-N	12.13	1.49	1.33
1	G	57	LYS	CA-C	11.99	1.68	1.52
1	G	181	GLY	C-O	-11.97	1.06	1.24
1	I	383	TRP	CE3-CZ3	11.64	1.73	1.38
1	C	57	LYS	CA-C	11.35	1.68	1.52
1	J	57	LYS	CA-C	10.91	1.67	1.53
1	F	57	LYS	CA-C	10.60	1.66	1.53
1	E	77	VAL	CB-CG1	10.22	1.86	1.52
1	K	550	LEU	CA-C	10.19	1.66	1.53
1	F	57	LYS	CA-CB	9.88	1.69	1.52
1	L	23	PRO	C-N	9.82	1.46	1.33
1	F	57	LYS	CB-CG	9.72	1.81	1.52
1	G	58	PRO	CA-C	9.40	1.60	1.52
1	C	57	LYS	CA-CB	9.15	1.66	1.53
1	I	77	VAL	CA-CB	-9.04	1.43	1.54
1	I	383	TRP	CG-CD2	8.96	1.59	1.43
1	I	57	LYS	CA-C	8.91	1.62	1.53
1	J	57	LYS	CA-CB	8.90	1.66	1.53
1	G	57	LYS	C-O	8.33	1.34	1.24
1	A	181	GLY	C-O	-8.22	1.13	1.24
1	H	24	PRO	CA-C	8.11	1.62	1.52
1	B	77	VAL	CA-CB	-7.98	1.44	1.53
1	G	57	LYS	CA-CB	7.54	1.65	1.53
1	I	57	LYS	CB-CG	7.25	1.74	1.52
1	F	428	VAL	CA-CB	-7.22	1.50	1.54
1	D	550	LEU	CA-C	6.79	1.61	1.52
1	I	24	PRO	N-CD	6.50	1.56	1.47
1	E	77	VAL	CA-C	6.41	1.60	1.52
1	I	24	PRO	N-CA	6.34	1.54	1.46
1	G	182	ASP	N-CA	6.32	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	77	VAL	CA-C	6.29	1.60	1.52
1	G	189	TRP	CE2-CZ2	-6.20	1.26	1.39
1	L	24	PRO	N-CA	-6.09	1.39	1.47
1	E	396	ILE	CA-CB	6.01	1.57	1.54
1	G	550	LEU	N-CA	-5.60	1.39	1.46
1	J	57	LYS	CB-CG	5.54	1.69	1.52
1	C	57	LYS	C-O	5.53	1.31	1.23
1	I	383	TRP	CG-CD1	5.41	1.50	1.36
1	I	57	LYS	CA-CB	5.39	1.62	1.53
1	L	326	MET	SD-CE	5.38	1.93	1.79
1	F	57	LYS	C-O	5.31	1.30	1.23
1	K	181	GLY	C-O	-5.21	1.17	1.24
1	H	77	VAL	CA-CB	-5.20	1.48	1.54
1	G	189	TRP	CE3-CZ3	-5.12	1.23	1.38
1	L	77	VAL	CA-C	5.11	1.59	1.52
1	G	186	ARG	CA-CB	5.01	1.61	1.53

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	550	LEU	CA-C-O	-25.60	93.51	120.90
1	G	550	LEU	O-C-N	21.68	144.63	122.09
1	G	181	GLY	N-CA-C	-16.07	94.02	114.92
1	G	303	PHE	N-CA-C	15.51	128.19	111.28
1	E	303	PHE	N-CA-C	14.48	130.20	112.54
1	H	303	PHE	N-CA-C	13.80	129.22	112.38
1	L	303	PHE	N-CA-C	13.75	129.84	113.20
1	D	303	PHE	N-CA-C	13.44	128.77	112.38
1	K	303	PHE	N-CA-C	13.17	128.60	112.54
1	A	303	PHE	N-CA-C	13.08	128.50	112.54
1	A	550	LEU	O-C-N	12.88	136.88	122.20
1	I	303	PHE	N-CA-C	12.54	128.78	113.23
1	E	23	PRO	CA-C-N	-10.77	108.36	119.99
1	E	23	PRO	C-N-CA	-10.77	108.36	119.99
1	I	24	PRO	CB-CA-C	-10.13	96.14	110.63
1	I	383	TRP	CE2-CD2-CE3	-9.48	109.32	118.80
1	B	24	PRO	CB-CA-C	-9.31	97.73	110.85
1	E	24	PRO	CB-CA-C	-8.99	98.18	110.85
1	F	57	LYS	CB-CA-C	8.88	122.44	109.11
1	K	550	LEU	N-CA-C	-8.77	99.41	112.04
1	A	550	LEU	CA-C-O	-8.68	110.47	120.20
1	G	181	GLY	CA-C-O	-8.27	109.81	119.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	233	SER	CA-C-N	8.14	127.82	119.19
1	H	233	SER	C-N-CA	8.14	127.82	119.19
1	H	23	PRO	CA-C-N	-8.07	111.28	119.99
1	H	23	PRO	C-N-CA	-8.07	111.28	119.99
1	E	304	LEU	N-CA-C	-7.81	104.27	113.88
1	E	24	PRO	N-CA-C	-7.75	98.08	111.32
1	L	84	PRO	CA-C-N	7.68	127.61	119.85
1	L	84	PRO	C-N-CA	7.68	127.61	119.85
1	I	57	LYS	CB-CA-C	7.62	121.39	109.42
1	I	24	PRO	N-CA-C	-7.50	99.16	111.68
1	G	181	GLY	O-C-N	-7.47	113.71	122.60
1	K	490	ILE	N-CA-C	-7.36	105.48	111.81
1	H	77	VAL	N-CA-CB	-7.24	102.74	111.21
1	E	366	TYR	CA-C-N	7.19	127.51	119.32
1	E	366	TYR	C-N-CA	7.19	127.51	119.32
1	A	510	ASN	N-CA-C	7.18	119.84	110.43
1	C	57	LYS	N-CA-C	-7.18	99.62	110.39
1	B	24	PRO	N-CA-C	-7.17	99.06	111.32
1	I	23	PRO	O-C-N	7.17	129.92	121.46
1	I	24	PRO	CA-N-CD	-7.07	102.10	112.00
1	I	23	PRO	CA-C-N	-7.05	112.67	120.14
1	I	23	PRO	C-N-CA	-7.05	112.67	120.14
1	J	57	LYS	O-C-N	-7.02	114.15	121.60
1	A	366	TYR	CA-C-N	6.93	128.50	119.84
1	A	366	TYR	C-N-CA	6.93	128.50	119.84
1	D	550	LEU	CA-C-O	-6.92	113.50	120.90
1	E	61	GLY	CA-C-N	6.90	127.78	120.12
1	E	61	GLY	C-N-CA	6.90	127.78	120.12
1	J	160	HIS	N-CA-C	6.86	119.34	111.11
1	F	57	LYS	N-CA-C	-6.81	100.30	110.24
1	G	550	LEU	CA-C-N	-6.79	109.74	120.60
1	G	550	LEU	C-N-CA	-6.79	109.74	120.60
1	E	23	PRO	O-C-N	6.79	129.47	121.46
1	I	383	TRP	CB-CG-CD2	6.78	136.29	126.80
1	K	304	LEU	N-CA-C	-6.73	105.07	113.55
1	H	52	GLY	CA-C-N	-6.70	117.77	122.59
1	H	52	GLY	C-N-CA	-6.70	117.77	122.59
1	D	61	GLY	CA-C-N	6.68	126.36	119.82
1	D	61	GLY	C-N-CA	6.68	126.36	119.82
1	H	510	ASN	N-CA-C	6.67	119.17	110.43
1	B	84	PRO	CA-C-N	6.64	127.03	119.92
1	B	84	PRO	C-N-CA	6.64	127.03	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	57	LYS	CB-CA-C	6.62	121.76	109.51
1	H	428	VAL	CB-CA-C	-6.61	107.42	113.70
1	C	61	GLY	CA-C-N	6.60	126.23	119.56
1	C	61	GLY	C-N-CA	6.60	126.23	119.56
1	K	101	PHE	N-CA-C	6.60	118.48	111.28
1	J	366	TYR	CA-C-N	6.60	128.09	119.84
1	J	366	TYR	C-N-CA	6.60	128.09	119.84
1	K	508	ASN	CA-C-N	6.54	125.78	118.97
1	K	508	ASN	C-N-CA	6.54	125.78	118.97
1	D	550	LEU	N-CA-C	-6.53	103.28	111.11
1	H	224	GLY	N-CA-C	-6.48	106.31	114.16
1	K	181	GLY	N-CA-C	-6.47	106.75	115.36
1	A	181	GLY	N-CA-C	-6.43	106.37	115.43
1	E	83	TYR	CA-C-N	6.43	124.29	119.66
1	E	83	TYR	C-N-CA	6.43	124.29	119.66
1	A	72	GLU	CA-C-N	6.42	126.37	119.76
1	A	72	GLU	C-N-CA	6.42	126.37	119.76
1	A	233	SER	CA-C-N	6.41	125.84	118.85
1	A	233	SER	C-N-CA	6.41	125.84	118.85
1	L	221	SER	CB-CA-C	-6.40	109.21	116.63
1	E	75	SER	N-CA-C	6.39	119.55	111.69
1	E	396	ILE	CB-CA-C	-6.36	107.65	113.70
1	B	23	PRO	O-C-N	6.36	128.96	121.46
1	E	77	VAL	N-CA-CB	-6.36	103.66	111.67
1	G	57	LYS	O-C-N	-6.34	114.02	121.32
1	C	160	HIS	N-CA-C	6.33	118.18	111.28
1	I	77	VAL	N-CA-C	6.33	117.91	108.23
1	K	233	SER	CA-C-N	6.30	125.93	119.56
1	K	233	SER	C-N-CA	6.30	125.93	119.56
1	E	77	VAL	N-CA-C	6.29	116.69	107.37
1	F	57	LYS	CA-CB-CG	6.29	126.69	114.10
1	I	66	THR	CA-C-N	6.26	126.83	120.38
1	I	66	THR	C-N-CA	6.26	126.83	120.38
1	L	304	LEU	N-CA-C	-6.24	104.63	112.93
1	B	194	GLN	N-CA-C	-6.14	104.67	111.36
1	B	75	SER	CA-C-N	-6.12	116.58	123.13
1	B	75	SER	C-N-CA	-6.12	116.58	123.13
1	G	181	GLY	CA-C-N	-6.12	112.68	122.53
1	G	181	GLY	C-N-CA	-6.12	112.68	122.53
1	I	383	TRP	CA-CB-CG	-6.09	102.02	113.60
1	C	114	GLU	N-CA-C	-6.09	104.76	111.82
1	J	57	LYS	CA-C-N	6.07	126.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	57	LYS	C-N-CA	6.07	126.63	120.38
1	G	194	GLN	N-CA-C	-6.00	104.86	111.82
1	L	366	TYR	CA-C-N	6.00	126.16	119.32
1	L	366	TYR	C-N-CA	6.00	126.16	119.32
1	I	452	ARG	CA-C-N	5.99	125.96	120.03
1	I	452	ARG	C-N-CA	5.99	125.96	120.03
1	D	304	LEU	N-CA-C	-5.95	106.06	113.55
1	D	194	GLN	N-CA-C	-5.93	104.50	110.97
1	I	304	LEU	N-CA-C	-5.93	105.04	112.93
1	K	75	SER	N-CA-C	5.92	119.56	112.93
1	H	311	ASP	CA-C-N	5.90	126.04	119.32
1	H	311	ASP	C-N-CA	5.90	126.04	119.32
1	J	221	SER	CB-CA-C	-5.88	109.78	116.54
1	A	61	GLY	CA-C-N	5.84	125.55	119.82
1	A	61	GLY	C-N-CA	5.84	125.55	119.82
1	B	75	SER	N-CA-C	5.84	117.73	111.36
1	L	507	GLY	N-CA-C	-5.84	107.20	115.43
1	G	95	GLN	N-CA-C	-5.78	105.06	111.36
1	B	233	SER	CA-C-N	5.78	125.40	119.56
1	B	233	SER	C-N-CA	5.78	125.40	119.56
1	E	76	PHE	CA-C-O	5.77	121.97	118.33
1	B	221	SER	CB-CA-C	-5.77	109.94	116.63
1	C	366	TYR	CA-C-N	5.76	127.04	119.84
1	C	366	TYR	C-N-CA	5.76	127.04	119.84
1	D	57	LYS	CA-C-N	5.74	126.29	120.38
1	D	57	LYS	C-N-CA	5.74	126.29	120.38
1	L	197	ALA	N-CA-C	-5.74	104.94	111.14
1	F	81	THR	N-CA-C	5.73	118.21	110.88
1	B	23	PRO	CA-C-N	-5.69	113.85	119.99
1	B	23	PRO	C-N-CA	-5.69	113.85	119.99
1	H	160	HIS	N-CA-C	5.67	117.92	111.11
1	F	61	GLY	CA-C-N	5.66	125.28	119.56
1	F	61	GLY	C-N-CA	5.66	125.28	119.56
1	I	84	PRO	CA-C-N	5.66	125.97	119.92
1	I	84	PRO	C-N-CA	5.66	125.97	119.92
1	I	221	SER	CB-CA-C	-5.66	109.54	117.23
1	H	221	SER	CB-CA-C	-5.65	110.04	116.54
1	C	57	LYS	CB-CA-C	5.65	119.67	109.45
1	B	24	PRO	CA-N-CD	-5.60	104.16	112.00
1	D	84	PRO	CA-C-N	5.60	126.39	120.11
1	D	84	PRO	C-N-CA	5.60	126.39	120.11
1	E	335	LEU	N-CA-C	5.60	117.06	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	303	PHE	CB-CA-C	-5.58	99.51	110.11
1	K	268	ILE	CB-CA-C	-5.55	104.94	111.94
1	D	66	THR	CA-C-N	5.53	123.70	119.66
1	D	66	THR	C-N-CA	5.53	123.70	119.66
1	H	194	GLN	N-CA-C	-5.52	105.17	111.07
1	I	366	TYR	CA-C-N	5.49	125.58	119.32
1	I	366	TYR	C-N-CA	5.49	125.58	119.32
1	D	160	HIS	N-CA-C	5.49	117.70	111.11
1	F	366	TYR	CA-C-N	5.48	126.69	119.84
1	F	366	TYR	C-N-CA	5.48	126.69	119.84
1	K	124	PRO	N-CA-C	-5.46	108.42	114.92
1	E	49	ILE	N-CA-C	5.46	115.45	107.37
1	B	76	PHE	CA-C-O	5.45	121.77	118.33
1	G	366	TYR	CA-C-N	5.44	126.16	120.12
1	G	366	TYR	C-N-CA	5.44	126.16	120.12
1	I	155	LEU	N-CA-C	5.43	117.63	111.11
1	G	324	ASP	N-CA-C	5.42	116.87	111.07
1	A	428	VAL	CB-CA-C	-5.41	108.56	113.70
1	I	147	GLY	N-CA-C	5.40	117.53	112.08
1	A	358	LEU	N-CA-C	5.40	117.61	111.02
1	H	304	LEU	N-CA-C	-5.39	106.75	113.55
1	F	316	GLN	CA-C-N	5.37	124.70	118.85
1	F	316	GLN	C-N-CA	5.37	124.70	118.85
1	E	72	GLU	CA-C-N	5.36	125.26	119.85
1	E	72	GLU	C-N-CA	5.36	125.26	119.85
1	K	61	GLY	CA-C-N	5.36	125.07	119.82
1	K	61	GLY	C-N-CA	5.36	125.07	119.82
1	C	221	SER	CB-CA-C	-5.35	109.95	117.23
1	I	442	ALA	CA-C-N	5.35	125.36	119.90
1	I	442	ALA	C-N-CA	5.35	125.36	119.90
1	C	325	GLY	N-CA-C	-5.35	107.41	114.95
1	C	428	VAL	CA-C-N	5.34	124.80	119.24
1	C	428	VAL	C-N-CA	5.34	124.80	119.24
1	J	510	ASN	N-CA-C	5.32	117.15	110.24
1	K	327	LEU	N-CA-C	-5.31	105.57	111.36
1	I	57	LYS	CB-CG-CD	5.30	123.49	111.30
1	E	57	LYS	CA-C-N	5.29	125.83	120.38
1	E	57	LYS	C-N-CA	5.29	125.83	120.38
1	K	66	THR	CA-C-N	5.29	125.83	120.38
1	K	66	THR	C-N-CA	5.29	125.83	120.38
1	L	77	VAL	CA-CB-CG2	5.28	119.38	110.40
1	I	383	TRP	CB-CG-CD1	-5.28	118.98	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	552	ALA	N-CA-C	-5.27	107.03	112.93
1	A	233	SER	N-CA-C	5.27	116.71	110.07
1	A	283	VAL	CB-CA-C	-5.27	105.03	112.14
1	H	181	GLY	N-CA-C	-5.27	107.84	115.27
1	H	57	LYS	CA-C-N	5.26	125.80	120.38
1	H	57	LYS	C-N-CA	5.26	125.80	120.38
1	L	233	SER	N-CA-C	5.25	116.49	109.83
1	K	517	TRP	CA-C-N	5.24	125.14	119.85
1	K	517	TRP	C-N-CA	5.24	125.14	119.85
1	J	296	GLU	N-CA-C	-5.24	105.48	111.14
1	A	84	PRO	CA-C-N	5.23	125.52	119.92
1	A	84	PRO	C-N-CA	5.23	125.52	119.92
1	B	366	TYR	CA-C-N	5.22	126.36	119.84
1	B	366	TYR	C-N-CA	5.22	126.36	119.84
1	H	30	HIS	N-CA-C	5.21	119.49	113.18
1	K	268	ILE	N-CA-C	-5.21	106.06	111.58
1	L	78	LYS	N-CA-C	5.21	116.74	108.67
1	G	31	GLY	N-CA-C	5.20	117.63	110.56
1	G	160	HIS	N-CA-C	5.19	116.75	111.14
1	C	57	LYS	N-CA-CB	-5.18	102.63	109.78
1	I	249	VAL	N-CA-C	5.17	115.13	108.82
1	K	366	TYR	CA-C-N	5.17	126.30	119.84
1	K	366	TYR	C-N-CA	5.17	126.30	119.84
1	D	311	ASP	CA-C-N	5.14	124.59	119.24
1	D	311	ASP	C-N-CA	5.14	124.59	119.24
1	I	24	PRO	N-CA-CB	5.14	108.14	103.15
1	J	75	SER	N-CA-C	5.14	119.26	112.89
1	E	75	SER	CA-C-N	-5.13	117.64	123.13
1	E	75	SER	C-N-CA	-5.13	117.64	123.13
1	I	31	GLY	N-CA-C	5.12	117.06	110.96
1	H	75	SER	N-CA-C	5.12	119.58	113.23
1	H	268	ILE	CB-CA-C	-5.12	105.33	112.04
1	A	311	ASP	CA-C-N	5.10	125.14	119.32
1	A	311	ASP	C-N-CA	5.10	125.14	119.32
1	G	325	GLY	N-CA-C	-5.09	107.77	114.95
1	K	160	HIS	N-CA-C	5.09	117.22	111.11
1	D	428	VAL	CB-CA-C	-5.08	108.87	113.70
1	I	186	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
1	B	77	VAL	N-CA-CB	-5.04	105.63	111.83
1	H	523	LYS	N-CA-C	-5.02	107.10	113.18
1	G	304	LEU	N-CA-C	-5.02	107.19	113.72
1	K	181	GLY	O-C-N	-5.01	116.02	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	24	PRO	O-C-N	-5.01	116.82	123.13
1	D	517	TRP	CA-C-N	5.00	124.98	120.03
1	D	517	TRP	C-N-CA	5.00	124.98	120.03

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	550	LEU	Mainchain
1	G	550	LEU	Mainchain
1	G	57	LYS	Mainchain
1	K	550	LEU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4131	240	0
1	B	4131	0	4130	193	0
1	C	4131	0	4130	213	0
1	D	4130	0	4130	221	0
1	E	4131	0	4131	215	0
1	F	4131	0	4130	198	0
1	G	4130	0	4129	198	0
1	H	4129	0	4131	216	0
1	I	4131	0	4131	240	0
1	J	4131	0	4129	227	0
1	K	4130	0	4130	234	0
1	L	4131	0	4131	245	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	3	0
2	G	14	0	13	1	0
2	H	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	14	0	13	0	0
2	J	14	0	13	1	0
2	K	14	0	13	2	0
2	L	14	0	13	0	0
3	A	42	0	36	13	0
3	B	21	0	18	5	0
3	D	21	0	18	8	0
3	E	21	0	18	2	0
3	F	21	0	18	1	0
3	G	21	0	18	6	0
3	H	21	0	18	1	0
3	I	21	0	18	6	0
3	J	21	0	18	5	0
3	K	21	0	18	7	0
3	L	21	0	18	7	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
4	I	10	0	0	1	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
5	A	18	0	10	2	0
5	B	18	0	11	6	0
5	C	17	0	10	4	0
5	D	18	0	11	3	0
5	E	18	0	10	0	0
5	F	17	0	10	0	0
5	G	18	0	10	1	0
5	H	18	0	10	1	0
5	I	18	0	10	1	0
5	J	17	0	10	0	0
5	K	18	0	10	0	0
5	L	18	0	10	1	0
6	A	43	0	0	11	0
6	B	30	0	0	5	0
6	C	33	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	49	0	0	9	0
6	E	38	0	0	16	0
6	F	42	0	0	4	0
6	G	41	0	0	8	0
6	H	37	0	0	8	0
6	I	34	0	0	10	0
6	J	38	0	0	9	0
6	K	50	0	0	11	0
6	L	39	0	0	12	0
All	All	50793	0	50057	2672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (2672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:12:BEZ:C2	5:B:12:BEZ:C3	1.76	1.62
1:B:24:PRO:C	1:B:24:PRO:CA	1.76	1.59
5:B:12:BEZ:C2	5:B:12:BEZ:C1	1.78	1.59
5:B:12:BEZ:C5	5:B:12:BEZ:C6	1.74	1.58
1:I:24:PRO:CA	1:I:24:PRO:C	1.77	1.57
5:B:12:BEZ:C1	5:B:12:BEZ:C6	1.78	1.57
1:E:24:PRO:C	1:E:24:PRO:CA	1.79	1.54
1:F:57:LYS:CB	1:F:57:LYS:CG	1.81	1.54
1:A:550:LEU:CA	1:A:550:LEU:C	1.75	1.53
5:B:12:BEZ:C3	5:B:12:BEZ:C4	1.85	1.53
5:D:2385:BEZ:C3	5:D:2385:BEZ:C4	1.82	1.53
5:D:2385:BEZ:C4	5:D:2385:BEZ:C5	1.81	1.51
5:B:12:BEZ:C5	5:B:12:BEZ:C4	1.84	1.51
1:E:77:VAL:CG1	1:E:77:VAL:CB	1.86	1.50
1:G:550:LEU:CA	1:G:550:LEU:C	1.87	1.47
1:H:77:VAL:CG1	1:H:77:VAL:CB	1.94	1.44
1:B:495:MET:HE1	1:B:533:THR:HG21	1.33	1.11
1:A:372:GLN:HB2	1:A:410:THR:HB	1.35	1.08
1:L:343:THR:HB	1:L:442:ALA:HB2	1.34	1.07
1:C:86:MET:HE3	1:C:110:LEU:HD13	1.37	1.03
1:L:379:MET:HE1	1:L:397:PRO:HG3	1.39	1.03
1:E:379:MET:HE1	1:E:397:PRO:HG3	1.36	1.02
1:H:199:ARG:HB3	1:H:199:ARG:HH11	1.27	1.00
1:H:319:LEU:HD23	1:H:319:LEU:H	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:THR:OG1	1:G:293:GLU:HG3	1.62	0.99
3:A:1181:SIA:HN5	3:A:1181:SIA:H92	1.27	0.97
1:I:134:PRO:HG2	1:I:163:VAL:HG12	1.46	0.97
1:L:25:VAL:HG22	1:L:34:LEU:HD23	1.44	0.96
1:G:303:PHE:O	1:G:317:PRO:O	1.84	0.94
1:C:421:ILE:HG22	1:C:425:MET:HE2	1.51	0.93
1:D:103:ASN:ND2	1:D:476:PHE:HB3	1.85	0.92
1:I:242:ARG:HG2	1:I:242:ARG:HH11	1.34	0.91
1:L:125:ALA:HB2	1:L:133:LEU:HD11	1.53	0.91
1:D:350:ILE:C	1:D:351:ASN:HD22	1.79	0.91
1:I:472:LEU:HD12	6:I:6117:HOH:O	1.71	0.91
1:F:215:VAL:H	1:F:241:HIS:HD2	1.16	0.90
1:G:86:MET:HE2	1:G:110:LEU:HD12	1.53	0.90
3:L:1282:SIA:H92	3:L:1282:SIA:H112	1.51	0.90
1:H:216:THR:HG23	1:H:242:ARG:HB2	1.52	0.89
3:L:1282:SIA:H7	6:L:6029:HOH:O	1.72	0.89
1:D:316:GLN:NE2	1:D:317:PRO:HD2	1.86	0.89
1:E:77:VAL:CG1	1:E:77:VAL:CA	2.51	0.89
1:D:241:HIS:O	1:D:242:ARG:HG3	1.72	0.88
1:J:124:PRO:HD3	1:J:158:ALA:HB1	1.53	0.88
1:J:134:PRO:HG2	1:J:163:VAL:HG12	1.54	0.88
1:G:404:LEU:HD23	1:G:413:LYS:HB3	1.56	0.88
1:K:68:PRO:HA	6:K:6330:HOH:O	1.73	0.88
1:C:319:LEU:HD23	1:C:319:LEU:H	1.39	0.87
1:K:343:THR:HA	6:K:6389:HOH:O	1.73	0.87
1:C:202:GLN:HE22	1:C:215:VAL:HG21	1.37	0.87
1:D:359:ILE:HB	1:D:360:PRO:HD3	1.57	0.87
1:I:24:PRO:C	1:I:24:PRO:CB	2.46	0.87
3:J:1082:SIA:H112	1:K:278:THR:HA	1.55	0.87
1:E:24:PRO:C	1:E:24:PRO:CB	2.48	0.86
1:B:24:PRO:C	1:B:24:PRO:CB	2.47	0.86
1:A:136:MET:HE3	1:A:504:ALA:HB2	1.57	0.86
1:D:276:THR:HB	1:D:282:MET:HE2	1.58	0.85
1:A:266:GLU:HG2	1:A:282:MET:HE1	1.55	0.85
1:G:105:LYS:HE2	1:G:106:GLU:HG2	1.59	0.85
3:A:1181:SIA:H92	3:A:1181:SIA:N5	1.91	0.85
1:E:355:PHE:CE1	1:E:360:PRO:HG3	2.11	0.84
1:I:105:LYS:HG3	1:I:106:GLU:H	1.42	0.84
1:C:268:ILE:HG12	1:C:301:MET:HE2	1.59	0.84
1:I:257:LYS:HG3	1:I:316:GLN:HE22	1.43	0.84
1:J:268:ILE:HG12	1:J:301:MET:HE2	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:HE3	1:B:504:ALA:HB2	1.58	0.83
1:A:276:THR:HG22	1:A:282:MET:HE2	1.60	0.83
1:I:303:PHE:O	1:I:317:PRO:O	1.96	0.83
1:J:317:PRO:HB3	1:J:387:PRO:HB2	1.60	0.83
1:K:25:VAL:HG22	1:K:34:LEU:CD2	2.07	0.83
1:J:139:ILE:HG12	1:J:168:ILE:HD11	1.61	0.83
1:E:327:LEU:HD23	1:E:328:LEU:HG	1.61	0.83
1:G:550:LEU:CA	1:G:551:PHE:N	2.41	0.82
1:F:357:TRP:O	1:F:360:PRO:HD2	1.79	0.82
1:C:216:THR:HG23	1:C:242:ARG:HB2	1.62	0.82
1:D:435:ARG:HB3	1:D:438:ARG:NH2	1.95	0.82
1:E:372:GLN:HB2	1:E:410:THR:HB	1.60	0.82
1:C:242:ARG:HG2	1:C:242:ARG:HH11	1.41	0.82
1:E:359:ILE:HB	1:E:360:PRO:HD3	1.62	0.81
3:A:1180:SIA:H112	1:B:278:THR:HG22	1.61	0.81
1:B:134:PRO:HG2	1:B:163:VAL:HG12	1.63	0.81
1:C:414:LYS:NZ	5:C:5014:BEZ:O2	2.12	0.81
1:D:244:ILE:HG12	1:D:347:MET:HB3	1.61	0.81
1:K:199:ARG:HB3	1:K:199:ARG:HH11	1.44	0.81
1:L:199:ARG:HB3	1:L:199:ARG:HH11	1.45	0.81
1:J:290:THR:OG1	1:J:293:GLU:HG3	1.80	0.81
1:L:382:LEU:HD23	1:L:396:ILE:HG23	1.63	0.81
1:J:357:TRP:O	1:J:360:PRO:HD2	1.79	0.80
1:F:131:ASN:O	1:F:132:ARG:HD2	1.81	0.80
1:K:431:VAL:HG21	1:K:540:LYS:HB2	1.63	0.80
1:H:495:MET:HE1	1:H:533:THR:OG1	1.81	0.80
1:E:134:PRO:HG2	1:E:163:VAL:HG12	1.64	0.79
1:D:262:LYS:NZ	2:F:2379:NAG:H82	1.97	0.79
1:A:220:GLU:HG3	1:A:472:LEU:HD21	1.64	0.79
1:C:357:TRP:O	1:C:360:PRO:HD2	1.81	0.79
1:E:141:GLY:CA	6:E:6472:HOH:O	2.30	0.79
1:J:86:MET:HE2	1:J:110:LEU:HB2	1.62	0.79
1:A:499:PHE:CE2	1:A:514:LEU:HD22	2.18	0.79
1:E:251:LEU:HD11	1:E:336:GLN:HE22	1.48	0.79
1:C:271:THR:HG22	1:C:297:THR:HG23	1.66	0.78
1:H:335:LEU:O	1:H:338:GLU:HB3	1.83	0.78
1:K:318:LEU:H	1:K:318:LEU:HD22	1.47	0.78
1:H:359:ILE:HB	1:H:360:PRO:HD3	1.65	0.78
1:I:86:MET:HE2	1:I:110:LEU:HB2	1.66	0.78
1:L:105:LYS:HG3	6:L:6432:HOH:O	1.82	0.78
1:B:25:VAL:HG22	1:B:34:LEU:HD23	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:GLU:HG3	1:F:291:GLU:HG3	1.65	0.78
1:A:410:THR:HA	1:A:413:LYS:HD2	1.63	0.78
1:F:134:PRO:HG2	1:F:163:VAL:HG12	1.65	0.78
1:F:456:SER:HB3	1:F:460:LYS:HE2	1.66	0.78
1:H:119:LEU:HB3	1:H:168:ILE:HG22	1.66	0.78
1:C:277:THR:HG22	1:C:278:THR:HG23	1.66	0.77
1:E:24:PRO:HG3	1:E:37:PHE:CE1	2.20	0.77
1:H:164:VAL:HG11	1:H:205:ILE:HD11	1.66	0.77
1:G:357:TRP:O	1:G:360:PRO:HD2	1.83	0.77
1:J:400:THR:HG23	1:J:404:LEU:HD12	1.66	0.77
1:A:223:GLY:O	1:A:227:VAL:HG23	1.84	0.77
1:G:517:TRP:CE3	1:G:527:LEU:HD23	2.20	0.77
1:D:403:TYR:O	1:D:416:LEU:HD13	1.83	0.76
1:F:528:GLN:HE21	1:F:536:ALA:HB2	1.48	0.76
1:L:87:CYS:HB3	6:L:6115:HOH:O	1.83	0.76
1:G:550:LEU:CA	1:G:550:LEU:O	2.32	0.76
1:L:200:TRP:O	1:L:204:ASN:HB2	1.85	0.76
1:L:303:PHE:O	1:L:317:PRO:O	2.02	0.76
1:D:86:MET:HE3	1:D:110:LEU:HB2	1.68	0.76
1:H:255:LEU:HA	1:H:318:LEU:HD11	1.68	0.76
1:H:304:LEU:HD12	1:H:364:MET:HE2	1.68	0.76
1:L:495:MET:HE1	1:L:533:THR:HG21	1.68	0.76
1:F:225:GLU:O	1:F:229:VAL:HG23	1.86	0.76
1:K:107:ASN:HD22	1:K:108:ILE:H	1.34	0.76
1:C:191:HIS:HA	1:C:194:GLN:OE1	1.85	0.76
1:F:105:LYS:HE2	1:F:106:GLU:HG2	1.66	0.76
1:A:241:HIS:O	1:A:242:ARG:HG3	1.85	0.76
3:D:2180:SIA:O10	3:D:2180:SIA:H92	1.85	0.76
1:F:253:SER:HA	6:F:6118:HOH:O	1.84	0.76
1:K:79:ASN:O	3:K:1182:SIA:H32	1.86	0.76
1:D:227:VAL:O	1:D:231:VAL:HG23	1.86	0.75
1:C:493:SER:O	1:C:497:MET:HG3	1.85	0.75
1:D:271:THR:HG22	1:D:297:THR:HG23	1.69	0.75
1:J:97:LEU:HD22	1:J:146:VAL:HG23	1.68	0.75
1:K:257:LYS:HE2	1:K:257:LYS:HA	1.66	0.75
1:D:266:GLU:HG2	1:D:282:MET:HE1	1.69	0.75
1:A:103:ASN:ND2	1:A:476:PHE:HB3	2.02	0.75
1:C:355:PHE:CE1	1:C:360:PRO:HG3	2.22	0.75
1:K:105:LYS:HG3	1:K:106:GLU:H	1.52	0.75
1:D:95:GLN:O	1:D:99:GLU:HG3	1.86	0.74
1:A:215:VAL:H	1:A:241:HIS:CD2	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:GLU:O	1:G:270:ILE:HG13	1.87	0.74
1:J:120:ASN:HB2	1:J:167:THR:OG1	1.87	0.74
1:I:236:ALA:HB1	1:I:240:PHE:HE1	1.51	0.74
1:I:242:ARG:HG2	1:I:242:ARG:NH1	2.02	0.74
1:J:353:GLN:NE2	1:J:465:ILE:H	1.86	0.74
1:B:527:LEU:HD11	1:B:533:THR:HG22	1.67	0.74
1:D:495:MET:HE1	1:D:533:THR:HB	1.70	0.74
1:E:141:GLY:HA3	6:E:6472:HOH:O	1.86	0.74
1:G:456:SER:HB3	1:G:460:LYS:HE2	1.69	0.74
1:K:139:ILE:HG12	1:K:168:ILE:HD11	1.69	0.74
1:G:164:VAL:HG11	1:G:205:ILE:HD11	1.68	0.73
1:H:241:HIS:O	1:H:242:ARG:HG3	1.87	0.73
1:B:317:PRO:HD2	6:B:6020:HOH:O	1.86	0.73
1:L:498:LYS:HD2	1:L:514:LEU:HD21	1.70	0.73
1:A:59:PRO:HD3	1:A:117:LEU:HD12	1.69	0.73
1:B:529:ILE:HA	1:B:533:THR:HG23	1.69	0.73
1:L:453:PRO:HG2	1:L:456:SER:OG	1.88	0.73
1:B:359:ILE:HB	1:B:360:PRO:HD3	1.70	0.73
1:G:242:ARG:HG2	1:G:242:ARG:HH11	1.52	0.73
1:A:161:GLU:HG3	1:A:497:MET:O	1.89	0.73
1:A:359:ILE:HB	1:A:360:PRO:HD3	1.69	0.73
1:H:262:LYS:HE3	1:H:279:SER:OG	1.89	0.73
1:I:322:VAL:HG12	1:I:323:ILE:N	2.03	0.72
1:K:83:TYR:CD1	1:K:150:SER:HB3	2.24	0.72
1:L:236:ALA:HA	1:L:239:LEU:HD12	1.71	0.72
1:D:529:ILE:HA	1:D:533:THR:HG23	1.71	0.72
1:F:135:VAL:HG21	1:F:205:ILE:HG12	1.71	0.72
1:L:242:ARG:HG2	1:L:242:ARG:HH11	1.51	0.72
1:L:348:VAL:O	1:L:446:MET:HA	1.89	0.72
1:L:88:THR:HG21	1:L:291:GLU:HG3	1.70	0.72
1:B:392:ALA:HB3	1:B:395:LEU:HG	1.69	0.72
1:K:428:VAL:HG13	1:K:544:VAL:HG22	1.71	0.72
1:L:89:GLN:HB2	1:L:146:VAL:HG12	1.70	0.72
1:L:128:THR:OG1	1:L:129:LYS:HE3	1.90	0.72
1:C:234:PRO:HA	1:C:341:PHE:HZ	1.55	0.72
1:H:168:ILE:HG21	1:H:197:ALA:HB1	1.70	0.72
1:C:403:TYR:O	1:C:416:LEU:HD13	1.90	0.72
1:L:367:PRO:HG2	1:L:381:LEU:HD21	1.72	0.72
1:A:90:ASP:HB3	1:A:93:ALA:HB3	1.71	0.72
1:C:86:MET:HE3	1:C:110:LEU:CD1	2.17	0.71
1:F:86:MET:HG3	1:F:112:LEU:HD23	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:VAL:HG13	1:H:205:ILE:HB	1.71	0.71
1:L:24:PRO:HG3	1:L:37:PHE:CZ	2.25	0.71
1:K:241:HIS:O	1:K:242:ARG:HG3	1.89	0.71
1:F:526:TYR:CD2	1:F:539:LEU:HB2	2.26	0.71
1:G:403:TYR:O	1:G:416:LEU:HD13	1.90	0.71
1:F:23:PRO:HB2	1:F:34:LEU:HD21	1.70	0.71
1:K:185:SER:HB2	1:K:283:VAL:HG21	1.72	0.71
1:E:24:PRO:HG3	1:E:37:PHE:CZ	2.26	0.71
1:K:495:MET:HE1	1:K:533:THR:HG21	1.72	0.71
1:L:403:TYR:CD1	1:L:420:LEU:HD23	2.26	0.71
1:A:26:VAL:CG1	1:A:207:SER:HB3	2.21	0.71
1:C:199:ARG:HB3	1:C:199:ARG:HH11	1.55	0.71
1:D:495:MET:HE1	1:D:533:THR:CB	2.21	0.71
1:A:550:LEU:CA	1:A:551:PHE:N	2.54	0.71
1:B:403:TYR:O	1:B:416:LEU:HD13	1.91	0.71
1:G:268:ILE:HG12	1:G:301:MET:HE2	1.73	0.71
1:J:463:THR:HG23	6:J:6348:HOH:O	1.90	0.71
1:K:85:PRO:HD3	3:K:1182:SIA:H91	1.72	0.71
1:B:24:PRO:C	1:B:24:PRO:N	2.49	0.70
1:D:34:LEU:HB3	1:D:79:ASN:HB3	1.72	0.70
1:D:229:VAL:HG13	1:D:328:LEU:HD11	1.73	0.70
1:I:359:ILE:HB	1:I:360:PRO:HD3	1.73	0.70
1:E:103:ASN:ND2	1:E:476:PHE:HB3	2.06	0.70
1:E:236:ALA:HB1	1:E:240:PHE:HE1	1.56	0.70
1:B:317:PRO:HG2	1:B:318:LEU:H	1.57	0.70
1:E:86:MET:HE2	1:E:110:LEU:HB2	1.72	0.70
1:C:242:ARG:HG2	1:C:242:ARG:NH1	2.05	0.70
1:F:86:MET:HE3	1:F:110:LEU:HB2	1.73	0.70
1:I:368:LEU:HD21	1:I:373:LEU:HD22	1.73	0.70
1:A:373:LEU:O	1:A:413:LYS:HD3	1.92	0.70
1:E:24:PRO:C	1:E:24:PRO:N	2.49	0.70
1:K:252:THR:HG22	1:K:254:VAL:HG12	1.72	0.70
1:E:103:ASN:HD22	1:E:476:PHE:HB3	1.55	0.70
1:F:105:LYS:HG3	1:F:106:GLU:H	1.56	0.70
1:K:229:VAL:HG13	1:K:328:LEU:HD11	1.74	0.70
1:A:341:PHE:HB2	6:A:6326:HOH:O	1.90	0.70
1:L:359:ILE:HB	1:L:360:PRO:HD3	1.71	0.70
1:E:77:VAL:CG1	1:E:77:VAL:C	2.65	0.69
1:K:131:ASN:C	1:K:132:ARG:HD2	2.16	0.69
1:D:290:THR:OG1	1:D:293:GLU:HG3	1.92	0.69
1:G:220:GLU:HG3	1:G:472:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:VAL:HG22	1:G:446:MET:HE1	1.73	0.69
1:L:396:ILE:HB	1:L:397:PRO:HD3	1.73	0.69
1:B:24:PRO:HG3	1:B:37:PHE:CZ	2.27	0.69
1:L:372:GLN:HE21	1:L:411:VAL:HG13	1.56	0.69
3:L:1282:SIA:H92	3:L:1282:SIA:C11	2.22	0.69
1:A:339:ARG:HG2	1:A:440:ALA:HA	1.75	0.69
3:A:1181:SIA:HN5	3:A:1181:SIA:C9	2.04	0.69
1:D:59:PRO:HD3	1:D:117:LEU:HD12	1.74	0.69
1:G:134:PRO:HG2	1:G:163:VAL:HG12	1.75	0.69
1:G:215:VAL:H	1:G:241:HIS:HD2	1.41	0.69
1:K:311:ASP:HB3	1:K:314:GLU:HG3	1.73	0.69
1:L:218:PHE:CB	1:L:244:ILE:HB	2.23	0.69
1:C:120:ASN:HB2	1:C:167:THR:OG1	1.92	0.69
1:I:25:VAL:HG22	1:I:34:LEU:CD2	2.23	0.69
1:H:60:LEU:HA	6:H:6248:HOH:O	1.92	0.68
1:H:428:VAL:HB	1:H:429:PRO:HD3	1.73	0.68
1:J:403:TYR:O	1:J:416:LEU:HD13	1.92	0.68
1:A:262:LYS:HB3	1:A:263:PRO:HD3	1.74	0.68
1:A:350:ILE:C	1:A:351:ASN:HD22	2.02	0.68
1:H:217:ILE:HG13	1:H:227:VAL:HG13	1.75	0.68
1:I:278:THR:OG1	1:I:281:VAL:HG23	1.93	0.68
1:K:330:LYS:HG3	1:K:335:LEU:HG	1.73	0.68
1:L:498:LYS:HD3	6:L:6137:HOH:O	1.92	0.68
1:A:226:SER:HA	1:A:229:VAL:HG23	1.76	0.68
1:B:236:ALA:HB1	1:B:240:PHE:HE1	1.57	0.68
1:B:382:LEU:HD23	1:B:396:ILE:HG23	1.75	0.68
3:D:2180:SIA:H92	3:D:2180:SIA:C10	2.24	0.68
3:D:2180:SIA:C11	1:E:278:THR:HG22	2.24	0.68
3:G:782:SIA:H112	1:H:278:THR:HA	1.75	0.68
1:C:343:THR:HA	6:C:6124:HOH:O	1.92	0.68
1:H:77:VAL:CG1	1:H:77:VAL:CA	2.70	0.68
1:I:277:THR:HG22	1:I:278:THR:HG23	1.75	0.68
1:J:277:THR:HG22	1:J:278:THR:HG23	1.76	0.68
1:K:262:LYS:HB3	1:K:263:PRO:HD3	1.75	0.68
1:D:357:TRP:CH2	1:D:361:MET:HE2	2.29	0.68
1:L:372:GLN:NE2	1:L:411:VAL:HG13	2.09	0.68
1:B:403:TYR:CD1	1:B:420:LEU:HD23	2.29	0.68
1:C:526:TYR:CD2	1:C:539:LEU:HB2	2.28	0.68
1:J:495:MET:HE1	1:J:533:THR:OG1	1.94	0.68
1:L:423:ASP:O	1:L:428:VAL:HG23	1.94	0.68
1:C:86:MET:HE2	1:C:148:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:THR:HG21	1:L:113:SER:HB2	1.76	0.68
1:K:85:PRO:HD3	3:K:1182:SIA:C9	2.24	0.68
1:I:24:PRO:C	1:I:24:PRO:N	2.52	0.67
1:I:322:VAL:HG12	1:I:323:ILE:H	1.58	0.67
1:L:495:MET:CE	1:L:533:THR:HG21	2.23	0.67
1:A:140:HIS:HD2	1:A:141:GLY:O	1.77	0.67
3:J:1082:SIA:H4	1:K:262:LYS:NZ	2.10	0.67
1:B:141:GLY:HA2	1:B:223:GLY:H	1.59	0.67
1:C:290:THR:OG1	1:C:293:GLU:HG3	1.94	0.67
1:F:439:ASP:C	1:F:441:GLY:H	2.01	0.67
1:G:114:GLU:HG3	1:G:291:GLU:HG3	1.76	0.67
1:L:392:ALA:HB3	1:L:395:LEU:HG	1.75	0.67
1:B:223:GLY:O	1:B:227:VAL:HG23	1.93	0.67
1:I:306:LEU:HD11	1:I:387:PRO:HG2	1.77	0.67
1:K:88:THR:HA	1:K:112:LEU:HD22	1.77	0.67
1:C:357:TRP:C	1:C:360:PRO:HD2	2.20	0.67
1:K:90:ASP:HB3	1:K:93:ALA:HB3	1.75	0.67
1:K:423:ASP:OD2	1:K:543:GLU:HG2	1.95	0.67
1:L:36:LYS:HB3	6:L:6146:HOH:O	1.94	0.67
1:D:51:LEU:O	1:D:80:ALA:HB1	1.95	0.67
1:D:396:ILE:HB	1:D:397:PRO:HD3	1.75	0.67
1:D:425:MET:HB2	1:D:426:PHE:CE1	2.30	0.67
1:E:117:LEU:HD21	1:E:193:ASP:OD2	1.94	0.67
1:E:403:TYR:O	1:E:416:LEU:HD13	1.95	0.67
1:H:151:THR:HG22	1:H:152:TYR:CD1	2.30	0.67
1:I:118:TYR:CE2	3:I:982:SIA:H92	2.29	0.67
1:I:403:TYR:O	1:I:416:LEU:HD13	1.95	0.67
1:K:372:GLN:HB2	1:K:410:THR:HB	1.77	0.67
1:B:78:LYS:HG3	3:B:1280:SIA:O1B	1.93	0.67
3:B:1280:SIA:H113	1:C:262:LYS:NZ	2.10	0.67
1:D:34:LEU:HD13	1:D:35:GLY:N	2.10	0.67
1:E:423:ASP:O	1:E:428:VAL:HG23	1.95	0.67
1:E:526:TYR:CE1	1:E:528:GLN:HG2	2.30	0.67
1:A:99:GLU:O	1:A:102:THR:HG22	1.94	0.67
1:B:276:THR:HB	1:B:282:MET:HE2	1.75	0.67
1:C:385:SER:C	1:C:387:PRO:HD2	2.19	0.67
1:H:83:TYR:CD1	1:H:150:SER:HB3	2.30	0.67
1:L:529:ILE:HA	1:L:533:THR:HG23	1.76	0.67
1:D:474:SER:HB3	1:D:496:VAL:HG21	1.76	0.66
1:H:349:GLY:HA3	1:H:447:TYR:CE1	2.30	0.66
1:K:232:LEU:HD21	1:K:336:GLN:HE21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:VAL:HG21	1:D:49:ILE:HD12	1.76	0.66
1:E:257:LYS:HE2	1:E:264:LEU:HD12	1.75	0.66
1:A:403:TYR:O	1:A:416:LEU:HD13	1.95	0.66
1:A:529:ILE:HD12	1:A:529:ILE:N	2.10	0.66
1:C:60:LEU:CD2	1:C:114:GLU:HB3	2.26	0.66
1:E:251:LEU:HD21	1:E:333:GLU:HG3	1.76	0.66
1:G:452:ARG:HG2	1:G:452:ARG:HH11	1.61	0.66
1:I:216:THR:HG23	1:I:242:ARG:HB2	1.77	0.66
1:A:349:GLY:HA3	1:A:447:TYR:CD1	2.30	0.66
1:G:97:LEU:HD22	1:G:146:VAL:HG23	1.76	0.66
1:G:140:HIS:HE1	6:G:6042:HOH:O	1.77	0.66
1:G:357:TRP:C	1:G:360:PRO:HD2	2.21	0.66
1:H:353:GLN:NE2	1:H:465:ILE:H	1.94	0.66
1:K:215:VAL:H	1:K:241:HIS:HD2	1.43	0.66
1:L:106:GLU:HG2	6:L:6432:HOH:O	1.96	0.66
1:F:403:TYR:O	1:F:416:LEU:HD13	1.96	0.66
1:J:133:LEU:HD22	1:J:162:ASN:O	1.94	0.66
1:J:382:LEU:HD11	1:J:391:ILE:HD12	1.77	0.66
1:L:257:LYS:HE2	1:L:316:GLN:OE1	1.95	0.66
1:A:420:LEU:HD13	1:A:420:LEU:C	2.20	0.66
1:F:131:ASN:C	1:F:132:ARG:HD2	2.21	0.66
1:H:199:ARG:HH11	1:H:199:ARG:CB	2.07	0.66
1:J:339:ARG:HG3	1:J:440:ALA:HA	1.77	0.66
1:F:120:ASN:HB2	1:F:167:THR:OG1	1.95	0.66
1:J:428:VAL:HB	1:J:429:PRO:HD3	1.76	0.66
1:I:266:GLU:O	1:I:270:ILE:HG13	1.96	0.66
1:J:131:ASN:O	1:J:132:ARG:HD2	1.95	0.66
1:J:237:LYS:HE3	1:J:342:HIS:HB3	1.79	0.66
1:K:467:ASP:HB3	1:K:470:ASP:OD2	1.96	0.66
1:C:215:VAL:H	1:C:241:HIS:HD2	1.43	0.65
1:G:268:ILE:HG12	1:G:301:MET:CE	2.26	0.65
1:B:355:PHE:CE1	1:B:360:PRO:HG3	2.31	0.65
1:D:264:LEU:HD22	1:D:268:ILE:HD11	1.78	0.65
1:L:379:MET:CE	1:L:397:PRO:HG3	2.23	0.65
1:B:495:MET:CE	1:B:533:THR:HG21	2.20	0.65
1:D:467:ASP:CG	1:D:468:HIS:H	2.05	0.65
1:G:48:ALA:HB3	1:G:123:THR:HG23	1.78	0.65
1:G:355:PHE:CE1	1:G:360:PRO:HG3	2.31	0.65
1:I:498:LYS:HB3	1:I:514:LEU:HD11	1.77	0.65
1:B:495:MET:HE1	1:B:533:THR:CG2	2.20	0.65
1:E:95:GLN:O	1:E:99:GLU:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:HIS:HA	1:G:194:GLN:OE1	1.97	0.65
1:K:304:LEU:O	1:K:364:MET:HE2	1.96	0.65
1:K:498:LYS:HB3	1:K:514:LEU:HD11	1.79	0.65
1:G:350:ILE:C	1:G:351:ASN:HD22	2.03	0.65
1:H:428:VAL:O	1:H:432:ILE:HG13	1.97	0.65
1:G:249:VAL:HG21	1:G:433:VAL:HG21	1.79	0.65
1:J:176:GLY:HA2	1:J:189:TRP:HB2	1.78	0.65
1:K:34:LEU:HD13	1:K:35:GLY:N	2.12	0.65
1:C:131:ASN:O	1:C:132:ARG:HD2	1.97	0.65
1:G:139:ILE:HG12	1:G:168:ILE:HD11	1.77	0.65
1:I:87:CYS:O	1:I:89:GLN:HG2	1.97	0.65
1:C:88:THR:HB	1:C:175:TRP:CZ3	2.32	0.65
1:A:529:ILE:HA	1:A:533:THR:HG23	1.78	0.64
1:A:271:THR:HG22	1:A:297:THR:HG23	1.79	0.64
1:A:550:LEU:C	1:A:550:LEU:CB	2.70	0.64
1:D:140:HIS:HD2	1:D:141:GLY:O	1.80	0.64
1:G:428:VAL:HB	1:G:429:PRO:HD3	1.79	0.64
1:F:164:VAL:HG11	1:F:205:ILE:HD11	1.79	0.64
1:G:492:LEU:O	1:G:496:VAL:HG23	1.96	0.64
1:H:201:VAL:O	1:H:205:ILE:HG22	1.96	0.64
1:J:429:PRO:O	1:J:433:VAL:HG23	1.98	0.64
1:K:227:VAL:O	1:K:231:VAL:HG23	1.97	0.64
1:B:404:LEU:HD23	1:B:404:LEU:N	2.13	0.64
1:H:64:ARG:O	1:H:66:THR:HG23	1.98	0.64
1:H:417:PHE:O	1:H:420:LEU:HB3	1.97	0.64
1:A:264:LEU:HD22	1:A:268:ILE:HD11	1.79	0.64
1:I:379:MET:HA	1:I:396:ILE:HG21	1.78	0.64
1:D:102:THR:OG1	1:D:104:ARG:HG3	1.98	0.64
1:F:331:THR:HB	1:F:333:GLU:OE1	1.98	0.64
3:F:682:SIA:H91	3:F:682:SIA:H113	1.80	0.64
1:A:349:GLY:HA3	1:A:447:TYR:CE1	2.31	0.64
1:D:97:LEU:HD13	5:D:2385:BEZ:H4	1.79	0.64
1:J:140:HIS:HE1	6:J:6125:HOH:O	1.79	0.64
1:A:88:THR:HG22	1:A:295:LEU:HD13	1.79	0.64
1:C:134:PRO:HG2	1:C:163:VAL:HG12	1.80	0.64
1:C:382:LEU:HD11	1:C:391:ILE:HD12	1.78	0.64
1:D:349:GLY:HA3	1:D:447:TYR:CE1	2.33	0.64
1:K:225:GLU:O	1:K:229:VAL:HG23	1.98	0.64
1:C:135:VAL:HG21	1:C:205:ILE:HG12	1.80	0.64
1:E:339:ARG:NH2	6:E:6307:HOH:O	2.30	0.64
1:F:395:LEU:HD13	1:F:550:LEU:HG	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:PRO:HD2	1:I:35:GLY:O	1.98	0.64
1:I:143:GLY:H	1:I:222:ALA:HB2	1.63	0.64
1:J:308:LEU:HA	1:J:384:LYS:HD3	1.79	0.64
1:D:425:MET:HB2	1:D:426:PHE:CD1	2.33	0.64
1:D:524:GLU:OE2	1:D:538:LYS:HG2	1.98	0.64
1:G:431:VAL:CG2	1:G:446:MET:HE1	2.28	0.64
1:K:215:VAL:H	1:K:241:HIS:CD2	2.16	0.64
1:K:431:VAL:O	1:K:435:ARG:HG3	1.98	0.63
1:C:132:ARG:HH11	1:C:132:ARG:HG2	1.63	0.63
1:D:445:TYR:CE1	1:D:519:GLU:HA	2.34	0.63
1:I:86:MET:HB3	1:I:148:ALA:HB2	1.79	0.63
1:A:227:VAL:O	1:A:231:VAL:HG23	1.98	0.63
1:H:495:MET:HE1	1:H:533:THR:CB	2.29	0.63
1:I:283:VAL:O	1:I:287:ARG:HG3	1.98	0.63
1:A:386:TYR:N	1:A:387:PRO:HD2	2.13	0.63
1:F:216:THR:HG23	1:F:242:ARG:HB2	1.81	0.63
1:I:157:LEU:HD13	1:I:497:MET:HG2	1.81	0.63
1:B:386:TYR:N	1:B:387:PRO:HD2	2.14	0.63
1:B:474:SER:HA	1:B:493:SER:HB2	1.81	0.63
1:D:173:GLY:HA3	6:D:6075:HOH:O	1.97	0.63
1:H:456:SER:HB3	1:H:460:LYS:HD3	1.79	0.63
1:L:149:ALA:HB2	1:L:168:ILE:O	1.98	0.63
1:K:328:LEU:HA	6:K:6425:HOH:O	1.98	0.63
1:F:215:VAL:H	1:F:241:HIS:CD2	2.07	0.63
1:B:262:LYS:HB3	1:B:263:PRO:HD3	1.79	0.63
1:C:218:PHE:HB3	1:C:244:ILE:HB	1.81	0.63
1:F:133:LEU:HD22	1:F:162:ASN:O	1.98	0.63
1:G:498:LYS:HD2	1:G:514:LEU:HD21	1.81	0.63
1:I:188:ASN:HD22	1:I:324:ASP:CG	2.06	0.63
1:J:343:THR:HB	1:J:442:ALA:HB2	1.80	0.63
1:J:386:TYR:N	1:J:387:PRO:HD2	2.14	0.63
1:H:241:HIS:C	1:H:242:ARG:HG3	2.22	0.63
1:L:400:THR:HG22	1:L:404:LEU:HD11	1.80	0.63
1:J:102:THR:HG21	1:J:107:ASN:HD22	1.64	0.62
1:J:119:LEU:HD12	1:J:119:LEU:O	1.98	0.62
1:L:23:PRO:HB2	1:L:34:LEU:HD21	1.81	0.62
1:D:318:LEU:O	1:D:319:LEU:C	2.42	0.62
1:K:107:ASN:HD22	1:K:108:ILE:N	1.96	0.62
1:K:197:ALA:O	1:K:201:VAL:HG23	1.99	0.62
1:K:264:LEU:O	1:K:268:ILE:HG13	1.99	0.62
1:K:359:ILE:HB	1:K:360:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:MET:HB3	1:F:218:PHE:CE1	2.34	0.62
1:L:190:GLY:O	1:L:194:GLN:HG3	1.99	0.62
1:L:220:GLU:HG2	1:L:221:SER:N	2.13	0.62
1:L:343:THR:HB	1:L:442:ALA:CB	2.20	0.62
1:I:379:MET:HE1	1:I:397:PRO:HG3	1.82	0.62
1:L:86:MET:HE2	1:L:110:LEU:HB2	1.81	0.62
1:L:134:PRO:HG2	1:L:163:VAL:HG12	1.82	0.62
1:C:386:TYR:N	1:C:387:PRO:HD2	2.14	0.62
1:F:428:VAL:HG13	1:F:544:VAL:HG22	1.82	0.62
1:G:86:MET:HE3	1:G:110:LEU:HB2	1.80	0.62
1:H:354:GLU:O	1:H:468:HIS:HB2	1.99	0.62
1:A:134:PRO:HG2	1:A:163:VAL:HG12	1.81	0.62
1:I:24:PRO:O	1:I:34:LEU:HD22	2.00	0.62
1:J:262:LYS:HB3	1:J:263:PRO:HD3	1.82	0.62
1:K:105:LYS:HG3	1:K:106:GLU:N	2.15	0.62
1:K:351:ASN:HD22	1:K:351:ASN:N	1.98	0.62
1:A:396:ILE:HB	1:A:397:PRO:HD3	1.81	0.62
1:B:403:TYR:CE1	1:B:420:LEU:HD23	2.34	0.62
1:F:242:ARG:HG2	1:F:242:ARG:HH11	1.65	0.62
2:K:4279:NAG:H81	1:L:260:ASP:HB2	1.82	0.62
1:F:386:TYR:N	1:F:387:PRO:HD2	2.14	0.62
1:A:215:VAL:H	1:A:241:HIS:HD2	1.48	0.62
3:D:2180:SIA:O10	3:D:2180:SIA:C9	2.47	0.62
1:G:350:ILE:O	1:G:448:GLU:HA	2.00	0.62
1:G:446:MET:HE2	1:G:539:LEU:HD23	1.82	0.62
1:K:244:ILE:HG12	1:K:347:MET:HB3	1.82	0.62
1:C:338:GLU:OE2	1:C:341:PHE:HB2	2.00	0.62
1:G:135:VAL:HG21	1:G:205:ILE:HG12	1.82	0.62
1:J:135:VAL:HG21	1:J:205:ILE:HG12	1.81	0.62
1:E:279:SER:O	1:E:283:VAL:HG23	1.99	0.61
1:G:64:ARG:O	1:G:65:PHE:HB2	1.98	0.61
1:H:95:GLN:O	1:H:99:GLU:HG3	2.00	0.61
1:H:399:ALA:HB2	1:H:550:LEU:HD21	1.82	0.61
1:A:550:LEU:CA	1:A:550:LEU:O	2.36	0.61
1:C:48:ALA:HB3	1:C:123:THR:HG23	1.81	0.61
1:H:383:TRP:C	1:H:385:SER:H	2.07	0.61
1:C:498:LYS:HD2	1:C:514:LEU:HD11	1.81	0.61
1:H:135:VAL:HG21	1:H:205:ILE:HG12	1.82	0.61
1:H:279:SER:HA	1:H:282:MET:HE2	1.81	0.61
1:L:254:VAL:HG13	1:L:255:LEU:HG	1.82	0.61
1:D:399:ALA:HB2	1:D:550:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:GLY:O	1:H:227:VAL:HG23	2.01	0.61
1:I:268:ILE:HG12	1:I:301:MET:HE2	1.83	0.61
1:K:119:LEU:HB3	1:K:168:ILE:HG22	1.82	0.61
1:K:396:ILE:HB	1:K:397:PRO:HD3	1.82	0.61
1:L:218:PHE:HB2	1:L:244:ILE:HB	1.82	0.61
1:A:232:LEU:HB3	1:A:335:LEU:HD13	1.82	0.61
1:C:198:LEU:O	1:C:201:VAL:HB	1.99	0.61
1:D:547:TRP:O	1:D:551:PHE:HB2	2.01	0.61
1:F:350:ILE:C	1:F:351:ASN:HD22	2.08	0.61
1:I:379:MET:SD	1:I:396:ILE:HG22	2.40	0.61
1:K:495:MET:HE1	1:K:533:THR:CB	2.30	0.61
1:L:38:VAL:HG21	1:L:49:ILE:HD12	1.83	0.61
1:B:264:LEU:O	1:B:268:ILE:HG13	2.01	0.61
1:C:331:THR:HB	1:C:333:GLU:OE1	2.00	0.61
1:F:130:LYS:C	1:F:131:ASN:HD22	2.09	0.61
1:H:350:ILE:C	1:H:351:ASN:HD22	2.08	0.61
1:I:431:VAL:HA	1:I:446:MET:HE1	1.83	0.61
1:A:131:ASN:O	1:A:132:ARG:HD2	2.00	0.61
1:A:529:ILE:HD12	1:A:529:ILE:H	1.65	0.61
1:E:343:THR:HA	6:E:6126:HOH:O	2.00	0.61
1:L:547:TRP:O	1:L:551:PHE:HB2	2.01	0.61
1:D:382:LEU:HD23	1:D:396:ILE:HG23	1.82	0.61
1:E:222:ALA:N	6:E:6472:HOH:O	2.04	0.61
1:I:257:LYS:HG3	1:I:316:GLN:NE2	2.14	0.61
1:E:333:GLU:H	1:E:333:GLU:CD	2.09	0.61
1:I:427:GLY:O	1:I:431:VAL:HG23	2.01	0.61
1:K:526:TYR:CD2	1:K:539:LEU:HB2	2.36	0.61
1:B:295:LEU:O	1:B:299:LEU:HG	2.01	0.60
1:C:316:GLN:HA	1:C:316:GLN:NE2	2.15	0.60
1:G:262:LYS:O	1:G:266:GLU:HG3	2.01	0.60
1:H:216:THR:HG23	1:H:242:ARG:CB	2.26	0.60
3:I:982:SIA:H7	6:I:6011:HOH:O	2.01	0.60
1:J:498:LYS:O	1:J:502:ASN:HB2	2.01	0.60
1:D:53:ILE:HB	1:D:119:LEU:HD12	1.83	0.60
1:D:103:ASN:HD22	1:D:476:PHE:HB3	1.65	0.60
1:D:262:LYS:HZ3	2:F:2379:NAG:H82	1.64	0.60
1:E:382:LEU:HD11	1:E:391:ILE:HD12	1.83	0.60
1:F:423:ASP:HA	1:F:427:GLY:HA3	1.83	0.60
1:F:87:CYS:HB2	1:F:172:LEU:HD12	1.83	0.60
1:F:499:PHE:CE2	1:F:514:LEU:HB3	2.35	0.60
1:J:23:PRO:HB2	1:J:34:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:312:PRO:HG2	1:J:383:TRP:NE1	2.15	0.60
1:K:83:TYR:HD1	1:K:150:SER:HB3	1.66	0.60
1:L:64:ARG:O	1:L:65:PHE:HB2	2.02	0.60
1:L:292:GLU:O	1:L:296:GLU:HG3	2.01	0.60
3:L:1282:SIA:O9	3:L:1282:SIA:N5	2.33	0.60
1:E:303:PHE:O	1:E:317:PRO:O	2.20	0.60
1:F:218:PHE:HB3	1:F:244:ILE:HB	1.84	0.60
3:I:982:SIA:H113	3:I:982:SIA:H8	1.84	0.60
1:J:333:GLU:H	1:J:333:GLU:CD	2.10	0.60
1:L:357:TRP:CZ2	1:L:361:MET:HE2	2.37	0.60
1:A:197:ALA:O	1:A:201:VAL:HG23	2.01	0.60
1:A:484:GLY:O	1:A:485:ALA:C	2.45	0.60
1:G:88:THR:HG22	1:G:295:LEU:HD13	1.82	0.60
1:I:127:LEU:H	1:I:127:LEU:HD12	1.65	0.60
1:I:223:GLY:O	1:I:227:VAL:HG23	2.02	0.60
1:I:357:TRP:CZ2	1:I:361:MET:HG3	2.36	0.60
1:I:379:MET:HA	1:I:396:ILE:CG2	2.32	0.60
1:J:190:GLY:O	1:J:194:GLN:HG3	2.02	0.60
1:F:262:LYS:HE3	1:F:279:SER:OG	2.02	0.60
1:F:271:THR:HG22	1:F:297:THR:HG23	1.84	0.60
1:A:252:THR:HG22	1:A:254:VAL:HG12	1.82	0.60
1:B:86:MET:HE3	1:B:110:LEU:HB2	1.84	0.60
1:E:364:MET:HE1	1:E:388:LEU:HD11	1.82	0.60
1:H:262:LYS:HB3	1:H:263:PRO:HD3	1.83	0.60
1:K:495:MET:CE	1:K:533:THR:HG21	2.31	0.60
1:A:382:LEU:HD23	1:A:396:ILE:HG23	1.84	0.60
1:E:33:VAL:HG12	1:E:34:LEU:N	2.17	0.60
1:H:420:LEU:HD13	1:H:421:ILE:N	2.17	0.60
1:I:103:ASN:HB2	1:I:478:ALA:HB2	1.83	0.60
1:I:215:VAL:H	1:I:241:HIS:HD2	1.50	0.60
1:A:88:THR:HB	1:A:175:TRP:CZ3	2.36	0.60
1:A:218:PHE:CB	1:A:244:ILE:HB	2.32	0.60
1:B:140:HIS:HD2	1:B:141:GLY:O	1.85	0.60
1:E:379:MET:SD	1:E:396:ILE:HG22	2.41	0.60
1:C:527:LEU:HD11	1:C:533:THR:HG22	1.82	0.59
1:E:353:GLN:O	1:E:467:ASP:HA	2.01	0.59
1:G:382:LEU:HD23	1:G:396:ILE:HG23	1.82	0.59
1:G:479:PRO:HB3	1:G:490:ILE:HG12	1.83	0.59
1:L:357:TRP:CH2	1:L:361:MET:HE2	2.37	0.59
1:C:316:GLN:NE2	1:C:317:PRO:HD2	2.16	0.59
1:E:77:VAL:C	1:E:77:VAL:HG12	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HD23	1:A:318:LEU:HD11	1.83	0.59
1:B:133:LEU:O	1:B:211:ASN:N	2.36	0.59
1:E:242:ARG:HG2	1:E:242:ARG:HH11	1.67	0.59
1:G:107:ASN:ND2	1:G:108:ILE:H	2.00	0.59
1:H:400:THR:HG23	1:H:404:LEU:HD12	1.83	0.59
1:I:409:ASP:O	1:I:413:LYS:HG3	2.03	0.59
1:L:428:VAL:HG13	1:L:544:VAL:HG22	1.85	0.59
1:C:63:LEU:HD11	6:C:6271:HOH:O	2.02	0.59
1:G:271:THR:HG22	1:G:297:THR:HG23	1.85	0.59
1:C:398:GLU:HB3	1:C:550:LEU:HD11	1.83	0.59
1:D:46:PRO:HA	6:D:6225:HOH:O	2.03	0.59
1:I:453:PRO:HG2	1:I:456:SER:OG	2.03	0.59
1:K:350:ILE:C	1:K:351:ASN:HD22	2.09	0.59
1:A:279:SER:HB2	3:A:1181:SIA:H111	1.84	0.59
1:H:194:GLN:OE1	1:H:226:SER:HB3	2.03	0.59
1:B:373:LEU:O	1:B:410:THR:HG22	2.02	0.59
1:C:138:TRP:HH2	1:C:220:GLU:HB2	1.67	0.59
1:C:355:PHE:CD1	1:C:360:PRO:HG3	2.37	0.59
1:E:304:LEU:HG	1:E:305:SER:N	2.18	0.59
1:G:400:THR:HG23	1:G:404:LEU:HD13	1.84	0.59
1:G:423:ASP:HA	1:G:427:GLY:HA3	1.84	0.59
1:H:34:LEU:HB2	1:H:77:VAL:CG1	2.32	0.59
1:I:538:LYS:HB3	1:I:541:ASP:HB2	1.84	0.59
1:J:526:TYR:CD2	1:J:539:LEU:HB2	2.38	0.59
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.67	0.59
1:C:546:PHE:O	1:C:549:ASN:HB2	2.02	0.59
1:E:190:GLY:O	1:E:194:GLN:HG3	2.03	0.59
1:G:78:LYS:HD3	3:G:782:SIA:H91	1.84	0.59
1:G:218:PHE:HB3	1:G:244:ILE:HB	1.84	0.59
1:H:545:ALA:O	1:H:549:ASN:ND2	2.36	0.59
1:I:253:SER:O	1:I:255:LEU:N	2.36	0.59
1:A:236:ALA:HA	1:A:239:LEU:HD12	1.84	0.59
1:D:264:LEU:O	1:D:268:ILE:HG13	2.03	0.59
1:H:131:ASN:O	1:H:209:GLY:HA2	2.03	0.59
1:B:134:PRO:CG	1:B:163:VAL:HG12	2.32	0.59
1:D:186:ARG:HD2	1:D:326:MET:HG3	1.85	0.59
1:H:227:VAL:O	1:H:231:VAL:HG23	2.03	0.59
1:H:352:LYS:HD2	1:H:448:GLU:OE1	2.03	0.59
1:I:461:PRO:HG2	1:I:464:VAL:HG23	1.85	0.59
1:A:226:SER:HA	1:A:229:VAL:CG2	2.32	0.58
1:C:99:GLU:HG2	1:C:107:ASN:OD1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:PRO:HB3	1:C:387:PRO:HB2	1.85	0.58
1:D:204:ASN:O	1:D:206:ALA:N	2.36	0.58
1:H:447:TYR:C	1:H:447:TYR:CD2	2.80	0.58
1:J:57:LYS:HB2	1:J:71:ALA:HA	1.84	0.58
1:K:86:MET:HE2	1:K:110:LEU:HB2	1.85	0.58
1:K:201:VAL:O	1:K:205:ILE:HG22	2.02	0.58
1:C:174:ILE:HA	1:C:319:LEU:HD11	1.85	0.58
1:C:428:VAL:HB	1:C:429:PRO:HD3	1.84	0.58
1:D:318:LEU:O	1:D:318:LEU:HD12	2.03	0.58
1:D:372:GLN:HB2	1:D:410:THR:C	2.28	0.58
1:E:547:TRP:O	1:E:551:PHE:HB2	2.02	0.58
1:G:29:VAL:HG23	1:G:204:ASN:OD1	2.03	0.58
1:J:105:LYS:HG3	1:J:106:GLU:H	1.67	0.58
1:K:278:THR:O	1:K:282:MET:HG3	2.03	0.58
1:L:118:TYR:CE2	3:L:1282:SIA:H91	2.38	0.58
1:L:386:TYR:N	1:L:387:PRO:HD2	2.18	0.58
1:D:423:ASP:O	1:D:428:VAL:HG23	2.03	0.58
1:K:318:LEU:HD22	1:K:318:LEU:N	2.17	0.58
1:B:357:TRP:CZ2	1:B:361:MET:HG3	2.39	0.58
1:D:34:LEU:HB3	1:D:79:ASN:HA	1.85	0.58
1:F:268:ILE:HG12	1:F:301:MET:HE2	1.85	0.58
1:H:351:ASN:HD22	1:H:351:ASN:N	2.01	0.58
1:I:396:ILE:HB	1:I:397:PRO:HD3	1.84	0.58
1:L:59:PRO:HD3	1:L:117:LEU:HD12	1.85	0.58
1:C:241:HIS:O	1:C:242:ARG:HG2	2.03	0.58
1:F:439:ASP:C	1:F:441:GLY:N	2.62	0.58
1:K:495:MET:HE1	1:K:533:THR:CG2	2.33	0.58
1:L:373:LEU:HD11	1:L:377:THR:HB	1.85	0.58
1:A:229:VAL:HG13	1:A:328:LEU:HD11	1.84	0.58
1:A:338:GLU:HB3	1:A:340:ASN:OD1	2.03	0.58
1:C:447:TYR:HA	1:C:527:LEU:O	2.04	0.58
1:F:385:SER:C	1:F:387:PRO:HD2	2.29	0.58
1:J:218:PHE:HB3	1:J:244:ILE:HB	1.86	0.58
1:K:202:GLN:HG2	6:K:6081:HOH:O	2.02	0.58
1:K:242:ARG:HG2	1:K:242:ARG:HH11	1.69	0.58
1:K:447:TYR:C	1:K:447:TYR:CD2	2.81	0.58
1:L:297:THR:HA	1:L:300:LYS:HE3	1.85	0.58
1:F:257:LYS:HE2	1:F:316:GLN:HE22	1.69	0.58
1:C:359:ILE:HB	1:C:360:PRO:HD3	1.86	0.58
1:D:252:THR:HG22	1:D:254:VAL:HG12	1.86	0.58
1:L:227:VAL:O	1:L:228:SER:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:LYS:HB3	1:L:263:PRO:HD3	1.85	0.58
1:C:350:ILE:O	1:C:448:GLU:HA	2.03	0.58
1:E:386:TYR:N	1:E:387:PRO:HD2	2.18	0.58
1:F:300:LYS:O	1:F:302:LYS:HG3	2.03	0.58
1:J:527:LEU:HD11	1:J:533:THR:HG22	1.86	0.58
1:K:343:THR:HB	1:K:442:ALA:HB2	1.86	0.58
1:A:550:LEU:C	1:A:550:LEU:N	2.57	0.58
1:E:131:ASN:O	1:E:132:ARG:HD2	2.04	0.58
1:F:332:PRO:O	1:F:336:GLN:HG2	2.04	0.58
1:I:131:ASN:O	1:I:132:ARG:HD2	2.04	0.58
1:I:311:ASP:OD1	1:I:313:ARG:HB2	2.04	0.58
1:J:306:LEU:HD22	1:J:366:TYR:CE1	2.39	0.58
1:J:385:SER:C	1:J:387:PRO:HD2	2.29	0.58
1:C:29:VAL:HG23	1:C:204:ASN:OD1	2.03	0.57
1:D:221:SER:HB3	6:D:6019:HOH:O	2.04	0.57
1:J:349:GLY:HA3	1:J:447:TYR:CE1	2.39	0.57
1:L:76:PHE:HD1	1:L:76:PHE:H	1.52	0.57
3:A:1180:SIA:O8	3:A:1180:SIA:O10	2.21	0.57
1:C:359:ILE:HG12	5:C:5013:BEZ:H3	1.86	0.57
1:D:355:PHE:CE1	1:D:360:PRO:HG3	2.39	0.57
1:E:467:ASP:CG	1:E:468:HIS:H	2.12	0.57
1:F:241:HIS:C	1:F:242:ARG:HG3	2.29	0.57
3:G:782:SIA:H7	6:G:6005:HOH:O	2.04	0.57
1:J:25:VAL:HG22	1:J:34:LEU:HD23	1.86	0.57
1:J:131:ASN:C	1:J:132:ARG:HD2	2.29	0.57
1:D:97:LEU:HD11	1:D:101:PHE:CE2	2.40	0.57
1:D:319:LEU:N	1:D:319:LEU:HD23	2.19	0.57
1:K:107:ASN:ND2	1:K:108:ILE:H	2.00	0.57
1:A:34:LEU:HD13	1:A:34:LEU:C	2.29	0.57
1:A:276:THR:CG2	1:A:282:MET:HE2	2.31	0.57
1:E:252:THR:HG22	1:E:254:VAL:HG12	1.86	0.57
1:E:438:ARG:HD2	1:E:521:ASN:C	2.29	0.57
1:L:338:GLU:HG2	1:L:340:ASN:H	1.68	0.57
1:E:186:ARG:HB3	1:E:324:ASP:HB2	1.87	0.57
1:H:97:LEU:HA	1:H:100:LEU:HD12	1.86	0.57
1:L:126:ASP:HB3	1:L:129:LYS:CG	2.34	0.57
1:L:262:LYS:HE3	1:L:282:MET:CE	2.35	0.57
1:D:218:PHE:HB3	1:D:244:ILE:HB	1.86	0.57
1:D:385:SER:O	1:D:389:VAL:HG22	2.04	0.57
3:D:2180:SIA:H92	3:D:2180:SIA:N5	2.19	0.57
1:G:124:PRO:HG3	1:G:158:ALA:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:LEU:HD21	1:G:381:LEU:HD12	1.86	0.57
1:J:86:MET:SD	1:J:110:LEU:HD22	2.45	0.57
1:J:164:VAL:HG11	1:J:205:ILE:HD11	1.86	0.57
1:K:237:LYS:O	1:K:238:ASN:HB2	2.03	0.57
1:K:253:SER:CB	1:K:258:LYS:HZ3	2.17	0.57
1:L:184:HIS:O	1:L:185:SER:HB2	2.05	0.57
1:L:367:PRO:CG	1:L:381:LEU:HD21	2.34	0.57
1:B:449:PHE:CE2	1:B:451:TYR:HB3	2.40	0.57
1:C:60:LEU:HD22	1:C:114:GLU:HB3	1.86	0.57
1:C:435:ARG:NE	1:C:524:GLU:OE1	2.38	0.57
1:F:191:HIS:HA	1:F:194:GLN:OE1	2.03	0.57
1:F:316:GLN:HA	1:F:316:GLN:HE21	1.69	0.57
1:H:56:ALA:HB3	1:H:117:LEU:HD13	1.86	0.57
1:J:491:ARG:HD2	6:J:6263:HOH:O	2.05	0.57
1:J:493:SER:O	1:J:497:MET:HG3	2.04	0.57
1:A:215:VAL:N	1:A:241:HIS:HD2	2.03	0.57
1:G:264:LEU:HD11	1:G:316:GLN:HG2	1.85	0.57
1:I:251:LEU:HD13	1:I:433:VAL:HG22	1.87	0.57
1:J:231:VAL:HA	1:J:240:PHE:HZ	1.69	0.57
1:J:254:VAL:HG13	1:J:255:LEU:H	1.70	0.57
1:J:308:LEU:CA	1:J:384:LYS:HD3	2.35	0.57
1:K:185:SER:HB2	1:K:283:VAL:CG2	2.35	0.57
1:L:192:LEU:HD23	1:L:327:LEU:HD12	1.87	0.57
1:A:428:VAL:HB	1:A:429:PRO:HD3	1.87	0.57
1:B:103:ASN:ND2	1:B:476:PHE:HB3	2.20	0.57
1:B:186:ARG:HB3	1:B:324:ASP:HB2	1.86	0.57
1:D:48:ALA:HB3	1:D:123:THR:HG23	1.87	0.57
1:D:318:LEU:O	1:D:320:GLY:N	2.38	0.57
1:G:199:ARG:HG2	1:G:199:ARG:HH11	1.70	0.57
1:H:319:LEU:HD23	1:H:319:LEU:N	2.07	0.57
1:L:218:PHE:HB3	1:L:244:ILE:HB	1.86	0.57
1:B:447:TYR:HB3	1:B:517:TRP:CZ2	2.40	0.56
1:D:304:LEU:O	1:D:364:MET:HE2	2.05	0.56
1:F:355:PHE:CE1	1:F:360:PRO:HG3	2.40	0.56
1:F:461:PRO:HG2	1:F:464:VAL:HG23	1.86	0.56
1:G:351:ASN:HD22	1:G:351:ASN:N	2.02	0.56
1:J:135:VAL:CG2	1:J:205:ILE:HG12	2.35	0.56
1:A:527:LEU:HD11	1:A:533:THR:HG22	1.86	0.56
1:H:215:VAL:H	1:H:241:HIS:HD2	1.53	0.56
1:K:353:GLN:OE1	1:K:464:VAL:HG13	2.05	0.56
1:K:550:LEU:C	1:K:552:ALA:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:343:THR:CB	1:L:442:ALA:HB2	2.23	0.56
1:A:211:ASN:C	1:A:213:GLY:H	2.13	0.56
1:A:278:THR:OG1	1:A:281:VAL:HG23	2.05	0.56
1:A:385:SER:O	1:A:389:VAL:HG22	2.05	0.56
1:E:77:VAL:CG1	1:E:77:VAL:CG2	2.81	0.56
1:F:495:MET:HE1	1:F:533:THR:HG21	1.87	0.56
1:H:59:PRO:HD3	1:H:117:LEU:HD12	1.88	0.56
1:I:358:LEU:HD23	1:I:468:HIS:HB3	1.86	0.56
1:J:24:PRO:HG3	1:J:37:PHE:CZ	2.40	0.56
1:K:63:LEU:HD21	1:K:69:GLN:NE2	2.21	0.56
1:B:428:VAL:HG13	1:B:544:VAL:HA	1.87	0.56
1:C:57:LYS:HD2	1:C:63:LEU:CD1	2.36	0.56
1:E:24:PRO:O	1:E:34:LEU:HD22	2.05	0.56
1:F:428:VAL:HB	1:F:429:PRO:HD3	1.87	0.56
1:G:355:PHE:CD1	1:G:360:PRO:HG3	2.40	0.56
1:H:161:GLU:HB3	1:H:501:ALA:HB2	1.88	0.56
1:A:367:PRO:HG2	1:A:381:LEU:HD21	1.88	0.56
1:A:393:LYS:HA	1:A:396:ILE:HG12	1.87	0.56
1:B:23:PRO:HB2	1:B:34:LEU:HD21	1.86	0.56
1:E:218:PHE:CB	1:E:244:ILE:HB	2.35	0.56
1:E:279:SER:HA	1:E:282:MET:HE3	1.88	0.56
1:H:382:LEU:HB2	1:H:417:PHE:HE1	1.68	0.56
1:L:24:PRO:HB3	1:L:127:LEU:HD12	1.87	0.56
1:L:469:GLY:O	1:L:472:LEU:HG	2.06	0.56
1:A:60:LEU:O	1:A:63:LEU:HB2	2.05	0.56
1:B:252:THR:HG22	1:B:254:VAL:HG12	1.88	0.56
1:G:358:LEU:HD23	1:G:468:HIS:HB3	1.86	0.56
1:G:393:LYS:C	1:G:395:LEU:H	2.14	0.56
1:I:421:ILE:CG2	1:I:425:MET:HE2	2.36	0.56
1:K:266:GLU:O	1:K:270:ILE:HG13	2.06	0.56
1:G:404:LEU:HD23	1:G:413:LYS:CB	2.34	0.56
1:H:77:VAL:CG1	1:H:77:VAL:CG2	2.81	0.56
1:I:426:PHE:C	1:I:429:PRO:HD2	2.31	0.56
1:C:119:LEU:O	1:C:119:LEU:HD12	2.05	0.56
1:H:161:GLU:HB3	1:H:501:ALA:CB	2.36	0.56
1:H:503:PHE:O	1:H:507:GLY:HA2	2.06	0.56
1:I:386:TYR:N	1:I:387:PRO:HD2	2.20	0.56
1:J:318:LEU:HD12	1:J:318:LEU:O	2.05	0.56
1:K:46:PRO:HA	6:K:6235:HOH:O	2.05	0.56
1:A:424:VAL:O	1:A:424:VAL:HG12	2.04	0.56
1:C:145:MET:SD	1:C:173:GLY:HA2	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ASP:HB3	1:E:93:ALA:HB3	1.87	0.56
1:F:86:MET:HE2	1:F:110:LEU:HD12	1.86	0.56
1:I:24:PRO:HG3	1:I:37:PHE:CZ	2.40	0.56
1:I:255:LEU:HD23	1:I:318:LEU:HD11	1.87	0.56
1:I:480:PHE:CE1	1:I:497:MET:HE1	2.41	0.56
1:E:447:TYR:C	1:E:447:TYR:CD2	2.84	0.56
1:G:136:MET:HB3	1:G:218:PHE:CE1	2.41	0.56
1:G:527:LEU:HD11	1:G:533:THR:HG22	1.89	0.56
1:I:56:ALA:HB3	1:I:117:LEU:HD13	1.86	0.56
1:I:95:GLN:O	1:I:99:GLU:HG3	2.05	0.56
1:B:24:PRO:HG3	1:B:37:PHE:CE1	2.41	0.55
1:C:431:VAL:HG22	1:C:446:MET:HE1	1.87	0.55
1:E:241:HIS:C	1:E:242:ARG:HG3	2.31	0.55
1:E:396:ILE:HB	1:E:397:PRO:HD3	1.88	0.55
1:H:172:LEU:HB2	6:H:6375:HOH:O	2.05	0.55
1:L:403:TYR:O	1:L:416:LEU:HD13	2.06	0.55
1:B:348:VAL:O	1:B:446:MET:HA	2.06	0.55
1:E:431:VAL:O	1:E:434:ALA:HB3	2.06	0.55
3:H:882:SIA:O4	3:H:882:SIA:C10	2.55	0.55
1:J:241:HIS:C	1:J:242:ARG:HG3	2.30	0.55
1:A:275:LYS:NZ	6:A:6039:HOH:O	2.36	0.55
1:A:316:GLN:NE2	1:A:317:PRO:HD2	2.21	0.55
1:F:197:ALA:O	1:F:201:VAL:HG23	2.06	0.55
1:G:428:VAL:HG13	1:G:544:VAL:HA	1.88	0.55
1:H:395:LEU:HD22	1:H:550:LEU:CD1	2.36	0.55
1:I:143:GLY:N	1:I:222:ALA:HB2	2.20	0.55
1:I:503:PHE:HD1	1:I:509:PRO:HD3	1.71	0.55
1:K:318:LEU:N	1:K:318:LEU:HD13	2.22	0.55
1:K:499:PHE:CZ	1:K:514:LEU:HD22	2.41	0.55
1:L:133:LEU:HD12	1:L:209:GLY:O	2.07	0.55
1:A:320:GLY:O	1:A:322:VAL:HG13	2.06	0.55
1:B:251:LEU:HD12	1:B:336:GLN:NE2	2.20	0.55
1:C:316:GLN:HA	1:C:316:GLN:HE21	1.70	0.55
3:L:1282:SIA:C7	6:L:6029:HOH:O	2.41	0.55
1:A:237:LYS:O	1:A:238:ASN:HB2	2.06	0.55
1:C:417:PHE:O	1:C:420:LEU:HB3	2.07	0.55
1:E:346:TYR:HB3	1:E:437:HIS:CD2	2.42	0.55
1:E:374:ASP:OD2	1:E:376:LYS:HB2	2.06	0.55
1:F:103:ASN:HA	1:F:482:LYS:HD2	1.88	0.55
1:F:485:ALA:HB3	6:F:6306:HOH:O	2.05	0.55
1:H:245:SER:HB3	1:H:248:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:ARG:O	1:K:66:THR:HG23	2.07	0.55
1:A:134:PRO:HG3	1:A:505:ARG:HG2	1.87	0.55
3:A:1181:SIA:N5	3:A:1181:SIA:C9	2.67	0.55
1:E:330:LYS:HB2	1:E:334:GLU:OE1	2.06	0.55
1:G:104:ARG:HD2	1:G:108:ILE:HG12	1.87	0.55
1:H:461:PRO:HG2	1:H:464:VAL:HG23	1.88	0.55
1:I:353:GLN:O	1:I:467:ASP:HA	2.06	0.55
1:I:495:MET:HE3	1:I:499:PHE:HE1	1.72	0.55
1:K:216:THR:HG23	1:K:242:ARG:HB2	1.87	0.55
1:K:264:LEU:HD22	1:K:268:ILE:HD11	1.89	0.55
1:L:357:TRP:C	1:L:360:PRO:HD2	2.31	0.55
1:A:308:LEU:HD21	1:A:367:PRO:HG3	1.89	0.55
1:E:363:LEU:C	1:E:365:SER:H	2.15	0.55
1:E:495:MET:HE3	1:E:499:PHE:HE1	1.70	0.55
1:J:202:GLN:HE22	1:J:215:VAL:HG21	1.72	0.55
1:J:432:ILE:HD11	1:J:544:VAL:HG13	1.87	0.55
1:K:368:LEU:HD11	1:K:418:LEU:HD21	1.88	0.55
1:C:77:VAL:O	1:C:77:VAL:HG12	2.06	0.55
1:C:104:ARG:HD2	1:C:108:ILE:HG12	1.89	0.55
1:G:318:LEU:HD12	1:G:318:LEU:O	2.06	0.55
1:I:24:PRO:HG3	1:I:37:PHE:CE1	2.42	0.55
1:I:176:GLY:HA2	1:I:189:TRP:HB2	1.88	0.55
1:B:445:TYR:CE1	1:B:519:GLU:HA	2.41	0.55
1:E:215:VAL:H	1:E:241:HIS:HD2	1.55	0.55
1:F:333:GLU:CD	1:F:333:GLU:H	2.15	0.55
1:H:323:ILE:HD12	1:H:331:THR:HA	1.89	0.55
1:B:95:GLN:HG2	1:B:99:GLU:OE2	2.07	0.55
1:D:290:THR:HG23	1:D:293:GLU:OE2	2.07	0.55
1:E:290:THR:OG1	1:E:293:GLU:HG3	2.07	0.55
1:F:316:GLN:NE2	1:F:317:PRO:HD2	2.21	0.55
1:F:457:SER:C	1:F:459:MET:H	2.15	0.55
1:F:499:PHE:CD2	1:F:514:LEU:HD13	2.42	0.55
1:H:134:PRO:HG2	1:H:163:VAL:HG12	1.89	0.55
1:I:301:MET:O	1:I:302:LYS:C	2.50	0.55
1:K:249:VAL:HB	1:K:433:VAL:HG21	1.89	0.55
1:L:372:GLN:HE22	1:L:411:VAL:HG22	1.72	0.55
1:C:373:LEU:HD21	1:C:414:LYS:HA	1.88	0.54
1:D:358:LEU:HD23	1:D:468:HIS:HB3	1.89	0.54
1:J:330:LYS:HB2	1:J:334:GLU:OE2	2.07	0.54
1:K:215:VAL:N	1:K:241:HIS:HD2	2.06	0.54
1:K:232:LEU:HD21	1:K:336:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TRP:CH2	1:A:361:MET:HE2	2.42	0.54
1:B:338:GLU:OE2	1:B:341:PHE:HB2	2.07	0.54
1:D:351:ASN:HD22	1:D:351:ASN:N	1.96	0.54
1:E:331:THR:OG1	1:E:334:GLU:HG3	2.07	0.54
1:H:319:LEU:H	1:H:319:LEU:CD2	2.01	0.54
1:H:370:GLU:HB2	1:H:372:GLN:HG2	1.89	0.54
1:B:266:GLU:O	1:B:270:ILE:HG13	2.07	0.54
1:C:249:VAL:HG23	1:C:251:LEU:H	1.72	0.54
1:C:353:GLN:HG3	1:C:465:ILE:O	2.06	0.54
1:D:186:ARG:HB3	1:D:324:ASP:HB2	1.90	0.54
1:G:268:ILE:HD11	1:G:319:LEU:HD21	1.89	0.54
1:J:357:TRP:C	1:J:360:PRO:HD2	2.33	0.54
1:A:97:LEU:HD11	1:A:101:PHE:CE2	2.42	0.54
1:A:339:ARG:CG	1:A:440:ALA:HA	2.37	0.54
3:D:2180:SIA:H112	1:E:278:THR:HG22	1.89	0.54
1:E:133:LEU:HB3	1:E:134:PRO:HD2	1.88	0.54
3:G:782:SIA:H4	1:H:262:LYS:NZ	2.22	0.54
1:I:71:ALA:HB1	6:I:6282:HOH:O	2.07	0.54
1:K:403:TYR:O	1:K:416:LEU:HD13	2.08	0.54
1:L:428:VAL:HG13	1:L:544:VAL:HG13	1.89	0.54
1:B:86:MET:CE	1:B:110:LEU:HB2	2.37	0.54
1:F:97:LEU:HD22	1:F:146:VAL:HG23	1.90	0.54
1:F:407:THR:HG22	1:F:409:ASP:H	1.72	0.54
1:H:428:VAL:HG21	1:H:547:TRP:CD1	2.43	0.54
1:K:28:THR:HB	1:K:204:ASN:OD1	2.08	0.54
1:A:380:SER:O	1:A:384:LYS:HG3	2.08	0.54
1:B:327:LEU:HD23	1:B:327:LEU:C	2.33	0.54
1:E:251:LEU:HD11	1:E:336:GLN:NE2	2.20	0.54
1:I:338:GLU:HG2	1:I:339:ARG:N	2.22	0.54
1:K:107:ASN:ND2	1:K:108:ILE:N	2.55	0.54
1:K:306:LEU:HG	1:K:307:ASP:N	2.23	0.54
1:L:47:VAL:HG13	1:L:123:THR:O	2.08	0.54
1:L:495:MET:HE1	1:L:533:THR:CG2	2.35	0.54
1:A:217:ILE:HG13	1:A:227:VAL:HG13	1.88	0.54
1:A:456:SER:HB3	1:A:460:LYS:HD3	1.88	0.54
1:D:386:TYR:N	1:D:387:PRO:HD2	2.23	0.54
1:F:449:PHE:CE2	1:F:451:TYR:HB3	2.42	0.54
1:G:143:GLY:O	1:G:144:LEU:HB2	2.07	0.54
1:G:216:THR:HG23	1:G:242:ARG:HB2	1.89	0.54
1:K:47:VAL:HG13	1:K:123:THR:O	2.07	0.54
1:B:243:ALA:C	1:B:244:ILE:HG13	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:LYS:HA	1:H:257:LYS:NZ	2.22	0.54
1:K:171:ARG:HB3	1:K:176:GLY:CA	2.37	0.54
1:K:429:PRO:O	1:K:433:VAL:HG23	2.08	0.54
1:B:447:TYR:C	1:B:447:TYR:CD2	2.86	0.54
1:I:279:SER:HA	1:I:282:MET:HE3	1.89	0.54
1:J:104:ARG:O	1:J:482:LYS:HE3	2.06	0.54
1:K:131:ASN:O	1:K:132:ARG:HD2	2.07	0.54
1:K:355:PHE:CE1	1:K:360:PRO:HG3	2.43	0.54
1:L:178:PHE:CZ	1:L:286:LEU:HD12	2.43	0.54
1:A:218:PHE:HB3	1:A:244:ILE:HB	1.90	0.54
3:B:1280:SIA:H113	1:C:262:LYS:HZ1	1.72	0.54
1:F:119:LEU:O	1:F:119:LEU:HD12	2.07	0.54
1:F:268:ILE:HG12	1:F:301:MET:CE	2.38	0.54
1:F:368:LEU:C	1:F:370:GLU:H	2.16	0.54
1:G:288:GLN:HG3	6:I:6384:HOH:O	2.07	0.54
1:A:414:LYS:HZ3	5:A:1385:BEZ:H2	1.72	0.53
1:D:262:LYS:HB3	1:D:263:PRO:HD3	1.88	0.53
1:H:431:VAL:HG22	1:H:446:MET:HE1	1.90	0.53
1:C:24:PRO:HD2	1:C:35:GLY:O	2.08	0.53
1:C:89:GLN:HB2	1:C:146:VAL:HG12	1.90	0.53
1:C:526:TYR:CE2	1:C:539:LEU:HB2	2.43	0.53
1:E:227:VAL:O	1:E:231:VAL:HG23	2.06	0.53
1:G:138:TRP:HH2	1:G:220:GLU:HB2	1.73	0.53
1:H:283:VAL:HG12	1:H:287:ARG:NH1	2.22	0.53
1:I:348:VAL:O	1:I:446:MET:HA	2.08	0.53
1:J:29:VAL:HG23	1:J:204:ASN:OD1	2.07	0.53
1:A:316:GLN:CD	1:A:317:PRO:HD2	2.33	0.53
1:A:317:PRO:HG2	1:A:318:LEU:H	1.72	0.53
1:A:478:ALA:N	1:A:479:PRO:CD	2.71	0.53
1:B:39:SER:OG	1:B:46:PRO:HB3	2.09	0.53
1:B:396:ILE:HB	1:B:397:PRO:HD3	1.89	0.53
1:C:218:PHE:CB	1:C:244:ILE:HB	2.38	0.53
1:C:371:GLY:HA2	1:C:414:LYS:HZ2	1.74	0.53
1:D:218:PHE:CB	1:D:244:ILE:HB	2.38	0.53
1:D:393:LYS:HA	1:D:396:ILE:HG12	1.91	0.53
1:G:87:CYS:O	1:G:89:GLN:HG2	2.07	0.53
1:J:339:ARG:CG	1:J:440:ALA:HA	2.39	0.53
1:K:495:MET:HE1	1:K:533:THR:OG1	2.08	0.53
1:B:333:GLU:H	1:B:333:GLU:CD	2.16	0.53
1:C:139:ILE:HG12	1:C:168:ILE:HD11	1.91	0.53
1:C:257:LYS:HE3	1:C:316:GLN:HE22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:CYS:O	1:E:118:TYR:N	2.40	0.53
1:E:348:VAL:O	1:E:446:MET:HA	2.08	0.53
1:F:357:TRP:C	1:F:360:PRO:HD2	2.32	0.53
1:H:532:ASN:ND2	1:H:532:ASN:H	2.06	0.53
1:I:527:LEU:HD23	1:I:529:ILE:HG12	1.90	0.53
1:L:199:ARG:HH11	1:L:199:ARG:CB	2.19	0.53
1:A:417:PHE:O	1:A:420:LEU:HB3	2.08	0.53
1:C:344:VAL:HG12	6:C:6160:HOH:O	2.08	0.53
1:F:41:GLU:HG3	1:F:41:GLU:O	2.09	0.53
1:H:290:THR:OG1	1:H:293:GLU:HG3	2.08	0.53
1:K:357:TRP:CZ2	1:K:361:MET:HG3	2.44	0.53
1:L:373:LEU:HD21	1:L:378:ALA:HA	1.90	0.53
1:G:248:GLY:N	6:G:6144:HOH:O	2.42	0.53
1:H:199:ARG:HB3	1:H:199:ARG:NH1	2.09	0.53
1:I:186:ARG:HB3	1:I:324:ASP:HB2	1.91	0.53
1:I:313:ARG:HD2	1:I:386:TYR:CE2	2.43	0.53
1:K:393:LYS:HA	1:K:396:ILE:HG12	1.91	0.53
1:A:352:LYS:HD2	1:A:448:GLU:OE1	2.09	0.53
1:A:510:ASN:HD21	1:A:517:TRP:H	1.55	0.53
1:B:495:MET:HE3	1:B:499:PHE:CE1	2.44	0.53
1:C:202:GLN:NE2	1:C:215:VAL:HG21	2.15	0.53
1:G:120:ASN:HB2	1:G:167:THR:OG1	2.08	0.53
1:I:132:ARG:HG2	1:I:132:ARG:HH11	1.74	0.53
1:K:143:GLY:O	1:K:144:LEU:HB2	2.08	0.53
1:L:264:LEU:O	1:L:268:ILE:HG13	2.09	0.53
1:A:312:PRO:O	1:A:315:SER:HB3	2.08	0.53
1:C:553:LYS:OXT	1:C:553:LYS:HD3	2.09	0.53
1:E:222:ALA:CB	6:E:6472:HOH:O	2.57	0.53
1:E:319:LEU:O	1:E:320:GLY:O	2.26	0.53
1:G:241:HIS:O	1:G:242:ARG:HG2	2.09	0.53
1:H:218:PHE:CB	1:H:244:ILE:HB	2.39	0.53
1:H:501:ALA:HB1	1:H:505:ARG:NH1	2.23	0.53
1:I:498:LYS:O	1:I:502:ASN:HB2	2.09	0.53
1:L:383:TRP:CZ3	1:L:393:LYS:HB2	2.43	0.53
1:B:59:PRO:HD3	1:B:117:LEU:HD12	1.91	0.53
1:K:477:GLY:HA2	1:K:493:SER:OG	2.09	0.53
1:A:215:VAL:N	1:A:241:HIS:CD2	2.76	0.53
1:B:343:THR:HB	1:B:442:ALA:HB2	1.90	0.53
1:C:111:LYS:H	1:C:111:LYS:HD2	1.74	0.53
1:D:104:ARG:O	1:D:482:LYS:HE2	2.09	0.53
1:E:453:PRO:HG3	1:E:470:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:ARG:O	1:G:65:PHE:CB	2.57	0.53
1:G:164:VAL:CG1	1:G:205:ILE:HD11	2.38	0.53
1:H:526:TYR:CD2	1:H:539:LEU:HB2	2.44	0.53
1:J:157:LEU:HD23	1:J:165:VAL:HG22	1.91	0.53
1:C:297:THR:O	1:C:301:MET:HG2	2.09	0.52
1:E:343:THR:HB	1:E:442:ALA:HB2	1.91	0.52
1:I:324:ASP:C	1:I:326:MET:H	2.16	0.52
1:K:241:HIS:C	1:K:242:ARG:HG3	2.34	0.52
1:E:478:ALA:N	1:E:479:PRO:CD	2.71	0.52
1:F:528:GLN:HE21	1:F:536:ALA:CB	2.21	0.52
1:G:217:ILE:CD1	1:G:227:VAL:HG13	2.39	0.52
1:H:63:LEU:HD21	1:H:69:GLN:HE21	1.74	0.52
1:K:132:ARG:HA	1:K:209:GLY:O	2.09	0.52
1:A:266:GLU:HG2	1:A:282:MET:CE	2.33	0.52
1:B:266:GLU:HG2	1:B:282:MET:HE1	1.91	0.52
1:F:358:LEU:O	1:F:363:LEU:HD12	2.09	0.52
1:I:423:ASP:OD1	1:I:540:LYS:HD2	2.09	0.52
1:K:104:ARG:NH1	1:K:153:ASP:HB2	2.25	0.52
1:L:323:ILE:HD12	1:L:330:LYS:O	2.09	0.52
1:D:527:LEU:HD11	1:D:533:THR:HG22	1.90	0.52
1:E:526:TYR:HE1	1:E:528:GLN:HG2	1.75	0.52
1:G:386:TYR:N	1:G:387:PRO:HD2	2.24	0.52
1:H:393:LYS:HA	1:H:396:ILE:HG12	1.91	0.52
1:H:425:MET:HB2	1:H:426:PHE:CD1	2.44	0.52
1:I:435:ARG:NH1	1:I:544:VAL:HG11	2.24	0.52
1:I:499:PHE:HD2	1:I:509:PRO:HB2	1.74	0.52
1:K:393:LYS:HA	1:K:396:ILE:CG1	2.40	0.52
1:K:493:SER:OG	1:K:497:MET:HE2	2.08	0.52
1:B:428:VAL:HG13	1:B:544:VAL:HG13	1.91	0.52
1:E:498:LYS:HD2	1:E:514:LEU:HD21	1.91	0.52
1:H:103:ASN:ND2	1:H:476:PHE:O	2.43	0.52
1:I:225:GLU:O	1:I:229:VAL:HG23	2.09	0.52
1:I:322:VAL:CG1	1:I:323:ILE:N	2.72	0.52
1:K:211:ASN:C	1:K:211:ASN:OD1	2.53	0.52
1:A:461:PRO:HG2	1:A:464:VAL:CG2	2.39	0.52
1:B:53:ILE:HD12	1:B:121:ILE:HD12	1.90	0.52
1:B:392:ALA:HB3	1:B:395:LEU:CG	2.38	0.52
1:D:467:ASP:N	1:D:470:ASP:OD2	2.41	0.52
1:E:385:SER:C	1:E:387:PRO:HD2	2.34	0.52
1:E:493:SER:O	1:E:497:MET:HG3	2.10	0.52
1:H:351:ASN:HB3	1:H:466:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:GLY:O	1:I:194:GLN:HG3	2.09	0.52
1:K:383:TRP:C	1:K:385:SER:H	2.17	0.52
1:A:423:ASP:OD2	1:A:543:GLU:HG2	2.09	0.52
1:B:420:LEU:CD2	1:B:547:TRP:HZ2	2.23	0.52
1:G:333:GLU:H	1:G:333:GLU:CD	2.18	0.52
1:I:310:GLY:O	1:I:312:PRO:HD3	2.10	0.52
1:I:431:VAL:HG12	1:I:435:ARG:HD2	1.91	0.52
1:I:435:ARG:O	1:I:438:ARG:HB3	2.10	0.52
1:J:79:ASN:OD1	2:J:4179:NAG:H3	2.09	0.52
1:J:360:PRO:O	1:J:366:TYR:HB2	2.10	0.52
1:K:95:GLN:O	1:K:99:GLU:HG3	2.09	0.52
1:K:180:THR:HG22	1:K:282:MET:HE3	1.92	0.52
1:A:328:LEU:HA	6:A:6261:HOH:O	2.08	0.52
1:B:236:ALA:HB1	1:B:240:PHE:CE1	2.42	0.52
1:D:156:ALA:O	1:D:157:LEU:C	2.52	0.52
1:D:499:PHE:CD2	1:D:514:LEU:HD13	2.44	0.52
1:F:324:ASP:OD2	1:F:324:ASP:N	2.40	0.52
1:G:97:LEU:HD22	1:G:146:VAL:CG2	2.40	0.52
1:H:386:TYR:N	1:H:387:PRO:HD2	2.24	0.52
1:H:396:ILE:HB	1:H:397:PRO:HD3	1.90	0.52
1:H:501:ALA:HB1	1:H:505:ARG:HH12	1.75	0.52
1:I:264:LEU:HD11	1:I:316:GLN:HG2	1.92	0.52
1:L:75:SER:O	1:L:76:PHE:O	2.26	0.52
1:L:103:ASN:HA	1:L:482:LYS:HE2	1.92	0.52
1:L:431:VAL:O	1:L:434:ALA:HB3	2.09	0.52
1:F:218:PHE:CB	1:F:244:ILE:HB	2.39	0.52
1:L:543:GLU:O	1:L:547:TRP:HD1	1.91	0.52
1:A:317:PRO:O	1:A:318:LEU:HB3	2.09	0.52
1:B:98:SER:O	1:B:107:ASN:ND2	2.43	0.52
1:C:221:SER:HA	1:C:247:SER:O	2.09	0.52
1:D:526:TYR:CD2	1:D:539:LEU:HB2	2.45	0.52
1:E:303:PHE:CZ	1:E:319:LEU:HD21	2.45	0.52
1:G:242:ARG:HD2	1:G:504:ALA:HA	1.92	0.52
1:G:478:ALA:N	1:G:479:PRO:CD	2.72	0.52
1:C:372:GLN:O	1:C:373:LEU:HB3	2.09	0.51
1:F:138:TRP:HE3	1:F:218:PHE:CD2	2.28	0.51
1:H:264:LEU:O	1:H:268:ILE:HG13	2.10	0.51
1:H:395:LEU:HD22	1:H:550:LEU:HD12	1.92	0.51
1:J:417:PHE:O	1:J:420:LEU:HB3	2.09	0.51
1:K:306:LEU:HG	1:K:307:ASP:H	1.74	0.51
1:L:215:VAL:N	1:L:241:HIS:HD2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ARG:HG3	1:D:491:ARG:HH11	1.75	0.51
1:F:205:ILE:HG13	1:F:210:GLY:HA3	1.92	0.51
1:F:254:VAL:HG13	1:F:255:LEU:N	2.25	0.51
1:J:59:PRO:HD3	1:J:117:LEU:HD12	1.93	0.51
1:A:34:LEU:HD13	1:A:35:GLY:O	2.11	0.51
1:A:83:TYR:CD1	1:A:150:SER:HB3	2.46	0.51
1:B:382:LEU:HD11	1:B:391:ILE:HD12	1.93	0.51
1:G:447:TYR:HB3	1:G:517:TRP:CZ2	2.45	0.51
1:H:526:TYR:CE2	1:H:539:LEU:HB2	2.45	0.51
1:I:345:PRO:HA	1:I:443:PRO:HB2	1.92	0.51
1:J:324:ASP:OD2	1:J:325:GLY:N	2.41	0.51
1:B:255:LEU:HD23	1:B:318:LEU:HD11	1.91	0.51
1:C:403:TYR:CG	1:C:420:LEU:HD23	2.45	0.51
1:D:87:CYS:O	1:D:89:GLN:HG2	2.11	0.51
1:E:220:GLU:HA	1:E:246:GLU:O	2.11	0.51
1:F:262:LYS:HB3	1:F:263:PRO:HD3	1.92	0.51
1:I:527:LEU:HD23	1:I:529:ILE:CG1	2.40	0.51
1:K:223:GLY:O	1:K:227:VAL:HG23	2.11	0.51
1:L:268:ILE:HD11	1:L:319:LEU:HD21	1.91	0.51
1:A:152:TYR:HB3	1:A:476:PHE:CE2	2.45	0.51
1:C:264:LEU:HG	1:C:316:GLN:HG2	1.92	0.51
1:C:290:THR:HG23	1:C:293:GLU:OE2	2.09	0.51
1:D:498:LYS:HD2	6:D:6232:HOH:O	2.10	0.51
1:E:355:PHE:CD1	1:E:360:PRO:HG3	2.44	0.51
1:F:539:LEU:HD12	1:F:540:LYS:H	1.74	0.51
1:G:221:SER:OG	5:G:3385:BEZ:H2	2.10	0.51
1:H:381:LEU:HD22	1:H:417:PHE:CE2	2.45	0.51
1:I:403:TYR:CG	1:I:420:LEU:HD23	2.45	0.51
1:K:138:TRP:O	6:K:6407:HOH:O	2.19	0.51
1:K:152:TYR:N	1:K:152:TYR:CD1	2.76	0.51
1:K:218:PHE:HB3	1:K:244:ILE:HB	1.92	0.51
1:K:318:LEU:O	1:K:319:LEU:C	2.50	0.51
1:L:110:LEU:HD11	1:L:150:SER:HB2	1.92	0.51
1:A:425:MET:O	1:A:429:PRO:HG2	2.10	0.51
1:C:193:ASP:O	1:C:194:GLN:C	2.54	0.51
1:C:262:LYS:HE3	1:C:279:SER:OG	2.10	0.51
1:D:264:LEU:HD22	1:D:268:ILE:CD1	2.40	0.51
1:J:456:SER:HB3	1:J:460:LYS:HE2	1.93	0.51
3:J:1082:SIA:H4	1:K:262:LYS:HZ3	1.74	0.51
1:K:25:VAL:HG22	1:K:34:LEU:HD23	1.88	0.51
1:K:221:SER:O	1:K:224:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:THR:OG1	1:L:293:GLU:HG3	2.10	0.51
1:A:316:GLN:NE2	1:A:316:GLN:HA	2.25	0.51
1:B:277:THR:HG22	1:B:278:THR:HG23	1.92	0.51
1:B:364:MET:HE1	1:B:388:LEU:HD21	1.93	0.51
1:E:142:GLY:N	6:E:6472:HOH:O	2.24	0.51
1:E:445:TYR:CE1	1:E:519:GLU:HA	2.46	0.51
1:E:493:SER:OG	1:E:497:MET:HE2	2.10	0.51
1:G:222:ALA:CB	6:G:6473:HOH:O	2.58	0.51
1:I:281:VAL:O	1:I:284:HIS:HB3	2.11	0.51
1:K:333:GLU:CD	1:K:333:GLU:H	2.19	0.51
1:A:24:PRO:HG3	1:A:37:PHE:CZ	2.45	0.51
1:A:26:VAL:CG2	1:A:127:LEU:HD13	2.41	0.51
1:A:184:HIS:HD2	1:A:279:SER:HB3	1.74	0.51
1:A:383:TRP:CE3	1:A:393:LYS:HB2	2.46	0.51
1:A:447:TYR:C	1:A:447:TYR:CD2	2.87	0.51
1:B:385:SER:C	1:B:387:PRO:HD2	2.34	0.51
1:C:499:PHE:CE2	1:C:514:LEU:HB3	2.46	0.51
1:F:202:GLN:NE2	1:F:212:PRO:O	2.44	0.51
1:F:293:GLU:O	1:F:296:GLU:HB3	2.10	0.51
1:F:445:TYR:CZ	1:F:509:PRO:HD2	2.45	0.51
1:F:539:LEU:HD12	1:F:540:LYS:N	2.26	0.51
1:G:132:ARG:HB3	1:G:211:ASN:HB2	1.91	0.51
1:I:200:TRP:CE2	1:I:204:ASN:ND2	2.79	0.51
1:I:539:LEU:O	1:I:541:ASP:N	2.44	0.51
1:J:218:PHE:CB	1:J:244:ILE:HB	2.41	0.51
1:J:359:ILE:HB	1:J:360:PRO:HD3	1.92	0.51
1:L:215:VAL:H	1:L:241:HIS:HD2	1.59	0.51
1:B:218:PHE:CB	1:B:244:ILE:HB	2.41	0.51
1:D:339:ARG:HH12	1:D:440:ALA:HB2	1.75	0.51
1:D:526:TYR:CE2	1:D:539:LEU:HB2	2.45	0.51
1:E:237:LYS:O	1:E:238:ASN:HB2	2.10	0.51
1:F:57:LYS:HB2	1:F:71:ALA:HA	1.93	0.51
3:G:782:SIA:H4	1:H:262:LYS:HZ1	1.75	0.51
1:H:255:LEU:HD23	1:H:318:LEU:CD1	2.41	0.51
1:I:171:ARG:HD2	1:I:175:TRP:O	2.11	0.51
1:J:218:PHE:HA	1:J:244:ILE:O	2.11	0.51
1:K:257:LYS:HB2	1:K:322:VAL:HG12	1.93	0.51
1:K:550:LEU:C	1:K:552:ALA:N	2.69	0.51
1:L:527:LEU:HD11	1:L:533:THR:HG22	1.92	0.51
1:A:495:MET:HE1	1:A:533:THR:CB	2.41	0.51
1:B:25:VAL:HG22	1:B:34:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HD21	1:C:217:ILE:CG2	2.41	0.51
1:D:260:ASP:OD2	1:D:263:PRO:HD3	2.12	0.51
1:D:266:GLU:HG2	1:D:282:MET:CE	2.41	0.51
1:E:317:PRO:HD2	6:E:6027:HOH:O	2.09	0.51
1:F:236:ALA:HB1	1:F:240:PHE:HE1	1.76	0.51
1:H:34:LEU:HB2	1:H:77:VAL:HG12	1.92	0.51
1:L:431:VAL:HA	1:L:446:MET:HE1	1.93	0.51
1:A:364:MET:HE1	1:A:388:LEU:HD21	1.93	0.50
1:B:86:MET:HG3	1:B:112:LEU:HD23	1.94	0.50
1:D:478:ALA:N	1:D:479:PRO:CD	2.74	0.50
1:F:40:LEU:O	1:F:41:GLU:C	2.55	0.50
1:F:414:LYS:HD2	1:F:414:LYS:C	2.36	0.50
1:I:24:PRO:C	1:I:24:PRO:HB2	2.35	0.50
1:I:194:GLN:OE1	1:I:226:SER:HB3	2.11	0.50
1:I:539:LEU:C	1:I:541:ASP:H	2.17	0.50
1:L:427:GLY:O	1:L:431:VAL:HG23	2.11	0.50
1:D:152:TYR:HB3	1:D:476:PHE:CE2	2.46	0.50
1:F:447:TYR:HB3	1:F:517:TRP:CZ2	2.46	0.50
1:F:510:ASN:OD1	1:F:516:HIS:HA	2.12	0.50
1:J:264:LEU:HG	1:J:316:GLN:HG2	1.93	0.50
1:J:478:ALA:N	1:J:479:PRO:CD	2.73	0.50
1:L:105:LYS:HG3	1:L:106:GLU:H	1.76	0.50
1:A:119:LEU:C	1:A:119:LEU:HD12	2.37	0.50
1:A:343:THR:HA	6:A:6423:HOH:O	2.11	0.50
1:B:141:GLY:HA2	1:B:223:GLY:N	2.26	0.50
1:D:255:LEU:HA	1:D:318:LEU:HD11	1.93	0.50
1:D:349:GLY:HA3	1:D:447:TYR:CD1	2.47	0.50
1:D:428:VAL:HG13	1:D:544:VAL:HA	1.93	0.50
1:G:131:ASN:HB2	1:G:209:GLY:HA2	1.93	0.50
1:H:312:PRO:HG3	1:H:384:LYS:HA	1.93	0.50
1:D:101:PHE:O	1:D:102:THR:C	2.53	0.50
1:E:91:PRO:HB3	1:E:112:LEU:HD11	1.93	0.50
1:E:426:PHE:C	1:E:429:PRO:HD2	2.37	0.50
1:F:104:ARG:HD2	1:F:108:ILE:HG12	1.93	0.50
1:F:452:ARG:NH2	1:F:460:LYS:O	2.45	0.50
1:G:86:MET:CE	1:G:110:LEU:HB2	2.40	0.50
1:H:193:ASP:O	1:H:196:ALA:HB3	2.11	0.50
1:H:244:ILE:HG12	1:H:347:MET:HB3	1.93	0.50
1:I:149:ALA:HB2	1:I:168:ILE:O	2.12	0.50
1:I:227:VAL:O	1:I:228:SER:C	2.55	0.50
1:I:491:ARG:HH11	1:I:491:ARG:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:THR:HG22	1:J:295:LEU:HD22	1.93	0.50
1:L:87:CYS:O	1:L:89:GLN:HG2	2.11	0.50
1:A:211:ASN:O	1:A:213:GLY:N	2.44	0.50
1:K:517:TRP:CE3	1:K:527:LEU:HD22	2.46	0.50
1:L:355:PHE:CE1	1:L:360:PRO:HG3	2.47	0.50
1:D:428:VAL:HB	1:D:429:PRO:HD3	1.94	0.50
1:F:88:THR:HB	1:F:175:TRP:CZ3	2.47	0.50
1:F:221:SER:OG	1:F:222:ALA:N	2.44	0.50
1:F:253:SER:O	1:F:254:VAL:C	2.54	0.50
1:J:88:THR:CG2	1:J:295:LEU:HD22	2.41	0.50
1:J:393:LYS:C	1:J:395:LEU:H	2.19	0.50
1:L:257:LYS:HE2	1:L:316:GLN:CD	2.37	0.50
1:A:237:LYS:HE3	1:A:342:HIS:HB2	1.92	0.50
1:B:90:ASP:HB3	1:B:93:ALA:HB3	1.94	0.50
1:C:319:LEU:H	1:C:319:LEU:CD2	2.17	0.50
1:D:231:VAL:O	1:D:231:VAL:HG12	2.12	0.50
1:D:456:SER:HB3	1:D:460:LYS:HD3	1.93	0.50
1:E:260:ASP:OD2	1:E:263:PRO:HD3	2.12	0.50
1:F:220:GLU:HG3	1:F:472:LEU:HD21	1.93	0.50
1:J:540:LYS:O	1:J:544:VAL:HG23	2.11	0.50
1:L:255:LEU:HD23	1:L:318:LEU:HD11	1.93	0.50
1:B:317:PRO:CD	6:B:6020:HOH:O	2.53	0.50
1:E:495:MET:HE1	1:E:533:THR:HG21	1.93	0.50
1:F:382:LEU:HD11	1:F:391:ILE:HD12	1.94	0.50
1:G:149:ALA:HB2	1:G:168:ILE:O	2.12	0.50
1:I:34:LEU:HB2	1:I:77:VAL:HG12	1.94	0.50
1:I:89:GLN:HA	6:I:6167:HOH:O	2.12	0.50
1:I:351:ASN:ND2	1:I:449:PHE:HB3	2.26	0.50
1:J:253:SER:O	1:J:254:VAL:C	2.54	0.50
1:L:63:LEU:C	1:L:66:THR:HG23	2.36	0.50
1:L:447:TYR:HB3	1:L:517:TRP:CZ2	2.47	0.50
1:C:293:GLU:O	1:C:296:GLU:HB2	2.12	0.50
1:D:186:ARG:HD3	1:D:324:ASP:HB2	1.94	0.50
1:E:221:SER:HB3	6:E:6472:HOH:O	2.11	0.50
1:H:49:ILE:HD13	1:H:122:TYR:HE2	1.76	0.50
1:H:87:CYS:HB3	6:H:6375:HOH:O	2.12	0.50
1:H:355:PHE:CE1	1:H:360:PRO:HG3	2.47	0.50
1:I:417:PHE:O	1:I:420:LEU:HB3	2.12	0.50
1:I:421:ILE:HG22	1:I:425:MET:HE2	1.93	0.50
1:K:252:THR:HG22	1:K:254:VAL:CG1	2.41	0.50
1:K:267:GLN:HE22	1:K:316:GLN:HG2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:CG2	1:A:295:LEU:HD13	2.40	0.49
1:A:461:PRO:HB2	1:A:463:THR:HG22	1.94	0.49
1:B:123:THR:HB	1:B:164:VAL:HG13	1.94	0.49
1:C:143:GLY:O	1:C:144:LEU:HB2	2.11	0.49
1:D:24:PRO:HG3	1:D:37:PHE:CZ	2.46	0.49
1:D:257:LYS:HB2	1:D:322:VAL:HG12	1.94	0.49
1:D:359:ILE:HB	1:D:360:PRO:CD	2.38	0.49
1:D:521:ASN:HD21	1:D:523:LYS:HD3	1.77	0.49
1:E:177:PHE:HB3	1:E:319:LEU:O	2.12	0.49
1:I:41:GLU:OE1	1:I:41:GLU:N	2.40	0.49
1:J:295:LEU:O	1:J:298:THR:HB	2.12	0.49
1:J:381:LEU:HD22	1:J:417:PHE:CE2	2.47	0.49
1:L:357:TRP:O	1:L:360:PRO:HD2	2.11	0.49
1:A:503:PHE:O	1:A:507:GLY:N	2.45	0.49
1:B:447:TYR:HB3	1:B:517:TRP:HZ2	1.77	0.49
1:F:368:LEU:HD13	1:F:418:LEU:HD21	1.94	0.49
1:H:121:ILE:HG12	1:H:166:VAL:HG22	1.93	0.49
1:I:349:GLY:HA3	1:I:447:TYR:CE1	2.47	0.49
1:J:99:GLU:HA	1:J:107:ASN:ND2	2.27	0.49
1:J:241:HIS:O	1:J:345:PRO:HD2	2.12	0.49
1:A:219:GLY:N	1:A:227:VAL:HG21	2.27	0.49
1:A:366:TYR:HD2	1:A:368:LEU:HG	1.76	0.49
1:C:392:ALA:HB3	1:C:395:LEU:HG	1.94	0.49
1:E:143:GLY:N	6:E:6469:HOH:O	2.40	0.49
1:F:57:LYS:CB	1:F:57:LYS:CD	2.77	0.49
1:F:257:LYS:HE2	1:F:316:GLN:NE2	2.27	0.49
1:F:546:PHE:O	1:F:549:ASN:HB2	2.13	0.49
1:H:129:LYS:HD2	6:H:6358:HOH:O	2.12	0.49
1:H:420:LEU:HD13	1:H:420:LEU:C	2.37	0.49
1:I:251:LEU:HD11	1:I:336:GLN:OE1	2.12	0.49
1:I:355:PHE:CE1	1:I:360:PRO:HG3	2.48	0.49
1:K:136:MET:HB3	1:K:218:PHE:CE1	2.48	0.49
1:K:242:ARG:HH11	1:K:242:ARG:CG	2.25	0.49
1:L:539:LEU:C	1:L:541:ASP:H	2.20	0.49
1:C:228:SER:O	1:C:232:LEU:HG	2.13	0.49
1:D:194:GLN:O	1:D:197:ALA:HB3	2.13	0.49
1:E:254:VAL:O	1:E:254:VAL:HG22	2.12	0.49
1:H:249:VAL:HB	1:H:433:VAL:HG21	1.93	0.49
1:H:350:ILE:O	1:H:448:GLU:HA	2.13	0.49
1:I:389:VAL:HB	1:I:424:VAL:HG11	1.93	0.49
1:K:487:GLU:HG3	1:K:491:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:252:THR:HG22	1:L:254:VAL:HG12	1.94	0.49
1:D:59:PRO:HD3	1:D:117:LEU:CD1	2.42	0.49
1:F:254:VAL:HG13	1:F:255:LEU:H	1.77	0.49
1:G:89:GLN:OE1	1:G:146:VAL:HB	2.12	0.49
1:H:34:LEU:C	1:H:34:LEU:HD13	2.38	0.49
1:H:56:ALA:CB	1:H:117:LEU:HD13	2.42	0.49
1:H:339:ARG:HH22	1:H:439:ASP:HB3	1.77	0.49
1:H:413:LYS:O	1:H:416:LEU:N	2.45	0.49
1:I:262:LYS:HB3	1:I:263:PRO:HD3	1.93	0.49
1:J:355:PHE:CE1	1:J:360:PRO:HG3	2.48	0.49
1:K:211:ASN:C	1:K:213:GLY:H	2.21	0.49
1:L:215:VAL:H	1:L:241:HIS:CD2	2.31	0.49
1:B:423:ASP:OD1	1:B:540:LYS:HD2	2.13	0.49
1:E:236:ALA:HB1	1:E:240:PHE:CE1	2.42	0.49
1:E:428:VAL:HG13	1:E:544:VAL:HA	1.94	0.49
1:F:139:ILE:HG12	1:F:168:ILE:HD11	1.95	0.49
1:G:348:VAL:O	1:G:446:MET:HA	2.12	0.49
1:I:322:VAL:CG1	1:I:323:ILE:H	2.25	0.49
1:J:161:GLU:CD	1:J:498:LYS:HG2	2.37	0.49
1:J:257:LYS:HE3	1:J:316:GLN:HE22	1.78	0.49
1:J:447:TYR:C	1:J:447:TYR:CD2	2.91	0.49
1:L:262:LYS:HE3	1:L:282:MET:HE1	1.95	0.49
1:A:151:THR:HG22	1:A:152:TYR:CD1	2.48	0.49
1:A:355:PHE:CE1	1:A:360:PRO:HG3	2.47	0.49
1:A:357:TRP:CZ2	1:A:361:MET:HG3	2.48	0.49
1:D:223:GLY:O	1:D:227:VAL:HG23	2.13	0.49
1:D:311:ASP:HB3	1:D:314:GLU:HG2	1.94	0.49
1:D:492:LEU:O	1:D:496:VAL:HG23	2.12	0.49
1:F:425:MET:HE3	1:F:426:PHE:CE1	2.47	0.49
1:H:323:ILE:CD1	1:H:331:THR:HA	2.42	0.49
1:J:64:ARG:O	1:J:65:PHE:HB2	2.13	0.49
1:L:25:VAL:HG22	1:L:34:LEU:CD2	2.31	0.49
1:L:178:PHE:O	1:L:178:PHE:CD1	2.65	0.49
1:L:236:ALA:HB1	1:L:240:PHE:HE1	1.77	0.49
1:D:79:ASN:O	3:D:2180:SIA:O7	2.28	0.49
1:E:357:TRP:CZ2	1:E:361:MET:HG3	2.47	0.49
1:G:121:ILE:HD11	1:G:200:TRP:HZ3	1.77	0.49
1:H:351:ASN:N	1:H:351:ASN:ND2	2.60	0.49
1:J:222:ALA:O	1:J:226:SER:OG	2.31	0.49
1:J:254:VAL:HG13	1:J:255:LEU:N	2.28	0.49
1:L:24:PRO:HG3	1:L:37:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:ARG:O	1:L:65:PHE:CB	2.61	0.49
1:A:134:PRO:HD3	6:A:6314:HOH:O	2.11	0.49
1:C:90:ASP:OD1	1:C:92:LYS:HG3	2.13	0.49
1:C:527:LEU:HD11	1:C:533:THR:CG2	2.42	0.49
1:D:103:ASN:ND2	1:D:476:PHE:O	2.46	0.49
1:I:431:VAL:HG21	1:I:540:LYS:HB2	1.94	0.49
1:J:393:LYS:HA	1:J:396:ILE:HG12	1.93	0.49
1:A:550:LEU:C	1:A:552:ALA:H	2.21	0.49
1:B:126:ASP:H	1:B:131:ASN:ND2	2.10	0.49
1:E:228:SER:O	1:E:231:VAL:HB	2.13	0.49
1:E:414:LYS:O	1:E:417:PHE:HB3	2.13	0.49
1:G:343:THR:HA	6:G:6372:HOH:O	2.13	0.49
1:H:423:ASP:OD2	1:H:543:GLU:HG2	2.13	0.49
1:K:372:GLN:HG3	1:K:410:THR:HB	1.95	0.49
1:A:103:ASN:ND2	1:A:476:PHE:O	2.46	0.48
1:A:461:PRO:C	1:A:463:THR:H	2.21	0.48
1:A:499:PHE:CE2	1:A:514:LEU:HB3	2.48	0.48
1:C:348:VAL:O	1:C:446:MET:HA	2.13	0.48
1:C:371:GLY:HA2	1:C:414:LYS:NZ	2.28	0.48
1:E:447:TYR:HB3	1:E:517:TRP:CZ2	2.48	0.48
1:F:111:LYS:HG3	6:F:6052:HOH:O	2.12	0.48
1:F:145:MET:HE2	1:F:303:PHE:CB	2.43	0.48
1:F:495:MET:CE	1:F:533:THR:HG21	2.43	0.48
1:H:87:CYS:O	1:H:88:THR:C	2.56	0.48
1:I:450:GLN:NE2	6:I:6101:HOH:O	2.43	0.48
1:L:447:TYR:C	1:L:447:TYR:CD2	2.91	0.48
1:B:113:SER:HB2	1:C:277:THR:HG21	1.94	0.48
1:D:176:GLY:HA2	1:D:189:TRP:HB2	1.95	0.48
1:D:283:VAL:O	1:D:287:ARG:HG3	2.13	0.48
1:E:425:MET:HE3	1:E:426:PHE:HE1	1.78	0.48
1:G:121:ILE:HD11	1:G:200:TRP:CZ3	2.48	0.48
1:H:58:PRO:O	1:H:60:LEU:N	2.44	0.48
1:H:140:HIS:C	1:H:140:HIS:CD2	2.91	0.48
1:H:349:GLY:HA3	1:H:447:TYR:CD1	2.48	0.48
1:J:86:MET:CB	1:J:148:ALA:HB2	2.43	0.48
1:L:311:ASP:HB3	1:L:314:GLU:OE1	2.13	0.48
1:D:372:GLN:HG3	1:D:410:THR:HB	1.95	0.48
1:E:312:PRO:HG2	1:E:383:TRP:NE1	2.28	0.48
1:F:355:PHE:CD1	1:F:360:PRO:HG3	2.48	0.48
1:G:199:ARG:HG2	1:G:199:ARG:NH1	2.28	0.48
1:G:456:SER:CB	1:G:460:LYS:HE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:495:MET:HE1	1:I:533:THR:HG21	1.94	0.48
1:K:491:ARG:HH11	1:K:491:ARG:HG3	1.78	0.48
1:L:353:GLN:HE22	1:L:465:ILE:H	1.61	0.48
1:B:60:LEU:CD2	1:B:114:GLU:HB3	2.43	0.48
1:B:218:PHE:N	1:B:218:PHE:CD1	2.81	0.48
1:D:131:ASN:O	1:D:209:GLY:HA2	2.13	0.48
1:D:449:PHE:CE2	1:D:471:GLU:HA	2.49	0.48
1:F:45:GLN:NE2	6:F:6068:HOH:O	2.46	0.48
1:F:134:PRO:CG	1:F:163:VAL:HG12	2.40	0.48
1:F:348:VAL:O	1:F:446:MET:HA	2.13	0.48
1:F:486:SER:O	1:F:490:ILE:HG13	2.13	0.48
1:G:452:ARG:HG2	1:G:452:ARG:NH1	2.27	0.48
1:I:450:GLN:HB2	6:I:6101:HOH:O	2.13	0.48
1:J:467:ASP:N	1:J:470:ASP:OD2	2.44	0.48
1:K:404:LEU:H	1:K:404:LEU:HD12	1.79	0.48
1:K:540:LYS:O	1:K:544:VAL:HG23	2.13	0.48
1:L:139:ILE:O	1:L:223:GLY:HA3	2.13	0.48
1:A:351:ASN:N	1:A:354:GLU:OE2	2.46	0.48
1:B:392:ALA:HB3	1:B:395:LEU:CD1	2.44	0.48
1:B:478:ALA:N	1:B:479:PRO:CD	2.77	0.48
1:C:27:ASP:CG	1:C:32:LYS:HG2	2.39	0.48
1:C:456:SER:HB3	1:C:460:LYS:HE2	1.94	0.48
1:D:85:PRO:HA	6:D:6246:HOH:O	2.13	0.48
1:D:91:PRO:HB3	1:D:112:LEU:HD11	1.95	0.48
1:E:254:VAL:O	1:E:318:LEU:HD11	2.14	0.48
1:J:86:MET:HB3	1:J:148:ALA:HB2	1.95	0.48
1:J:392:ALA:HB3	1:J:395:LEU:HD12	1.95	0.48
3:J:1082:SIA:H4	1:K:262:LYS:HZ1	1.74	0.48
1:K:427:GLY:O	1:K:431:VAL:HG23	2.13	0.48
1:K:471:GLU:OE1	1:K:471:GLU:N	2.46	0.48
1:L:160:HIS:NE2	1:L:480:PHE:CD2	2.81	0.48
1:L:199:ARG:O	1:L:202:GLN:HB2	2.13	0.48
1:L:379:MET:HE1	1:L:397:PRO:CG	2.28	0.48
1:C:409:ASP:OD2	1:C:412:LYS:HE2	2.13	0.48
1:D:204:ASN:O	1:D:205:ILE:C	2.57	0.48
1:D:447:TYR:HB3	1:D:517:TRP:CZ2	2.48	0.48
1:I:316:GLN:OE1	1:I:317:PRO:HD2	2.14	0.48
1:B:24:PRO:C	1:B:24:PRO:HB2	2.37	0.48
1:B:218:PHE:HB3	1:B:244:ILE:HB	1.96	0.48
1:C:246:GLU:HG2	1:C:447:TYR:OH	2.14	0.48
1:E:521:ASN:HB2	1:E:522:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:SER:C	1:G:371:GLY:H	2.22	0.48
1:J:242:ARG:HG2	1:J:242:ARG:HH11	1.78	0.48
1:K:526:TYR:CE1	1:K:539:LEU:HD13	2.49	0.48
1:L:301:MET:HE3	1:L:303:PHE:CZ	2.49	0.48
1:G:176:GLY:O	1:G:189:TRP:HB2	2.14	0.48
1:G:369:SER:C	1:G:371:GLY:N	2.72	0.48
1:H:253:SER:O	1:H:254:VAL:C	2.56	0.48
1:I:447:TYR:HB3	1:I:517:TRP:CZ2	2.49	0.48
1:K:206:ALA:HA	1:K:210:GLY:O	2.14	0.48
1:L:353:GLN:NE2	1:L:465:ILE:H	2.11	0.48
1:A:138:TRP:CD2	1:A:476:PHE:HZ	2.32	0.48
1:A:264:LEU:O	1:A:268:ILE:HG13	2.14	0.48
1:A:519:GLU:O	1:A:521:ASN:N	2.42	0.48
1:C:304:LEU:HD11	5:C:5013:BEZ:H5	1.96	0.48
1:D:417:PHE:O	1:D:420:LEU:HB3	2.13	0.48
1:E:218:PHE:HB3	1:E:244:ILE:HB	1.95	0.48
1:E:527:LEU:HD23	1:E:529:ILE:CG1	2.44	0.48
1:E:527:LEU:HD23	1:E:529:ILE:HG12	1.95	0.48
1:F:495:MET:HE1	1:F:533:THR:OG1	2.13	0.48
1:G:107:ASN:ND2	1:G:108:ILE:N	2.62	0.48
1:G:122:TYR:HB2	1:G:165:VAL:HB	1.96	0.48
1:H:330:LYS:HG3	1:H:335:LEU:CD2	2.43	0.48
1:K:40:LEU:O	1:K:41:GLU:C	2.57	0.48
1:K:257:LYS:NZ	1:K:317:PRO:HB3	2.28	0.48
1:K:325:GLY:HA2	1:K:329:LEU:HA	1.96	0.48
1:L:53:ILE:HG21	1:L:200:TRP:CZ2	2.49	0.48
1:L:374:ASP:OD2	1:L:376:LYS:HB2	2.13	0.48
1:B:191:HIS:HB3	1:B:327:LEU:HD11	1.95	0.48
3:B:1280:SIA:H113	1:C:262:LYS:HZ3	1.78	0.48
1:D:34:LEU:HB3	1:D:79:ASN:CB	2.42	0.48
1:D:90:ASP:HB3	1:D:93:ALA:HB3	1.96	0.48
1:D:194:GLN:O	1:D:195:VAL:C	2.56	0.48
1:E:380:SER:O	1:E:383:TRP:HB3	2.13	0.48
1:F:88:THR:CG2	1:F:295:LEU:HD22	2.44	0.48
1:F:452:ARG:NE	1:F:462:LYS:HA	2.29	0.48
1:F:476:PHE:O	1:F:477:GLY:C	2.56	0.48
1:H:220:GLU:HA	1:H:246:GLU:O	2.12	0.48
1:H:333:GLU:CD	1:H:333:GLU:H	2.21	0.48
1:J:134:PRO:CG	1:J:163:VAL:HG12	2.34	0.48
1:L:407:THR:C	1:L:409:ASP:H	2.21	0.48
1:A:68:PRO:HG3	1:A:193:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:HD22	1:B:476:PHE:HB3	1.79	0.47
1:B:119:LEU:C	1:B:119:LEU:HD12	2.39	0.47
1:C:140:HIS:HD2	1:C:141:GLY:O	1.97	0.47
1:D:317:PRO:HG2	1:D:318:LEU:H	1.79	0.47
1:G:191:HIS:NE2	1:G:321:THR:OG1	2.41	0.47
1:H:215:VAL:N	1:H:241:HIS:HD2	2.11	0.47
1:I:55:PHE:CE1	1:I:197:ALA:HB2	2.49	0.47
1:I:428:VAL:N	1:I:429:PRO:CD	2.77	0.47
1:J:268:ILE:HG12	1:J:301:MET:CE	2.35	0.47
1:L:202:GLN:HG2	6:L:6395:HOH:O	2.14	0.47
1:A:461:PRO:HG2	1:A:464:VAL:HG23	1.96	0.47
1:B:211:ASN:HD22	1:B:214:SER:CB	2.26	0.47
1:C:452:ARG:NE	1:C:462:LYS:HA	2.29	0.47
1:E:184:HIS:O	1:E:185:SER:HB2	2.14	0.47
1:E:321:THR:HG22	1:E:322:VAL:N	2.28	0.47
1:G:316:GLN:NE2	1:G:316:GLN:HA	2.29	0.47
1:H:180:THR:HG22	1:H:282:MET:HE3	1.96	0.47
1:H:215:VAL:H	1:H:241:HIS:CD2	2.32	0.47
1:H:262:LYS:N	1:H:263:PRO:CD	2.78	0.47
1:H:532:ASN:ND2	1:H:532:ASN:N	2.60	0.47
1:I:28:THR:HG23	1:I:31:GLY:O	2.14	0.47
1:I:357:TRP:O	1:I:360:PRO:HD2	2.14	0.47
1:I:385:SER:C	1:I:387:PRO:HD2	2.38	0.47
1:J:312:PRO:HG2	1:J:383:TRP:CE2	2.50	0.47
1:K:59:PRO:HD3	1:K:117:LEU:HD12	1.96	0.47
1:L:498:LYS:CD	6:L:6137:HOH:O	2.59	0.47
1:D:172:LEU:HB2	6:D:6033:HOH:O	2.14	0.47
1:D:319:LEU:HG	1:D:319:LEU:O	2.13	0.47
1:D:381:LEU:HA	1:D:384:LYS:HD2	1.95	0.47
1:F:540:LYS:O	1:F:544:VAL:HG23	2.13	0.47
1:H:171:ARG:HB3	1:H:176:GLY:CA	2.44	0.47
1:H:194:GLN:HE22	1:H:226:SER:CB	2.26	0.47
1:B:453:PRO:HG2	1:B:456:SER:OG	2.14	0.47
1:C:228:SER:CB	1:C:250:ALA:H	2.27	0.47
1:D:283:VAL:HG12	1:D:287:ARG:NH1	2.28	0.47
1:E:33:VAL:CG1	1:E:34:LEU:N	2.78	0.47
1:F:420:LEU:HD22	1:F:547:TRP:HZ2	1.79	0.47
1:G:56:ALA:C	1:G:71:ALA:HB2	2.39	0.47
1:H:34:LEU:HD13	1:H:35:GLY:N	2.28	0.47
1:I:217:ILE:O	1:I:243:ALA:HA	2.15	0.47
1:I:414:LYS:O	1:I:417:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:LEU:HD21	1:J:193:ASP:OD2	2.14	0.47
1:K:386:TYR:C	1:K:388:LEU:H	2.23	0.47
1:B:132:ARG:HG3	1:B:211:ASN:HB2	1.97	0.47
1:D:495:MET:HE3	1:D:515:PRO:HD2	1.96	0.47
1:E:149:ALA:HB2	1:E:168:ILE:O	2.15	0.47
1:F:145:MET:HE2	1:F:303:PHE:HB2	1.96	0.47
1:G:264:LEU:CD1	1:G:316:GLN:HG2	2.44	0.47
1:J:88:THR:HA	1:J:112:LEU:HD22	1.97	0.47
1:J:403:TYR:CG	1:J:420:LEU:HD23	2.49	0.47
1:J:421:ILE:HG22	1:J:425:MET:HE2	1.97	0.47
1:K:78:LYS:HE2	1:L:182:ASP:HB3	1.97	0.47
1:K:97:LEU:HG	1:K:101:PHE:CD2	2.50	0.47
1:A:40:LEU:O	1:A:41:GLU:C	2.58	0.47
1:A:225:GLU:O	1:A:229:VAL:HG23	2.14	0.47
1:B:185:SER:HA	6:B:6123:HOH:O	2.14	0.47
1:D:23:PRO:HA	1:D:24:PRO:HD3	1.77	0.47
1:D:297:THR:O	1:D:301:MET:HG2	2.13	0.47
1:E:28:THR:HG23	1:E:31:GLY:O	2.14	0.47
1:E:487:GLU:HA	1:E:490:ILE:HD12	1.96	0.47
1:G:450:GLN:HG2	1:G:450:GLN:O	2.13	0.47
1:I:34:LEU:HD22	1:I:34:LEU:HA	1.61	0.47
1:I:241:HIS:C	1:I:242:ARG:CG	2.88	0.47
1:L:316:GLN:HE21	1:L:316:GLN:HA	1.79	0.47
1:L:453:PRO:HG2	1:L:456:SER:HG	1.76	0.47
3:L:1282:SIA:H113	3:L:1282:SIA:H31	1.95	0.47
1:A:95:GLN:O	1:A:99:GLU:HG3	2.15	0.47
1:D:409:ASP:O	1:D:413:LYS:HG3	2.15	0.47
1:D:426:PHE:CD1	1:D:426:PHE:N	2.82	0.47
1:E:113:SER:HB2	1:F:277:THR:HG21	1.95	0.47
1:E:136:MET:HA	1:E:216:THR:O	2.15	0.47
1:E:276:THR:O	1:E:277:THR:C	2.57	0.47
1:F:499:PHE:CE2	1:F:514:LEU:HD13	2.50	0.47
1:I:34:LEU:HD13	1:I:35:GLY:N	2.30	0.47
1:I:220:GLU:HA	1:I:246:GLU:O	2.15	0.47
1:I:242:ARG:NH1	1:I:242:ARG:CG	2.72	0.47
1:I:264:LEU:O	1:I:268:ILE:HG13	2.13	0.47
1:I:495:MET:HE1	1:I:533:THR:CB	2.45	0.47
1:J:55:PHE:O	1:J:56:ALA:HB2	2.13	0.47
1:J:103:ASN:O	1:J:482:LYS:HG3	2.14	0.47
1:K:26:VAL:CG1	1:K:207:SER:HB3	2.44	0.47
1:K:312:PRO:HG2	1:K:383:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:447:TYR:HB3	1:K:517:TRP:CZ2	2.50	0.47
3:K:1182:SIA:C7	3:K:1182:SIA:O2	2.62	0.47
1:L:262:LYS:HE3	1:L:282:MET:HE2	1.96	0.47
1:L:286:LEU:HD23	1:L:286:LEU:HA	1.70	0.47
1:B:266:GLU:HG2	1:B:282:MET:CE	2.45	0.47
1:C:403:TYR:CD1	1:C:420:LEU:HD23	2.49	0.47
3:D:2180:SIA:H111	1:E:278:THR:HG22	1.96	0.47
1:E:242:ARG:HH11	1:E:242:ARG:CG	2.28	0.47
1:E:495:MET:HE3	1:E:499:PHE:CE1	2.50	0.47
1:G:306:LEU:HD22	1:G:366:TYR:CE1	2.49	0.47
1:G:438:ARG:HH12	1:G:524:GLU:HG2	1.80	0.47
1:H:487:GLU:HG3	1:H:491:ARG:HD2	1.97	0.47
1:I:199:ARG:HG2	1:I:199:ARG:HH11	1.80	0.47
1:I:478:ALA:N	1:I:479:PRO:CD	2.78	0.47
1:J:461:PRO:HB2	6:J:6348:HOH:O	2.14	0.47
1:K:237:LYS:HE3	1:K:342:HIS:HB2	1.97	0.47
1:L:211:ASN:C	1:L:213:GLY:H	2.23	0.47
1:L:428:VAL:N	1:L:429:PRO:CD	2.77	0.47
1:A:138:TRP:HH2	1:A:220:GLU:HB2	1.80	0.47
1:A:382:LEU:HB2	1:A:417:PHE:HE1	1.80	0.47
1:B:467:ASP:CG	1:B:468:HIS:H	2.21	0.47
1:C:138:TRP:CZ3	1:C:219:GLY:HA2	2.50	0.47
1:C:540:LYS:O	1:C:544:VAL:HG23	2.15	0.47
1:G:121:ILE:HG12	1:G:166:VAL:HG13	1.97	0.47
1:H:330:LYS:HG3	1:H:335:LEU:HD21	1.97	0.47
1:H:413:LYS:O	1:H:414:LYS:C	2.58	0.47
1:H:413:LYS:O	1:H:416:LEU:HB2	2.14	0.47
1:L:304:LEU:O	1:L:364:MET:HE3	2.14	0.47
1:L:312:PRO:HD2	1:L:383:TRP:CZ2	2.50	0.47
1:L:495:MET:HE1	1:L:533:THR:CB	2.45	0.47
1:A:198:LEU:HB3	1:A:239:LEU:HB3	1.97	0.47
1:D:395:LEU:HD22	1:D:550:LEU:CD1	2.44	0.47
1:D:487:GLU:OE2	1:D:491:ARG:HG2	2.15	0.47
1:E:290:THR:HG23	1:E:293:GLU:OE2	2.15	0.47
1:F:225:GLU:O	1:F:225:GLU:HG2	2.14	0.47
1:G:86:MET:HG3	1:G:112:LEU:HD23	1.95	0.47
1:G:431:VAL:HG22	1:G:446:MET:CE	2.43	0.47
1:G:461:PRO:HG2	1:G:464:VAL:CG2	2.45	0.47
1:H:278:THR:O	1:H:282:MET:HG3	2.15	0.47
1:H:383:TRP:C	1:H:385:SER:N	2.71	0.47
1:I:142:GLY:HA3	1:I:146:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:325:GLY:O	1:I:329:LEU:HD23	2.15	0.47
1:I:526:TYR:CE2	1:I:536:ALA:HB3	2.50	0.47
1:J:258:LYS:HA	6:J:6129:HOH:O	2.14	0.47
1:L:242:ARG:HG2	1:L:242:ARG:NH1	2.24	0.47
1:L:478:ALA:N	1:L:479:PRO:CD	2.78	0.47
1:A:78:LYS:HE3	1:B:183:GLU:OE2	2.16	0.46
1:A:383:TRP:C	1:A:385:SER:H	2.21	0.46
1:A:386:TYR:N	1:A:387:PRO:CD	2.78	0.46
1:A:540:LYS:O	1:A:544:VAL:HG23	2.15	0.46
1:E:59:PRO:HD3	1:E:117:LEU:HD12	1.97	0.46
1:E:227:VAL:O	1:E:228:SER:C	2.56	0.46
1:F:350:ILE:O	1:F:448:GLU:HA	2.15	0.46
1:F:396:ILE:HB	1:F:397:PRO:HD3	1.96	0.46
1:F:431:VAL:HG21	1:F:540:LYS:HB2	1.96	0.46
1:F:477:GLY:HA2	1:F:493:SER:OG	2.15	0.46
1:G:332:PRO:O	1:G:336:GLN:HG2	2.15	0.46
1:H:491:ARG:HH11	1:H:491:ARG:HG3	1.80	0.46
1:J:45:GLN:NE2	1:J:46:PRO:HD2	2.30	0.46
1:K:142:GLY:O	1:K:144:LEU:N	2.48	0.46
1:K:257:LYS:HE2	1:K:257:LYS:CA	2.40	0.46
1:K:290:THR:OG1	1:K:293:GLU:HG3	2.14	0.46
1:K:317:PRO:C	1:K:318:LEU:HD13	2.40	0.46
1:L:64:ARG:HH11	1:L:294:LEU:CD1	2.28	0.46
1:L:141:GLY:HA2	1:L:223:GLY:H	1.80	0.46
1:L:143:GLY:N	6:L:6474:HOH:O	2.43	0.46
1:L:480:PHE:N	1:L:480:PHE:CD1	2.82	0.46
1:A:241:HIS:CD2	1:A:241:HIS:N	2.83	0.46
1:C:97:LEU:HD22	1:C:146:VAL:HG23	1.97	0.46
1:D:395:LEU:HD22	1:D:550:LEU:HD12	1.98	0.46
1:E:383:TRP:C	1:E:385:SER:H	2.23	0.46
1:F:222:ALA:HA	1:F:255:LEU:HD11	1.98	0.46
1:G:218:PHE:CB	1:G:244:ILE:HB	2.44	0.46
1:G:428:VAL:HG13	1:G:544:VAL:HG22	1.97	0.46
1:H:340:ASN:HD22	1:H:340:ASN:N	2.12	0.46
1:I:121:ILE:HD11	1:I:200:TRP:CZ3	2.50	0.46
1:J:59:PRO:C	1:J:60:LEU:HD23	2.40	0.46
1:K:278:THR:HG23	1:K:281:VAL:CG2	2.46	0.46
1:L:105:LYS:HG3	1:L:106:GLU:N	2.31	0.46
1:L:525:GLY:HA2	1:L:537:GLN:HA	1.97	0.46
3:A:1181:SIA:C7	6:A:6003:HOH:O	2.63	0.46
1:B:264:LEU:O	1:B:264:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:C	1:C:195:VAL:N	2.72	0.46
1:C:381:LEU:HB3	1:C:417:PHE:CZ	2.51	0.46
1:C:396:ILE:HB	1:C:397:PRO:HD3	1.97	0.46
1:C:478:ALA:C	1:C:480:PHE:H	2.23	0.46
1:E:218:PHE:HA	1:E:244:ILE:O	2.15	0.46
1:E:218:PHE:HB2	1:E:244:ILE:HB	1.97	0.46
1:E:242:ARG:HD3	1:E:503:PHE:O	2.16	0.46
1:F:179:SER:HB2	1:F:187:GLY:HA3	1.96	0.46
1:G:72:GLU:HB3	6:G:6098:HOH:O	2.15	0.46
1:G:190:GLY:O	1:G:193:ASP:HB2	2.15	0.46
1:G:236:ALA:HB1	1:G:240:PHE:HE1	1.80	0.46
1:G:242:ARG:HG2	1:G:242:ARG:NH1	2.24	0.46
1:H:84:PRO:HA	1:H:85:PRO:HD3	1.79	0.46
1:J:104:ARG:HD2	1:J:108:ILE:HG12	1.97	0.46
1:J:252:THR:O	1:J:253:SER:C	2.57	0.46
1:J:453:PRO:HG2	1:J:456:SER:OG	2.15	0.46
1:K:180:THR:HB	1:K:279:SER:OG	2.15	0.46
1:L:220:GLU:C	1:L:224:GLY:H	2.23	0.46
1:L:256:VAL:O	1:L:256:VAL:HG12	2.15	0.46
1:L:428:VAL:CG1	1:L:544:VAL:HG13	2.46	0.46
1:B:381:LEU:O	1:B:382:LEU:C	2.58	0.46
1:B:469:GLY:O	1:B:470:ASP:C	2.58	0.46
1:E:132:ARG:HG2	1:E:132:ARG:HH11	1.80	0.46
1:E:191:HIS:CD2	1:E:321:THR:HG23	2.50	0.46
1:E:438:ARG:HD2	1:E:521:ASN:HA	1.97	0.46
1:G:132:ARG:CB	1:G:211:ASN:HB2	2.45	0.46
1:G:427:GLY:O	1:G:428:VAL:C	2.57	0.46
1:I:257:LYS:CG	1:I:316:GLN:HE22	2.22	0.46
1:J:179:SER:HA	1:J:185:SER:O	2.15	0.46
1:J:357:TRP:O	1:J:358:LEU:C	2.58	0.46
1:K:178:PHE:CZ	1:K:286:LEU:HD12	2.50	0.46
1:K:201:VAL:HG13	1:K:205:ILE:HB	1.97	0.46
1:K:251:LEU:O	1:K:253:SER:N	2.49	0.46
1:L:403:TYR:CE2	1:L:420:LEU:HA	2.50	0.46
1:A:101:PHE:O	1:A:102:THR:C	2.59	0.46
1:A:406:GLY:O	1:A:407:THR:C	2.58	0.46
1:C:135:VAL:CG2	1:C:205:ILE:HG12	2.45	0.46
1:D:57:LYS:HD3	1:D:63:LEU:HD11	1.96	0.46
1:F:316:GLN:HA	1:F:316:GLN:NE2	2.30	0.46
1:F:318:LEU:HD12	1:F:318:LEU:O	2.15	0.46
1:G:385:SER:C	1:G:387:PRO:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:LEU:HD12	1:I:251:LEU:N	2.29	0.46
1:I:292:GLU:HG3	1:I:293:GLU:N	2.31	0.46
1:J:261:VAL:O	1:J:262:LYS:C	2.59	0.46
1:J:364:MET:HE1	1:J:388:LEU:HD11	1.97	0.46
1:L:400:THR:HG22	1:L:404:LEU:CD1	2.45	0.46
1:A:499:PHE:HE2	1:A:514:LEU:HB3	1.81	0.46
1:C:25:VAL:HG22	1:C:34:LEU:HD23	1.97	0.46
1:C:386:TYR:N	1:C:387:PRO:CD	2.78	0.46
1:D:65:PHE:O	1:D:66:THR:CG2	2.63	0.46
1:D:254:VAL:HG13	1:D:255:LEU:HD12	1.96	0.46
1:D:480:PHE:CD1	1:D:480:PHE:N	2.83	0.46
1:F:135:VAL:CG2	1:F:205:ILE:HG12	2.41	0.46
1:F:487:GLU:HG3	1:F:491:ARG:NH2	2.31	0.46
1:H:452:ARG:HG2	1:H:452:ARG:HH11	1.79	0.46
1:I:526:TYR:CD2	1:I:539:LEU:HB2	2.51	0.46
1:J:316:GLN:NE2	1:J:317:PRO:HD2	2.30	0.46
1:K:96:LEU:O	1:K:100:LEU:HD12	2.15	0.46
1:K:499:PHE:CE2	1:K:514:LEU:HD22	2.51	0.46
1:A:264:LEU:HD22	1:A:268:ILE:CD1	2.46	0.46
1:A:367:PRO:HB2	1:A:381:LEU:HD11	1.96	0.46
1:A:467:ASP:HB3	1:A:470:ASP:OD2	2.16	0.46
1:B:253:SER:O	1:B:254:VAL:C	2.58	0.46
1:C:101:PHE:CE1	1:C:358:LEU:HD21	2.51	0.46
1:D:87:CYS:O	1:D:88:THR:C	2.57	0.46
1:D:311:ASP:HB3	1:D:314:GLU:CG	2.45	0.46
1:D:372:GLN:HB2	1:D:410:THR:O	2.14	0.46
1:D:467:ASP:CG	1:D:468:HIS:N	2.73	0.46
1:D:549:ASN:O	1:D:550:LEU:C	2.58	0.46
1:E:87:CYS:HB3	6:E:6367:HOH:O	2.15	0.46
1:E:355:PHE:CE2	1:E:421:ILE:HG21	2.51	0.46
1:F:242:ARG:HD3	1:F:503:PHE:O	2.16	0.46
1:F:526:TYR:CE2	1:F:539:LEU:HB2	2.50	0.46
1:G:261:VAL:O	1:G:262:LYS:C	2.59	0.46
1:G:447:TYR:C	1:G:447:TYR:CD2	2.94	0.46
1:G:453:PRO:HG2	1:G:456:SER:OG	2.15	0.46
1:H:24:PRO:O	1:H:34:LEU:HD22	2.15	0.46
1:I:137:VAL:HA	1:I:166:VAL:O	2.16	0.46
1:I:287:ARG:HD2	4:I:3285:SO4:O3	2.16	0.46
1:I:358:LEU:O	1:I:363:LEU:HG	2.16	0.46
1:I:524:GLU:OE2	1:I:538:LYS:HG2	2.16	0.46
1:J:119:LEU:HD12	1:J:119:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:242:ARG:CG	1:K:242:ARG:NH1	2.79	0.46
1:L:186:ARG:HB3	1:L:324:ASP:HB2	1.96	0.46
1:L:380:SER:O	1:L:383:TRP:HB3	2.15	0.46
1:A:368:LEU:HD11	1:A:418:LEU:HD21	1.98	0.46
1:A:524:GLU:OE2	1:A:538:LYS:HG2	2.15	0.46
1:B:227:VAL:O	1:B:228:SER:C	2.59	0.46
1:C:55:PHE:CE1	1:C:197:ALA:HB2	2.51	0.46
1:C:89:GLN:OE1	1:C:146:VAL:HA	2.16	0.46
1:C:330:LYS:HB3	1:C:330:LYS:HE2	1.74	0.46
1:E:51:LEU:HD13	1:E:83:TYR:CE1	2.51	0.46
1:F:31:GLY:HA3	1:F:74:TRP:NE1	2.31	0.46
1:F:478:ALA:N	1:F:479:PRO:CD	2.79	0.46
1:I:343:THR:HB	1:I:442:ALA:CB	2.46	0.46
1:J:381:LEU:HD22	1:J:417:PHE:CZ	2.51	0.46
1:K:308:LEU:HD21	1:K:367:PRO:HG2	1.98	0.46
1:K:351:ASN:N	1:K:351:ASN:ND2	2.63	0.46
1:K:543:GLU:O	1:K:544:VAL:C	2.58	0.46
1:A:549:ASN:O	1:A:550:LEU:C	2.59	0.46
1:B:84:PRO:HA	1:B:85:PRO:HD3	1.80	0.46
1:B:104:ARG:HD2	1:B:108:ILE:HG12	1.98	0.46
1:C:101:PHE:CZ	1:C:358:LEU:HD21	2.51	0.46
1:D:156:ALA:O	1:D:159:ALA:N	2.49	0.46
1:D:320:GLY:O	1:D:322:VAL:HG13	2.15	0.46
1:E:363:LEU:C	1:E:365:SER:N	2.73	0.46
1:F:439:ASP:O	1:F:441:GLY:N	2.49	0.46
1:G:218:PHE:HA	1:G:244:ILE:O	2.16	0.46
1:H:38:VAL:HG21	1:H:49:ILE:HD12	1.97	0.46
1:J:88:THR:HB	1:J:175:TRP:CZ3	2.50	0.46
1:J:330:LYS:HG3	1:J:335:LEU:HG	1.98	0.46
1:K:221:SER:O	1:K:222:ALA:C	2.59	0.46
1:B:160:HIS:NE2	1:B:480:PHE:CD2	2.83	0.46
1:B:352:LYS:HD3	1:B:450:GLN:HG3	1.98	0.46
1:E:51:LEU:HD13	1:E:83:TYR:CD1	2.51	0.46
1:E:348:VAL:O	1:E:446:MET:HG2	2.16	0.46
1:E:359:ILE:HA	1:E:363:LEU:HD12	1.97	0.46
1:F:404:LEU:O	1:F:406:GLY:N	2.49	0.46
1:G:372:GLN:NE2	1:G:410:THR:OG1	2.49	0.46
1:I:135:VAL:HG21	1:I:205:ILE:HG12	1.98	0.46
1:J:140:HIS:CE1	1:J:170:TYR:CE1	3.03	0.46
1:J:421:ILE:O	1:J:425:MET:HG3	2.16	0.46
1:L:64:ARG:NH1	1:L:289:LYS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:CA	1:A:229:VAL:HG23	2.44	0.45
1:B:24:PRO:O	1:B:34:LEU:HD22	2.16	0.45
1:B:403:TYR:HB3	1:B:404:LEU:HD23	1.97	0.45
1:D:64:ARG:HG2	1:D:65:PHE:CE1	2.52	0.45
1:E:435:ARG:O	1:E:438:ARG:HB3	2.15	0.45
1:F:420:LEU:CD2	1:F:547:TRP:HZ2	2.29	0.45
1:G:23:PRO:HB2	1:G:34:LEU:HD21	1.97	0.45
1:G:425:MET:HE3	1:G:426:PHE:CE1	2.50	0.45
1:H:105:LYS:HG3	1:H:106:GLU:H	1.81	0.45
1:I:477:GLY:C	1:I:479:PRO:CD	2.89	0.45
1:I:494:LYS:HA	1:I:497:MET:HE3	1.97	0.45
1:J:59:PRO:HD3	1:J:117:LEU:CD1	2.46	0.45
1:L:318:LEU:HD12	1:L:318:LEU:O	2.16	0.45
1:L:495:MET:HE1	1:L:533:THR:OG1	2.17	0.45
1:A:184:HIS:O	1:A:283:VAL:HG21	2.16	0.45
1:B:332:PRO:C	1:B:334:GLU:H	2.25	0.45
1:C:107:ASN:ND2	1:C:108:ILE:H	2.14	0.45
1:H:30:HIS:HD2	6:H:6446:HOH:O	1.97	0.45
1:H:194:GLN:O	1:H:195:VAL:C	2.59	0.45
1:H:492:LEU:O	1:H:496:VAL:HG23	2.17	0.45
1:I:211:ASN:C	1:I:213:GLY:H	2.24	0.45
1:J:138:TRP:HH2	1:J:220:GLU:HB2	1.80	0.45
1:J:386:TYR:N	1:J:387:PRO:CD	2.79	0.45
1:K:171:ARG:HB3	1:K:176:GLY:HA3	1.99	0.45
1:L:112:LEU:O	1:L:113:SER:HB2	2.15	0.45
1:L:126:ASP:HB3	1:L:129:LYS:HG2	1.96	0.45
1:L:154:GLY:O	1:L:155:LEU:C	2.59	0.45
1:L:522:GLN:HB2	6:L:6288:HOH:O	2.16	0.45
1:B:420:LEU:HD21	1:B:547:TRP:CZ2	2.51	0.45
1:E:453:PRO:HG2	1:E:456:SER:OG	2.15	0.45
1:E:495:MET:CE	1:E:533:THR:HG21	2.46	0.45
1:G:197:ALA:O	1:G:201:VAL:HG23	2.16	0.45
1:H:161:GLU:CB	1:H:501:ALA:HB2	2.46	0.45
1:H:357:TRP:CZ2	1:H:361:MET:HG3	2.51	0.45
1:H:383:TRP:O	1:H:385:SER:N	2.50	0.45
1:I:404:LEU:HD22	1:I:413:LYS:O	2.15	0.45
1:J:349:GLY:HA3	1:J:447:TYR:CZ	2.51	0.45
1:K:161:GLU:HG3	1:K:501:ALA:HB2	1.98	0.45
1:L:386:TYR:C	1:L:388:LEU:H	2.24	0.45
1:A:173:GLY:O	1:A:174:ILE:C	2.57	0.45
1:A:324:ASP:OD2	1:A:325:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TRP:CH2	1:B:361:MET:HE2	2.52	0.45
1:B:547:TRP:O	1:B:551:PHE:HB2	2.17	0.45
1:E:133:LEU:HD12	1:E:209:GLY:O	2.16	0.45
1:H:221:SER:O	1:H:222:ALA:C	2.59	0.45
1:H:426:PHE:O	1:H:427:GLY:C	2.58	0.45
1:I:25:VAL:HG22	1:I:34:LEU:HD23	1.95	0.45
1:L:90:ASP:HB3	1:L:93:ALA:HB3	1.99	0.45
1:L:435:ARG:O	1:L:438:ARG:HB3	2.16	0.45
1:L:539:LEU:C	1:L:541:ASP:N	2.73	0.45
1:C:45:GLN:HB2	1:L:488:GLU:HG3	1.99	0.45
1:G:262:LYS:HB3	1:G:263:PRO:HD3	1.99	0.45
1:G:335:LEU:O	1:G:338:GLU:HG2	2.17	0.45
1:H:143:GLY:O	1:H:144:LEU:HB2	2.16	0.45
1:H:318:LEU:O	1:H:318:LEU:HD12	2.16	0.45
1:J:121:ILE:HD11	1:J:200:TRP:HZ3	1.81	0.45
1:K:34:LEU:HB3	1:K:79:ASN:HA	1.98	0.45
1:L:84:PRO:HA	1:L:85:PRO:HD3	1.78	0.45
1:A:152:TYR:CD1	1:A:152:TYR:N	2.85	0.45
1:A:529:ILE:N	1:A:529:ILE:CD1	2.80	0.45
1:A:547:TRP:CZ3	1:A:550:LEU:HD23	2.52	0.45
1:B:378:ALA:O	1:B:379:MET:C	2.60	0.45
1:B:386:TYR:N	1:B:387:PRO:CD	2.80	0.45
1:C:51:LEU:HD13	1:C:83:TYR:CD1	2.52	0.45
1:C:119:LEU:HD12	1:C:119:LEU:C	2.42	0.45
1:C:237:LYS:O	1:C:238:ASN:HB2	2.16	0.45
1:D:31:GLY:HA3	1:D:74:TRP:NE1	2.30	0.45
1:G:105:LYS:CE	1:G:106:GLU:HG2	2.38	0.45
1:H:499:PHE:CE1	1:H:514:LEU:HD22	2.51	0.45
1:J:223:GLY:O	1:J:227:VAL:HG23	2.16	0.45
1:K:85:PRO:HD3	3:K:1182:SIA:H92	1.96	0.45
1:A:88:THR:HB	1:A:175:TRP:CH2	2.51	0.45
1:A:343:THR:HB	1:A:442:ALA:HB2	1.99	0.45
1:C:142:GLY:HA3	1:C:146:VAL:O	2.17	0.45
1:C:264:LEU:CG	1:C:316:GLN:HG2	2.47	0.45
1:D:264:LEU:CD2	1:D:268:ILE:HD11	2.46	0.45
1:D:471:GLU:OE1	1:D:471:GLU:N	2.45	0.45
1:E:84:PRO:HA	1:E:85:PRO:HD3	1.85	0.45
1:I:431:VAL:O	1:I:434:ALA:HB3	2.16	0.45
1:J:339:ARG:O	1:J:341:PHE:N	2.50	0.45
1:K:199:ARG:HB3	1:K:199:ARG:NH1	2.24	0.45
1:K:386:TYR:N	1:K:387:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:425:MET:HE3	1:K:426:PHE:CE1	2.52	0.45
1:B:218:PHE:N	1:B:218:PHE:HD1	2.15	0.45
1:B:320:GLY:O	1:B:322:VAL:HG13	2.17	0.45
1:C:24:PRO:HG3	1:C:37:PHE:CZ	2.51	0.45
1:E:119:LEU:C	1:E:119:LEU:HD12	2.42	0.45
1:I:56:ALA:CB	1:I:117:LEU:HD13	2.47	0.45
3:I:982:SIA:O9	6:I:6011:HOH:O	2.09	0.45
1:J:48:ALA:HB3	1:J:123:THR:HG23	1.99	0.45
1:J:60:LEU:HD23	1:J:60:LEU:N	2.32	0.45
1:K:372:GLN:HB2	1:K:410:THR:C	2.42	0.45
1:A:221:SER:O	1:A:224:GLY:N	2.50	0.45
1:A:366:TYR:C	1:A:368:LEU:H	2.25	0.45
1:B:218:PHE:HA	1:B:244:ILE:O	2.16	0.45
1:C:86:MET:HG2	1:C:110:LEU:HB3	1.99	0.45
1:C:471:GLU:OE1	1:C:472:LEU:HG	2.17	0.45
1:D:119:LEU:HD12	1:D:119:LEU:O	2.17	0.45
1:D:132:ARG:HB3	1:D:211:ASN:HB2	1.98	0.45
1:G:40:LEU:O	1:G:41:GLU:C	2.59	0.45
1:G:231:VAL:HA	1:G:240:PHE:HZ	1.81	0.45
1:G:236:ALA:O	1:G:239:LEU:HB2	2.17	0.45
1:H:218:PHE:HB2	1:H:244:ILE:HB	1.98	0.45
1:I:61:GLY:C	1:I:63:LEU:H	2.25	0.45
1:I:105:LYS:HG3	1:I:106:GLU:N	2.21	0.45
1:J:64:ARG:HH11	1:J:287:ARG:HA	1.82	0.45
1:J:173:GLY:O	1:J:174:ILE:C	2.60	0.45
1:J:204:ASN:O	1:J:206:ALA:N	2.49	0.45
1:K:383:TRP:CE3	1:K:393:LYS:HB2	2.52	0.45
1:L:191:HIS:O	1:L:195:VAL:HG23	2.17	0.45
1:A:495:MET:HE1	1:A:533:THR:HB	1.98	0.45
1:B:218:PHE:HB3	1:B:244:ILE:HD12	1.98	0.45
1:B:363:LEU:C	1:B:365:SER:H	2.25	0.45
1:C:24:PRO:HG3	1:C:37:PHE:CE1	2.52	0.45
1:C:107:ASN:HB3	6:C:6463:HOH:O	2.16	0.45
1:C:124:PRO:HD3	1:C:158:ALA:HB1	1.99	0.45
1:D:97:LEU:HD11	1:D:101:PHE:CZ	2.52	0.45
1:G:217:ILE:HD12	1:G:227:VAL:HG13	1.99	0.45
1:G:317:PRO:O	1:G:318:LEU:CB	2.64	0.45
1:G:393:LYS:O	1:G:395:LEU:N	2.47	0.45
1:H:151:THR:HG22	1:H:152:TYR:CE1	2.52	0.45
1:I:65:PHE:O	1:I:189:TRP:CZ2	2.70	0.45
1:J:161:GLU:OE2	1:J:498:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:271:THR:HG22	1:J:297:THR:HG23	1.99	0.45
3:J:1082:SIA:C11	1:K:278:THR:HA	2.38	0.45
1:K:61:GLY:HA3	1:K:62:PRO:HD2	1.84	0.45
1:K:478:ALA:N	1:K:479:PRO:CD	2.80	0.45
1:L:254:VAL:HG11	5:L:4380:BEZ:H4	1.99	0.45
1:L:396:ILE:O	1:L:399:ALA:HB3	2.16	0.45
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.32	0.44
1:C:372:GLN:NE2	1:C:410:THR:OG1	2.50	0.44
1:C:526:TYR:CE1	1:C:528:GLN:HG2	2.52	0.44
1:F:404:LEU:C	1:F:406:GLY:N	2.76	0.44
1:H:526:TYR:CE1	1:H:539:LEU:HD13	2.52	0.44
1:I:377:THR:O	1:I:380:SER:HB3	2.17	0.44
1:J:221:SER:OG	1:J:222:ALA:N	2.48	0.44
1:J:374:ASP:O	1:J:375:GLN:C	2.60	0.44
1:J:528:GLN:HE21	1:J:536:ALA:HB2	1.81	0.44
1:L:38:VAL:CG2	1:L:49:ILE:HD12	2.46	0.44
1:A:211:ASN:C	1:A:213:GLY:N	2.75	0.44
1:A:312:PRO:HG2	1:A:383:TRP:NE1	2.32	0.44
1:B:34:LEU:HB3	1:B:79:ASN:HA	1.99	0.44
1:B:354:GLU:HB2	1:B:422:ALA:HB1	1.98	0.44
1:C:271:THR:CG2	1:C:297:THR:HG23	2.41	0.44
1:D:68:PRO:HA	6:D:6276:HOH:O	2.18	0.44
1:D:225:GLU:O	1:D:229:VAL:HG23	2.18	0.44
1:D:400:THR:HG23	1:D:404:LEU:HD12	1.98	0.44
1:E:461:PRO:HG2	1:E:464:VAL:HG23	1.99	0.44
1:F:245:SER:HB3	1:F:248:GLY:O	2.17	0.44
1:F:420:LEU:C	1:F:420:LEU:HD13	2.42	0.44
1:G:34:LEU:C	1:G:34:LEU:HD13	2.42	0.44
1:G:393:LYS:O	1:G:396:ILE:HG12	2.18	0.44
1:G:446:MET:CE	1:G:539:LEU:HD23	2.46	0.44
1:G:471:GLU:HG2	1:G:472:LEU:N	2.31	0.44
1:H:184:HIS:HD2	1:H:279:SER:HB2	1.82	0.44
1:I:539:LEU:C	1:I:541:ASP:N	2.75	0.44
1:J:145:MET:HE1	1:J:303:PHE:CD1	2.53	0.44
1:J:382:LEU:HD23	1:J:396:ILE:HG23	1.99	0.44
1:K:173:GLY:O	1:K:177:PHE:N	2.47	0.44
1:K:176:GLY:C	1:K:177:PHE:CD2	2.95	0.44
1:K:372:GLN:HB2	1:K:410:THR:O	2.17	0.44
1:L:131:ASN:O	1:L:132:ARG:HD2	2.17	0.44
1:L:544:VAL:HG12	1:L:548:THR:OG1	2.17	0.44
1:A:201:VAL:O	1:A:205:ILE:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LYS:HG2	1:B:238:ASN:ND2	2.32	0.44
1:C:498:LYS:O	1:C:502:ASN:HB2	2.17	0.44
1:D:188:ASN:O	1:D:189:TRP:C	2.59	0.44
1:D:339:ARG:N	1:D:339:ARG:HD2	2.31	0.44
1:E:314:GLU:O	1:E:315:SER:C	2.60	0.44
1:G:369:SER:O	1:G:371:GLY:N	2.50	0.44
1:I:76:PHE:CD1	1:I:76:PHE:N	2.86	0.44
1:I:260:ASP:O	1:I:263:PRO:HD2	2.17	0.44
1:J:102:THR:CG2	1:J:107:ASN:HD22	2.29	0.44
1:J:510:ASN:ND2	1:J:517:TRP:O	2.50	0.44
1:K:278:THR:HG23	1:K:281:VAL:HG21	1.99	0.44
1:K:309:GLN:OE1	1:K:309:GLN:N	2.50	0.44
1:A:191:HIS:CD2	1:A:321:THR:HG23	2.52	0.44
1:B:171:ARG:HG3	1:B:193:ASP:OD2	2.18	0.44
1:B:540:LYS:O	1:B:543:GLU:HB2	2.18	0.44
1:C:194:GLN:HE22	1:C:226:SER:CB	2.30	0.44
1:C:241:HIS:C	1:C:242:ARG:HG2	2.42	0.44
1:D:199:ARG:NH1	1:D:202:GLN:HE22	2.14	0.44
1:D:373:LEU:HG	1:D:378:ALA:HB2	1.98	0.44
1:D:461:PRO:C	1:D:463:THR:H	2.25	0.44
1:F:198:LEU:HD21	1:F:217:ILE:CG2	2.48	0.44
1:F:279:SER:C	1:F:281:VAL:N	2.72	0.44
1:G:133:LEU:HD22	1:G:162:ASN:O	2.17	0.44
1:G:388:LEU:HD22	1:G:425:MET:SD	2.58	0.44
1:H:355:PHE:CZ	1:H:360:PRO:HG3	2.53	0.44
1:H:385:SER:C	1:H:387:PRO:HD2	2.43	0.44
1:H:399:ALA:HB2	1:H:550:LEU:CD2	2.45	0.44
1:H:437:HIS:HD2	1:H:444:THR:OG1	2.01	0.44
1:I:55:PHE:CD2	1:I:119:LEU:HD23	2.52	0.44
1:K:218:PHE:CB	1:K:244:ILE:HB	2.48	0.44
1:L:339:ARG:HH11	1:L:339:ARG:HG3	1.82	0.44
1:A:84:PRO:HA	1:A:85:PRO:HD3	1.72	0.44
1:A:138:TRP:CH2	1:A:220:GLU:HB2	2.53	0.44
1:A:529:ILE:H	1:A:529:ILE:CD1	2.30	0.44
1:C:193:ASP:O	1:C:195:VAL:N	2.50	0.44
1:C:241:HIS:C	1:C:242:ARG:CG	2.90	0.44
1:E:278:THR:O	1:E:279:SER:C	2.61	0.44
1:H:103:ASN:ND2	1:H:481:LEU:HD12	2.33	0.44
1:I:104:ARG:O	1:I:482:LYS:HE2	2.17	0.44
1:I:241:HIS:O	1:I:242:ARG:HG2	2.18	0.44
1:I:416:LEU:O	1:I:419:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:538:LYS:HB3	1:J:541:ASP:HB2	1.99	0.44
1:K:245:SER:HB3	1:K:248:GLY:O	2.18	0.44
1:L:102:THR:HG23	1:L:103:ASN:N	2.32	0.44
1:L:339:ARG:HG2	1:L:440:ALA:HA	2.00	0.44
1:L:414:LYS:O	1:L:417:PHE:HB3	2.18	0.44
1:A:245:SER:HB3	1:A:248:GLY:O	2.18	0.44
1:A:418:LEU:C	1:A:420:LEU:N	2.76	0.44
1:C:357:TRP:CH2	1:C:361:MET:HE2	2.52	0.44
1:C:517:TRP:CE3	1:C:527:LEU:HD23	2.53	0.44
1:E:495:MET:HE1	1:E:533:THR:OG1	2.18	0.44
1:F:376:LYS:HB2	1:F:376:LYS:HE3	1.80	0.44
1:F:457:SER:C	1:F:459:MET:N	2.76	0.44
1:G:152:TYR:HE2	1:G:472:LEU:HD13	1.81	0.44
1:H:255:LEU:HD23	1:H:318:LEU:HD11	1.99	0.44
1:K:217:ILE:HG13	1:K:227:VAL:HG13	1.99	0.44
1:K:383:TRP:C	1:K:385:SER:N	2.75	0.44
1:L:461:PRO:HG2	1:L:464:VAL:HG23	2.00	0.44
1:B:242:ARG:HG2	1:B:242:ARG:HH11	1.83	0.44
1:B:374:ASP:OD2	1:B:376:LYS:HB2	2.18	0.44
3:B:1280:SIA:C10	3:B:1280:SIA:HO4	2.31	0.44
1:C:230:LEU:O	1:C:236:ALA:HB3	2.17	0.44
1:D:144:LEU:HB3	1:D:177:PHE:CE2	2.52	0.44
1:D:198:LEU:HB3	1:D:239:LEU:HB3	2.00	0.44
1:D:242:ARG:HD3	1:D:503:PHE:O	2.18	0.44
1:D:426:PHE:O	1:D:427:GLY:C	2.61	0.44
1:E:24:PRO:C	1:E:24:PRO:HB2	2.38	0.44
3:E:582:SIA:C7	3:E:582:SIA:O2	2.66	0.44
1:F:45:GLN:NE2	1:F:46:PRO:HD2	2.32	0.44
1:F:338:GLU:OE2	1:F:341:PHE:HB2	2.17	0.44
1:G:220:GLU:HB2	1:G:472:LEU:HD21	1.99	0.44
1:H:104:ARG:HB3	1:H:104:ARG:HH11	1.83	0.44
1:H:161:GLU:HG3	1:H:501:ALA:HB2	2.00	0.44
1:I:211:ASN:ND2	1:I:214:SER:HB2	2.33	0.44
1:I:503:PHE:C	1:I:505:ARG:H	2.25	0.44
1:J:224:GLY:O	1:J:227:VAL:HB	2.18	0.44
1:J:350:ILE:C	1:J:351:ASN:HD22	2.26	0.44
1:J:427:GLY:O	1:J:428:VAL:C	2.59	0.44
1:K:519:GLU:O	1:K:521:ASN:N	2.50	0.44
1:L:24:PRO:HD2	1:L:35:GLY:O	2.17	0.44
1:A:353:GLN:NE2	1:A:465:ILE:H	2.16	0.44
1:A:414:LYS:NZ	5:A:1385:BEZ:H2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LEU:HD23	1:A:529:ILE:HD11	1.99	0.44
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.82	0.44
1:B:373:LEU:O	1:B:413:LYS:HD2	2.18	0.44
1:C:23:PRO:HB2	1:C:34:LEU:HD21	1.99	0.44
1:C:197:ALA:O	1:C:201:VAL:HG23	2.18	0.44
1:D:140:HIS:CD2	1:D:140:HIS:C	2.96	0.44
1:D:197:ALA:O	1:D:201:VAL:HG23	2.17	0.44
1:D:472:LEU:O	1:D:473:PHE:C	2.60	0.44
1:E:278:THR:OG1	1:E:281:VAL:HG23	2.18	0.44
1:F:51:LEU:HD13	1:F:83:TYR:CE1	2.53	0.44
1:G:52:GLY:HA2	1:G:118:TYR:HB3	1.98	0.44
1:G:467:ASP:HB3	1:G:470:ASP:OD2	2.18	0.44
1:H:26:VAL:CG1	1:H:207:SER:HB3	2.48	0.44
1:H:218:PHE:HB3	1:H:244:ILE:HB	1.99	0.44
1:I:447:TYR:CD2	1:I:447:TYR:C	2.96	0.44
1:J:136:MET:HB3	1:J:218:PHE:CE1	2.53	0.44
1:J:462:LYS:N	6:J:6348:HOH:O	2.50	0.44
1:L:257:LYS:HE2	1:L:316:GLN:NE2	2.33	0.44
1:A:34:LEU:C	1:A:34:LEU:CD1	2.91	0.44
1:A:237:LYS:HE3	1:A:342:HIS:CB	2.47	0.44
1:B:187:GLY:O	1:B:188:ASN:HB2	2.18	0.44
1:B:241:HIS:C	1:B:242:ARG:HG3	2.42	0.44
1:C:316:GLN:NE2	1:C:316:GLN:CA	2.76	0.44
1:C:353:GLN:O	1:C:467:ASP:HA	2.17	0.44
1:D:188:ASN:OD1	1:D:322:VAL:HG22	2.17	0.44
1:E:428:VAL:N	1:E:429:PRO:CD	2.80	0.44
1:G:135:VAL:CG2	1:G:205:ILE:HG12	2.47	0.44
1:L:119:LEU:C	1:L:119:LEU:HD12	2.43	0.44
1:L:233:SER:HA	1:L:234:PRO:HD3	1.90	0.44
1:A:87:CYS:O	1:A:88:THR:C	2.59	0.43
1:A:424:VAL:O	1:A:424:VAL:CG1	2.65	0.43
1:B:140:HIS:HE1	6:B:6392:HOH:O	2.01	0.43
1:B:221:SER:OG	6:B:6470:HOH:O	2.12	0.43
1:E:366:TYR:HE2	1:E:417:PHE:HE2	1.66	0.43
1:G:251:LEU:HD12	1:G:433:VAL:HG22	1.99	0.43
1:H:498:LYS:HB3	1:H:514:LEU:HD11	1.99	0.43
1:I:38:VAL:HG21	1:I:49:ILE:HD12	1.99	0.43
1:J:477:GLY:HA2	1:J:493:SER:OG	2.17	0.43
1:K:420:LEU:C	1:K:420:LEU:HD13	2.43	0.43
1:L:106:GLU:HG3	1:L:106:GLU:O	2.16	0.43
1:L:236:ALA:HB1	1:L:240:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:O	1:A:418:LEU:HG	2.18	0.43
1:B:104:ARG:O	1:B:482:LYS:HE3	2.18	0.43
1:E:428:VAL:O	1:E:429:PRO:C	2.60	0.43
1:E:467:ASP:CG	1:E:468:HIS:N	2.77	0.43
1:F:124:PRO:HG3	1:F:158:ALA:O	2.17	0.43
1:G:306:LEU:HD22	1:G:366:TYR:CD1	2.52	0.43
1:G:491:ARG:HG3	1:G:491:ARG:HH11	1.83	0.43
1:G:538:LYS:HB3	1:G:541:ASP:HB2	2.00	0.43
1:H:343:THR:HA	6:H:6072:HOH:O	2.17	0.43
1:H:359:ILE:CB	1:H:360:PRO:HD3	2.43	0.43
1:I:126:ASP:OD2	1:I:129:LYS:HE2	2.18	0.43
1:I:170:TYR:CD1	1:I:170:TYR:N	2.86	0.43
1:J:393:LYS:C	1:J:395:LEU:N	2.76	0.43
1:K:188:ASN:N	6:K:6038:HOH:O	2.37	0.43
1:L:544:VAL:O	1:L:545:ALA:C	2.61	0.43
1:A:222:ALA:HA	1:A:255:LEU:CD1	2.48	0.43
1:A:385:SER:C	1:A:387:PRO:HD2	2.43	0.43
1:B:211:ASN:HD22	1:B:214:SER:HB3	1.83	0.43
1:B:220:GLU:HA	1:B:246:GLU:O	2.18	0.43
1:B:366:TYR:HA	1:B:367:PRO:HD3	1.74	0.43
1:B:435:ARG:O	1:B:438:ARG:HB3	2.18	0.43
1:B:543:GLU:O	1:B:544:VAL:C	2.60	0.43
1:C:420:LEU:CD2	1:C:547:TRP:HZ2	2.31	0.43
1:D:33:VAL:HA	1:D:78:LYS:O	2.18	0.43
1:D:495:MET:HE1	1:D:533:THR:CG2	2.48	0.43
1:G:152:TYR:N	1:G:152:TYR:CD1	2.86	0.43
1:G:176:GLY:HA2	1:G:189:TRP:HB2	2.00	0.43
1:G:361:MET:SD	1:G:363:LEU:HD23	2.58	0.43
1:G:379:MET:HE2	1:G:397:PRO:HA	2.00	0.43
1:H:120:ASN:HB2	1:H:167:THR:OG1	2.18	0.43
1:H:296:GLU:O	1:H:300:LYS:HG3	2.18	0.43
1:H:382:LEU:HB2	1:H:417:PHE:CE1	2.51	0.43
1:H:450:GLN:HG2	1:H:529:ILE:O	2.19	0.43
1:I:140:HIS:NE2	1:I:147:GLY:HA3	2.33	0.43
1:I:495:MET:CE	1:I:533:THR:HG21	2.48	0.43
1:I:526:TYR:CE1	1:I:528:GLN:HG2	2.53	0.43
1:J:24:PRO:HG3	1:J:37:PHE:CE1	2.53	0.43
1:J:164:VAL:CG1	1:J:205:ILE:HD11	2.47	0.43
1:K:87:CYS:O	1:K:88:THR:C	2.62	0.43
1:K:144:LEU:HD13	1:K:177:PHE:CE1	2.53	0.43
1:A:237:LYS:CG	6:A:6099:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:OG1	1:A:293:GLU:HG3	2.19	0.43
1:B:327:LEU:HD23	1:B:327:LEU:O	2.17	0.43
1:C:34:LEU:HD13	1:C:34:LEU:C	2.42	0.43
1:C:97:LEU:CD2	1:C:146:VAL:HG23	2.48	0.43
1:C:300:LYS:NZ	6:C:6102:HOH:O	2.42	0.43
1:C:551:PHE:C	1:C:553:LYS:H	2.25	0.43
1:E:543:GLU:O	1:E:544:VAL:C	2.60	0.43
1:F:29:VAL:HG23	1:F:204:ASN:OD1	2.19	0.43
1:F:335:LEU:C	1:F:337:ALA:H	2.26	0.43
1:H:59:PRO:HD3	1:H:117:LEU:CD1	2.47	0.43
1:H:266:GLU:O	1:H:270:ILE:HG13	2.19	0.43
1:H:316:GLN:HA	1:H:316:GLN:NE2	2.33	0.43
1:H:403:TYR:O	1:H:416:LEU:HD13	2.18	0.43
1:I:355:PHE:HD1	1:I:418:LEU:HD22	1.83	0.43
1:I:364:MET:HE1	1:I:388:LEU:HD21	2.00	0.43
1:I:445:TYR:CE1	1:I:519:GLU:HA	2.53	0.43
1:K:84:PRO:HA	3:K:1182:SIA:H91	1.99	0.43
1:K:420:LEU:HD13	1:K:421:ILE:N	2.33	0.43
1:L:129:LYS:HG2	1:L:129:LYS:H	1.53	0.43
1:B:304:LEU:O	1:B:364:MET:HG2	2.18	0.43
1:D:152:TYR:N	1:D:152:TYR:CD1	2.86	0.43
1:D:249:VAL:HB	1:D:433:VAL:HG21	2.01	0.43
1:D:551:PHE:C	1:D:553:LYS:H	2.26	0.43
1:E:343:THR:HB	1:E:442:ALA:CB	2.49	0.43
1:G:138:TRP:CH2	1:G:220:GLU:HB2	2.53	0.43
1:G:419:ASP:O	1:G:420:LEU:C	2.61	0.43
1:I:52:GLY:HA3	3:I:982:SIA:O9	2.19	0.43
1:I:249:VAL:HB	1:I:433:VAL:HG21	2.00	0.43
1:J:104:ARG:CZ	1:J:153:ASP:HB2	2.48	0.43
1:J:143:GLY:O	1:J:144:LEU:HB2	2.17	0.43
1:J:157:LEU:HD13	1:J:475:VAL:O	2.18	0.43
1:J:366:TYR:CE2	1:J:381:LEU:HD21	2.53	0.43
1:J:428:VAL:HG22	1:J:544:VAL:HA	2.01	0.43
1:J:447:TYR:HB3	1:J:517:TRP:CZ2	2.53	0.43
1:J:488:GLU:HA	1:J:491:ARG:NH1	2.34	0.43
1:K:319:LEU:HB2	6:K:6148:HOH:O	2.18	0.43
1:A:195:VAL:HG22	1:A:230:LEU:HD22	2.00	0.43
1:A:257:LYS:NZ	1:A:257:LYS:HA	2.34	0.43
1:C:478:ALA:N	1:C:479:PRO:CD	2.81	0.43
1:D:170:TYR:N	6:D:6060:HOH:O	2.51	0.43
1:E:139:ILE:HD12	1:E:227:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ASP:O	1:E:263:PRO:HD2	2.18	0.43
1:E:409:ASP:O	1:E:413:LYS:HG3	2.19	0.43
1:F:218:PHE:HA	1:F:244:ILE:O	2.19	0.43
1:G:332:PRO:HD2	1:G:333:GLU:OE2	2.18	0.43
1:I:52:GLY:HA2	1:I:118:TYR:HB3	2.00	0.43
1:I:368:LEU:CD1	1:I:418:LEU:HD21	2.48	0.43
1:I:526:TYR:HE2	6:I:6336:HOH:O	2.00	0.43
1:I:547:TRP:O	1:I:551:PHE:HB2	2.18	0.43
1:J:190:GLY:O	1:J:193:ASP:HB2	2.19	0.43
1:K:143:GLY:N	1:K:222:ALA:HB2	2.34	0.43
1:A:529:ILE:HA	1:A:533:THR:CG2	2.46	0.43
1:B:242:ARG:HH11	1:B:242:ARG:CG	2.31	0.43
1:B:492:LEU:O	1:B:495:MET:HB3	2.19	0.43
1:C:357:TRP:O	1:C:360:PRO:CD	2.59	0.43
1:D:204:ASN:C	1:D:206:ALA:N	2.77	0.43
1:D:237:LYS:O	1:D:238:ASN:HB2	2.18	0.43
1:D:253:SER:O	1:D:254:VAL:C	2.61	0.43
1:E:221:SER:CB	6:E:6472:HOH:O	2.66	0.43
1:E:431:VAL:O	1:E:435:ARG:HG3	2.19	0.43
1:F:222:ALA:HA	1:F:255:LEU:CD1	2.48	0.43
1:G:317:PRO:O	1:G:318:LEU:HB3	2.18	0.43
1:H:174:ILE:HA	1:H:319:LEU:HD11	2.00	0.43
1:H:498:LYS:NZ	6:H:6303:HOH:O	2.43	0.43
1:I:499:PHE:CD2	1:I:509:PRO:HB2	2.53	0.43
1:J:89:GLN:O	1:J:90:ASP:C	2.59	0.43
1:K:528:GLN:O	1:K:533:THR:HA	2.19	0.43
1:L:101:PHE:O	1:L:102:THR:O	2.37	0.43
1:A:211:ASN:C	1:A:211:ASN:OD1	2.60	0.43
1:B:301:MET:HB3	1:B:303:PHE:CE2	2.54	0.43
1:D:26:VAL:HG12	1:D:27:ASP:N	2.33	0.43
1:D:306:LEU:HD22	1:D:366:TYR:CE1	2.53	0.43
1:D:450:GLN:CD	1:D:528:GLN:HG2	2.44	0.43
1:F:31:GLY:HA3	1:F:74:TRP:CE2	2.54	0.43
1:F:50:PHE:CD1	1:F:50:PHE:N	2.85	0.43
1:F:290:THR:HG23	1:F:293:GLU:OE2	2.19	0.43
1:H:326:MET:HE3	1:H:326:MET:HB3	1.90	0.43
1:H:517:TRP:CE3	1:H:527:LEU:HD22	2.54	0.43
1:I:486:SER:C	1:I:488:GLU:N	2.76	0.43
1:J:184:HIS:CE1	1:J:280:ALA:HB2	2.54	0.43
1:J:215:VAL:H	1:J:241:HIS:HD2	1.67	0.43
1:J:351:ASN:ND2	1:J:449:PHE:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:297:THR:O	1:K:301:MET:HG2	2.18	0.43
1:L:88:THR:HB	1:L:175:TRP:CZ3	2.54	0.43
1:L:266:GLU:O	1:L:270:ILE:HG13	2.19	0.43
1:L:431:VAL:HG21	1:L:540:LYS:HB2	2.00	0.43
1:A:134:PRO:HG3	1:A:505:ARG:CG	2.47	0.43
1:A:249:VAL:HB	1:A:433:VAL:HG21	2.01	0.43
1:A:264:LEU:HD13	1:A:319:LEU:HD23	2.00	0.43
1:A:279:SER:HB2	3:A:1181:SIA:C11	2.48	0.43
1:A:312:PRO:HG2	1:A:383:TRP:CD1	2.54	0.43
1:A:499:PHE:CZ	1:A:514:LEU:HD22	2.52	0.43
3:A:1180:SIA:C11	1:B:278:THR:HG22	2.41	0.43
1:B:125:ALA:HB2	1:B:133:LEU:HD12	2.01	0.43
1:C:140:HIS:CE1	1:C:170:TYR:CE1	3.07	0.43
1:D:445:TYR:CD1	1:D:519:GLU:HA	2.54	0.43
1:D:497:MET:O	1:D:498:LYS:C	2.61	0.43
1:F:366:TYR:HB3	1:F:368:LEU:HG	2.00	0.43
1:F:539:LEU:O	1:F:540:LYS:C	2.61	0.43
1:G:351:ASN:N	1:G:351:ASN:ND2	2.65	0.43
1:H:257:LYS:HB2	1:H:322:VAL:HG12	2.01	0.43
1:I:90:ASP:OD1	1:I:91:PRO:HD2	2.18	0.43
1:I:379:MET:O	1:I:383:TRP:HB2	2.18	0.43
1:J:308:LEU:HD12	1:J:309:GLN:HG2	2.00	0.43
1:K:129:LYS:O	1:K:130:LYS:C	2.62	0.43
1:L:218:PHE:HA	1:L:244:ILE:O	2.19	0.43
1:L:361:MET:SD	1:L:363:LEU:HD23	2.59	0.43
1:A:136:MET:HB3	1:A:218:PHE:CE1	2.54	0.43
1:A:366:TYR:CD2	1:A:367:PRO:HD2	2.54	0.43
1:B:230:LEU:O	1:B:236:ALA:HB3	2.19	0.43
1:C:215:VAL:H	1:C:241:HIS:CD2	2.30	0.43
1:C:450:GLN:O	1:C:450:GLN:HG2	2.19	0.43
1:D:186:ARG:HG3	1:D:186:ARG:NH1	2.34	0.43
1:D:241:HIS:C	1:D:242:ARG:HG3	2.42	0.43
1:D:353:GLN:OE1	1:D:464:VAL:HG13	2.19	0.43
1:D:386:TYR:C	1:D:388:LEU:H	2.26	0.43
1:E:141:GLY:HA2	1:E:222:ALA:HB3	2.01	0.43
1:E:251:LEU:CD1	1:E:336:GLN:HE22	2.27	0.43
1:F:199:ARG:HG2	1:F:199:ARG:HH11	1.84	0.43
1:F:353:GLN:O	1:F:467:ASP:HA	2.18	0.43
1:G:89:GLN:HE22	1:G:147:GLY:N	2.16	0.43
1:H:221:SER:O	1:H:224:GLY:N	2.51	0.43
1:H:543:GLU:O	1:H:544:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:425:MET:O	1:I:429:PRO:HG2	2.19	0.43
1:I:517:TRP:CE3	1:I:527:LEU:HD22	2.54	0.43
1:J:436:ASN:HD22	1:J:436:ASN:HA	1.64	0.43
1:L:508:ASN:OD1	1:L:510:ASN:HB2	2.19	0.43
1:A:149:ALA:CB	1:A:169:GLN:HG3	2.49	0.42
1:A:218:PHE:HB2	1:A:244:ILE:HB	2.00	0.42
1:A:242:ARG:HD2	1:A:504:ALA:HA	2.01	0.42
1:A:308:LEU:HB2	6:A:6331:HOH:O	2.19	0.42
1:B:51:LEU:HD13	1:B:83:TYR:CE1	2.54	0.42
1:B:455:PHE:HZ	1:B:479:PRO:HA	1.84	0.42
1:B:530:GLY:O	1:B:531:ALA:C	2.61	0.42
1:C:133:LEU:HD22	1:C:162:ASN:O	2.19	0.42
1:C:545:ALA:O	1:C:546:PHE:C	2.62	0.42
1:E:423:ASP:OD2	1:E:543:GLU:HG2	2.19	0.42
1:F:34:LEU:HD13	1:F:34:LEU:C	2.43	0.42
1:F:277:THR:HG22	1:F:278:THR:HG23	2.01	0.42
1:G:51:LEU:HD13	1:G:83:TYR:CD1	2.53	0.42
1:G:486:SER:O	1:G:490:ILE:HG13	2.19	0.42
1:H:416:LEU:HD23	1:H:416:LEU:HA	1.84	0.42
3:I:982:SIA:O8	3:I:982:SIA:N5	2.51	0.42
1:J:296:GLU:O	1:J:297:THR:C	2.62	0.42
1:K:354:GLU:O	1:K:468:HIS:HB2	2.19	0.42
1:L:367:PRO:CB	1:L:381:LEU:HD21	2.49	0.42
1:A:269:ALA:O	1:A:270:ILE:C	2.61	0.42
1:A:420:LEU:C	1:A:420:LEU:CD1	2.92	0.42
1:A:549:ASN:C	1:A:550:LEU:C	2.87	0.42
1:B:308:LEU:HB2	1:B:309:GLN:OE1	2.19	0.42
1:B:348:VAL:O	1:B:446:MET:HG2	2.20	0.42
1:D:217:ILE:HD12	1:D:230:LEU:HD12	2.00	0.42
1:E:284:HIS:O	1:E:287:ARG:HB2	2.20	0.42
1:E:386:TYR:N	1:E:387:PRO:CD	2.82	0.42
1:E:442:ALA:HA	1:E:443:PRO:HD3	1.92	0.42
1:F:51:LEU:HD13	1:F:83:TYR:CD1	2.54	0.42
1:F:332:PRO:HA	1:F:335:LEU:HB2	2.01	0.42
1:F:373:LEU:HD21	1:F:378:ALA:HB2	2.01	0.42
1:G:220:GLU:CG	1:G:472:LEU:HD21	2.45	0.42
1:H:87:CYS:HB3	6:H:6073:HOH:O	2.17	0.42
1:I:24:PRO:HD2	1:I:35:GLY:C	2.45	0.42
1:I:26:VAL:HG23	1:I:50:PHE:CZ	2.54	0.42
1:I:88:THR:HG21	1:I:291:GLU:HG3	2.00	0.42
1:I:474:SER:HB3	1:I:493:SER:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:477:GLY:C	1:I:479:PRO:HD2	2.43	0.42
1:J:324:ASP:CG	1:J:325:GLY:H	2.24	0.42
1:J:332:PRO:C	1:J:334:GLU:H	2.26	0.42
1:J:479:PRO:HB3	1:J:490:ILE:HG12	2.01	0.42
1:J:499:PHE:HD2	1:J:499:PHE:HA	1.72	0.42
1:L:26:VAL:HG23	1:L:50:PHE:CZ	2.54	0.42
1:L:184:HIS:O	1:L:283:VAL:HG21	2.18	0.42
1:L:372:GLN:NE2	1:L:411:VAL:HG22	2.34	0.42
1:B:197:ALA:O	1:B:200:TRP:N	2.52	0.42
1:C:190:GLY:O	1:C:194:GLN:HG3	2.20	0.42
1:D:58:PRO:O	1:D:60:LEU:N	2.48	0.42
1:D:226:SER:O	1:D:227:VAL:C	2.62	0.42
1:D:351:ASN:N	1:D:351:ASN:ND2	2.61	0.42
1:D:418:LEU:C	1:D:420:LEU:N	2.77	0.42
1:F:176:GLY:HA2	1:F:189:TRP:HB2	2.02	0.42
1:G:145:MET:HE2	1:G:303:PHE:HB2	2.01	0.42
1:G:393:LYS:C	1:G:395:LEU:N	2.77	0.42
1:G:517:TRP:HA	1:G:518:PRO:HD2	1.93	0.42
1:H:487:GLU:OE2	1:H:491:ARG:NH1	2.50	0.42
1:I:145:MET:HE1	1:I:303:PHE:HD1	1.83	0.42
1:J:28:THR:HB	1:J:204:ASN:OD1	2.18	0.42
1:J:382:LEU:HD11	1:J:391:ILE:CD1	2.46	0.42
1:K:372:GLN:HE21	1:K:372:GLN:HB3	1.63	0.42
1:L:329:LEU:HD13	1:L:335:LEU:HD21	2.00	0.42
1:L:485:ALA:HB1	1:L:489:GLU:OE2	2.19	0.42
1:A:103:ASN:HD22	1:A:476:PHE:HB3	1.80	0.42
1:C:132:ARG:HG2	1:C:132:ARG:NH1	2.32	0.42
1:C:193:ASP:O	1:C:196:ALA:N	2.52	0.42
1:C:251:LEU:HD11	1:C:336:GLN:HE22	1.83	0.42
1:F:228:SER:CB	1:F:250:ALA:H	2.33	0.42
1:G:226:SER:O	1:G:230:LEU:HG	2.19	0.42
1:H:45:GLN:HA	1:H:46:PRO:HD2	1.92	0.42
1:I:133:LEU:O	1:I:211:ASN:N	2.48	0.42
1:I:517:TRP:CG	1:I:527:LEU:HD13	2.53	0.42
1:J:49:ILE:HG12	1:J:122:TYR:CD2	2.55	0.42
1:K:134:PRO:HG2	1:K:163:VAL:HG12	2.01	0.42
1:A:170:TYR:CD1	1:A:170:TYR:N	2.87	0.42
1:A:206:ALA:HA	1:A:210:GLY:O	2.19	0.42
1:B:154:GLY:O	1:B:155:LEU:C	2.63	0.42
1:B:241:HIS:O	1:B:344:VAL:HB	2.20	0.42
1:B:261:VAL:O	1:B:262:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TRP:CE2	1:B:361:MET:HG3	2.55	0.42
1:B:420:LEU:HD21	1:B:547:TRP:HZ2	1.82	0.42
1:B:499:PHE:CE2	1:B:514:LEU:HB3	2.54	0.42
1:D:344:VAL:O	1:D:345:PRO:C	2.62	0.42
1:E:254:VAL:HG23	1:E:387:PRO:O	2.19	0.42
1:E:445:TYR:HA	6:E:6035:HOH:O	2.20	0.42
1:F:264:LEU:O	1:F:268:ILE:HG13	2.19	0.42
1:F:510:ASN:ND2	1:F:517:TRP:O	2.48	0.42
1:G:222:ALA:HB2	6:G:6473:HOH:O	2.18	0.42
1:H:499:PHE:HD2	1:H:509:PRO:HB2	1.84	0.42
1:I:84:PRO:HA	1:I:85:PRO:HD3	1.81	0.42
1:J:36:LYS:HE3	1:J:38:VAL:CG2	2.49	0.42
1:K:279:SER:HA	1:K:282:MET:HE2	2.01	0.42
1:L:61:GLY:C	1:L:63:LEU:H	2.27	0.42
1:A:220:GLU:HA	1:A:246:GLU:O	2.19	0.42
1:C:136:MET:HB3	1:C:218:PHE:CE1	2.55	0.42
1:C:221:SER:HB2	1:C:468:HIS:NE2	2.35	0.42
1:C:276:THR:HG22	1:C:282:MET:SD	2.60	0.42
1:D:294:LEU:HD23	1:D:294:LEU:HA	1.87	0.42
1:E:24:PRO:CA	1:E:25:VAL:N	2.66	0.42
1:E:52:GLY:N	1:E:120:ASN:OD1	2.49	0.42
1:E:176:GLY:HA2	1:E:189:TRP:HB2	2.01	0.42
1:E:520:TYR:CE2	1:E:524:GLU:HG2	2.54	0.42
1:F:357:TRP:O	1:F:358:LEU:C	2.63	0.42
1:F:404:LEU:HD22	1:F:413:LYS:O	2.19	0.42
1:F:492:LEU:O	1:F:496:VAL:HG23	2.19	0.42
1:I:330:LYS:HE2	1:I:330:LYS:HB3	1.96	0.42
1:I:480:PHE:HE1	1:I:497:MET:HE1	1.83	0.42
1:K:44:ALA:N	6:K:6380:HOH:O	2.52	0.42
1:K:191:HIS:HB2	1:K:327:LEU:HD22	2.01	0.42
3:K:1182:SIA:H6	6:L:6046:HOH:O	2.19	0.42
1:L:102:THR:OG1	1:L:103:ASN:N	2.52	0.42
1:B:145:MET:HE2	1:B:303:PHE:HB2	2.00	0.42
1:B:226:SER:O	1:B:230:LEU:HG	2.20	0.42
1:D:180:THR:OG1	1:D:182:ASP:OD2	2.21	0.42
1:E:221:SER:OG	6:E:6469:HOH:O	1.90	0.42
1:G:428:VAL:HG21	1:G:547:TRP:CD1	2.55	0.42
1:H:97:LEU:HD11	1:H:101:PHE:CE2	2.54	0.42
1:H:357:TRP:CH2	1:H:361:MET:HE3	2.55	0.42
1:J:279:SER:C	1:J:281:VAL:N	2.77	0.42
1:L:76:PHE:CD1	1:L:76:PHE:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:428:VAL:HB	1:L:429:PRO:HD3	2.01	0.42
1:A:400:THR:O	1:A:404:LEU:HB2	2.19	0.42
1:B:316:GLN:H	1:B:316:GLN:CD	2.28	0.42
1:C:51:LEU:HD13	1:C:83:TYR:CE1	2.55	0.42
1:C:428:VAL:HG13	1:C:544:VAL:HG22	2.00	0.42
1:D:84:PRO:HA	1:D:85:PRO:HD3	1.77	0.42
1:D:262:LYS:CE	2:F:2379:NAG:H82	2.49	0.42
1:D:332:PRO:O	1:D:336:GLN:HG3	2.19	0.42
1:D:435:ARG:HB3	1:D:438:ARG:HH22	1.80	0.42
1:G:249:VAL:CG2	1:G:433:VAL:HG21	2.46	0.42
2:G:3179:NAG:H81	6:G:6010:HOH:O	2.19	0.42
1:I:184:HIS:O	1:I:185:SER:HB2	2.19	0.42
1:I:190:GLY:O	1:I:193:ASP:HB2	2.20	0.42
1:J:400:THR:CG2	1:J:404:LEU:HD12	2.43	0.42
1:J:517:TRP:CE3	1:J:527:LEU:HD23	2.54	0.42
1:K:63:LEU:HD23	1:K:63:LEU:HA	1.74	0.42
1:K:220:GLU:HA	1:K:246:GLU:HB2	2.01	0.42
1:K:314:GLU:O	1:K:316:GLN:N	2.53	0.42
1:L:144:LEU:HG	1:L:222:ALA:HB1	2.02	0.42
1:L:301:MET:O	1:L:302:LYS:C	2.62	0.42
1:L:366:TYR:HA	1:L:367:PRO:HD3	1.89	0.42
1:A:83:TYR:HD1	1:A:150:SER:HB3	1.85	0.42
1:A:131:ASN:O	1:A:209:GLY:HA2	2.19	0.42
1:A:399:ALA:C	1:A:401:GLU:N	2.77	0.42
1:A:526:TYR:CD2	1:A:539:LEU:HB2	2.55	0.42
1:B:297:THR:O	1:B:301:MET:HG2	2.19	0.42
1:B:355:PHE:HD1	1:B:418:LEU:HD22	1.85	0.42
1:B:400:THR:HG23	1:B:404:LEU:CD1	2.49	0.42
1:C:126:ASP:H	1:C:131:ASN:ND2	2.18	0.42
1:D:186:ARG:HG3	1:D:186:ARG:HH11	1.84	0.42
1:E:297:THR:C	1:E:299:LEU:N	2.75	0.42
1:F:386:TYR:N	1:F:387:PRO:CD	2.82	0.42
1:F:464:VAL:HG12	1:F:467:ASP:HB2	2.01	0.42
1:G:429:PRO:O	1:G:430:SER:C	2.63	0.42
1:G:543:GLU:C	1:G:545:ALA:N	2.76	0.42
1:I:218:PHE:N	1:I:218:PHE:CD1	2.88	0.42
1:I:338:GLU:CD	1:I:341:PHE:HB2	2.45	0.42
1:J:121:ILE:HD11	1:J:200:TRP:CZ3	2.55	0.42
1:J:452:ARG:NE	1:J:462:LYS:HA	2.35	0.42
1:K:132:ARG:HB3	1:K:211:ASN:HB2	2.01	0.42
1:K:325:GLY:HA2	1:K:329:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:MET:O	1:L:87:CYS:C	2.61	0.42
1:L:268:ILE:HG12	1:L:301:MET:HE2	2.00	0.42
1:A:109:PRO:O	1:A:110:LEU:HD23	2.20	0.42
1:A:237:LYS:HG2	6:A:6099:HOH:O	2.19	0.42
1:A:311:ASP:HA	1:A:312:PRO:HD3	1.94	0.42
1:C:194:GLN:NE2	1:C:226:SER:HB3	2.35	0.42
1:C:319:LEU:HD23	1:C:319:LEU:N	2.21	0.42
1:C:357:TRP:O	1:C:358:LEU:C	2.62	0.42
1:D:379:MET:HG2	1:D:400:THR:HG21	2.02	0.42
1:E:54:PRO:HD3	6:E:6015:HOH:O	2.20	0.42
1:E:61:GLY:HA3	1:E:62:PRO:HD2	1.83	0.42
1:E:403:TYR:CG	1:E:420:LEU:HD23	2.54	0.42
1:F:268:ILE:HD11	1:F:319:LEU:HD23	2.01	0.42
1:F:428:VAL:HG13	1:F:544:VAL:HG13	2.02	0.42
1:I:292:GLU:HA	6:I:6339:HOH:O	2.19	0.42
1:J:268:ILE:HD11	1:J:319:LEU:HD22	2.02	0.42
1:A:132:ARG:HB3	1:A:211:ASN:HB2	2.02	0.41
1:A:180:THR:HB	1:A:279:SER:OG	2.20	0.41
1:A:279:SER:O	1:A:283:VAL:HG23	2.20	0.41
1:A:395:LEU:O	1:A:396:ILE:C	2.63	0.41
1:A:425:MET:HE3	1:A:425:MET:HB3	1.87	0.41
1:B:33:VAL:HG12	1:B:34:LEU:N	2.35	0.41
1:C:132:ARG:O	1:C:211:ASN:HB2	2.20	0.41
1:C:149:ALA:HB1	1:C:167:THR:HB	2.02	0.41
1:C:269:ALA:O	1:C:274:CYS:HB2	2.20	0.41
1:C:349:GLY:HA3	1:C:447:TYR:CE1	2.55	0.41
1:C:477:GLY:HA2	1:C:493:SER:OG	2.19	0.41
1:D:226:SER:O	1:D:229:VAL:N	2.52	0.41
1:E:262:LYS:HG3	1:E:266:GLU:OE2	2.19	0.41
1:E:274:CYS:SG	1:E:289:LYS:HE3	2.60	0.41
1:H:191:HIS:CD2	1:H:321:THR:HG23	2.55	0.41
1:H:313:ARG:HG2	1:H:386:TYR:CE2	2.54	0.41
1:I:304:LEU:O	1:I:364:MET:HE3	2.20	0.41
1:J:185:SER:HA	6:J:6164:HOH:O	2.19	0.41
1:K:78:LYS:HE2	1:L:182:ASP:CB	2.50	0.41
1:K:319:LEU:HD23	1:K:319:LEU:N	2.35	0.41
1:K:372:GLN:HB2	1:K:410:THR:CB	2.44	0.41
1:K:425:MET:HB2	1:K:426:PHE:CD1	2.55	0.41
1:A:363:LEU:C	1:A:365:SER:H	2.29	0.41
1:B:145:MET:CE	1:B:303:PHE:HD1	2.32	0.41
1:C:25:VAL:HG22	1:C:34:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:HIS:HB2	1:C:152:TYR:CE1	2.54	0.41
1:C:216:THR:CG2	1:C:242:ARG:HB2	2.41	0.41
1:C:301:MET:O	1:C:302:LYS:HB2	2.20	0.41
1:E:540:LYS:HA	1:E:543:GLU:OE2	2.20	0.41
1:F:88:THR:HG22	1:F:295:LEU:HD13	2.02	0.41
1:G:218:PHE:N	1:G:218:PHE:CD1	2.88	0.41
1:I:133:LEU:HB3	1:I:134:PRO:HD2	2.02	0.41
1:I:332:PRO:O	1:I:333:GLU:C	2.62	0.41
1:J:51:LEU:HD13	1:J:83:TYR:CD1	2.55	0.41
1:J:132:ARG:HB3	1:J:211:ASN:HB2	2.02	0.41
1:K:51:LEU:O	1:K:80:ALA:HB1	2.20	0.41
1:L:386:TYR:N	1:L:387:PRO:CD	2.82	0.41
1:A:508:ASN:OD1	1:A:510:ASN:HB2	2.18	0.41
1:A:526:TYR:CE2	1:A:539:LEU:HB2	2.55	0.41
1:B:135:VAL:HG21	1:B:205:ILE:HG12	2.02	0.41
1:B:194:GLN:OE1	1:B:226:SER:HB3	2.20	0.41
1:B:435:ARG:NH1	1:B:544:VAL:HG11	2.35	0.41
1:C:86:MET:CE	1:C:110:LEU:HD13	2.27	0.41
1:C:234:PRO:HA	1:C:341:PHE:CZ	2.44	0.41
1:E:140:HIS:CD2	1:E:141:GLY:O	2.74	0.41
1:E:143:GLY:N	1:E:222:ALA:HB2	2.35	0.41
1:E:343:THR:CB	1:E:442:ALA:HB2	2.51	0.41
1:F:140:HIS:HB2	1:F:152:TYR:HE1	1.85	0.41
1:F:157:LEU:O	1:F:158:ALA:C	2.62	0.41
1:G:182:ASP:O	1:G:184:HIS:N	2.53	0.41
1:H:204:ASN:O	1:H:206:ALA:N	2.54	0.41
1:I:312:PRO:CG	1:I:384:LYS:HA	2.50	0.41
1:I:477:GLY:HA2	1:I:493:SER:OG	2.20	0.41
1:J:216:THR:HG23	1:J:242:ARG:HB2	2.01	0.41
1:J:332:PRO:C	1:J:334:GLU:N	2.77	0.41
1:J:447:TYR:HA	1:J:527:LEU:O	2.21	0.41
1:J:502:ASN:HB3	1:J:509:PRO:O	2.21	0.41
1:L:116:CYS:O	1:L:118:TYR:N	2.50	0.41
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.78	0.41
1:A:272:ALA:O	1:A:289:LYS:HE3	2.20	0.41
1:B:393:LYS:HA	1:B:396:ILE:HG12	2.03	0.41
1:D:86:MET:CE	1:D:110:LEU:HD12	2.49	0.41
1:D:403:TYR:CG	1:D:420:LEU:HD23	2.54	0.41
1:F:367:PRO:C	1:F:369:SER:H	2.29	0.41
1:G:455:PHE:O	1:G:456:SER:C	2.61	0.41
1:H:306:LEU:HD22	1:H:366:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:ALA:HB3	1:I:123:THR:HG23	2.01	0.41
1:I:221:SER:OG	5:I:3380:BEZ:H2	2.21	0.41
1:J:86:MET:CE	1:J:110:LEU:HD13	2.50	0.41
1:J:133:LEU:CD2	1:J:134:PRO:HD2	2.50	0.41
1:K:315:SER:O	1:K:316:GLN:C	2.63	0.41
1:K:366:TYR:HA	1:K:367:PRO:HD3	1.84	0.41
1:L:195:VAL:HG13	1:L:239:LEU:CD1	2.51	0.41
1:L:221:SER:O	1:L:224:GLY:N	2.53	0.41
1:L:426:PHE:C	1:L:429:PRO:HD2	2.45	0.41
1:B:34:LEU:C	1:B:34:LEU:HD13	2.45	0.41
1:B:486:SER:O	1:B:490:ILE:HG13	2.21	0.41
1:C:102:THR:OG1	1:C:104:ARG:HG2	2.20	0.41
1:C:143:GLY:N	5:C:5013:BEZ:O2	2.53	0.41
1:D:143:GLY:O	1:D:144:LEU:HB2	2.21	0.41
1:D:149:ALA:HB2	1:D:169:GLN:HG3	2.03	0.41
1:E:107:ASN:HD22	1:E:108:ILE:H	1.68	0.41
1:E:139:ILE:O	1:E:223:GLY:HA3	2.19	0.41
1:E:431:VAL:HG22	1:E:446:MET:HE1	2.02	0.41
1:F:426:PHE:O	1:F:430:SER:HB2	2.20	0.41
1:G:251:LEU:CD2	1:G:333:GLU:HG3	2.50	0.41
1:H:104:ARG:HD2	1:H:108:ILE:HG12	2.01	0.41
1:I:76:PHE:H	1:I:76:PHE:HD1	1.67	0.41
1:I:386:TYR:N	1:I:387:PRO:CD	2.84	0.41
1:I:543:GLU:OE2	1:I:543:GLU:N	2.46	0.41
1:J:343:THR:HB	1:J:442:ALA:CB	2.49	0.41
1:J:355:PHE:CD1	1:J:360:PRO:HG3	2.55	0.41
1:J:479:PRO:HG2	1:J:493:SER:HB2	2.02	0.41
1:K:449:PHE:CE2	1:K:471:GLU:HA	2.56	0.41
1:K:506:ASN:ND2	6:K:6453:HOH:O	2.38	0.41
1:L:33:VAL:HG12	1:L:34:LEU:N	2.35	0.41
1:L:354:GLU:O	1:L:468:HIS:HB2	2.20	0.41
1:A:233:SER:HA	1:A:234:PRO:HD3	1.74	0.41
1:B:145:MET:HE1	1:B:303:PHE:HD1	1.84	0.41
1:B:346:TYR:HB3	1:B:437:HIS:CD2	2.56	0.41
1:B:503:PHE:HD1	1:B:509:PRO:HD3	1.85	0.41
1:C:125:ALA:HB1	1:C:131:ASN:HD22	1.85	0.41
1:D:398:GLU:CD	1:D:550:LEU:HD13	2.45	0.41
1:E:179:SER:HB2	1:E:187:GLY:HA3	2.02	0.41
1:E:438:ARG:HD2	1:E:521:ASN:CA	2.50	0.41
1:F:359:ILE:HB	1:F:360:PRO:HD3	2.02	0.41
1:F:368:LEU:C	1:F:370:GLU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:GLN:HA	1:G:316:GLN:HE21	1.85	0.41
1:G:383:TRP:HA	1:G:383:TRP:CE3	2.55	0.41
1:G:526:TYR:CE1	1:G:528:GLN:HG2	2.56	0.41
1:I:47:VAL:HG13	1:I:123:THR:C	2.46	0.41
1:I:257:LYS:HA	1:I:257:LYS:HD3	1.88	0.41
1:I:431:VAL:HA	1:I:446:MET:CE	2.49	0.41
1:J:206:ALA:HA	1:J:210:GLY:O	2.21	0.41
1:J:216:THR:HA	1:J:242:ARG:O	2.20	0.41
1:J:237:LYS:HE3	1:J:342:HIS:CB	2.49	0.41
1:J:311:ASP:HA	1:J:312:PRO:HD3	1.95	0.41
1:J:366:TYR:HA	1:J:367:PRO:HD3	1.73	0.41
1:J:420:LEU:HD22	1:J:547:TRP:HZ2	1.85	0.41
1:K:131:ASN:O	1:K:209:GLY:HA2	2.21	0.41
1:K:400:THR:HG23	1:K:404:LEU:HD13	2.02	0.41
1:L:446:MET:CE	1:L:539:LEU:HD23	2.51	0.41
1:L:482:LYS:HB3	1:L:483:GLU:H	1.60	0.41
1:A:550:LEU:C	1:A:552:ALA:N	2.79	0.41
1:B:113:SER:OG	1:C:281:VAL:HG21	2.21	0.41
1:B:276:THR:O	1:B:277:THR:C	2.64	0.41
1:B:428:VAL:HB	1:B:429:PRO:HD3	2.02	0.41
1:C:324:ASP:OD2	1:C:324:ASP:N	2.52	0.41
1:D:372:GLN:HA	1:D:414:LYS:HB2	2.02	0.41
1:E:52:GLY:HA3	3:E:582:SIA:O9	2.19	0.41
1:E:351:ASN:O	1:E:352:LYS:C	2.63	0.41
1:G:114:GLU:CG	1:G:291:GLU:HG3	2.49	0.41
1:J:71:ALA:HB1	6:J:6057:HOH:O	2.20	0.41
1:J:97:LEU:CD2	1:J:146:VAL:HG23	2.45	0.41
1:J:151:THR:HG22	1:J:152:TYR:N	2.36	0.41
1:K:105:LYS:CG	1:K:106:GLU:H	2.28	0.41
1:L:101:PHE:CD2	1:L:472:LEU:HD11	2.56	0.41
1:L:374:ASP:OD1	1:L:377:THR:HB	2.19	0.41
1:L:452:ARG:HB2	1:L:465:ILE:HG12	2.03	0.41
1:A:205:ILE:HD12	1:A:205:ILE:HA	1.79	0.41
1:B:304:LEU:HD22	1:B:304:LEU:HA	1.87	0.41
1:C:194:GLN:HE22	1:C:226:SER:HB3	1.86	0.41
1:D:40:LEU:HD13	1:D:155:LEU:HD21	2.02	0.41
1:D:328:LEU:HD23	1:D:328:LEU:HA	1.94	0.41
1:D:352:LYS:HD2	1:D:448:GLU:OE1	2.21	0.41
1:E:121:ILE:HD11	1:E:200:TRP:CZ3	2.56	0.41
1:E:169:GLN:HE21	1:E:169:GLN:HB3	1.59	0.41
1:E:469:GLY:O	1:E:472:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:492:LEU:HD12	1:E:492:LEU:O	2.20	0.41
1:F:186:ARG:HB3	1:F:324:ASP:HB2	2.02	0.41
1:F:352:LYS:HD2	1:F:450:GLN:HG3	2.01	0.41
1:H:475:VAL:O	1:H:497:MET:HG2	2.20	0.41
1:I:137:VAL:O	1:I:218:PHE:CD1	2.74	0.41
1:I:379:MET:HE1	1:I:397:PRO:CG	2.51	0.41
1:I:538:LYS:HB3	1:I:541:ASP:CB	2.50	0.41
1:J:198:LEU:O	1:J:201:VAL:HB	2.21	0.41
1:L:404:LEU:N	1:L:404:LEU:HD23	2.36	0.41
1:A:135:VAL:HA	1:A:164:VAL:HG23	2.03	0.41
3:A:1181:SIA:H7	6:A:6003:HOH:O	2.21	0.41
1:B:43:PHE:HZ	1:B:160:HIS:ND1	2.18	0.41
1:C:103:ASN:HB2	1:C:478:ALA:HB2	2.03	0.41
1:D:45:GLN:C	6:D:6225:HOH:O	2.64	0.41
1:D:186:ARG:HD3	1:D:324:ASP:O	2.21	0.41
1:D:326:MET:HE3	1:D:326:MET:HB3	1.99	0.41
1:D:402:LYS:HG2	1:D:546:PHE:CE1	2.56	0.41
1:E:72:GLU:HA	1:E:73:PRO:HD2	1.92	0.41
1:E:262:LYS:HB3	1:E:263:PRO:HD3	2.03	0.41
1:F:86:MET:CE	1:F:110:LEU:HB2	2.46	0.41
1:F:138:TRP:CH2	1:F:220:GLU:HB2	2.56	0.41
1:F:339:ARG:HG3	1:F:440:ALA:HA	2.03	0.41
1:F:381:LEU:HD23	1:F:381:LEU:HA	1.94	0.41
1:F:506:ASN:O	1:F:507:GLY:C	2.62	0.41
1:G:324:ASP:OD2	1:G:324:ASP:N	2.51	0.41
1:G:366:TYR:HA	1:G:367:PRO:HD3	1.85	0.41
3:G:782:SIA:O10	3:G:782:SIA:O8	2.39	0.41
1:H:381:LEU:HD22	1:H:417:PHE:CZ	2.55	0.41
1:I:112:LEU:O	1:I:113:SER:HB2	2.20	0.41
1:I:179:SER:O	1:I:265:ALA:HB2	2.21	0.41
1:I:225:GLU:O	1:I:226:SER:C	2.64	0.41
1:I:324:ASP:C	1:I:326:MET:N	2.78	0.41
1:I:431:VAL:HG11	1:I:544:VAL:HG21	2.02	0.41
1:I:452:ARG:HA	1:I:453:PRO:HD2	1.94	0.41
1:I:503:PHE:C	1:I:505:ARG:N	2.79	0.41
1:J:45:GLN:NE2	6:J:6143:HOH:O	2.48	0.41
1:J:149:ALA:HB1	1:J:167:THR:HB	2.03	0.41
1:J:403:TYR:CE2	1:J:420:LEU:HA	2.55	0.41
1:K:311:ASP:HA	1:K:312:PRO:HD3	1.96	0.41
1:K:368:LEU:CD1	1:K:418:LEU:HD21	2.50	0.41
1:K:382:LEU:HD13	1:K:420:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:384:LYS:HE2	6:K:6420:HOH:O	2.19	0.41
2:K:4279:NAG:H81	1:L:260:ASP:CB	2.48	0.41
1:L:134:PRO:HG3	1:L:505:ARG:HG3	2.03	0.41
1:L:184:HIS:O	1:L:185:SER:CB	2.69	0.41
1:L:205:ILE:HD12	1:L:205:ILE:HA	1.84	0.41
1:L:236:ALA:O	1:L:239:LEU:HB2	2.21	0.41
1:L:540:LYS:O	1:L:541:ASP:C	2.63	0.41
1:A:104:ARG:NH1	1:A:153:ASP:HB2	2.36	0.41
1:A:407:THR:HG21	1:A:412:LYS:HD2	2.03	0.41
1:B:51:LEU:HA	1:B:120:ASN:OD1	2.20	0.41
1:B:141:GLY:CA	1:B:223:GLY:H	2.28	0.41
1:C:140:HIS:CD2	1:C:147:GLY:HA3	2.56	0.41
1:E:222:ALA:HB3	6:E:6472:HOH:O	2.18	0.41
1:E:477:GLY:HA2	1:E:493:SER:OG	2.20	0.41
1:F:24:PRO:HG3	1:F:37:PHE:CZ	2.56	0.41
1:F:351:ASN:HD22	1:F:351:ASN:N	2.14	0.41
1:F:498:LYS:HB3	1:F:514:LEU:HD11	2.02	0.41
1:F:498:LYS:HE2	1:F:514:LEU:HD11	2.03	0.41
1:G:379:MET:O	1:G:396:ILE:HG21	2.21	0.41
1:G:457:SER:C	1:G:459:MET:H	2.27	0.41
1:H:77:VAL:CG1	1:H:77:VAL:C	2.93	0.41
1:H:188:ASN:O	1:H:189:TRP:C	2.61	0.41
1:I:125:ALA:HB2	1:I:133:LEU:HD12	2.03	0.41
1:J:389:VAL:HG23	1:J:391:ILE:HG13	2.03	0.41
1:J:393:LYS:O	1:J:396:ILE:HG12	2.21	0.41
1:K:180:THR:OG1	1:K:182:ASP:OD2	2.29	0.41
1:K:296:GLU:O	1:K:300:LYS:HG3	2.21	0.41
1:L:137:VAL:HB	1:L:217:ILE:HG22	2.04	0.41
1:L:269:ALA:O	1:L:274:CYS:HB2	2.20	0.41
1:A:420:LEU:HD13	1:A:421:ILE:N	2.36	0.40
3:A:1181:SIA:H113	3:A:1181:SIA:H31	2.03	0.40
1:B:38:VAL:HG21	1:B:49:ILE:HD12	2.03	0.40
1:B:357:TRP:O	1:B:358:LEU:C	2.63	0.40
1:C:400:THR:HG23	1:C:404:LEU:HD12	2.03	0.40
1:D:399:ALA:HB2	1:D:550:LEU:CD2	2.50	0.40
1:E:57:LYS:HA	1:E:58:PRO:HD3	1.91	0.40
1:E:124:PRO:HD3	1:E:158:ALA:HB1	2.03	0.40
1:E:126:ASP:H	1:E:131:ASN:HD22	1.68	0.40
1:F:220:GLU:O	1:F:221:SER:C	2.65	0.40
1:G:144:LEU:HD22	1:G:177:PHE:CZ	2.56	0.40
1:G:529:ILE:HA	1:G:533:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:ILE:HD11	1:H:503:PHE:CD2	2.55	0.40
1:H:257:LYS:HA	1:H:257:LYS:HZ2	1.85	0.40
1:J:194:GLN:HE22	1:J:226:SER:HB3	1.86	0.40
1:J:442:ALA:HA	1:J:443:PRO:HD3	1.92	0.40
1:K:290:THR:HG23	1:K:293:GLU:HG3	2.03	0.40
1:L:140:HIS:CD2	1:L:147:GLY:HA3	2.56	0.40
1:L:143:GLY:O	1:L:144:LEU:HB2	2.20	0.40
1:L:257:LYS:CE	1:L:316:GLN:HE22	2.34	0.40
1:L:482:LYS:O	1:L:483:GLU:HG3	2.21	0.40
1:A:45:GLN:HE22	1:A:124:PRO:HB2	1.86	0.40
1:A:97:LEU:HD11	1:A:101:PHE:HE2	1.83	0.40
1:B:79:ASN:ND2	2:B:1279:NAG:H82	2.37	0.40
1:B:528:GLN:O	1:B:533:THR:HA	2.21	0.40
1:C:452:ARG:HA	1:C:453:PRO:HD2	1.91	0.40
1:C:489:GLU:O	1:C:490:ILE:C	2.63	0.40
1:D:319:LEU:N	1:D:319:LEU:CD2	2.83	0.40
1:D:447:TYR:CD2	1:D:447:TYR:C	2.99	0.40
1:D:495:MET:CE	1:D:533:THR:HG21	2.51	0.40
1:D:520:TYR:CZ	1:D:524:GLU:HG2	2.56	0.40
1:E:107:ASN:ND2	1:E:108:ILE:H	2.20	0.40
1:E:223:GLY:O	1:E:224:GLY:C	2.64	0.40
1:E:377:THR:O	1:E:380:SER:HB3	2.21	0.40
1:F:417:PHE:O	1:F:420:LEU:HB3	2.21	0.40
1:G:23:PRO:HA	1:G:24:PRO:HD3	1.78	0.40
1:G:372:GLN:HB2	1:G:410:THR:HB	2.03	0.40
1:G:375:GLN:HE21	1:G:375:GLN:HB3	1.56	0.40
1:H:221:SER:OG	5:H:3386:BEZ:H2	2.20	0.40
1:H:439:ASP:C	1:H:441:GLY:H	2.29	0.40
1:J:36:LYS:HE3	1:J:38:VAL:HG21	2.03	0.40
1:K:372:GLN:CB	1:K:410:THR:HB	2.50	0.40
1:L:218:PHE:CD1	1:L:218:PHE:N	2.89	0.40
1:A:26:VAL:HG11	1:A:207:SER:HB3	2.00	0.40
1:B:133:LEU:HB3	1:B:134:PRO:HD2	2.03	0.40
1:C:89:GLN:OE1	1:C:146:VAL:CA	2.69	0.40
1:C:457:SER:C	1:C:459:MET:H	2.30	0.40
1:D:351:ASN:N	1:D:354:GLU:OE2	2.54	0.40
1:E:357:TRP:O	1:E:360:PRO:HD2	2.21	0.40
1:E:431:VAL:HG12	1:E:435:ARG:HE	1.87	0.40
1:E:517:TRP:HA	1:E:518:PRO:HD2	1.96	0.40
1:F:240:PHE:CD1	1:F:240:PHE:N	2.90	0.40
1:G:297:THR:O	1:G:301:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:ARG:HD3	1:H:324:ASP:HB2	2.02	0.40
1:I:375:GLN:O	1:I:379:MET:HG2	2.21	0.40
1:J:138:TRP:CZ3	1:J:219:GLY:HA2	2.56	0.40
1:J:231:VAL:HG22	1:J:240:PHE:HE2	1.86	0.40
1:J:233:SER:HA	1:J:234:PRO:HD3	1.92	0.40
1:J:474:SER:HB3	1:J:496:VAL:HG21	2.02	0.40
1:J:488:GLU:O	1:J:491:ARG:HB3	2.22	0.40
1:K:205:ILE:HG13	1:K:210:GLY:HA3	2.03	0.40
1:K:253:SER:O	1:K:254:VAL:C	2.63	0.40
1:K:456:SER:HB3	1:K:460:LYS:HD3	2.02	0.40
1:L:64:ARG:HH11	1:L:294:LEU:HD12	1.85	0.40
1:L:491:ARG:HH11	1:L:491:ARG:HG3	1.87	0.40
1:A:257:LYS:HB2	1:A:322:VAL:HG12	2.02	0.40
1:B:539:LEU:C	1:B:541:ASP:H	2.29	0.40
1:C:40:LEU:O	1:C:41:GLU:C	2.64	0.40
1:C:89:GLN:OE1	1:C:146:VAL:HB	2.21	0.40
1:C:551:PHE:C	1:C:553:LYS:N	2.77	0.40
1:D:34:LEU:HB3	1:D:79:ASN:CA	2.51	0.40
1:D:134:PRO:HG2	1:D:163:VAL:HG12	2.02	0.40
1:E:283:VAL:HG12	1:E:287:ARG:NH1	2.36	0.40
1:E:449:PHE:CE2	1:E:451:TYR:HB3	2.56	0.40
1:G:383:TRP:O	1:G:386:TYR:HB2	2.21	0.40
1:H:62:PRO:C	1:H:64:ARG:H	2.29	0.40
1:H:204:ASN:C	1:H:206:ALA:N	2.79	0.40
1:H:225:GLU:O	1:H:229:VAL:HG23	2.21	0.40
1:H:236:ALA:HA	1:H:239:LEU:HD12	2.01	0.40
1:H:480:PHE:CD1	1:H:480:PHE:N	2.89	0.40
1:H:551:PHE:C	1:H:553:LYS:H	2.28	0.40
1:I:61:GLY:HA3	1:I:62:PRO:HD2	1.83	0.40
1:I:89:GLN:NE2	1:I:147:GLY:O	2.54	0.40
1:I:117:LEU:HD21	1:I:193:ASP:OD2	2.22	0.40
1:I:236:ALA:O	1:I:237:LYS:C	2.64	0.40
1:I:350:ILE:C	1:I:351:ASN:HD22	2.30	0.40
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.85	0.40
1:K:97:LEU:HD11	1:K:101:PHE:CE2	2.57	0.40
1:L:23:PRO:HB3	1:L:35:GLY:O	2.21	0.40
1:L:241:HIS:C	1:L:242:ARG:CG	2.94	0.40
1:L:297:THR:O	1:L:301:MET:HG2	2.21	0.40
1:L:493:SER:O	1:L:497:MET:HG3	2.21	0.40
1:A:252:THR:HG22	1:A:254:VAL:CG1	2.50	0.40
3:A:1181:SIA:H8	6:A:6003:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PRO:HA	1:C:24:PRO:HD3	1.85	0.40
1:C:268:ILE:HG12	1:C:301:MET:CE	2.39	0.40
1:C:415:ASP:HA	1:C:418:LEU:HD12	2.03	0.40
1:E:333:GLU:O	1:E:334:GLU:C	2.63	0.40
1:F:27:ASP:HA	1:F:32:LYS:HA	2.03	0.40
1:F:242:ARG:HG2	1:F:242:ARG:NH1	2.34	0.40
1:F:375:GLN:HE21	1:F:375:GLN:HB3	1.61	0.40
1:H:180:THR:O	1:H:262:LYS:HD3	2.22	0.40
1:H:366:TYR:C	1:H:368:LEU:H	2.30	0.40
1:H:447:TYR:HB3	1:H:517:TRP:CZ2	2.56	0.40
1:J:79:ASN:O	1:J:81:THR:N	2.54	0.40
1:J:83:TYR:CD1	1:J:150:SER:HB3	2.57	0.40
1:J:312:PRO:HG2	1:J:383:TRP:CD1	2.57	0.40
1:J:330:LYS:NZ	1:J:330:LYS:HB3	2.36	0.40
1:K:23:PRO:HA	1:K:24:PRO:HD3	1.80	0.40
1:K:143:GLY:O	1:K:144:LEU:CB	2.70	0.40
1:K:176:GLY:HA2	1:K:189:TRP:HB2	2.03	0.40
1:K:182:ASP:OD2	1:K:182:ASP:N	2.52	0.40
1:K:225:GLU:O	1:K:228:SER:HB3	2.22	0.40
1:K:428:VAL:HB	1:K:429:PRO:HD3	2.03	0.40
1:L:133:LEU:O	1:L:211:ASN:N	2.54	0.40
1:L:220:GLU:HA	1:L:246:GLU:O	2.22	0.40
1:L:278:THR:OG1	1:L:281:VAL:HG23	2.22	0.40
1:L:367:PRO:HB2	1:L:381:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/532 (100%)	451 (85%)	67 (13%)	12 (2%)	5 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	530/532 (100%)	448 (84%)	65 (12%)	17 (3%)	3	22
1	C	530/532 (100%)	467 (88%)	54 (10%)	9 (2%)	7	36
1	D	530/532 (100%)	454 (86%)	60 (11%)	16 (3%)	3	23
1	E	530/532 (100%)	438 (83%)	80 (15%)	12 (2%)	5	29
1	F	530/532 (100%)	464 (88%)	51 (10%)	15 (3%)	4	25
1	G	530/532 (100%)	445 (84%)	62 (12%)	23 (4%)	2	16
1	H	530/532 (100%)	449 (85%)	71 (13%)	10 (2%)	6	34
1	I	530/532 (100%)	451 (85%)	60 (11%)	19 (4%)	3	20
1	J	530/532 (100%)	444 (84%)	74 (14%)	12 (2%)	5	29
1	K	530/532 (100%)	451 (85%)	64 (12%)	15 (3%)	4	25
1	L	530/532 (100%)	434 (82%)	80 (15%)	16 (3%)	3	23
All	All	6360/6384 (100%)	5396 (85%)	788 (12%)	176 (3%)	4	25

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	SER
1	B	358	LEU
1	E	185	SER
1	E	358	LEU
1	E	456	SER
1	F	238	ASN
1	F	253	SER
1	F	531	ALA
1	G	105	LYS
1	I	76	PHE
1	I	185	SER
1	I	254	VAL
1	I	308	LEU
1	I	540	LYS
1	J	253	SER
1	J	340	ASN
1	L	76	PHE
1	L	102	THR
1	L	185	SER
1	L	308	LEU
1	A	102	THR
1	A	185	SER

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Mol	Chain	Res	Type
1	A	427	GLY
1	B	308	LEU
1	B	340	ASN
1	B	427	GLY
1	B	456	SER
1	B	538	LYS
1	C	105	LYS
1	C	357	TRP
1	C	427	GLY
1	D	185	SER
1	D	205	ILE
1	D	317	PRO
1	D	427	GLY
1	D	467	ASP
1	D	484	GLY
1	E	320	GLY
1	E	427	GLY
1	E	520	TYR
1	F	105	LYS
1	F	185	SER
1	F	358	LEU
1	F	427	GLY
1	G	127	LEU
1	G	140	HIS
1	G	205	ILE
1	G	253	SER
1	G	307	ASP
1	G	427	GLY
1	G	538	LYS
1	H	427	GLY
1	I	253	SER
1	I	302	LYS
1	J	127	LEU
1	J	254	VAL
1	J	427	GLY
1	K	252	THR
1	K	406	GLY
1	K	427	GLY
1	L	103	ASN
1	L	427	GLY
1	A	317	PRO
1	A	367	PRO

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Mol	Chain	Res	Type
1	A	485	ALA
1	B	105	LYS
1	B	182	ASP
1	B	254	VAL
1	B	302	LYS
1	C	185	SER
1	C	545	ALA
1	D	319	LEU
1	D	358	LEU
1	D	538	LYS
1	E	538	LYS
1	F	254	VAL
1	F	315	SER
1	F	406	GLY
1	F	520	TYR
1	G	76	PHE
1	G	79	ASN
1	G	183	GLU
1	G	306	LEU
1	G	312	PRO
1	G	394	GLU
1	H	102	THR
1	H	185	SER
1	H	252	THR
1	H	384	LYS
1	H	484	GLY
1	I	142	GLY
1	I	358	LEU
1	I	397	PRO
1	I	406	GLY
1	I	510	ASN
1	J	41	GLU
1	J	185	SER
1	J	315	SER
1	K	102	THR
1	K	143	GLY
1	K	340	ASN
1	K	482	LYS
1	K	551	PHE
1	L	75	SER
1	L	358	LEU
1	L	482	LYS

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Mol	Chain	Res	Type
1	B	80	ALA
1	D	156	ALA
1	D	340	ASN
1	E	127	LEU
1	E	254	VAL
1	E	364	MET
1	E	400	THR
1	G	65	PHE
1	G	156	ALA
1	G	318	LEU
1	G	370	GLU
1	G	456	SER
1	H	156	ALA
1	I	467	ASP
1	J	105	LYS
1	J	205	ILE
1	K	76	PHE
1	K	407	THR
1	L	79	ASN
1	L	369	SER
1	L	409	ASP
1	L	540	LYS
1	A	212	PRO
1	A	253	SER
1	A	540	LYS
1	B	397	PRO
1	B	470	ASP
1	B	520	TYR
1	C	148	ALA
1	C	253	SER
1	C	479	PRO
1	D	127	LEU
1	D	406	GLY
1	E	406	GLY
1	G	308	LEU
1	G	340	ASN
1	G	368	LEU
1	H	254	VAL
1	I	105	LYS
1	I	538	LYS
1	J	255	LEU
1	K	185	SER

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Mol	Chain	Res	Type
1	L	260	ASP
1	C	205	ILE
1	D	76	PHE
1	F	41	GLU
1	F	440	ALA
1	J	142	GLY
1	K	315	SER
1	K	367	PRO
1	L	275	LYS
1	D	254	VAL
1	F	477	GLY
1	G	406	GLY
1	H	544	VAL
1	I	205	ILE
1	K	254	VAL
1	L	254	VAL
1	B	317	PRO
1	H	143	GLY
1	I	62	PRO
1	K	142	GLY
1	D	515	PRO
1	I	427	GLY
1	A	143	GLY
1	B	227	VAL
1	A	90	ASP
1	A	142	GLY
1	F	405	GLY
1	I	124	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/448 (100%)	423 (94%)	25 (6%)	17 50
1	B	448/448 (100%)	423 (94%)	25 (6%)	17 50
1	C	448/448 (100%)	419 (94%)	29 (6%)	14 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	448/448 (100%)	419 (94%)	29 (6%)	14 45
1	E	448/448 (100%)	418 (93%)	30 (7%)	13 44
1	F	448/448 (100%)	429 (96%)	19 (4%)	25 58
1	G	448/448 (100%)	417 (93%)	31 (7%)	13 43
1	H	448/448 (100%)	425 (95%)	23 (5%)	20 53
1	I	448/448 (100%)	420 (94%)	28 (6%)	15 46
1	J	448/448 (100%)	424 (95%)	24 (5%)	18 51
1	K	448/448 (100%)	417 (93%)	31 (7%)	13 43
1	L	448/448 (100%)	415 (93%)	33 (7%)	11 40
All	All	5376/5376 (100%)	5049 (94%)	327 (6%)	15 47

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	78	LYS
1	A	86	MET
1	A	104	ARG
1	A	106	GLU
1	A	124	PRO
1	A	151	THR
1	A	164	VAL
1	A	221	SER
1	A	229	VAL
1	A	241	HIS
1	A	257	LYS
1	A	264	LEU
1	A	279	SER
1	A	304	LEU
1	A	338	GLU
1	A	344	VAL
1	A	347	MET
1	A	381	LEU
1	A	390	CYS
1	A	420	LEU
1	A	425	MET
1	A	522	GLN
1	A	529	ILE
1	A	553	LYS

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Mol	Chain	Res	Type
1	B	24	PRO
1	B	69	GLN
1	B	88	THR
1	B	132	ARG
1	B	162	ASN
1	B	215	VAL
1	B	218	PHE
1	B	225	GLU
1	B	249	VAL
1	B	251	LEU
1	B	257	LYS
1	B	261	VAL
1	B	292	GLU
1	B	304	LEU
1	B	306	LEU
1	B	329	LEU
1	B	338	GLU
1	B	379	MET
1	B	404	LEU
1	B	410	THR
1	B	411	VAL
1	B	506	ASN
1	B	523	LYS
1	B	542	LYS
1	B	551	PHE
1	C	57	LYS
1	C	86	MET
1	C	88	THR
1	C	92	LYS
1	C	105	LYS
1	C	123	THR
1	C	132	ARG
1	C	150	SER
1	C	151	THR
1	C	162	ASN
1	C	164	VAL
1	C	182	ASP
1	C	199	ARG
1	C	218	PHE
1	C	225	GLU
1	C	242	ARG
1	C	247	SER

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Mol	Chain	Res	Type
1	C	264	LEU
1	C	318	LEU
1	C	319	LEU
1	C	338	GLU
1	C	366	TYR
1	C	370	GLU
1	C	375	GLN
1	C	463	THR
1	C	471	GLU
1	C	499	PHE
1	C	506	ASN
1	C	523	LYS
1	D	79	ASN
1	D	102	THR
1	D	104	ARG
1	D	119	LEU
1	D	150	SER
1	D	151	THR
1	D	202	GLN
1	D	221	SER
1	D	225	GLU
1	D	242	ARG
1	D	255	LEU
1	D	261	VAL
1	D	262	LYS
1	D	264	LEU
1	D	278	THR
1	D	304	LEU
1	D	318	LEU
1	D	319	LEU
1	D	339	ARG
1	D	351	ASN
1	D	372	GLN
1	D	455	PHE
1	D	458	ASP
1	D	462	LYS
1	D	499	PHE
1	D	523	LYS
1	D	532	ASN
1	D	534	GLN
1	D	551	PHE
1	E	24	PRO

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Mol	Chain	Res	Type
1	E	25	VAL
1	E	28	THR
1	E	66	THR
1	E	69	GLN
1	E	79	ASN
1	E	104	ARG
1	E	106	GLU
1	E	124	PRO
1	E	151	THR
1	E	218	PHE
1	E	225	GLU
1	E	245	SER
1	E	264	LEU
1	E	298	THR
1	E	304	LEU
1	E	316	GLN
1	E	318	LEU
1	E	338	GLU
1	E	367	PRO
1	E	375	GLN
1	E	404	LEU
1	E	408	ASP
1	E	410	THR
1	E	420	LEU
1	E	459	MET
1	E	471	GLU
1	E	483	GLU
1	E	512	GLU
1	E	523	LYS
1	F	57	LYS
1	F	66	THR
1	F	69	GLN
1	F	162	ASN
1	F	172	LEU
1	F	182	ASP
1	F	220	GLU
1	F	225	GLU
1	F	264	LEU
1	F	270	ILE
1	F	275	LYS
1	F	293	GLU
1	F	319	LEU

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Mol	Chain	Res	Type
1	F	383	TRP
1	F	394	GLU
1	F	432	ILE
1	F	489	GLU
1	F	523	LYS
1	F	534	GLN
1	G	34	LEU
1	G	69	GLN
1	G	92	LYS
1	G	111	LYS
1	G	132	ARG
1	G	151	THR
1	G	162	ASN
1	G	172	LEU
1	G	174	ILE
1	G	182	ASP
1	G	202	GLN
1	G	218	PHE
1	G	225	GLU
1	G	242	ARG
1	G	257	LYS
1	G	264	LEU
1	G	278	THR
1	G	279	SER
1	G	292	GLU
1	G	335	LEU
1	G	347	MET
1	G	366	TYR
1	G	375	GLN
1	G	383	TRP
1	G	420	LEU
1	G	458	ASP
1	G	489	GLU
1	G	499	PHE
1	G	512	GLU
1	G	523	LYS
1	G	534	GLN
1	H	24	PRO
1	H	39	SER
1	H	79	ASN
1	H	104	ARG
1	H	132	ARG

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Mol	Chain	Res	Type
1	H	151	THR
1	H	168	ILE
1	H	195	VAL
1	H	199	ARG
1	H	225	GLU
1	H	242	ARG
1	H	257	LYS
1	H	276	THR
1	H	278	THR
1	H	292	GLU
1	H	319	LEU
1	H	366	TYR
1	H	370	GLU
1	H	419	ASP
1	H	420	LEU
1	H	479	PRO
1	H	532	ASN
1	H	541	ASP
1	I	24	PRO
1	I	27	ASP
1	I	28	THR
1	I	78	LYS
1	I	79	ASN
1	I	81	THR
1	I	82	SER
1	I	104	ARG
1	I	124	PRO
1	I	132	ARG
1	I	162	ASN
1	I	182	ASP
1	I	218	PHE
1	I	220	GLU
1	I	225	GLU
1	I	242	ARG
1	I	264	LEU
1	I	292	GLU
1	I	304	LEU
1	I	309	GLN
1	I	313	ARG
1	I	333	GLU
1	I	338	GLU
1	I	372	GLN

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Mol	Chain	Res	Type
1	I	374	ASP
1	I	423	ASP
1	I	471	GLU
1	I	506	ASN
1	J	60	LEU
1	J	88	THR
1	J	110	LEU
1	J	113	SER
1	J	150	SER
1	J	151	THR
1	J	162	ASN
1	J	182	ASP
1	J	215	VAL
1	J	218	PHE
1	J	225	GLU
1	J	226	SER
1	J	264	LEU
1	J	279	SER
1	J	304	LEU
1	J	318	LEU
1	J	319	LEU
1	J	330	LYS
1	J	342	HIS
1	J	366	TYR
1	J	375	GLN
1	J	457	SER
1	J	471	GLU
1	J	499	PHE
1	K	33	VAL
1	K	34	LEU
1	K	39	SER
1	K	41	GLU
1	K	63	LEU
1	K	78	LYS
1	K	88	THR
1	K	104	ARG
1	K	151	THR
1	K	199	ARG
1	K	207	SER
1	K	214	SER
1	K	225	GLU
1	K	242	ARG

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Mol	Chain	Res	Type
1	K	264	LEU
1	K	278	THR
1	K	292	GLU
1	K	304	LEU
1	K	307	ASP
1	K	309	GLN
1	K	316	GLN
1	K	318	LEU
1	K	361	MET
1	K	372	GLN
1	K	381	LEU
1	K	388	LEU
1	K	420	LEU
1	K	425	MET
1	K	455	PHE
1	K	471	GLU
1	K	523	LYS
1	L	24	PRO
1	L	28	THR
1	L	66	THR
1	L	79	ASN
1	L	81	THR
1	L	88	THR
1	L	129	LYS
1	L	132	ARG
1	L	133	LEU
1	L	135	VAL
1	L	162	ASN
1	L	163	VAL
1	L	182	ASP
1	L	199	ARG
1	L	203	ASP
1	L	218	PHE
1	L	220	GLU
1	L	225	GLU
1	L	264	LEU
1	L	302	LYS
1	L	304	LEU
1	L	329	LEU
1	L	338	GLU
1	L	375	GLN
1	L	400	THR

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Mol	Chain	Res	Type
1	L	404	LEU
1	L	411	VAL
1	L	420	LEU
1	L	471	GLU
1	L	491	ARG
1	L	497	MET
1	L	523	LYS
1	L	551	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	140	HIS
1	A	162	ASN
1	A	184	HIS
1	A	241	HIS
1	A	316	GLN
1	A	351	ASN
1	A	372	GLN
1	A	450	GLN
1	A	510	ASN
1	A	537	GLN
1	B	107	ASN
1	B	131	ASN
1	B	140	HIS
1	B	162	ASN
1	B	169	GLN
1	B	184	HIS
1	B	211	ASN
1	B	267	GLN
1	B	351	ASN
1	B	436	ASN
1	B	468	HIS
1	B	532	ASN
1	B	537	GLN
1	C	107	ASN
1	C	131	ASN
1	C	140	HIS
1	C	162	ASN
1	C	202	GLN
1	C	238	ASN

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Mol	Chain	Res	Type
1	C	241	HIS
1	C	336	GLN
1	C	351	ASN
1	C	372	GLN
1	C	436	ASN
1	C	537	GLN
1	D	30	HIS
1	D	69	GLN
1	D	131	ASN
1	D	140	HIS
1	D	162	ASN
1	D	202	GLN
1	D	241	HIS
1	D	351	ASN
1	D	372	GLN
1	D	436	ASN
1	D	437	HIS
1	D	450	GLN
1	D	521	ASN
1	D	522	GLN
1	D	528	GLN
1	D	537	GLN
1	E	69	GLN
1	E	107	ASN
1	E	131	ASN
1	E	140	HIS
1	E	162	ASN
1	E	169	GLN
1	E	184	HIS
1	E	241	HIS
1	E	316	GLN
1	E	336	GLN
1	E	351	ASN
1	E	372	GLN
1	E	375	GLN
1	E	436	ASN
1	E	528	GLN
1	E	532	ASN
1	E	534	GLN
1	E	537	GLN
1	F	45	GLN
1	F	95	GLN

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Mol	Chain	Res	Type
1	F	131	ASN
1	F	160	HIS
1	F	184	HIS
1	F	211	ASN
1	F	241	HIS
1	F	316	GLN
1	F	351	ASN
1	F	375	GLN
1	F	436	ASN
1	F	450	GLN
1	F	502	ASN
1	F	528	GLN
1	F	534	GLN
1	F	537	GLN
1	G	45	GLN
1	G	95	GLN
1	G	107	ASN
1	G	140	HIS
1	G	162	ASN
1	G	169	GLN
1	G	241	HIS
1	G	316	GLN
1	G	351	ASN
1	G	372	GLN
1	G	375	GLN
1	G	528	GLN
1	G	534	GLN
1	G	537	GLN
1	H	30	HIS
1	H	45	GLN
1	H	69	GLN
1	H	162	ASN
1	H	184	HIS
1	H	241	HIS
1	H	316	GLN
1	H	340	ASN
1	H	351	ASN
1	H	353	GLN
1	H	372	GLN
1	H	375	GLN
1	H	436	ASN
1	H	437	HIS

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Mol	Chain	Res	Type
1	H	522	GLN
1	H	528	GLN
1	H	532	ASN
1	H	534	GLN
1	H	537	GLN
1	H	549	ASN
1	I	45	GLN
1	I	69	GLN
1	I	107	ASN
1	I	162	ASN
1	I	184	HIS
1	I	241	HIS
1	I	309	GLN
1	I	336	GLN
1	I	342	HIS
1	I	351	ASN
1	I	372	GLN
1	I	375	GLN
1	I	436	ASN
1	I	437	HIS
1	I	450	GLN
1	I	468	HIS
1	I	528	GLN
1	I	534	GLN
1	I	537	GLN
1	J	30	HIS
1	J	45	GLN
1	J	69	GLN
1	J	107	ASN
1	J	131	ASN
1	J	140	HIS
1	J	238	ASN
1	J	241	HIS
1	J	309	GLN
1	J	336	GLN
1	J	351	ASN
1	J	353	GLN
1	J	372	GLN
1	J	436	ASN
1	J	450	GLN
1	J	528	GLN
1	J	534	GLN

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Mol	Chain	Res	Type
1	J	537	GLN
1	J	549	ASN
1	K	30	HIS
1	K	69	GLN
1	K	107	ASN
1	K	140	HIS
1	K	162	ASN
1	K	238	ASN
1	K	241	HIS
1	K	267	GLN
1	K	288	GLN
1	K	316	GLN
1	K	336	GLN
1	K	340	ASN
1	K	351	ASN
1	K	372	GLN
1	K	436	ASN
1	K	450	GLN
1	K	534	GLN
1	K	537	GLN
1	L	107	ASN
1	L	162	ASN
1	L	241	HIS
1	L	316	GLN
1	L	336	GLN
1	L	351	ASN
1	L	372	GLN
1	L	375	GLN
1	L	436	ASN
1	L	468	HIS
1	L	534	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

72 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BEZ	I	3380	-	9,9,9	1.55	1 (11%)	11,11,11	1.62	4 (36%)
5	BEZ	K	4387	-	9,9,9	3.36	6 (66%)	11,11,11	1.24	2 (18%)
4	SO4	I	3285	-	4,4,4	0.43	0	6,6,6	0.12	0
3	SIA	D	2180	-	21,21,21	0.91	0	24,31,31	1.00	1 (4%)
2	NAG	H	3279	1	14,14,15	0.76	0	17,19,21	0.88	0
5	BEZ	D	2385	-	9,9,9	14.32	9 (100%)	11,11,11	3.19	9 (81%)
5	BEZ	E	2387	-	9,9,9	1.57	1 (11%)	11,11,11	1.47	4 (36%)
4	SO4	B	1284	-	4,4,4	0.42	0	6,6,6	0.05	0
2	NAG	E	2279	1	14,14,15	0.55	0	17,19,21	1.10	1 (5%)
3	SIA	I	982	-	21,21,21	0.85	1 (4%)	24,31,31	1.00	2 (8%)
5	BEZ	G	3385	-	9,9,9	1.86	1 (11%)	11,11,11	1.71	4 (36%)
2	NAG	L	4379	1	14,14,15	0.57	0	17,19,21	0.85	1 (5%)
3	SIA	A	1180	-	21,21,21	0.82	0	24,31,31	1.07	1 (4%)
4	SO4	C	1285	-	4,4,4	0.43	0	6,6,6	0.11	0
4	SO4	F	2185	-	4,4,4	0.42	0	6,6,6	0.19	0
5	BEZ	D	2386	-	9,9,9	3.61	7 (77%)	11,11,11	1.26	1 (9%)
5	BEZ	F	5023	1	8,8,9	2.33	5 (62%)	9,9,11	0.70	0
4	SO4	A	1184	-	4,4,4	0.36	0	6,6,6	0.08	0
5	BEZ	J	5041	1	8,8,9	2.37	4 (50%)	9,9,11	0.69	0
4	SO4	H	3385	-	4,4,4	0.43	0	6,6,6	0.13	0
5	BEZ	K	4386	-	9,9,9	1.68	1 (11%)	11,11,11	1.41	2 (18%)
5	BEZ	G	3386	-	9,9,9	5.57	7 (77%)	11,11,11	4.35	6 (54%)
4	SO4	D	2384	-	4,4,4	0.45	0	6,6,6	0.16	0
5	BEZ	H	3387	-	9,9,9	4.05	5 (55%)	11,11,11	5.05	7 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	F	2285	-	4,4,4	0.42	0	6,6,6	0.12	0
4	SO4	D	2184	-	4,4,4	0.38	0	6,6,6	0.08	0
4	SO4	J	4185	-	4,4,4	0.42	0	6,6,6	0.26	0
2	NAG	G	3179	1	14,14,15	0.85	0	17,19,21	0.93	1 (5%)
2	NAG	A	1179	1	14,14,15	0.70	0	17,19,21	0.73	1 (5%)
5	BEZ	H	3386	-	9,9,9	1.62	1 (11%)	11,11,11	1.55	3 (27%)
3	SIA	B	1280	-	21,21,21	0.84	0	24,31,31	1.36	4 (16%)
2	NAG	K	4279	1	14,14,15	0.86	0	17,19,21	0.69	0
5	BEZ	C	5014	-	9,9,9	2.30	3 (33%)	11,11,11	1.55	2 (18%)
5	BEZ	J	5042	-	9,9,9	5.25	4 (44%)	11,11,11	3.14	3 (27%)
5	BEZ	E	2386	-	9,9,9	1.50	1 (11%)	11,11,11	1.36	2 (18%)
5	BEZ	I	3381	-	9,9,9	2.18	5 (55%)	11,11,11	0.89	1 (9%)
2	NAG	D	2179	1	14,14,15	0.73	0	17,19,21	0.68	1 (5%)
4	SO4	K	4284	-	4,4,4	0.40	0	6,6,6	0.08	0
2	NAG	F	2379	1	14,14,15	1.24	2 (14%)	17,19,21	1.61	4 (23%)
2	NAG	J	4179	1	14,14,15	0.81	0	17,19,21	1.38	4 (23%)
3	SIA	F	682	-	21,21,21	1.16	3 (14%)	24,31,31	1.12	3 (12%)
4	SO4	L	4285	-	4,4,4	0.42	0	6,6,6	0.07	0
5	BEZ	B	1386	-	9,9,9	2.42	4 (44%)	11,11,11	0.92	1 (9%)
4	SO4	H	3284	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	J	4384	-	4,4,4	0.44	0	6,6,6	0.09	0
3	SIA	G	782	-	21,21,21	0.97	0	24,31,31	1.06	1 (4%)
3	SIA	L	1282	-	21,21,21	0.88	0	24,31,31	1.20	2 (8%)
4	SO4	B	1385	-	4,4,4	0.38	0	6,6,6	0.12	0
4	SO4	A	1384	-	4,4,4	0.41	0	6,6,6	0.10	0
3	SIA	A	1181	-	21,21,21	1.10	2 (9%)	24,31,31	1.00	1 (4%)
4	SO4	G	3184	-	4,4,4	0.38	0	6,6,6	0.13	0
5	BEZ	L	4381	-	9,9,9	1.47	1 (11%)	11,11,11	1.40	3 (27%)
4	SO4	K	4385	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SIA	E	582	-	21,21,21	0.90	1 (4%)	24,31,31	1.20	2 (8%)
2	NAG	C	1379	1	14,14,15	0.69	0	17,19,21	0.89	1 (5%)
2	NAG	I	3379	1	14,14,15	0.65	0	17,19,21	0.94	1 (5%)
5	BEZ	B	12	-	9,9,9	19.07	9 (100%)	11,11,11	4.13	4 (36%)
3	SIA	K	1182	-	21,21,21	0.95	1 (4%)	24,31,31	1.12	2 (8%)
2	NAG	B	1279	1	14,14,15	0.68	0	17,19,21	0.84	1 (5%)
3	SIA	J	1082	-	21,21,21	1.07	2 (9%)	24,31,31	1.12	2 (8%)
4	SO4	G	3384	-	4,4,4	0.41	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	I	3185	-	4,4,4	0.38	0	6,6,6	0.16	0
5	BEZ	A	1385	-	9,9,9	4.58	4 (44%)	11,11,11	2.07	1 (9%)
5	BEZ	F	5024	-	9,9,9	2.00	3 (33%)	11,11,11	1.04	1 (9%)
3	SIA	H	882	-	21,21,21	1.09	2 (9%)	24,31,31	1.15	3 (12%)
4	SO4	E	2385	-	4,4,4	0.38	0	6,6,6	0.15	0
5	BEZ	A	11	-	9,9,9	3.48	6 (66%)	11,11,11	1.80	4 (36%)
5	BEZ	C	5013	1	8,8,9	2.33	4 (50%)	9,9,11	0.83	1 (11%)
5	BEZ	L	4380	-	9,9,9	1.69	1 (11%)	11,11,11	1.24	2 (18%)
4	SO4	E	2284	-	4,4,4	0.41	0	6,6,6	0.16	0
4	SO4	C	1185	-	4,4,4	0.42	0	6,6,6	0.20	0
4	SO4	J	4184	-	4,4,4	0.39	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BEZ	I	3380	-	-	0/4/4/4	0/1/1/1
5	BEZ	K	4387	-	-	0/4/4/4	0/1/1/1
3	SIA	D	2180	-	-	7/20/38/38	0/1/1/1
2	NAG	H	3279	1	-	5/6/23/26	0/1/1/1
5	BEZ	D	2385	-	-	0/4/4/4	0/1/1/1
5	BEZ	E	2387	-	-	0/4/4/4	0/1/1/1
2	NAG	E	2279	1	-	2/6/23/26	0/1/1/1
3	SIA	I	982	-	-	12/20/38/38	0/1/1/1
5	BEZ	G	3385	-	-	0/4/4/4	0/1/1/1
2	NAG	L	4379	1	-	6/6/23/26	0/1/1/1
3	SIA	A	1180	-	-	7/20/38/38	0/1/1/1
5	BEZ	D	2386	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5023	1	-	0/2/2/4	0/1/1/1
5	BEZ	J	5041	1	-	0/2/2/4	0/1/1/1
5	BEZ	K	4386	-	-	0/4/4/4	0/1/1/1
5	BEZ	G	3386	-	-	0/4/4/4	0/1/1/1
5	BEZ	H	3387	-	-	0/4/4/4	0/1/1/1
2	NAG	G	3179	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	1179	1	-	5/6/23/26	0/1/1/1
5	BEZ	H	3386	-	-	0/4/4/4	0/1/1/1
3	SIA	B	1280	-	-	9/20/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	4279	1	1/1/5/7	3/6/23/26	0/1/1/1
5	BEZ	C	5014	-	-	0/4/4/4	0/1/1/1
5	BEZ	J	5042	-	-	2/4/4/4	0/1/1/1
5	BEZ	I	3381	-	-	0/4/4/4	0/1/1/1
2	NAG	D	2179	1	-	2/6/23/26	0/1/1/1
2	NAG	F	2379	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	J	4179	1	1/1/5/7	4/6/23/26	0/1/1/1
3	SIA	F	682	-	-	9/20/38/38	0/1/1/1
5	BEZ	B	1386	-	-	0/4/4/4	0/1/1/1
3	SIA	G	782	-	-	9/20/38/38	0/1/1/1
3	SIA	L	1282	-	-	9/20/38/38	0/1/1/1
3	SIA	A	1181	-	-	8/20/38/38	0/1/1/1
5	BEZ	L	4381	-	-	0/4/4/4	0/1/1/1
3	SIA	E	582	-	-	10/20/38/38	0/1/1/1
2	NAG	C	1379	1	-	3/6/23/26	0/1/1/1
2	NAG	I	3379	1	-	2/6/23/26	0/1/1/1
5	BEZ	B	12	-	-	0/4/4/4	0/1/1/1
3	SIA	K	1182	-	-	14/20/38/38	0/1/1/1
2	NAG	B	1279	1	1/1/5/7	4/6/23/26	0/1/1/1
3	SIA	J	1082	-	-	11/20/38/38	0/1/1/1
5	BEZ	A	1385	-	-	0/4/4/4	0/1/1/1
5	BEZ	F	5024	-	-	0/4/4/4	0/1/1/1
3	SIA	H	882	-	-	7/20/38/38	0/1/1/1
5	BEZ	C	5013	1	-	0/2/2/4	0/1/1/1
5	BEZ	A	11	-	-	0/4/4/4	0/1/1/1
5	BEZ	E	2386	-	-	0/4/4/4	0/1/1/1
5	BEZ	L	4380	-	-	0/4/4/4	0/1/1/1

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	12	BEZ	C6-C1	25.95	1.78	1.39
5	B	12	BEZ	C2-C1	25.70	1.78	1.39
5	B	12	BEZ	C3-C2	22.14	1.76	1.38
5	B	12	BEZ	C4-C3	21.53	1.85	1.38
5	B	12	BEZ	C5-C4	21.16	1.84	1.38
5	B	12	BEZ	C5-C6	21.08	1.74	1.38
5	D	2385	BEZ	C4-C3	19.90	1.82	1.38
5	D	2385	BEZ	C5-C4	19.85	1.81	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2385	BEZ	C3-C2	19.12	1.71	1.38
5	D	2385	BEZ	C5-C6	16.75	1.67	1.38
5	D	2385	BEZ	C2-C1	13.23	1.59	1.39
5	D	2385	BEZ	C6-C1	12.13	1.57	1.39
5	J	5042	BEZ	C2-C1	11.15	1.56	1.39
5	G	3386	BEZ	C1-C	9.77	1.70	1.49
5	A	1385	BEZ	C2-C1	9.33	1.53	1.39
5	J	5042	BEZ	C6-C1	9.19	1.53	1.39
5	G	3386	BEZ	C2-C1	-8.31	1.26	1.39
5	A	1385	BEZ	C6-C1	8.15	1.51	1.39
5	G	3386	BEZ	C6-C1	-8.12	1.27	1.39
5	H	3387	BEZ	C1-C	8.08	1.66	1.49
5	B	12	BEZ	C1-C	7.38	1.65	1.49
5	D	2385	BEZ	C1-C	6.99	1.64	1.49
5	C	5014	BEZ	C1-C	5.55	1.61	1.49
5	D	2385	BEZ	O1-C	5.55	1.38	1.22
5	A	11	BEZ	C5-C4	5.47	1.50	1.38
5	B	12	BEZ	O1-C	5.46	1.38	1.22
5	K	4387	BEZ	C5-C4	5.36	1.50	1.38
5	K	4387	BEZ	C4-C3	5.31	1.49	1.38
5	H	3387	BEZ	C4-C3	-5.26	1.26	1.38
5	D	2386	BEZ	C5-C4	5.19	1.49	1.38
5	A	11	BEZ	C4-C3	5.10	1.49	1.38
5	J	5042	BEZ	C1-C	5.10	1.60	1.49
5	D	2386	BEZ	C4-C3	5.00	1.49	1.38
5	H	3387	BEZ	C2-C1	-4.85	1.32	1.39
5	G	3385	BEZ	C1-C	4.73	1.59	1.49
5	D	2386	BEZ	C1-C	4.50	1.59	1.49
5	A	1385	BEZ	C1-C	4.18	1.58	1.49
5	D	2386	BEZ	C5-C6	4.02	1.45	1.38
5	C	5013	BEZ	O2-C	-4.00	1.24	1.41
5	B	1386	BEZ	C6-C1	3.96	1.45	1.39
5	G	3386	BEZ	C5-C4	3.94	1.46	1.38
5	A	11	BEZ	C1-C	3.93	1.57	1.49
5	H	3386	BEZ	C1-C	3.91	1.57	1.49
5	J	5041	BEZ	O2-C	-3.85	1.25	1.41
5	A	11	BEZ	C5-C6	3.83	1.45	1.38
5	H	3387	BEZ	C6-C1	-3.83	1.33	1.39
5	A	1385	BEZ	O1-C	3.79	1.33	1.22
5	K	4386	BEZ	C1-C	3.74	1.57	1.49
5	K	4387	BEZ	C5-C6	3.62	1.45	1.38
5	G	3386	BEZ	O1-C	3.60	1.33	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	4387	BEZ	C1-C	3.58	1.57	1.49
5	F	5023	BEZ	O2-C	-3.58	1.26	1.41
5	A	11	BEZ	C3-C2	3.53	1.45	1.38
5	I	3380	BEZ	C1-C	3.52	1.56	1.49
5	B	1386	BEZ	C2-C1	3.49	1.44	1.39
5	E	2386	BEZ	C1-C	3.46	1.56	1.49
5	D	2386	BEZ	C3-C2	3.42	1.44	1.38
2	F	2379	NAG	C1-C2	3.38	1.56	1.52
5	I	3381	BEZ	C2-C1	3.33	1.44	1.39
5	E	2387	BEZ	C1-C	3.31	1.56	1.49
5	G	3386	BEZ	C4-C3	3.23	1.45	1.38
5	H	3387	BEZ	C5-C4	-3.10	1.31	1.38
5	B	12	BEZ	O2-C	3.04	1.39	1.30
5	J	5041	BEZ	C6-C1	2.97	1.44	1.38
5	L	4381	BEZ	C1-C	2.93	1.55	1.49
5	L	4380	BEZ	C1-C	2.92	1.55	1.49
5	F	5024	BEZ	C1-C	2.91	1.55	1.49
5	J	5042	BEZ	O1-C	2.89	1.31	1.22
5	D	2385	BEZ	O2-C	2.89	1.39	1.30
5	G	3386	BEZ	C3-C2	-2.86	1.34	1.38
5	J	5041	BEZ	C2-C1	2.85	1.44	1.38
5	C	5013	BEZ	C2-C1	2.80	1.44	1.38
5	I	3381	BEZ	C6-C1	2.79	1.43	1.39
5	D	2386	BEZ	C6-C1	2.79	1.43	1.39
3	K	1182	SIA	C4-C5	2.70	1.55	1.53
5	K	4387	BEZ	C3-C2	2.63	1.43	1.38
5	D	2386	BEZ	C2-C1	2.62	1.43	1.39
5	B	1386	BEZ	C1-C	2.61	1.55	1.49
5	F	5023	BEZ	C6-C1	2.58	1.44	1.38
3	F	682	SIA	O6-C2	2.50	1.45	1.43
5	F	5023	BEZ	C3-C2	2.47	1.43	1.38
5	C	5013	BEZ	C6-C1	2.47	1.43	1.38
5	F	5024	BEZ	C2-C1	2.45	1.43	1.39
5	F	5023	BEZ	C2-C1	2.40	1.43	1.38
5	K	4387	BEZ	C6-C1	2.37	1.43	1.39
5	F	5023	BEZ	C5-C6	2.36	1.42	1.38
3	A	1181	SIA	C4-C5	2.35	1.55	1.53
5	F	5024	BEZ	C6-C1	2.32	1.42	1.39
3	E	582	SIA	C4-C5	2.32	1.55	1.53
5	I	3381	BEZ	C1-C	2.29	1.54	1.49
3	H	882	SIA	C7-C6	2.28	1.55	1.52
3	F	682	SIA	C4-C5	2.26	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	882	SIA	C6-C5	2.20	1.56	1.53
3	A	1181	SIA	C6-C5	2.16	1.56	1.53
5	I	3381	BEZ	C3-C2	2.16	1.42	1.38
3	J	1082	SIA	O6-C2	2.13	1.45	1.43
3	J	1082	SIA	C4-C5	2.11	1.55	1.53
3	I	982	SIA	C3-C2	2.10	1.54	1.51
5	B	1386	BEZ	C4-C3	2.10	1.42	1.38
5	C	5014	BEZ	C6-C1	2.09	1.42	1.39
5	J	5041	BEZ	C5-C4	2.08	1.42	1.38
2	F	2379	NAG	C4-C5	2.07	1.57	1.53
5	C	5014	BEZ	C4-C3	2.06	1.42	1.38
5	A	11	BEZ	C6-C1	2.06	1.42	1.39
5	C	5013	BEZ	C5-C4	2.05	1.42	1.38
5	I	3381	BEZ	C5-C6	2.03	1.42	1.38
3	F	682	SIA	C3-C2	2.01	1.54	1.51

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3387	BEZ	O2-C-O1	-13.35	94.64	123.35
5	B	12	BEZ	O2-C-O1	11.24	147.52	123.35
5	J	5042	BEZ	C6-C1-C2	-8.15	108.20	118.57
5	G	3386	BEZ	C5-C4-C3	-7.58	109.49	119.87
5	H	3387	BEZ	O2-C-C1	7.31	133.59	114.84
5	G	3386	BEZ	C3-C2-C1	7.26	127.50	120.36
5	G	3386	BEZ	C5-C6-C1	7.15	127.39	120.36
5	D	2385	BEZ	O2-C-O1	6.39	137.09	123.35
5	A	1385	BEZ	C6-C1-C2	-6.19	110.70	118.57
5	B	12	BEZ	O1-C-C1	-5.39	107.33	121.46
5	B	12	BEZ	O2-C-C1	-4.47	103.38	114.84
5	G	3386	BEZ	O2-C-O1	-4.25	114.21	123.35
5	J	5042	BEZ	C3-C2-C1	-4.06	116.37	120.36
5	G	3386	BEZ	C6-C1-C2	-4.05	113.41	118.57
5	A	11	BEZ	C5-C4-C3	-3.92	114.51	119.87
5	H	3387	BEZ	O1-C-C1	3.89	131.66	121.46
5	J	5042	BEZ	C5-C6-C1	-3.64	116.78	120.36
2	F	2379	NAG	O5-C1-C2	-3.55	105.80	111.29
5	D	2385	BEZ	C4-C3-C2	-3.52	115.89	120.24
5	D	2385	BEZ	C5-C6-C1	3.51	123.82	120.36
2	J	4179	NAG	O5-C1-C2	-3.47	105.92	111.29
3	E	582	SIA	O1A-C1-C2	-3.41	118.17	123.85
5	D	2385	BEZ	O1-C-C1	-3.39	112.56	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1280	SIA	O1A-C1-C2	-3.35	118.26	123.85
5	H	3387	BEZ	C4-C3-C2	3.33	124.35	120.24
2	F	2379	NAG	C1-C2-N2	3.30	115.64	110.43
2	E	2279	NAG	C2-N2-C7	-3.29	118.49	122.90
2	I	3379	NAG	C2-N2-C7	-3.28	118.50	122.90
3	L	1282	SIA	O1A-C1-C2	-3.22	118.48	123.85
5	C	5014	BEZ	O2-C-O1	-3.20	116.47	123.35
3	A	1181	SIA	O1A-C1-C2	-3.19	118.54	123.85
3	H	882	SIA	O1A-C1-C2	-3.17	118.57	123.85
3	F	682	SIA	O1A-C1-C2	-3.12	118.64	123.85
5	G	3386	BEZ	O2-C-C1	3.12	122.85	114.84
3	A	1180	SIA	O1A-C1-C2	-3.05	118.76	123.85
3	G	782	SIA	O1A-C1-C2	-3.05	118.76	123.85
3	K	1182	SIA	O1A-C1-C2	-3.03	118.80	123.85
3	D	2180	SIA	O1A-C1-C2	-2.97	118.89	123.85
5	G	3385	BEZ	O2-C-O1	-2.97	116.97	123.35
3	J	1082	SIA	O1A-C1-C2	-2.93	118.97	123.85
5	H	3387	BEZ	C5-C4-C3	-2.91	115.88	119.87
5	H	3387	BEZ	C5-C6-C1	-2.88	117.53	120.36
5	I	3380	BEZ	C3-C2-C1	2.87	123.19	120.36
5	D	2385	BEZ	C4-C5-C6	-2.86	116.71	120.24
3	J	1082	SIA	C9-C8-C7	-2.83	106.40	112.17
3	B	1280	SIA	C9-C8-C7	-2.80	106.46	112.17
2	B	1279	NAG	C2-N2-C7	-2.79	119.17	122.90
3	I	982	SIA	O1A-C1-C2	-2.78	119.21	123.85
3	F	682	SIA	O6-C6-C7	2.77	110.98	106.65
5	D	2385	BEZ	C6-C1-C2	2.76	122.08	118.57
5	H	3386	BEZ	O2-C-O1	-2.75	117.44	123.35
5	G	3385	BEZ	O2-C-C1	2.73	121.83	114.84
5	C	5014	BEZ	C6-C1-C2	-2.72	115.10	118.57
5	I	3380	BEZ	O2-C-O1	-2.69	117.57	123.35
3	B	1280	SIA	C3-C2-C1	-2.68	107.87	112.84
3	B	1280	SIA	O6-C6-C7	2.55	110.64	106.65
2	L	4379	NAG	C2-N2-C7	-2.52	119.52	122.90
5	E	2386	BEZ	O2-C-O1	-2.52	117.94	123.35
5	E	2387	BEZ	C3-C2-C1	2.50	122.82	120.36
2	F	2379	NAG	C3-C4-C5	2.50	114.76	110.23
5	D	2385	BEZ	C5-C4-C3	-2.42	116.55	119.87
5	D	2385	BEZ	C3-C2-C1	2.42	122.75	120.36
2	J	4179	NAG	C1-C2-N2	2.42	114.25	110.43
5	K	4386	BEZ	O2-C-C1	2.41	121.03	114.84
5	G	3385	BEZ	C3-C2-C1	2.41	122.73	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	3380	BEZ	O2-C-C1	2.41	121.02	114.84
5	K	4386	BEZ	O2-C-O1	-2.37	118.27	123.35
2	A	1179	NAG	C2-N2-C7	-2.36	119.74	122.90
5	H	3386	BEZ	O2-C-C1	2.34	120.85	114.84
5	D	2386	BEZ	C5-C4-C3	-2.32	116.70	119.87
5	E	2387	BEZ	O2-C-O1	-2.31	118.38	123.35
3	I	982	SIA	C9-C8-C7	-2.31	107.46	112.17
5	A	11	BEZ	C5-C6-C1	2.31	122.63	120.36
5	G	3385	BEZ	C5-C6-C1	2.31	122.63	120.36
5	L	4380	BEZ	O2-C-C1	2.31	120.75	114.84
5	L	4381	BEZ	O2-C-O1	-2.30	118.41	123.35
5	B	12	BEZ	C4-C3-C2	-2.29	117.42	120.24
2	C	1379	NAG	C2-N2-C7	-2.27	119.86	122.90
5	H	3387	BEZ	C4-C5-C6	2.26	123.03	120.24
5	C	5013	BEZ	O2-C-C1	2.24	119.95	112.07
2	J	4179	NAG	C2-N2-C7	-2.24	119.90	122.90
5	K	4387	BEZ	C5-C4-C3	-2.21	116.85	119.87
3	E	582	SIA	O6-C6-C7	2.20	110.09	106.65
2	D	2179	NAG	C2-N2-C7	-2.19	119.96	122.90
5	E	2386	BEZ	O2-C-C1	2.18	120.42	114.84
5	A	11	BEZ	C3-C2-C1	2.17	122.50	120.36
5	A	11	BEZ	C6-C1-C2	-2.16	115.83	118.57
5	L	4381	BEZ	C5-C6-C1	2.15	122.48	120.36
5	L	4381	BEZ	O2-C-C1	2.15	120.35	114.84
3	H	882	SIA	C3-C2-C1	-2.14	108.86	112.84
2	J	4179	NAG	C4-C3-C2	-2.13	107.90	111.02
5	E	2387	BEZ	O2-C-C1	2.12	120.28	114.84
5	D	2385	BEZ	O2-C-C1	-2.12	109.40	114.84
3	K	1182	SIA	C3-C4-C5	2.11	112.99	109.72
3	L	1282	SIA	C3-C2-C1	-2.10	108.95	112.84
3	F	682	SIA	C3-C2-C1	-2.10	108.95	112.84
5	F	5024	BEZ	O2-C-C1	2.09	120.21	114.84
5	L	4380	BEZ	O2-C-O1	-2.09	118.86	123.35
2	F	2379	NAG	O7-C7-C8	-2.07	118.36	122.05
5	H	3386	BEZ	C5-C6-C1	2.07	122.40	120.36
5	I	3381	BEZ	O2-C-C1	2.05	120.10	114.84
2	G	3179	NAG	O5-C1-C2	-2.04	108.14	111.29
5	E	2387	BEZ	C5-C6-C1	2.03	122.36	120.36
5	K	4387	BEZ	C5-C6-C1	2.03	122.36	120.36
3	H	882	SIA	O6-C6-C7	2.01	109.79	106.65
5	I	3380	BEZ	C5-C6-C1	2.01	122.34	120.36
5	B	1386	BEZ	O2-C-C1	2.01	119.98	114.84

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1279	NAG	C1
2	F	2379	NAG	C1
2	G	3179	NAG	C1
2	J	4179	NAG	C1
2	K	4279	NAG	C1

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1179	NAG	C8-C7-N2-C2
2	A	1179	NAG	O7-C7-N2-C2
2	B	1279	NAG	C1-C2-N2-C7
2	B	1279	NAG	C8-C7-N2-C2
2	B	1279	NAG	O7-C7-N2-C2
2	C	1379	NAG	C8-C7-N2-C2
2	C	1379	NAG	O7-C7-N2-C2
2	E	2279	NAG	C8-C7-N2-C2
2	E	2279	NAG	O7-C7-N2-C2
2	F	2379	NAG	C8-C7-N2-C2
2	F	2379	NAG	O7-C7-N2-C2
2	G	3179	NAG	C8-C7-N2-C2
2	G	3179	NAG	O7-C7-N2-C2
2	H	3279	NAG	C8-C7-N2-C2
2	H	3279	NAG	O7-C7-N2-C2
2	I	3379	NAG	C8-C7-N2-C2
2	I	3379	NAG	O7-C7-N2-C2
2	J	4179	NAG	C8-C7-N2-C2
2	J	4179	NAG	O7-C7-N2-C2
2	K	4279	NAG	C8-C7-N2-C2
2	K	4279	NAG	O7-C7-N2-C2
2	L	4379	NAG	C8-C7-N2-C2
2	L	4379	NAG	O7-C7-N2-C2
3	A	1180	SIA	C5-C6-C7-C8
3	A	1180	SIA	C5-C6-C7-O7
3	A	1180	SIA	O6-C6-C7-C8
3	A	1180	SIA	O6-C6-C7-O7
3	A	1180	SIA	C11-C10-N5-C5
3	A	1180	SIA	O10-C10-N5-C5
3	A	1181	SIA	C4-C5-N5-C10
3	A	1181	SIA	C5-C6-C7-C8
3	A	1181	SIA	C5-C6-C7-O7
3	A	1181	SIA	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1181	SIA	O6-C6-C7-O7
3	A	1181	SIA	C11-C10-N5-C5
3	A	1181	SIA	O10-C10-N5-C5
3	B	1280	SIA	C4-C5-N5-C10
3	B	1280	SIA	C5-C6-C7-C8
3	B	1280	SIA	C5-C6-C7-O7
3	B	1280	SIA	O6-C6-C7-C8
3	B	1280	SIA	O6-C6-C7-O7
3	B	1280	SIA	C11-C10-N5-C5
3	B	1280	SIA	O10-C10-N5-C5
3	D	2180	SIA	C5-C6-C7-C8
3	D	2180	SIA	C5-C6-C7-O7
3	D	2180	SIA	O6-C6-C7-C8
3	D	2180	SIA	O6-C6-C7-O7
3	D	2180	SIA	C11-C10-N5-C5
3	D	2180	SIA	O10-C10-N5-C5
3	E	582	SIA	C5-C6-C7-C8
3	E	582	SIA	C5-C6-C7-O7
3	E	582	SIA	O6-C6-C7-C8
3	E	582	SIA	O6-C6-C7-O7
3	E	582	SIA	C6-C7-C8-C9
3	E	582	SIA	C6-C7-C8-O8
3	E	582	SIA	O7-C7-C8-C9
3	E	582	SIA	O7-C7-C8-O8
3	E	582	SIA	C11-C10-N5-C5
3	E	582	SIA	O10-C10-N5-C5
3	F	682	SIA	O1B-C1-C2-O2
3	F	682	SIA	O6-C6-C7-O7
3	F	682	SIA	C11-C10-N5-C5
3	F	682	SIA	O10-C10-N5-C5
3	G	782	SIA	C5-C6-C7-C8
3	G	782	SIA	C5-C6-C7-O7
3	G	782	SIA	O6-C6-C7-C8
3	G	782	SIA	O6-C6-C7-O7
3	G	782	SIA	C11-C10-N5-C5
3	G	782	SIA	O10-C10-N5-C5
3	H	882	SIA	C4-C5-N5-C10
3	H	882	SIA	C5-C6-C7-C8
3	H	882	SIA	C5-C6-C7-O7
3	H	882	SIA	O6-C6-C7-C8
3	H	882	SIA	O6-C6-C7-O7
3	H	882	SIA	C11-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
3	H	882	SIA	O10-C10-N5-C5
3	I	982	SIA	C5-C6-C7-C8
3	I	982	SIA	C5-C6-C7-O7
3	I	982	SIA	O6-C6-C7-C8
3	I	982	SIA	O6-C6-C7-O7
3	I	982	SIA	C11-C10-N5-C5
3	I	982	SIA	O10-C10-N5-C5
3	J	1082	SIA	O1B-C1-C2-O2
3	J	1082	SIA	C5-C6-C7-C8
3	J	1082	SIA	C5-C6-C7-O7
3	J	1082	SIA	O6-C6-C7-C8
3	J	1082	SIA	O6-C6-C7-O7
3	J	1082	SIA	C11-C10-N5-C5
3	J	1082	SIA	O10-C10-N5-C5
3	K	1182	SIA	O1A-C1-C2-O2
3	K	1182	SIA	O1A-C1-C2-O6
3	K	1182	SIA	O1B-C1-C2-O2
3	K	1182	SIA	O1B-C1-C2-O6
3	K	1182	SIA	C5-C6-C7-C8
3	K	1182	SIA	C5-C6-C7-O7
3	K	1182	SIA	O6-C6-C7-C8
3	K	1182	SIA	O6-C6-C7-O7
3	K	1182	SIA	C11-C10-N5-C5
3	K	1182	SIA	O10-C10-N5-C5
3	L	1282	SIA	C4-C5-N5-C10
3	L	1282	SIA	C5-C6-C7-C8
3	L	1282	SIA	C5-C6-C7-O7
3	L	1282	SIA	O6-C6-C7-C8
3	L	1282	SIA	O6-C6-C7-O7
3	L	1282	SIA	C11-C10-N5-C5
3	L	1282	SIA	O10-C10-N5-C5
2	A	1179	NAG	O5-C5-C6-O6
2	A	1179	NAG	C4-C5-C6-O6
2	G	3179	NAG	O5-C5-C6-O6
3	K	1182	SIA	C7-C8-C9-O9
2	G	3179	NAG	C4-C5-C6-O6
3	K	1182	SIA	C6-C5-N5-C10
2	J	4179	NAG	C4-C5-C6-O6
3	K	1182	SIA	O8-C8-C9-O9
2	C	1379	NAG	O5-C5-C6-O6
3	I	982	SIA	C7-C8-C9-O9
2	D	2179	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	J	4179	NAG	O5-C5-C6-O6
3	J	1082	SIA	C7-C8-C9-O9
2	D	2179	NAG	O7-C7-N2-C2
3	F	682	SIA	C4-C5-N5-C10
3	I	982	SIA	C4-C5-N5-C10
3	K	1182	SIA	C4-C5-N5-C10
2	K	4279	NAG	O5-C5-C6-O6
3	L	1282	SIA	C7-C8-C9-O9
3	A	1181	SIA	C7-C8-C9-O9
3	I	982	SIA	O8-C8-C9-O9
2	H	3279	NAG	C4-C5-C6-O6
5	J	5042	BEZ	O1-C-C1-C6
3	F	682	SIA	O1A-C1-C2-C3
3	F	682	SIA	O1B-C1-C2-C3
3	G	782	SIA	O1B-C1-C2-C3
3	J	1082	SIA	O1B-C1-C2-C3
2	L	4379	NAG	C3-C2-N2-C7
2	H	3279	NAG	O5-C5-C6-O6
5	J	5042	BEZ	O2-C-C1-C2
3	I	982	SIA	C6-C5-N5-C10
2	L	4379	NAG	C4-C5-C6-O6
3	F	682	SIA	C6-C5-N5-C10
3	B	1280	SIA	C7-C8-C9-O9
3	D	2180	SIA	O7-C7-C8-O8
3	L	1282	SIA	O8-C8-C9-O9
2	L	4379	NAG	C1-C2-N2-C7
3	F	682	SIA	C5-C6-C7-O7
2	A	1179	NAG	C3-C2-N2-C7
2	H	3279	NAG	C3-C2-N2-C7
3	I	982	SIA	O7-C7-C8-C9
3	A	1180	SIA	O1B-C1-C2-O6
3	G	782	SIA	O1B-C1-C2-O2
2	B	1279	NAG	C4-C5-C6-O6
3	J	1082	SIA	O8-C8-C9-O9
3	B	1280	SIA	O1B-C1-C2-C3
3	G	782	SIA	O1A-C1-C2-C3
3	J	1082	SIA	O1A-C1-C2-C3
2	L	4379	NAG	O5-C5-C6-O6
3	I	982	SIA	O7-C7-C8-O8

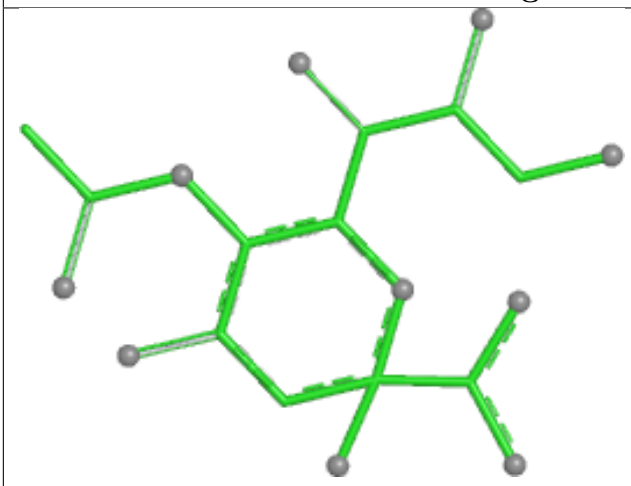
There are no ring outliers.

27 monomers are involved in 89 short contacts:

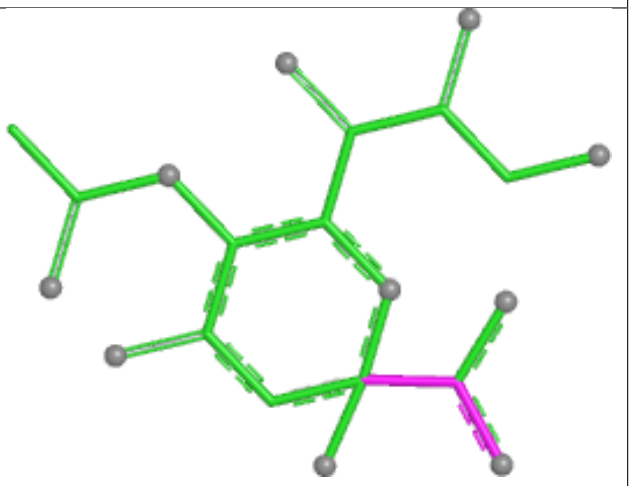
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	3380	BEZ	1	0
4	I	3285	SO4	1	0
3	D	2180	SIA	8	0
5	D	2385	BEZ	3	0
3	I	982	SIA	6	0
5	G	3385	BEZ	1	0
3	A	1180	SIA	3	0
2	G	3179	NAG	1	0
5	H	3386	BEZ	1	0
3	B	1280	SIA	5	0
2	K	4279	NAG	2	0
5	C	5014	BEZ	1	0
2	F	2379	NAG	3	0
2	J	4179	NAG	1	0
3	F	682	SIA	1	0
3	G	782	SIA	6	0
3	L	1282	SIA	7	0
3	A	1181	SIA	10	0
3	E	582	SIA	2	0
5	B	12	BEZ	6	0
3	K	1182	SIA	7	0
2	B	1279	NAG	1	0
3	J	1082	SIA	5	0
5	A	1385	BEZ	2	0
3	H	882	SIA	1	0
5	C	5013	BEZ	3	0
5	L	4380	BEZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

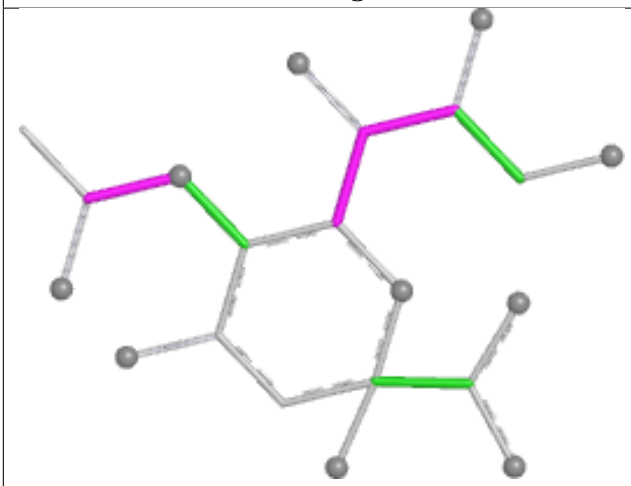
Ligand SIA D 2180



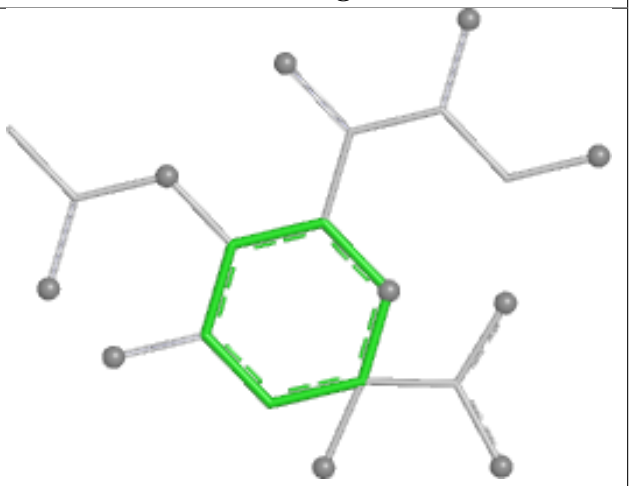
Bond lengths



Bond angles

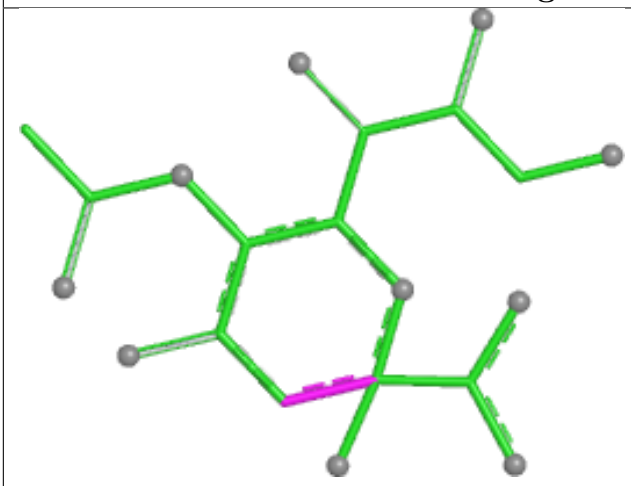


Torsions

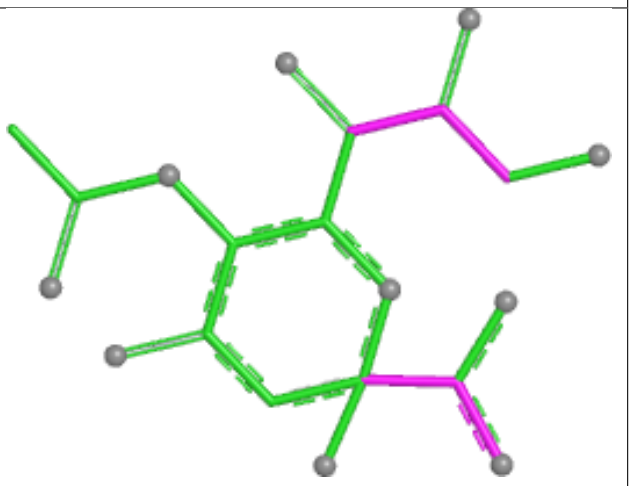


Rings

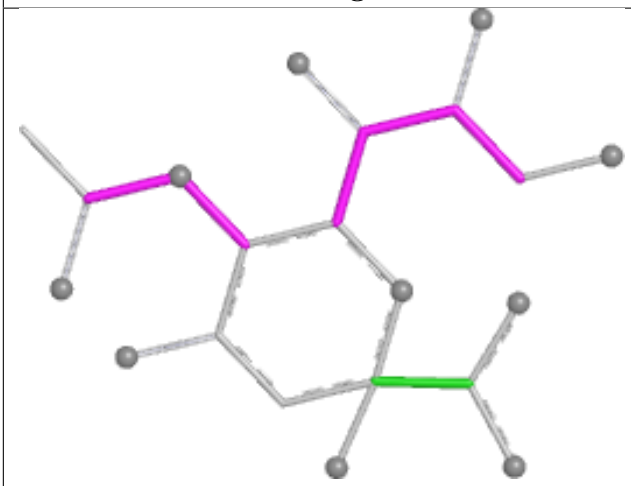
Ligand SIA I 982



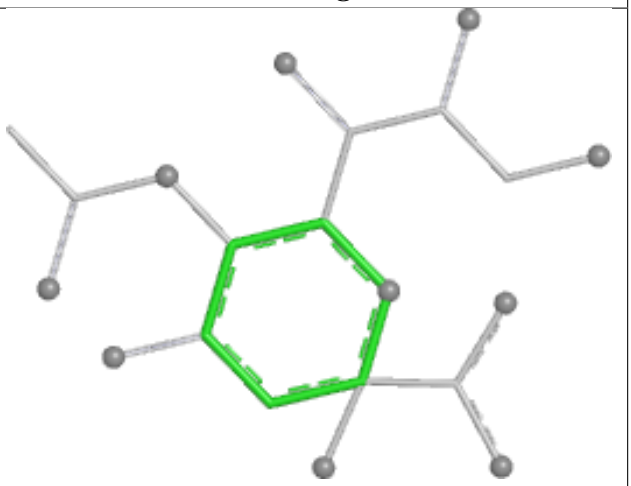
Bond lengths



Bond angles

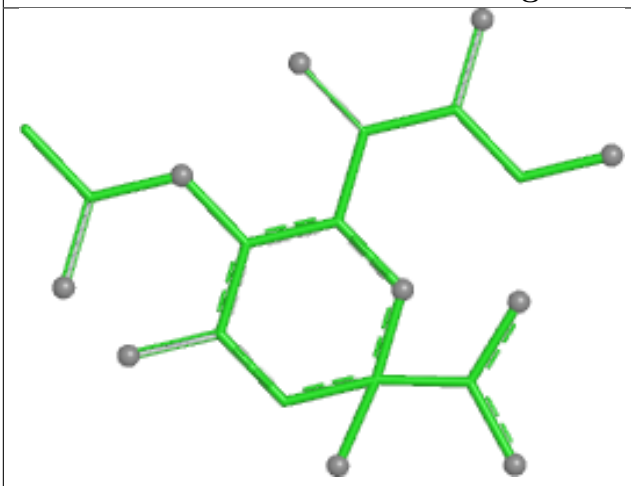


Torsions

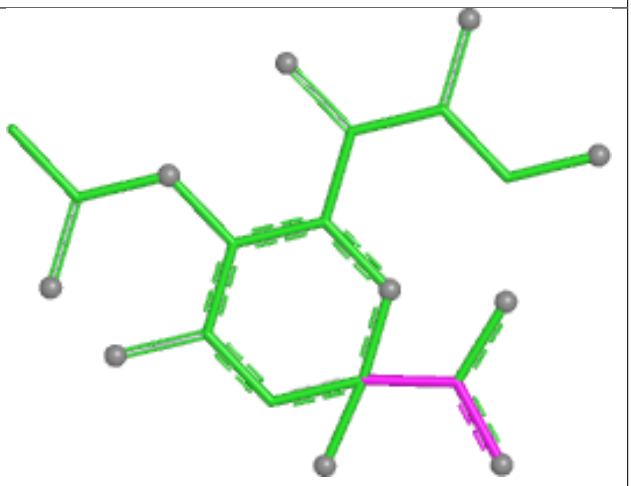


Rings

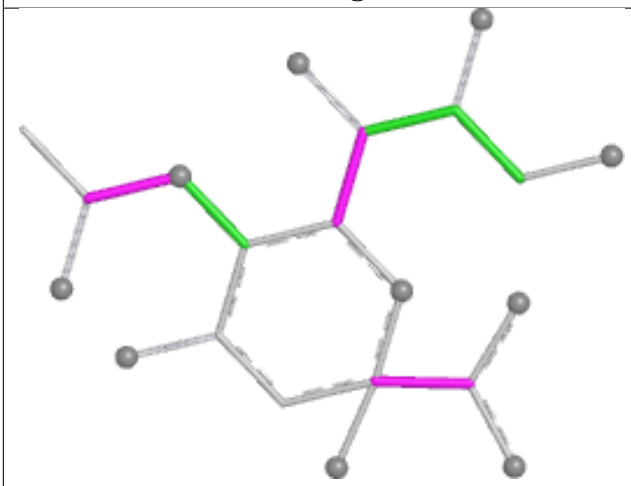
Ligand SIA A 1180



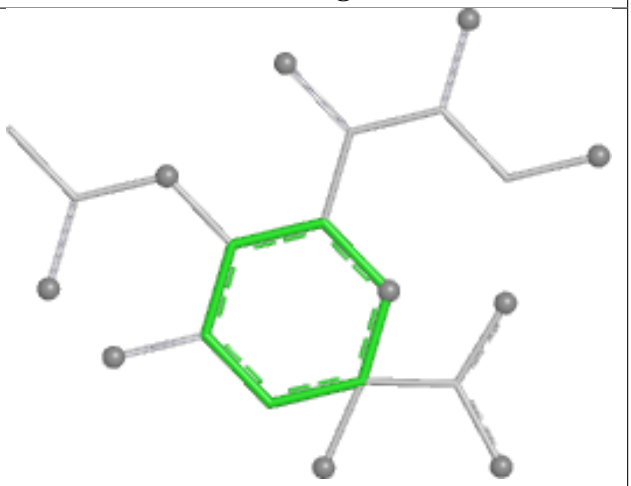
Bond lengths



Bond angles

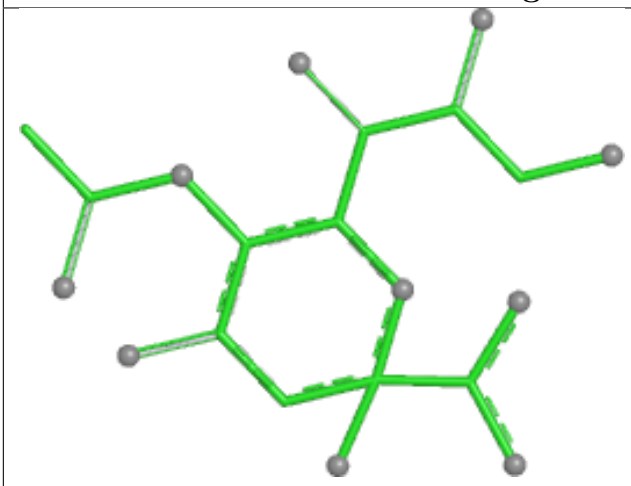


Torsions

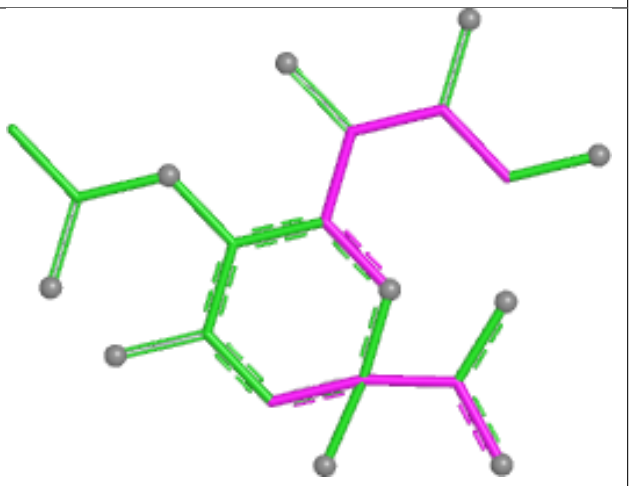


Rings

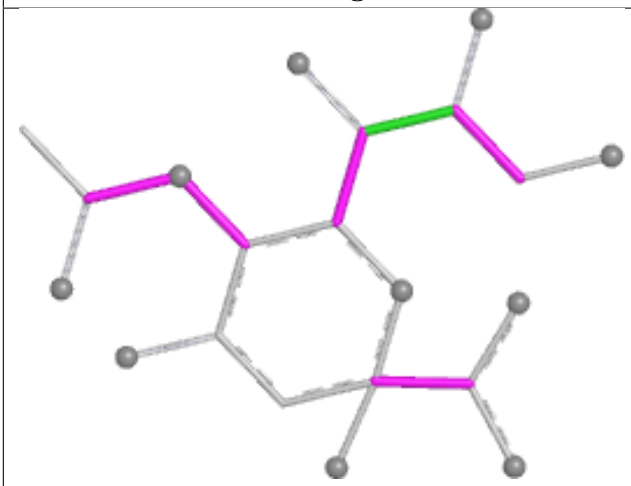
Ligand SIA B 1280



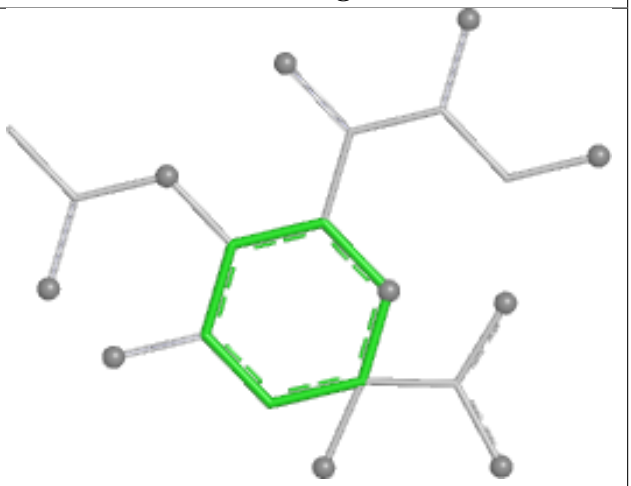
Bond lengths



Bond angles

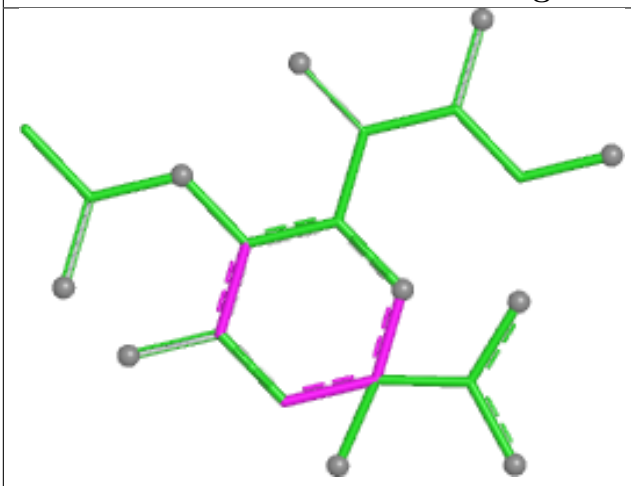


Torsions

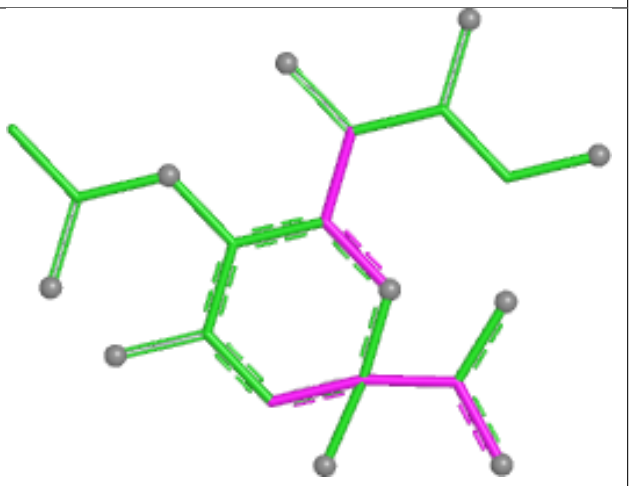


Rings

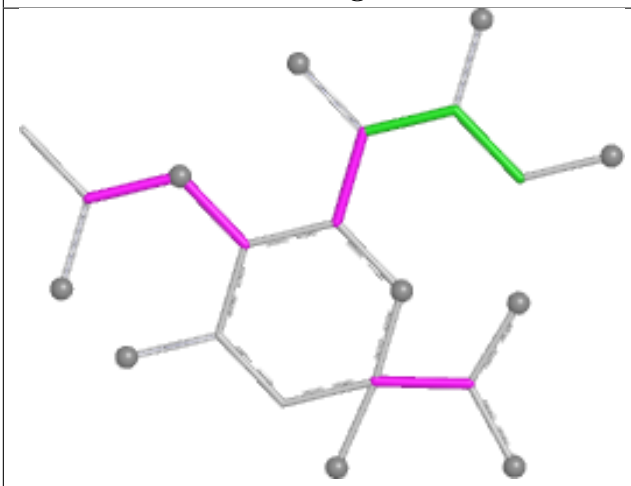
Ligand SIA F 682



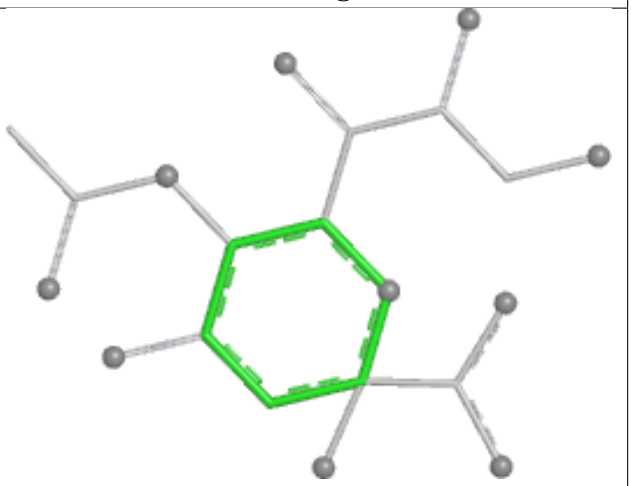
Bond lengths



Bond angles

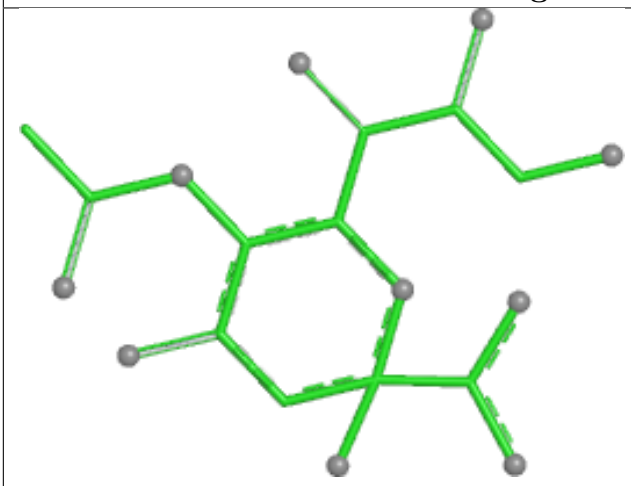


Torsions

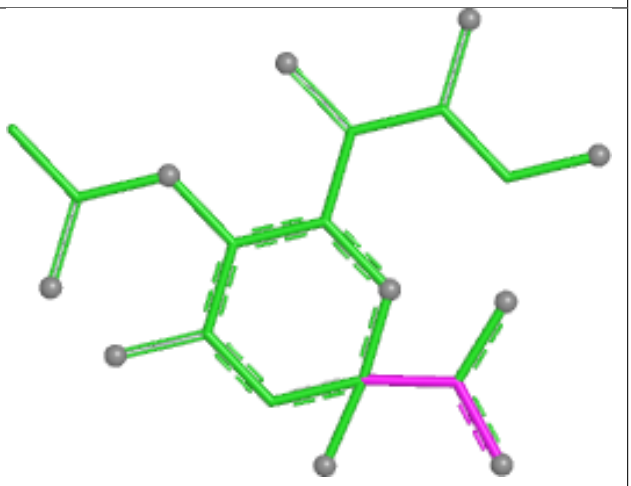


Rings

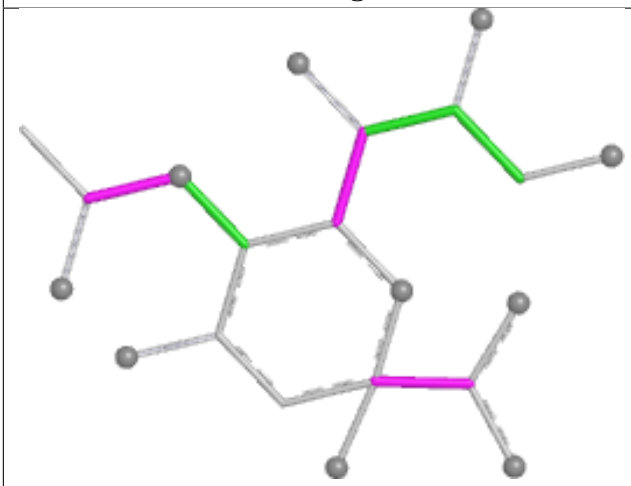
Ligand SIA G 782



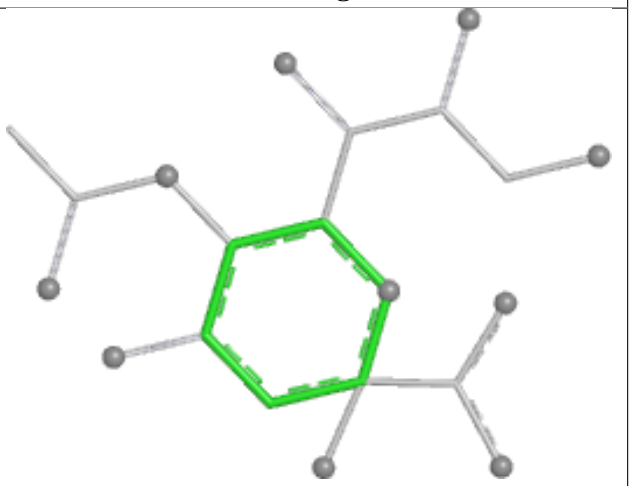
Bond lengths



Bond angles

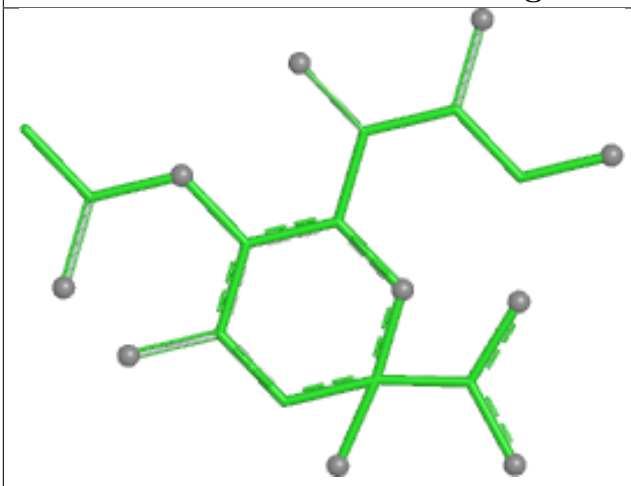


Torsions

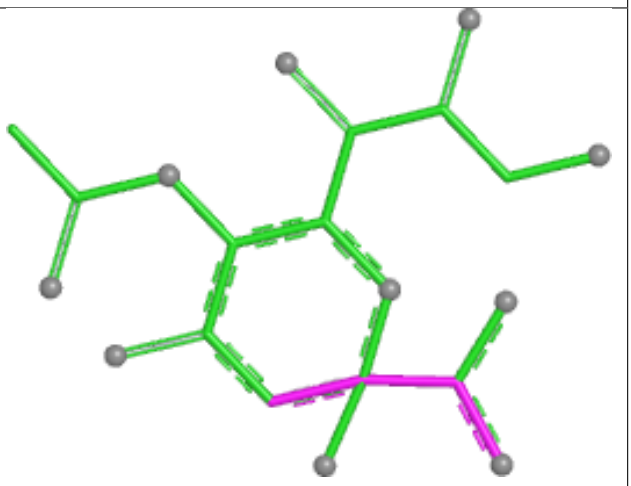


Rings

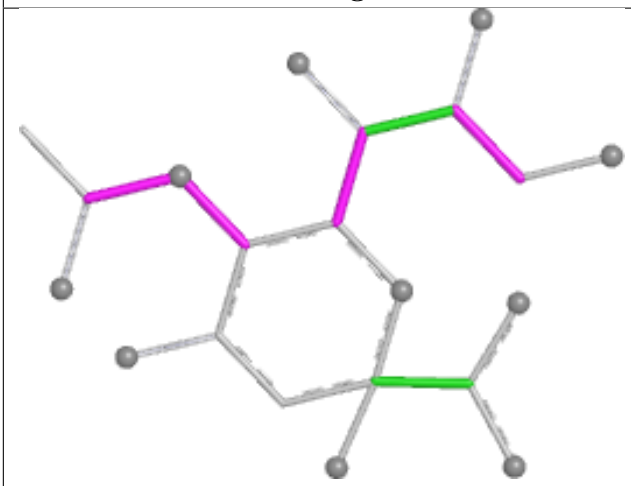
Ligand SIA L 1282



Bond lengths



Bond angles



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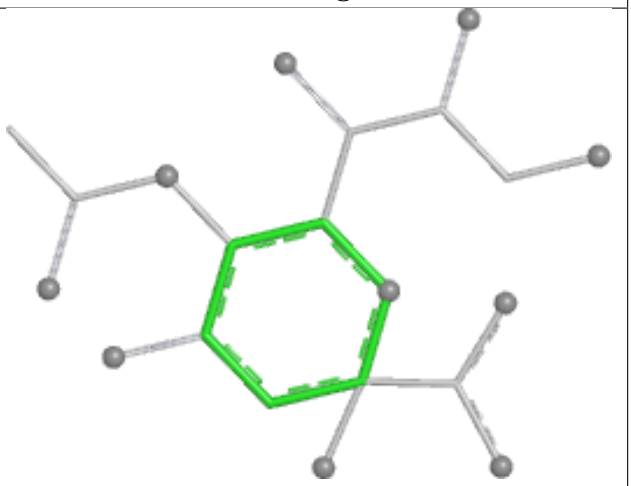
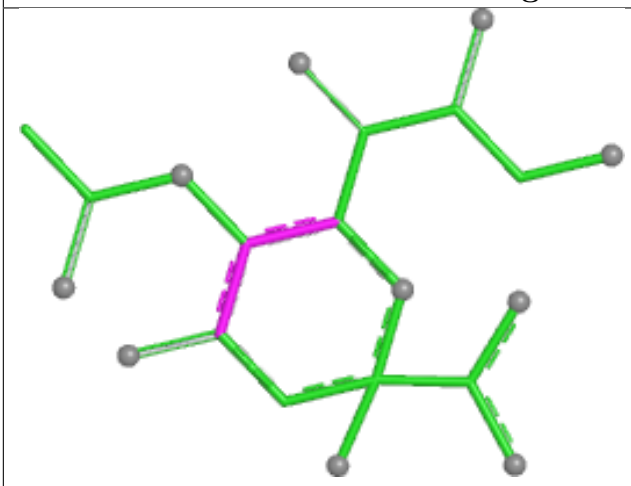
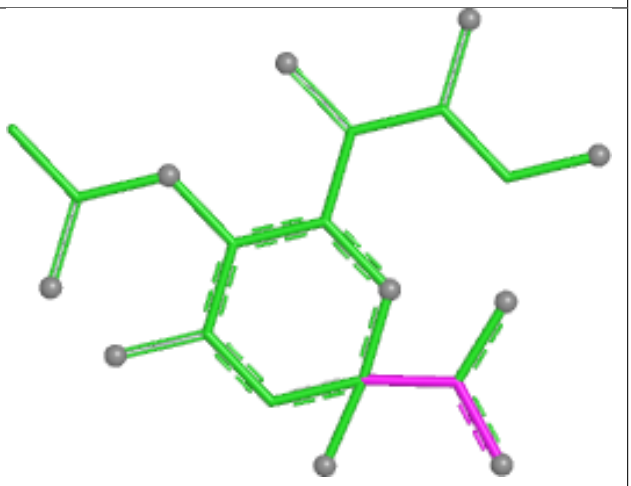


Rings

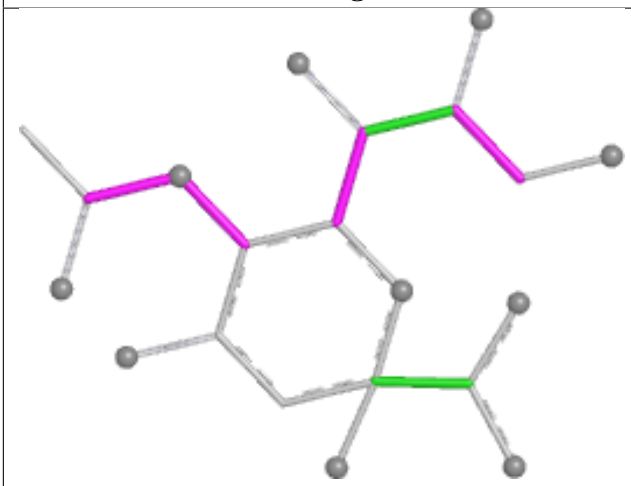
Ligand SIA A 1181



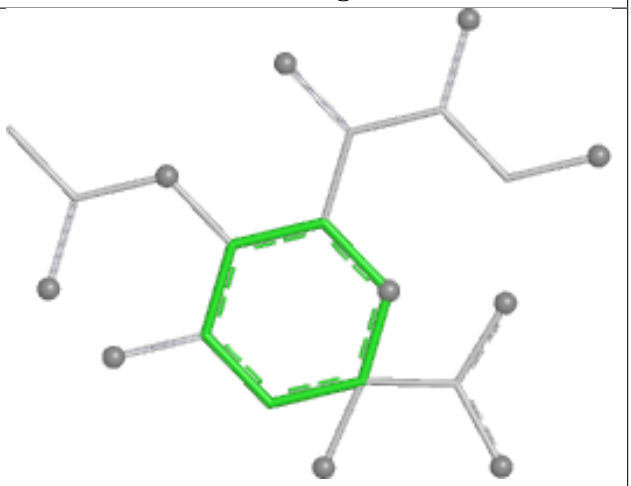
Bond lengths



Bond angles

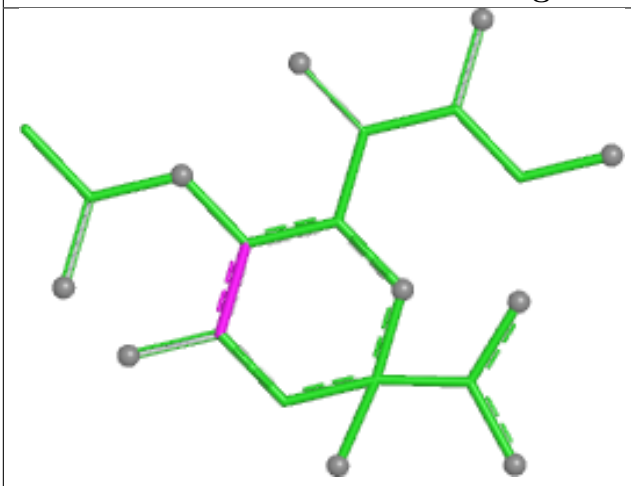


Torsions

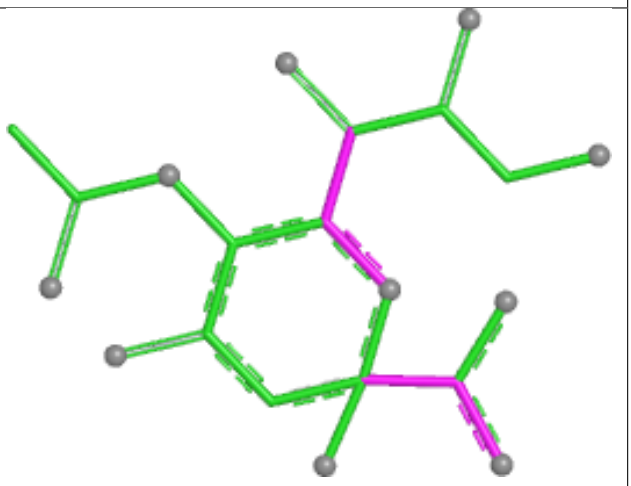


Rings

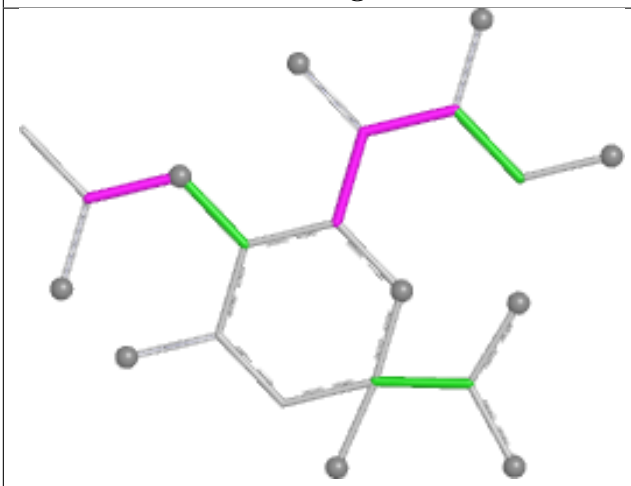
Ligand SIA E 582



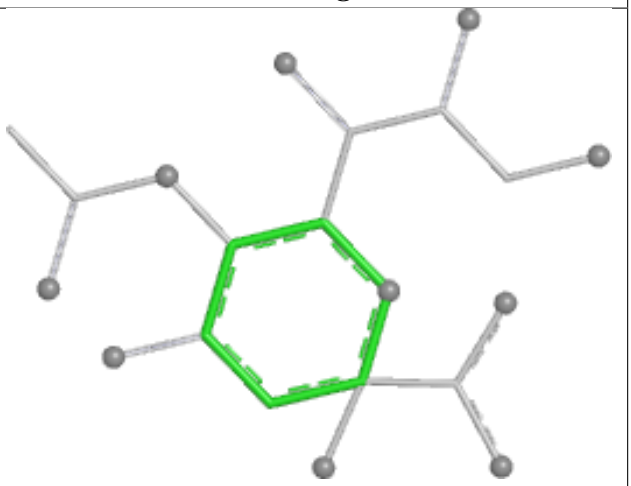
Bond lengths



Bond angles

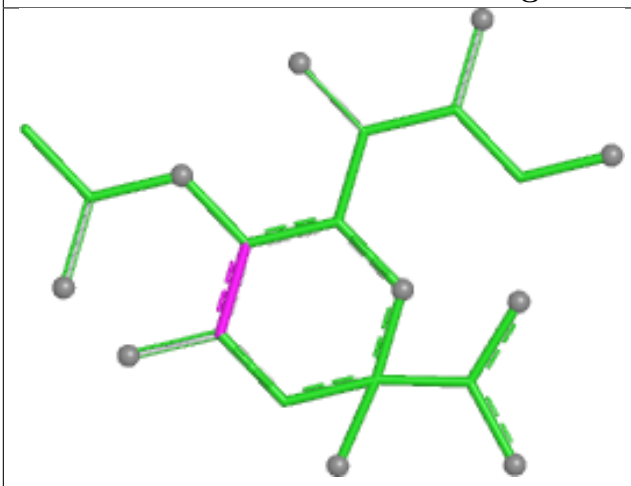


Torsions

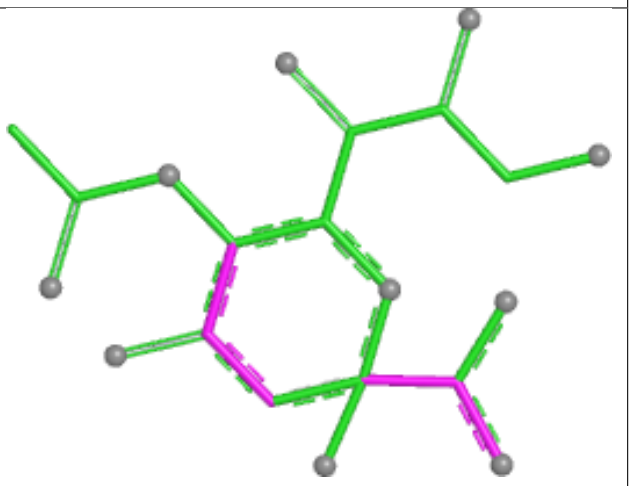


Rings

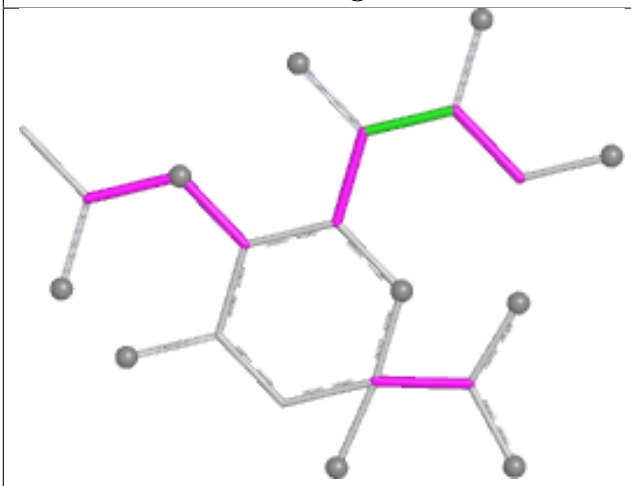
Ligand SIA K 1182



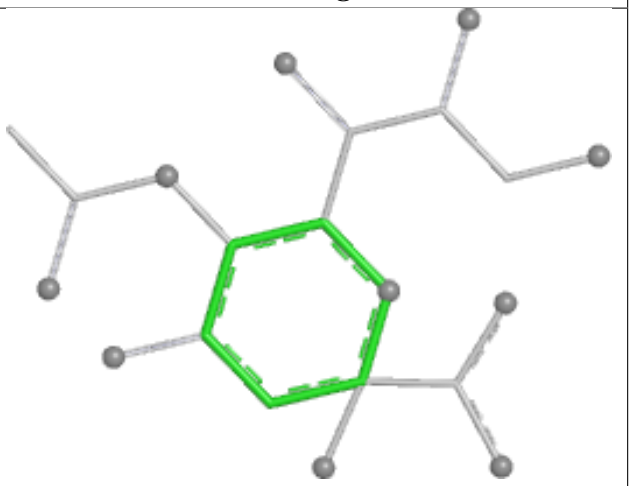
Bond lengths



Bond angles

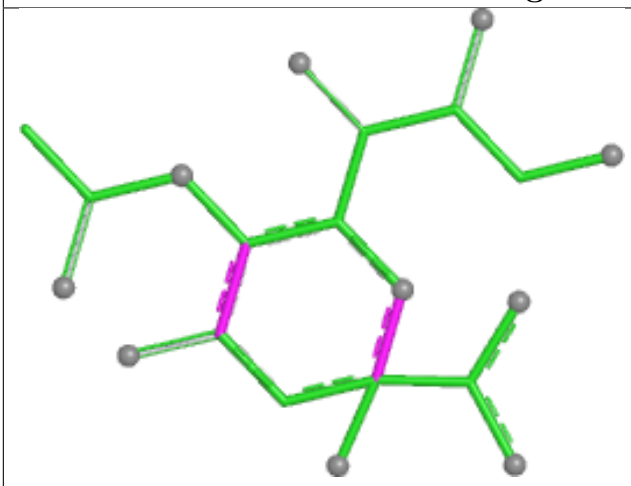


Torsions

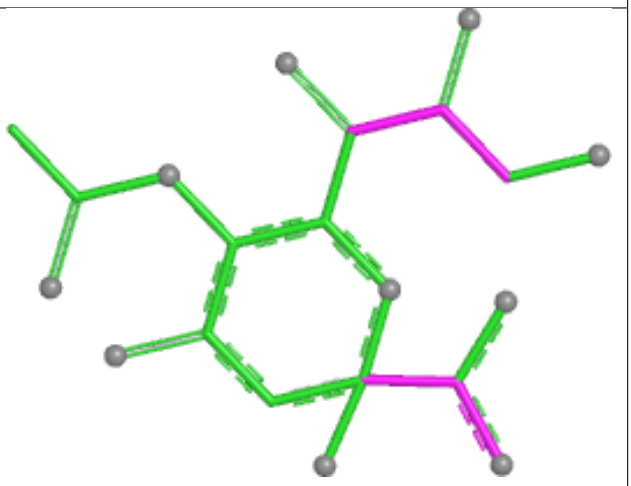


Rings

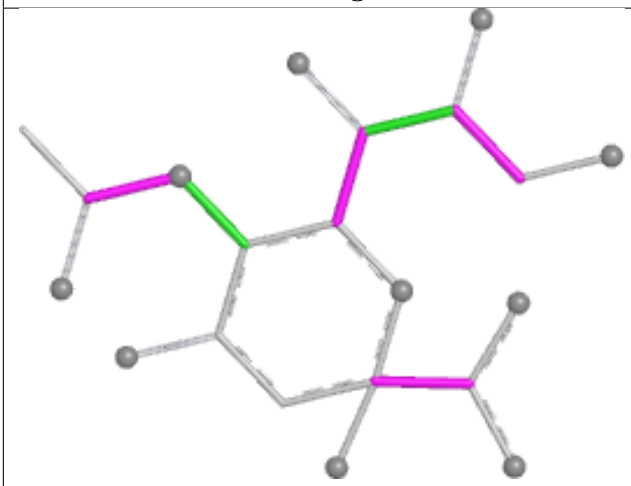
Ligand SIA J 1082



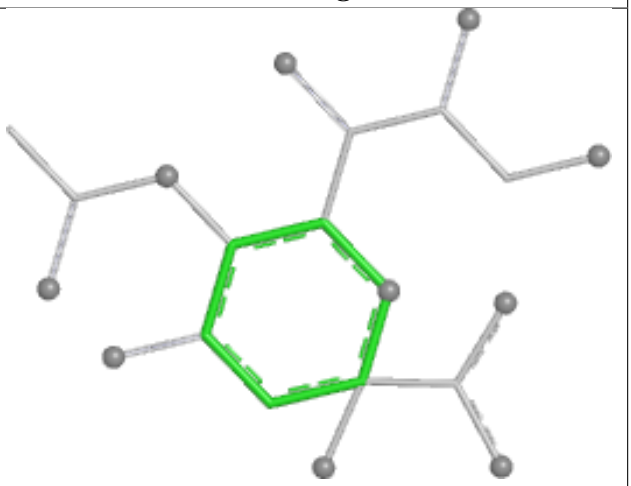
Bond lengths



Bond angles

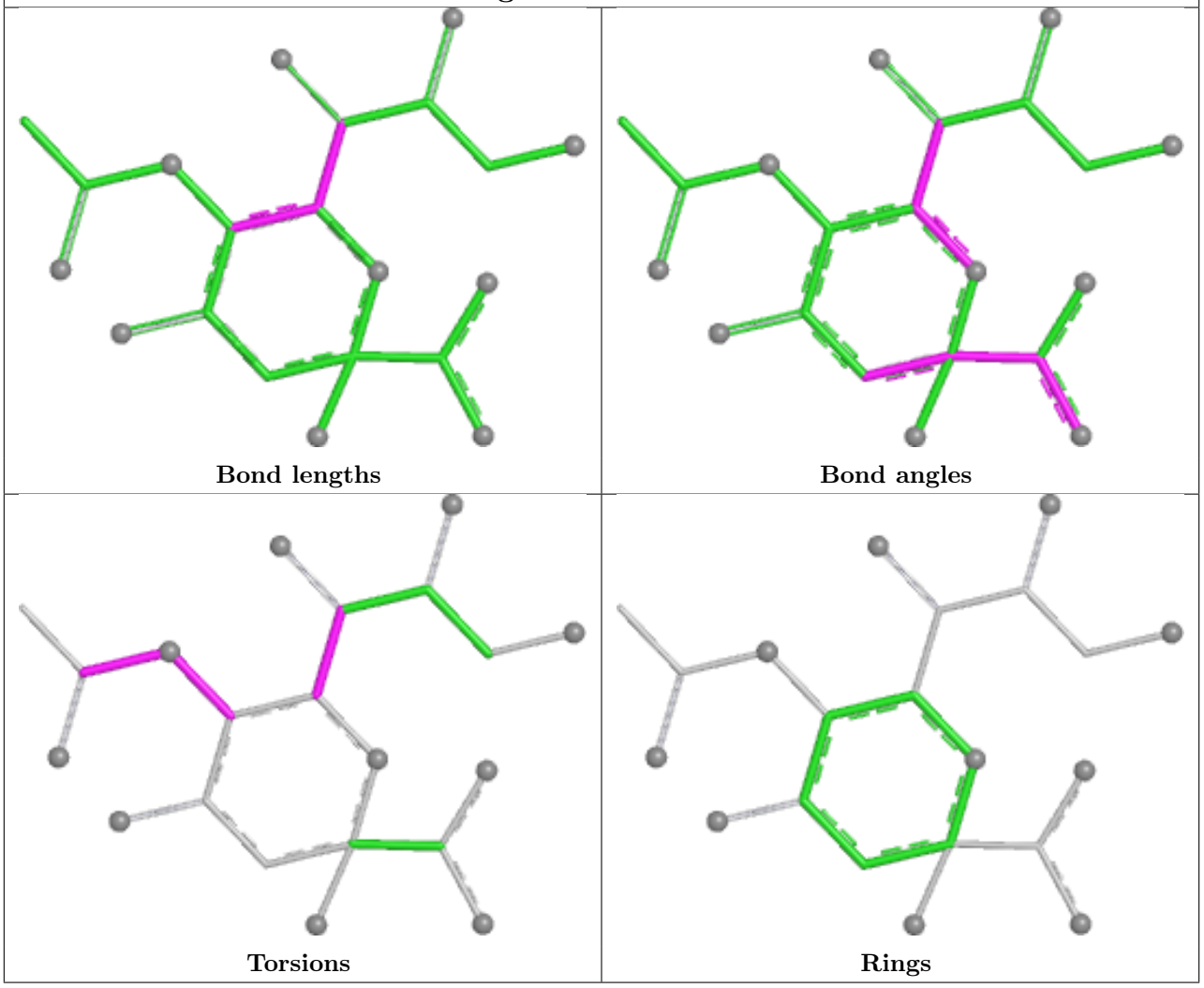


Torsions



Rings

Ligand SIA H 882



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	550:LEU	C	551:PHE	N	1.00

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	532/532 (100%)	-1.77	0	100	100	2, 25, 69, 83	0
1	B	532/532 (100%)	-1.76	0	100	100	4, 29, 74, 86	0
1	C	532/532 (100%)	-1.76	0	100	100	2, 26, 64, 85	0
1	D	532/532 (100%)	-1.77	0	100	100	2, 25, 70, 84	0
1	E	532/532 (100%)	-1.76	0	100	100	4, 30, 73, 86	0
1	F	532/532 (100%)	-1.76	0	100	100	3, 26, 65, 81	0
1	G	532/532 (100%)	-1.77	0	100	100	3, 26, 67, 85	0
1	H	532/532 (100%)	-1.74	0	100	100	2, 27, 71, 84	0
1	I	532/532 (100%)	-1.73	0	100	100	3, 31, 74, 85	0
1	J	532/532 (100%)	-1.78	0	100	100	2, 26, 64, 83	0
1	K	532/532 (100%)	-1.74	0	100	100	3, 27, 71, 85	0
1	L	532/532 (100%)	-1.75	0	100	100	2, 31, 73, 83	0
All	All	6384/6384 (100%)	-1.76	0	100	100	2, 27, 70, 86	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	1179	14/15	0.96	0.08	70,76,78,78	0
2	NAG	D	2179	14/15	0.96	0.06	70,76,78,79	0
5	BEZ	L	4381	9/9	0.96	0.06	54,55,55,55	0
4	SO4	C	1185	5/5	0.97	0.08	100,100,101,101	0
5	BEZ	E	2386	9/9	0.97	0.07	47,47,49,50	0
5	BEZ	L	4380	9/9	0.97	0.08	59,59,60,60	0
2	NAG	B	1279	14/15	0.97	0.05	59,64,68,70	0
2	NAG	H	3279	14/15	0.98	0.05	63,66,69,69	0
2	NAG	I	3379	14/15	0.98	0.05	57,61,62,63	0
2	NAG	J	4179	14/15	0.98	0.05	69,75,78,78	0
2	NAG	K	4279	14/15	0.98	0.04	63,67,71,71	0
2	NAG	L	4379	14/15	0.98	0.04	56,59,62,63	0
3	SIA	B	1280	21/21	0.98	0.05	45,61,66,67	0
2	NAG	C	1379	14/15	0.98	0.05	59,64,68,68	0
5	BEZ	A	1385	9/9	0.98	0.07	49,50,52,52	0
5	BEZ	B	1386	9/9	0.98	0.06	54,55,56,56	0
5	BEZ	C	5014	9/9	0.98	0.08	36,40,40,41	0
5	BEZ	D	2386	9/9	0.98	0.07	44,45,46,46	0
2	NAG	E	2279	14/15	0.98	0.04	57,60,62,63	0
5	BEZ	E	2387	9/9	0.98	0.06	42,43,43,44	0
5	BEZ	F	5024	9/9	0.98	0.11	42,44,46,46	0
5	BEZ	H	3387	9/9	0.98	0.07	41,43,45,46	0
5	BEZ	I	3381	9/9	0.98	0.08	52,52,53,54	0
5	BEZ	J	5042	9/9	0.98	0.09	44,45,46,46	0
5	BEZ	K	4387	9/9	0.98	0.09	36,39,40,41	0
2	NAG	F	2379	14/15	0.98	0.04	59,64,66,66	0
2	NAG	G	3179	14/15	0.98	0.04	67,72,75,75	0
4	SO4	B	1385	5/5	0.99	0.03	96,97,97,98	0
3	SIA	A	1181	21/21	0.99	0.04	44,57,67,68	0
4	SO4	D	2184	5/5	0.99	0.10	100,100,101,101	0
4	SO4	D	2384	5/5	0.99	0.07	76,77,77,77	0
4	SO4	E	2385	5/5	0.99	0.04	94,94,94,95	0
4	SO4	F	2185	5/5	0.99	0.04	106,106,106,106	0
4	SO4	F	2285	5/5	0.99	0.06	80,80,81,81	0
4	SO4	G	3184	5/5	0.99	0.06	86,86,87,88	0
4	SO4	G	3384	5/5	0.99	0.06	81,81,81,81	0
4	SO4	H	3284	5/5	0.99	0.12	84,84,85,85	0

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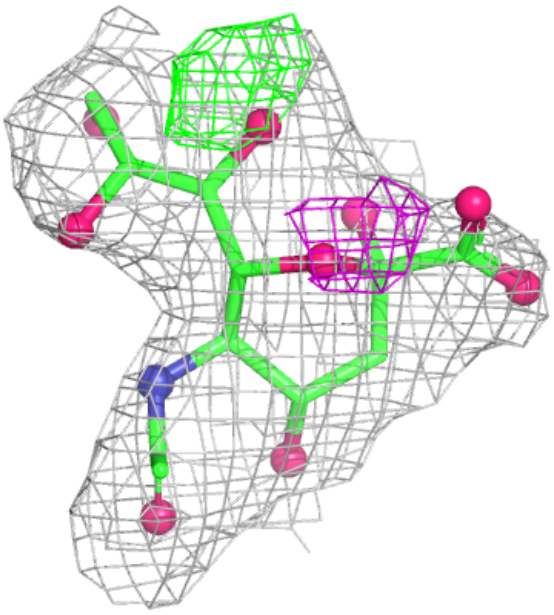
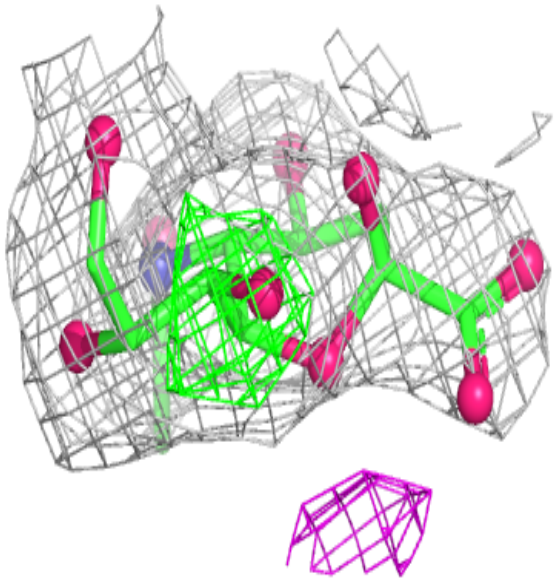
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	H	3385	5/5	0.99	0.05	97,97,97,97	0
4	SO4	I	3185	5/5	0.99	0.07	95,95,96,96	0
4	SO4	I	3285	5/5	0.99	0.05	79,79,79,80	0
4	SO4	J	4185	5/5	0.99	0.06	96,96,97,97	0
4	SO4	J	4384	5/5	0.99	0.04	84,85,85,86	0
4	SO4	K	4284	5/5	0.99	0.10	85,85,86,86	0
4	SO4	K	4385	5/5	0.99	0.08	97,98,98,99	0
4	SO4	L	4285	5/5	0.99	0.05	74,74,75,75	0
5	BEZ	A	11	9/9	0.99	0.05	49,51,52,52	0
3	SIA	A	1180	21/21	0.99	0.05	64,71,74,75	0
3	SIA	D	2180	21/21	0.99	0.04	57,69,72,73	0
5	BEZ	B	12	9/9	0.99	0.09	52,53,54,55	0
5	BEZ	C	5013	8/9	0.99	0.08	40,44,46,46	0
3	SIA	E	582	21/21	0.99	0.04	42,60,70,70	0
5	BEZ	D	2385	9/9	0.99	0.09	51,51,53,53	0
3	SIA	F	682	21/21	0.99	0.04	52,56,62,62	0
3	SIA	G	782	21/21	0.99	0.04	61,69,73,74	0
3	SIA	H	882	21/21	0.99	0.03	52,66,69,70	0
5	BEZ	F	5023	8/9	0.99	0.06	46,49,50,51	0
3	SIA	I	982	21/21	0.99	0.03	51,60,64,65	0
5	BEZ	G	3385	9/9	0.99	0.09	58,59,60,60	0
5	BEZ	G	3386	9/9	0.99	0.09	45,47,48,49	0
5	BEZ	H	3386	9/9	0.99	0.09	49,51,51,51	0
3	SIA	J	1082	21/21	0.99	0.05	59,71,76,77	0
5	BEZ	I	3380	9/9	0.99	0.07	53,53,54,55	0
3	SIA	K	1182	21/21	0.99	0.03	60,63,67,69	0
5	BEZ	J	5041	8/9	0.99	0.04	41,45,45,46	0
3	SIA	L	1282	21/21	0.99	0.05	50,55,63,65	0
5	BEZ	K	4386	9/9	0.99	0.05	48,49,50,50	0
4	SO4	A	1184	5/5	0.99	0.08	94,94,94,95	0
4	SO4	A	1384	5/5	0.99	0.09	76,76,77,77	0
4	SO4	B	1284	5/5	0.99	0.04	80,80,81,81	0
4	SO4	J	4184	5/5	1.00	0.03	94,94,95,95	0
4	SO4	E	2284	5/5	1.00	0.03	85,86,86,86	0
4	SO4	C	1285	5/5	1.00	0.04	76,76,77,77	0

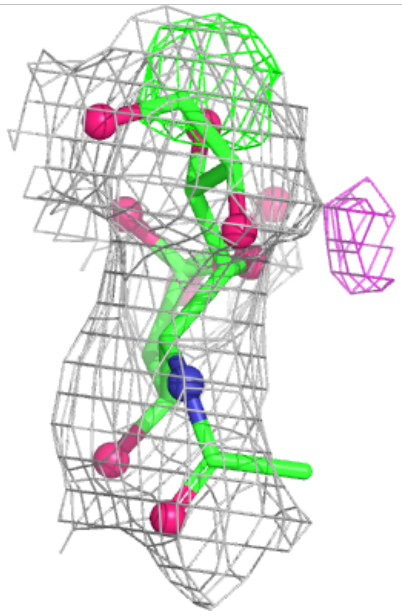
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA B 1280:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

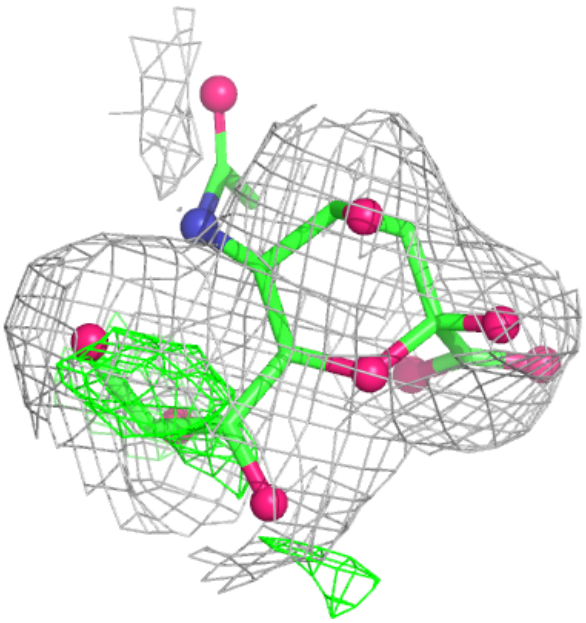


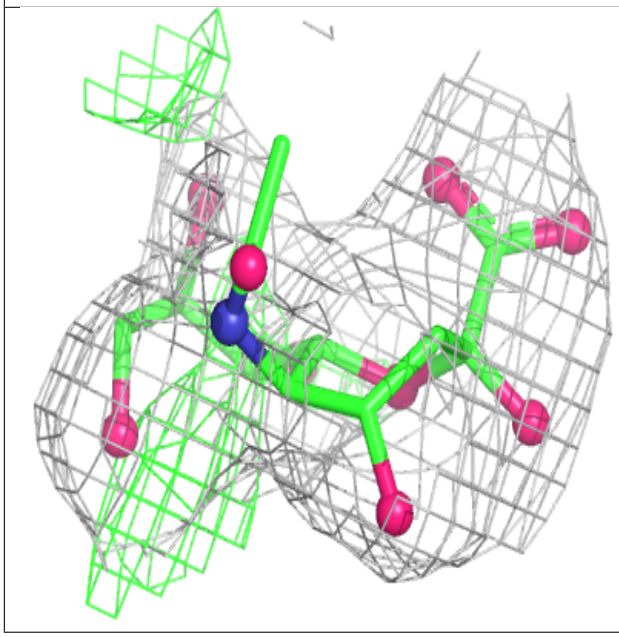


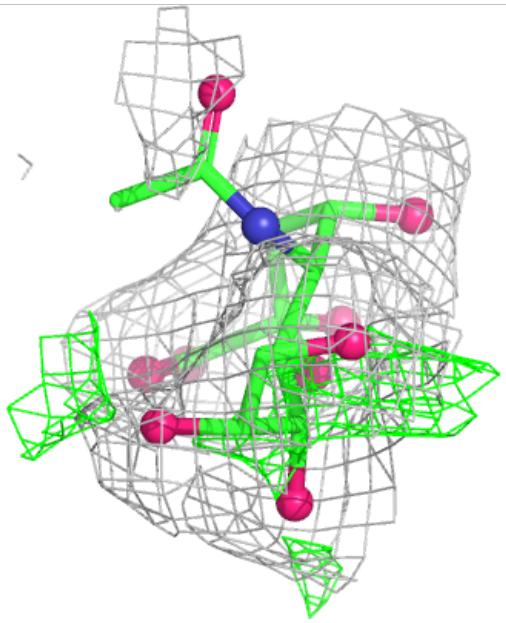


Electron density around SIA A 1181:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

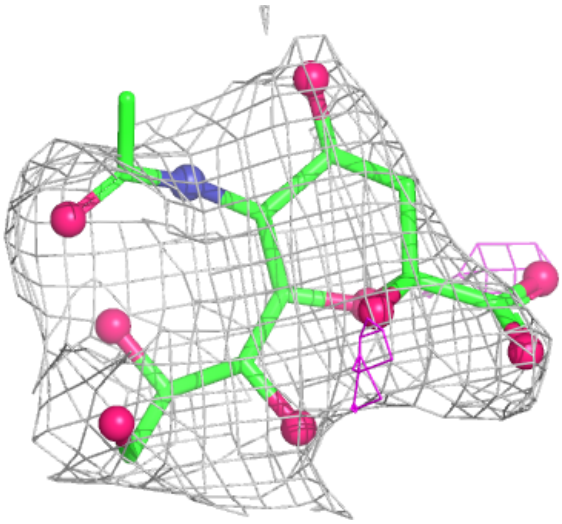


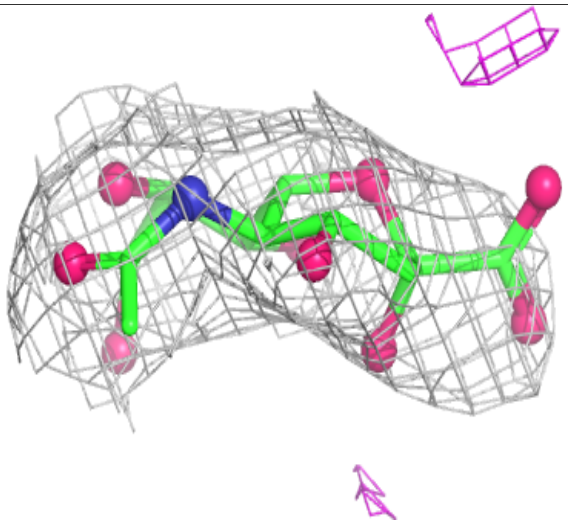


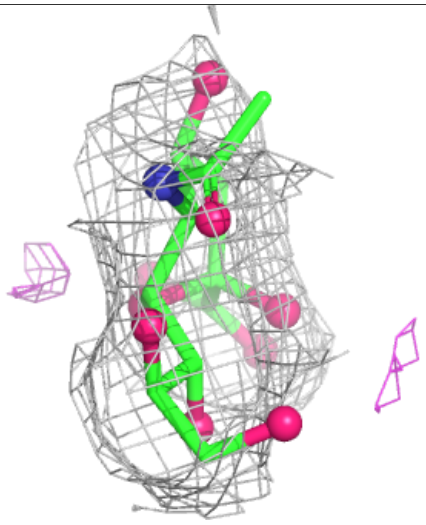


Electron density around SIA A 1180:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

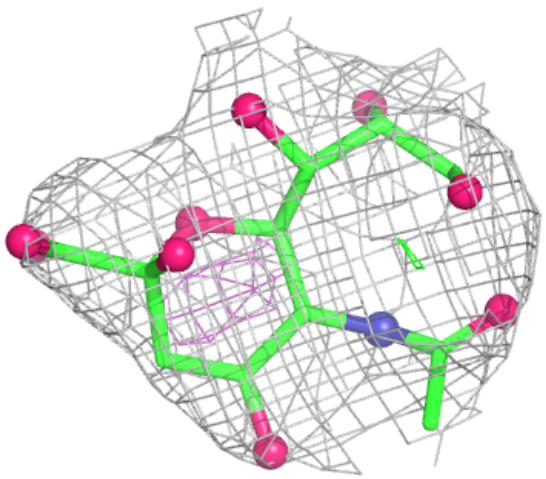


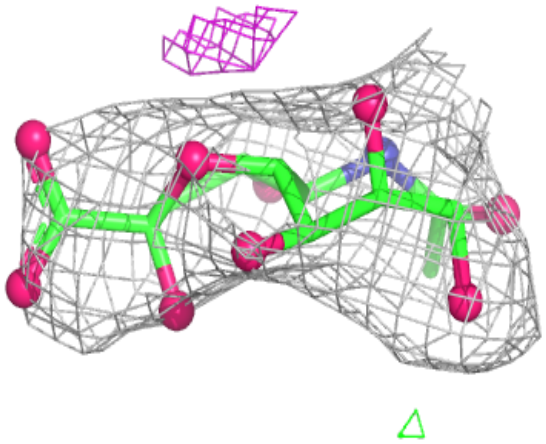


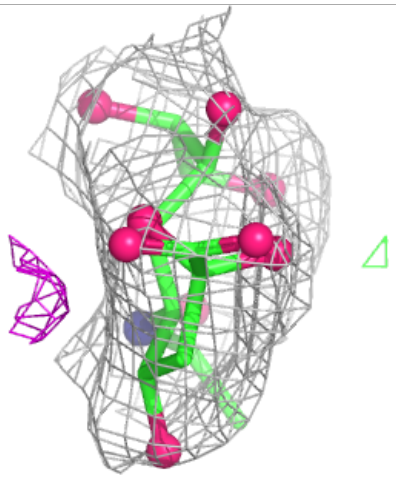


Electron density around SIA D 2180:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

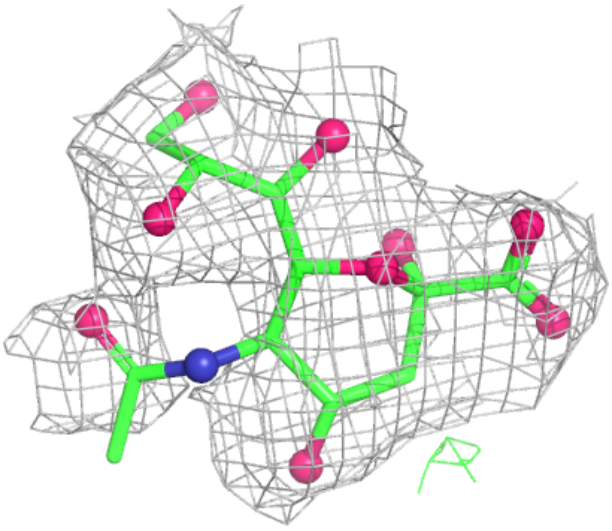


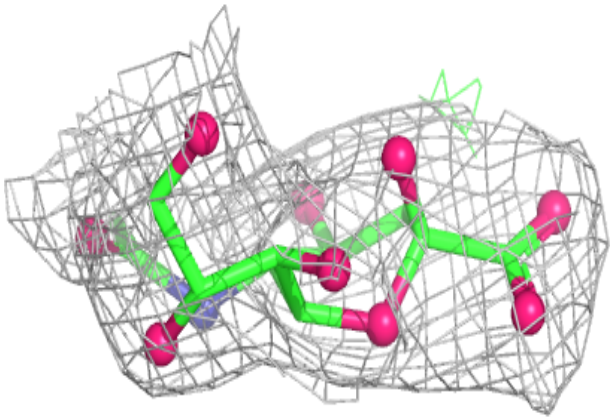


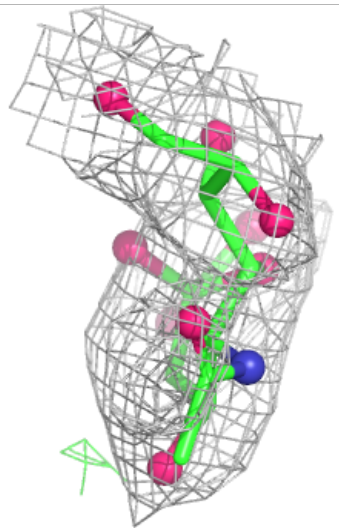


Electron density around SIA E 582:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

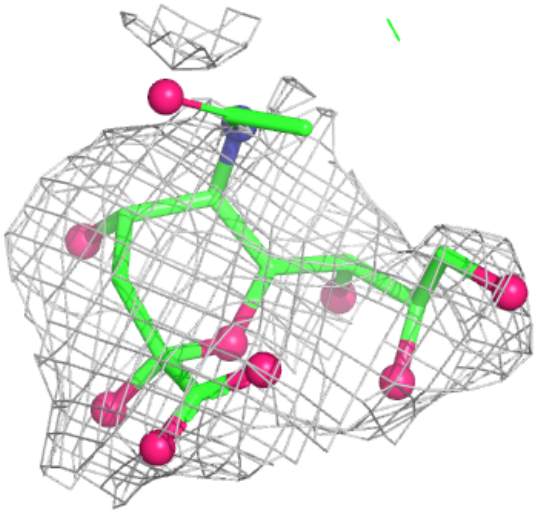


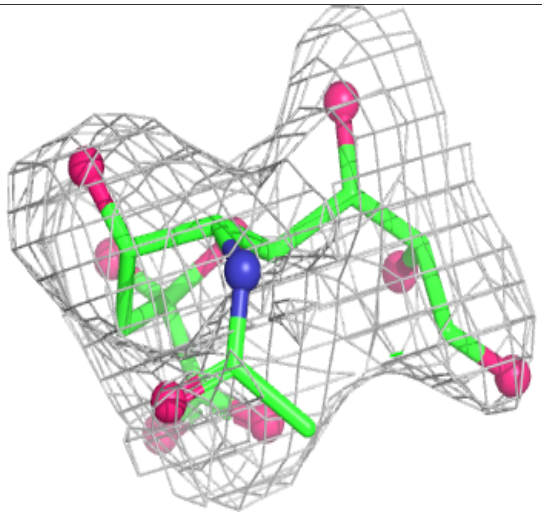


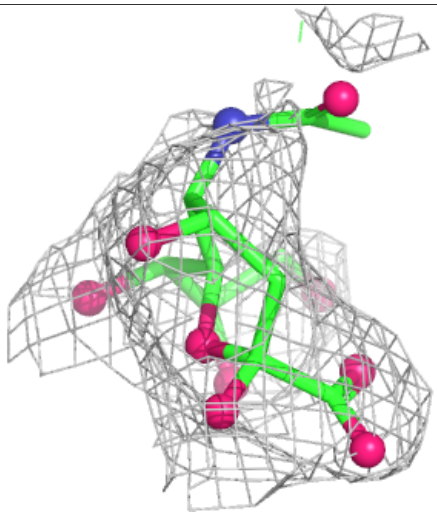


Electron density around SIA F 682:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

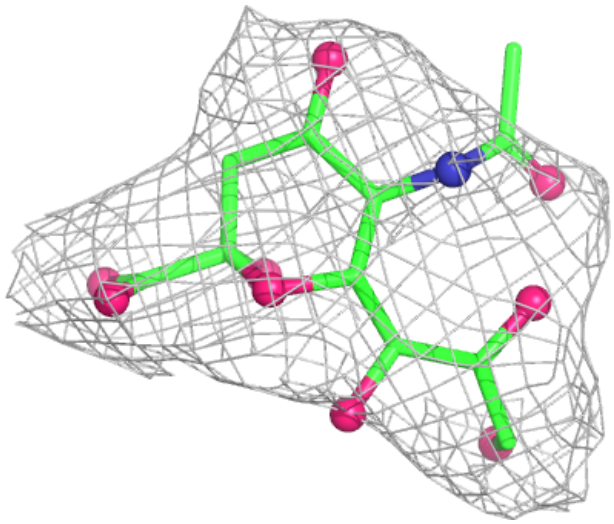


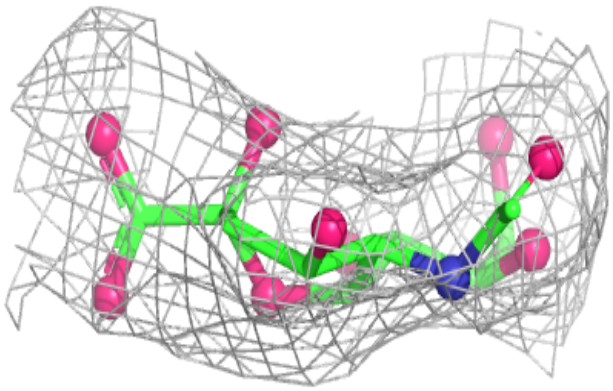


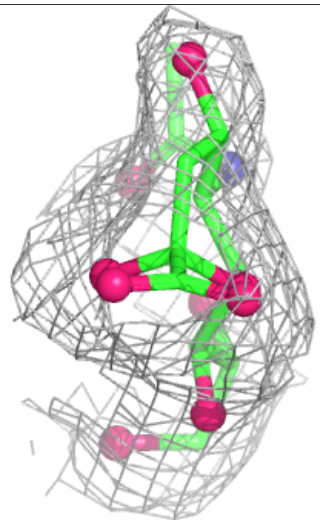


Electron density around SIA G 782:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

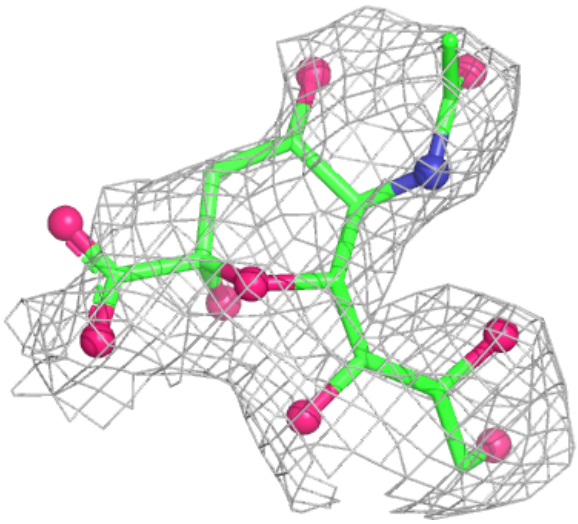


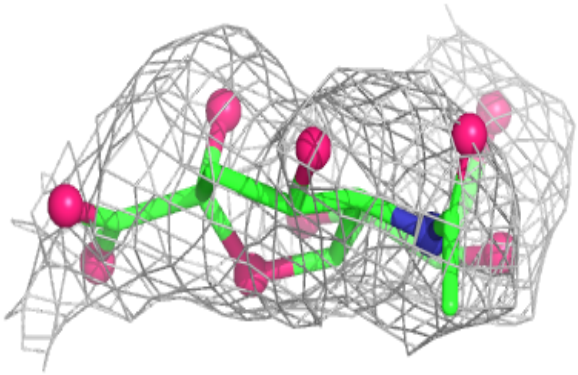


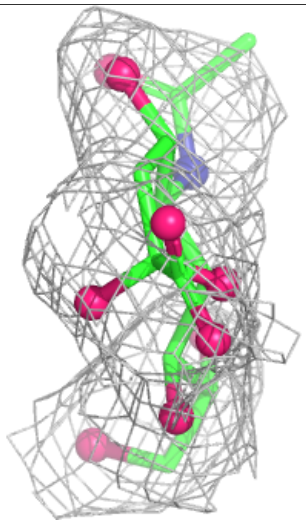


Electron density around SIA H 882:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

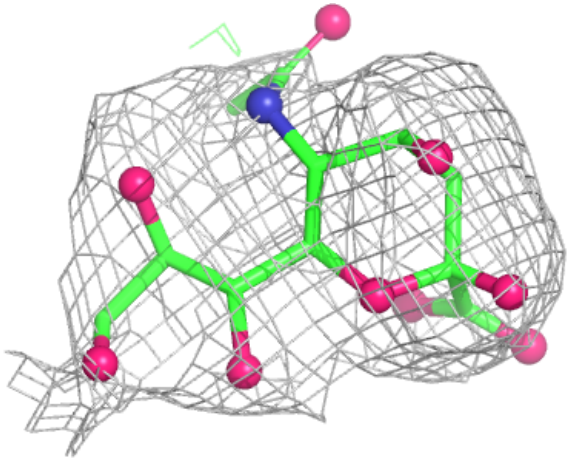


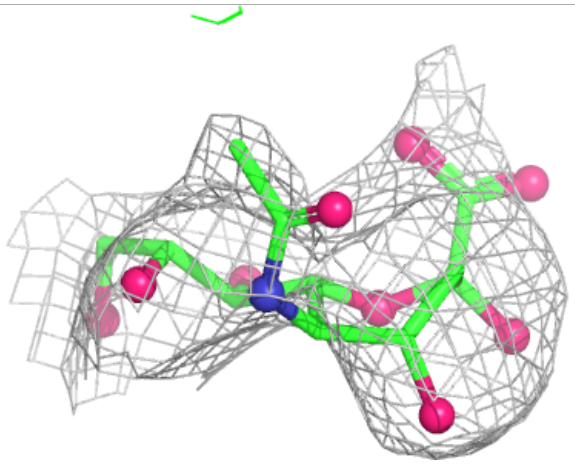


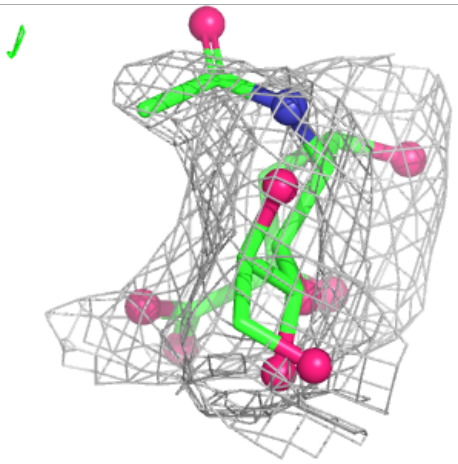


Electron density around SIA I 982:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

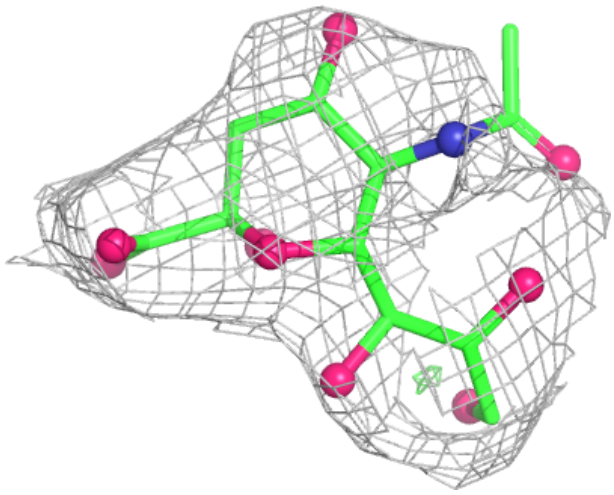


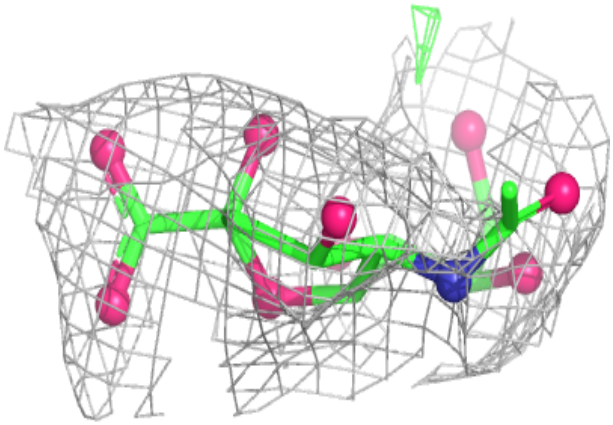


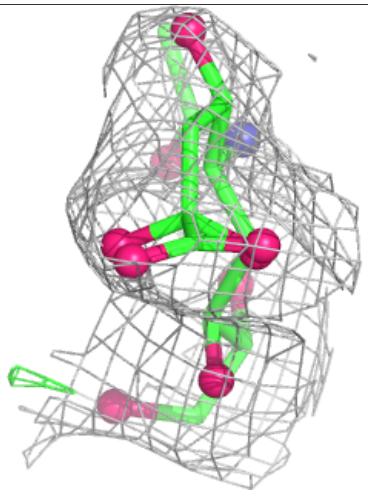


Electron density around SIA J 1082:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

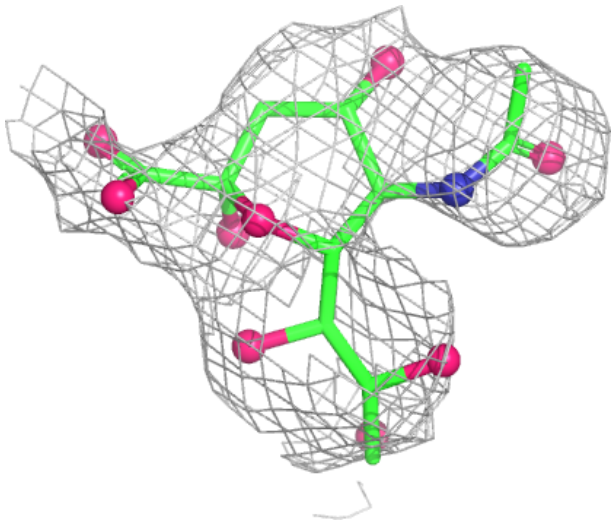


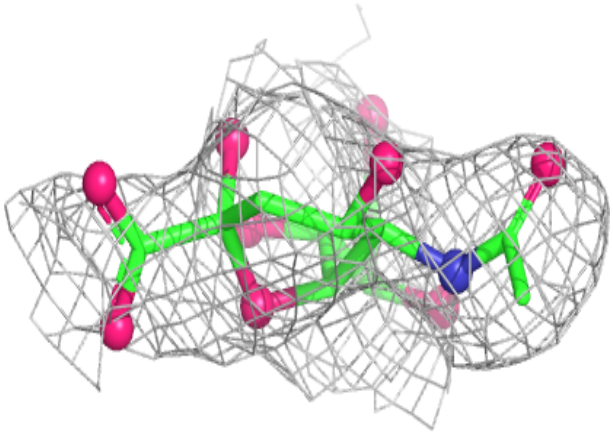


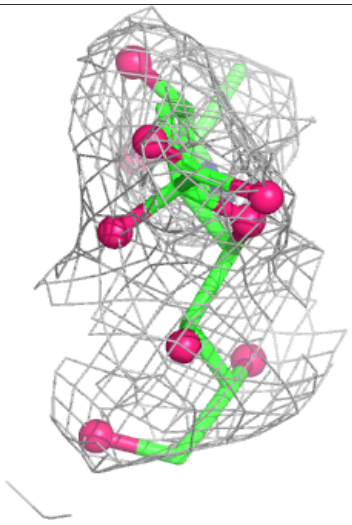


Electron density around SIA K 1182:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

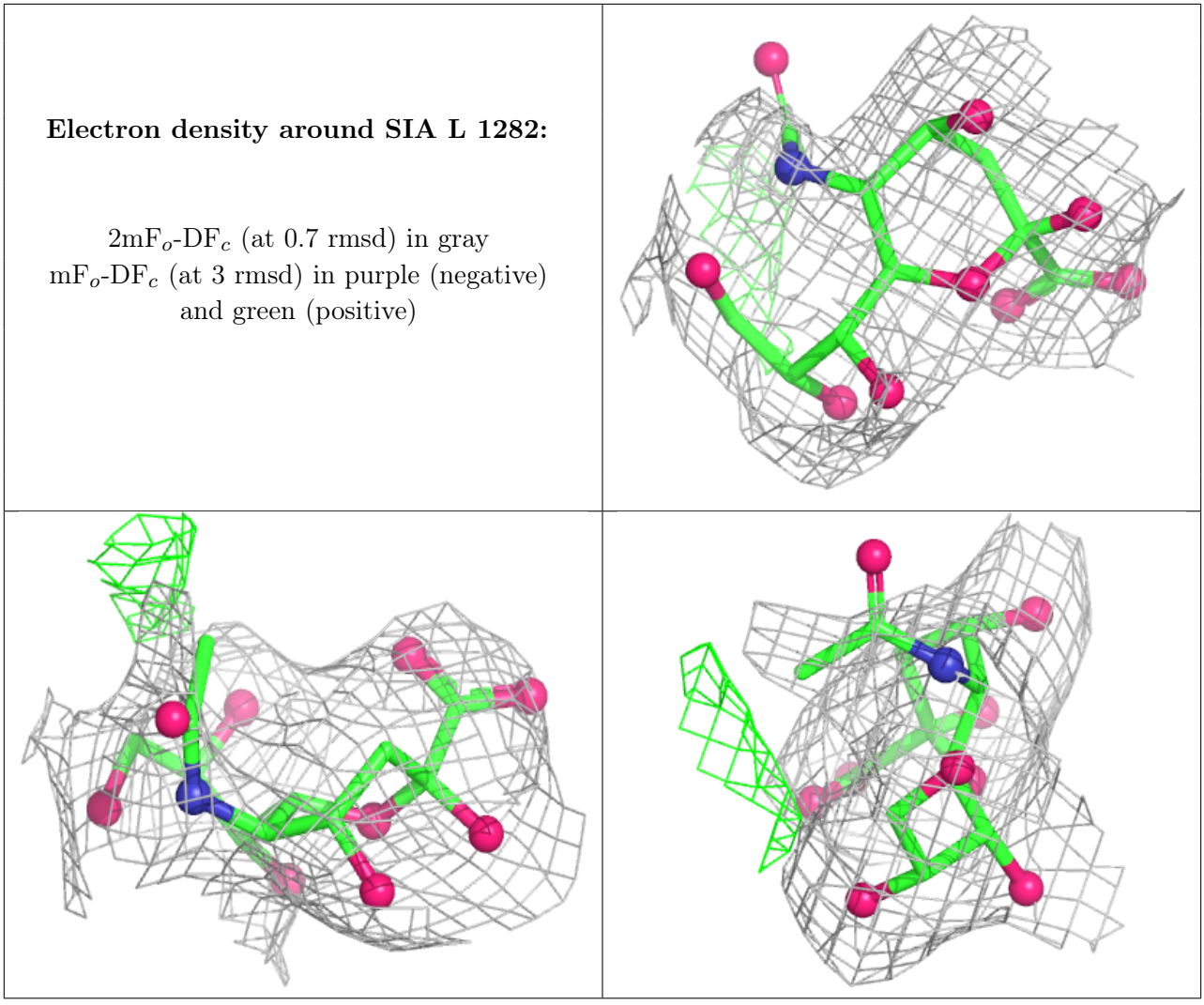






Electron density around SIA L 1282:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.