



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:35 AM UTC

PDB ID : 2VPY / pdb_00002vpy
Title : Polysulfide reductase with bound quinone inhibitor, pentachlorophenol (PCP)
Authors : Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on : 2008-03-09
Resolution : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

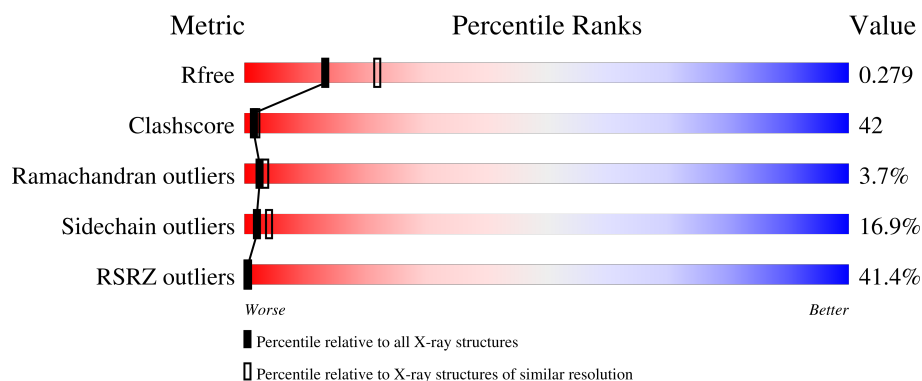
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	765	
1	E	765	
2	B	195	
2	F	195	
3	C	253	

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Mol	Chain	Length	Quality of chain
3	G	253	<p>65% 53% 33% 11%</p>

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
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	PCI	C	1252	-	-	X	-
7	PCI	G	1251	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20217 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

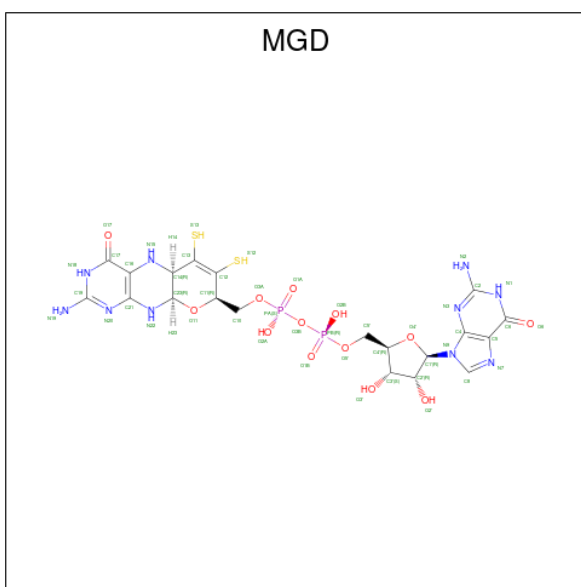
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

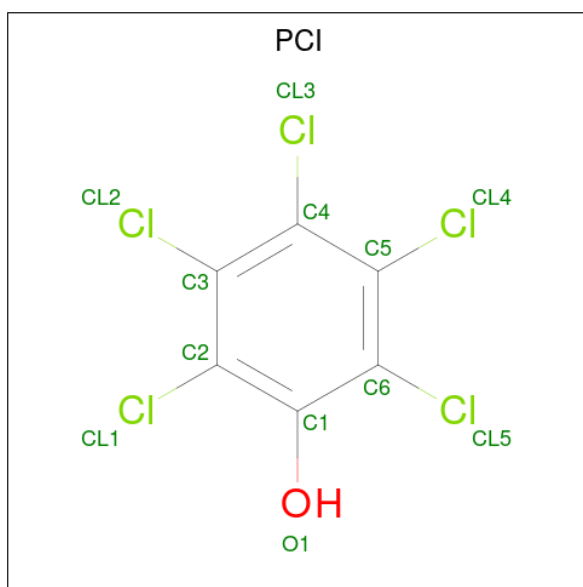


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is PENTACHLOROPHENOL (CCD ID: PCI) (formula: C₆HCl₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	Cl	O	0	0
			12	6	5	1		
7	G	1	Total	C	Cl	O	0	0
			12	6	5	1		

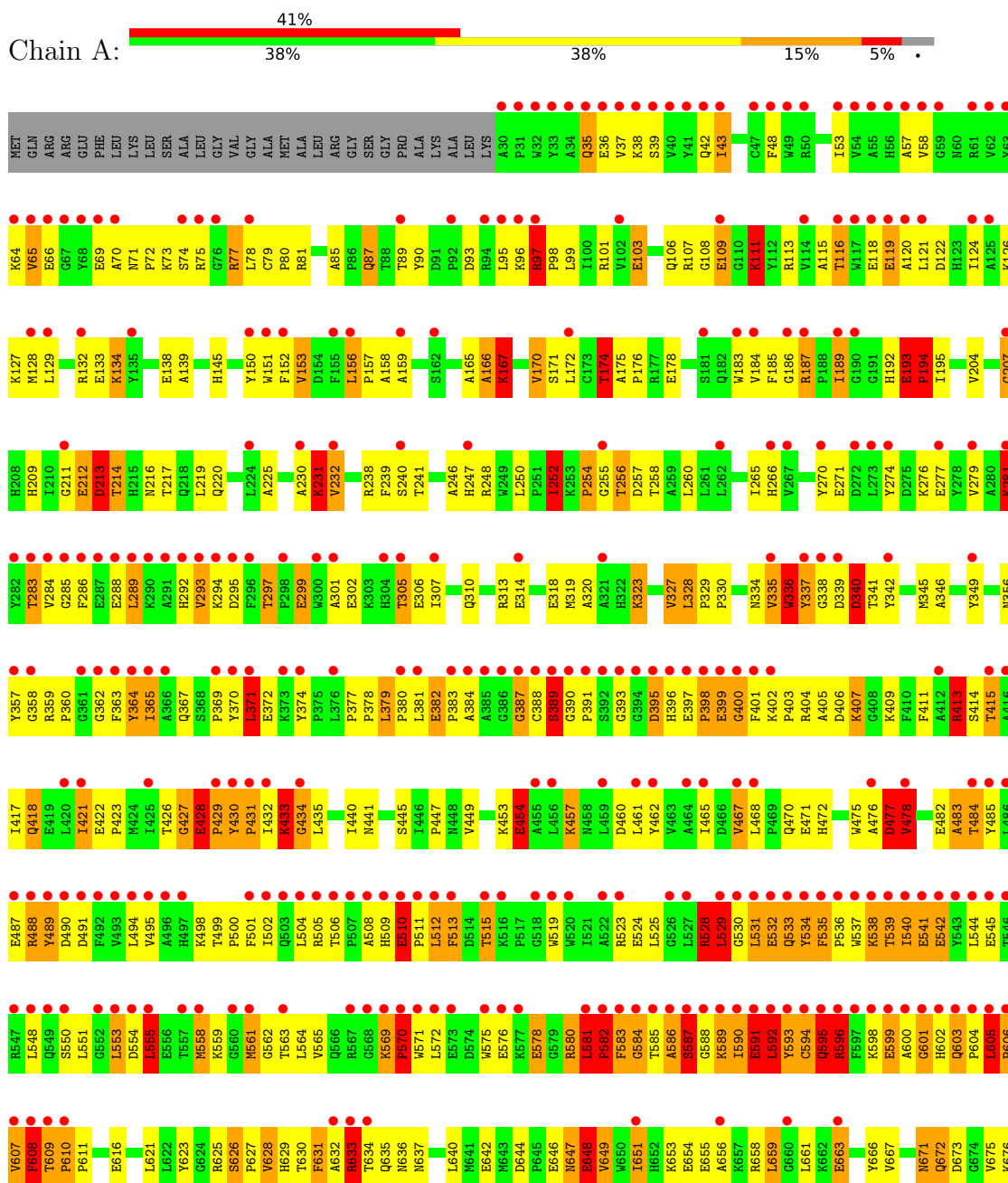
- Molecule 8 is water.

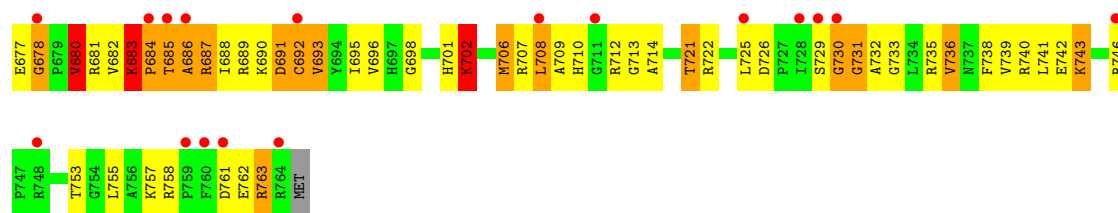
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	387	Total	O	0	0
			387	387		
8	B	150	Total	O	0	0
			150	150		
8	C	90	Total	O	0	0
			90	90		
8	E	452	Total	O	0	0
			452	452		
8	F	129	Total	O	0	0
			129	129		
8	G	77	Total	O	0	0
			77	77		

3 Residue-property plots

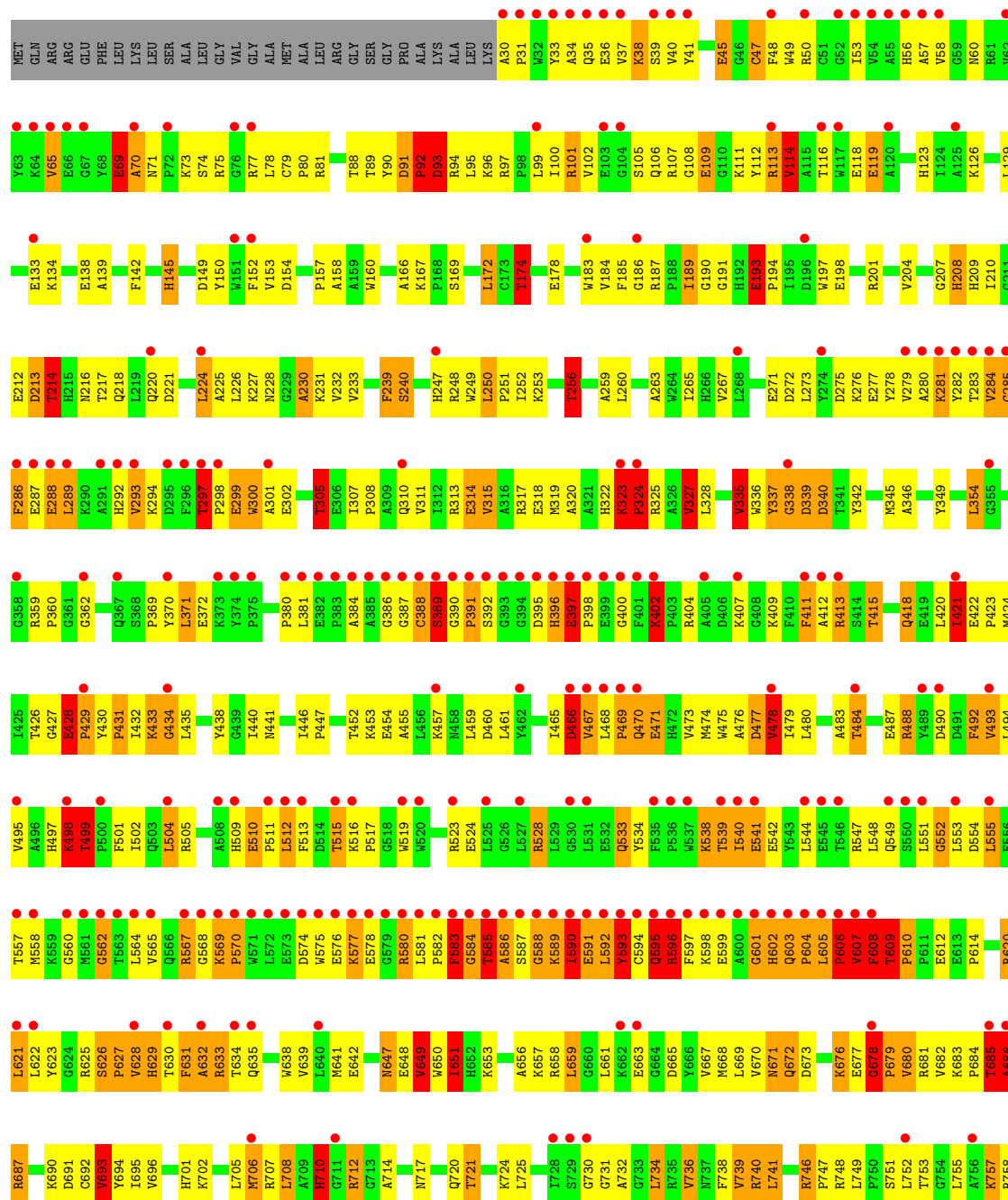
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

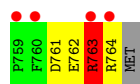
• Molecule 1: THIOSULFATE REDUCTASE



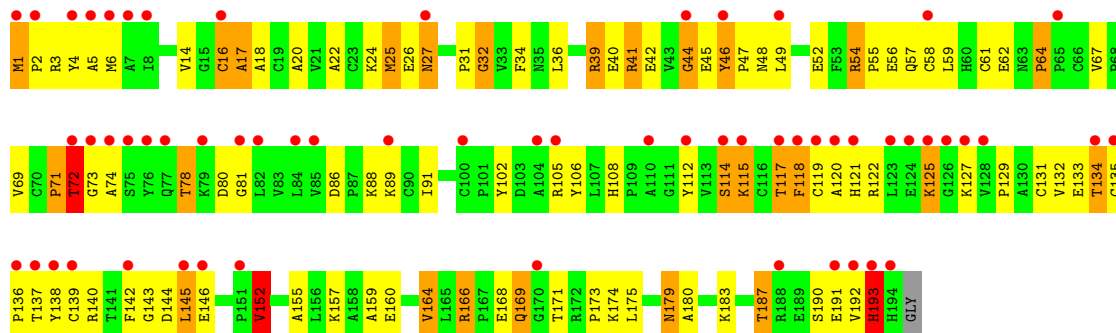


● Molecule 1: THIOSULFATE REDUCTASE

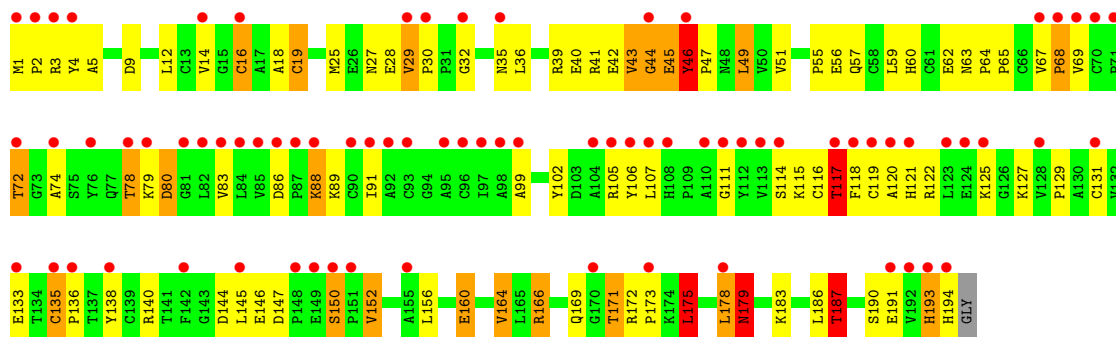
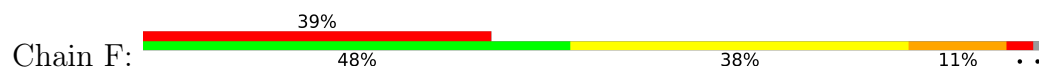




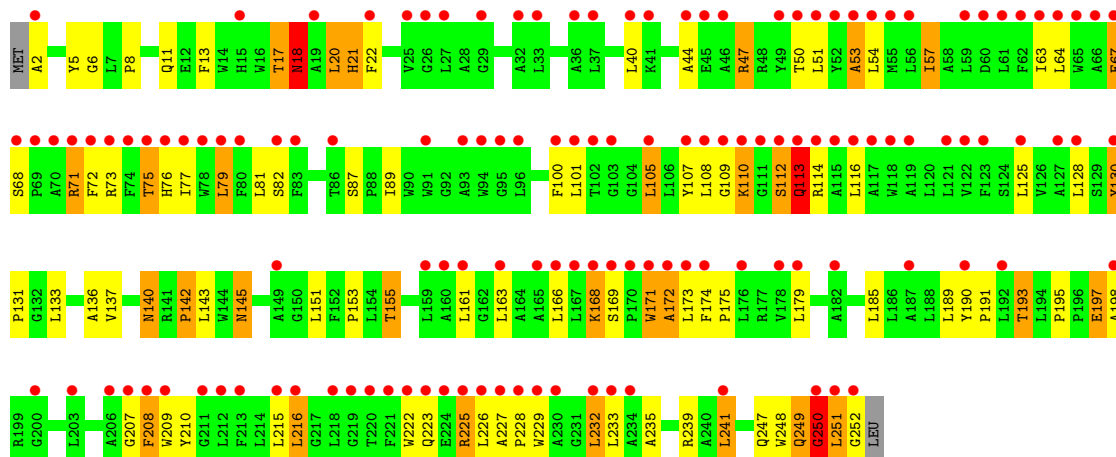
● Molecule 2: NRFC PROTEIN



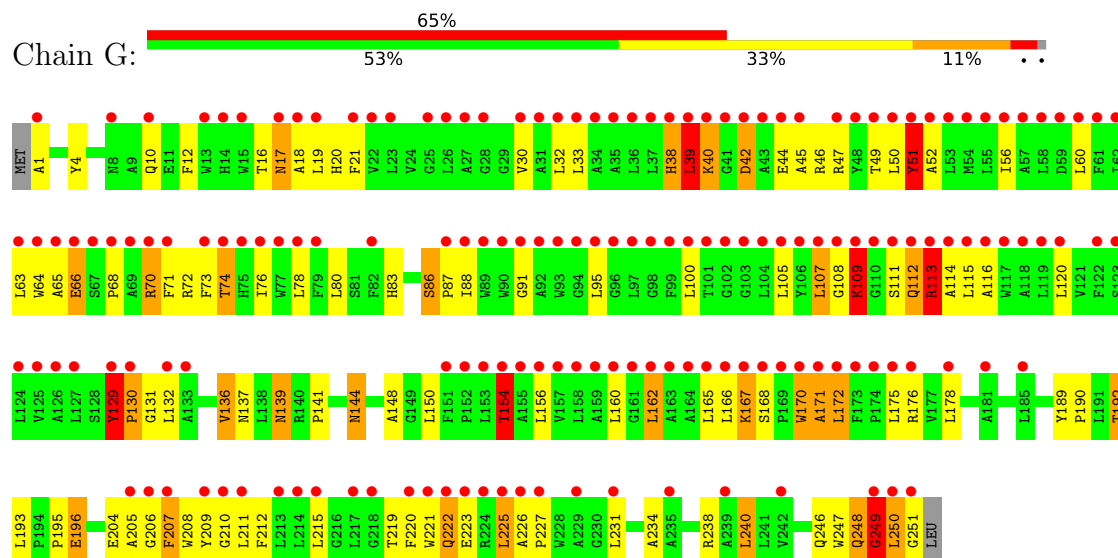
● Molecule 2: NRFC PROTEIN



● Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



● Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.12Å 165.19Å 243.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 2.50 39.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.58-2.50) 98.7 (39.58-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.289 0.277 , 0.279	Depositor DCC
R_{free} test set	3224 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20217	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MGD, SF4, MO, PCI

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	1.06	23/6079 (0.4%)	1.58	130/8267 (1.6%)
1	E	1.21	44/6079 (0.7%)	1.77	184/8267 (2.2%)
2	B	0.94	3/1512 (0.2%)	1.63	29/2058 (1.4%)
2	F	0.99	4/1512 (0.3%)	1.73	38/2058 (1.8%)
3	C	1.01	9/2016 (0.4%)	1.32	22/2764 (0.8%)
3	G	0.88	3/2016 (0.1%)	1.52	35/2764 (1.3%)
All	All	1.07	86/19214 (0.4%)	1.63	438/26178 (1.7%)

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	E	0	2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	323	LYS	C-O	17.65	1.46	1.24
1	E	592	LEU	CG-CD1	16.93	2.08	1.52
3	C	114	ARG	NE-CZ	14.03	1.48	1.33
1	E	240	SER	CA-CB	-11.88	1.35	1.53
1	E	324	PRO	CA-C	11.68	1.69	1.52
1	E	387	GLY	C-N	10.54	1.48	1.33
1	E	594	CYS	C-O	-9.66	1.12	1.24
1	E	685	THR	CA-C	9.51	1.65	1.52
1	E	593	TYR	CA-C	-9.37	1.40	1.52
1	A	364	TYR	C-O	-9.09	1.12	1.24
1	E	583	PHE	CA-C	8.96	1.64	1.52
1	E	421	ILE	CA-CB	-8.67	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	230	ALA	C-O	-8.59	1.12	1.23
1	A	581	LEU	CA-C	8.54	1.60	1.52
1	E	478	VAL	CA-CB	8.19	1.65	1.54
3	C	114	ARG	CZ-NH1	8.16	1.44	1.32
1	E	388	CYS	CA-CB	-8.13	1.39	1.53
1	E	324	PRO	CG-CD	8.03	1.78	1.50
1	E	231	LYS	CA-CB	-7.98	1.41	1.53
1	E	324	PRO	N-CA	7.79	1.57	1.47
1	E	586	ALA	CA-CB	-7.76	1.43	1.53
2	F	135	CYS	CB-SG	7.72	2.06	1.81
1	E	114	VAL	CA-CB	7.63	1.62	1.54
1	E	594	CYS	CA-C	7.53	1.62	1.52
3	G	109	LYS	C-N	7.48	1.44	1.33
1	A	401	PHE	N-CA	7.41	1.55	1.46
1	E	594	CYS	N-CA	-7.40	1.37	1.46
1	E	586	ALA	CA-C	7.34	1.59	1.53
3	C	195	PRO	CA-C	7.23	1.56	1.52
1	E	387	GLY	C-O	-7.19	1.14	1.23
1	A	648	GLU	CA-C	7.11	1.60	1.52
1	E	595	GLN	CA-CB	-6.97	1.41	1.53
1	A	97	ARG	NE-CZ	6.93	1.40	1.33
1	E	585	THR	CA-C	6.86	1.61	1.52
1	E	388	CYS	CA-C	-6.85	1.43	1.52
1	E	763	ARG	C-N	-6.76	1.23	1.33
1	E	446	ILE	CA-CB	6.73	1.59	1.54
1	E	239	PHE	C-O	-6.65	1.15	1.23
1	A	365	ILE	CA-CB	6.53	1.63	1.54
1	E	324	PRO	CA-CB	6.52	1.63	1.53
1	A	534	TYR	CA-C	6.45	1.60	1.52
1	A	583	PHE	C-O	6.40	1.32	1.24
2	F	91	ILE	CA-CB	6.36	1.62	1.54
1	A	601	GLY	CA-C	-6.33	1.43	1.51
3	C	63	ILE	CA-CB	6.32	1.61	1.54
1	A	648	GLU	CB-CG	6.29	1.71	1.52
3	C	114	ARG	CD-NE	6.29	1.55	1.46
1	A	583	PHE	N-CA	6.24	1.54	1.46
1	E	608	PHE	CA-C	6.15	1.61	1.52
1	E	585	THR	CA-CB	6.08	1.63	1.53
2	B	67	VAL	CA-CB	6.07	1.61	1.54
3	C	18	ASN	CG-OD1	5.94	1.34	1.23
1	A	581	LEU	N-CA	5.91	1.51	1.45
1	E	388	CYS	N-CA	-5.89	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	594	CYS	C-N	-5.88	1.25	1.33
3	C	251	LEU	C-N	-5.85	1.25	1.33
1	A	401	PHE	CA-CB	-5.83	1.45	1.53
1	E	583	PHE	CA-CB	-5.83	1.43	1.53
1	E	324	PRO	N-CD	5.81	1.55	1.47
1	E	493	VAL	CA-CB	5.70	1.61	1.54
2	F	51	VAL	CA-CB	5.69	1.61	1.54
1	A	649	VAL	CA-CB	5.68	1.60	1.54
2	F	193	HIS	C-N	-5.64	1.25	1.33
1	E	686	ALA	N-CA	5.61	1.53	1.46
1	A	528	ARG	CA-C	5.57	1.60	1.52
3	C	63	ILE	CA-C	5.55	1.58	1.52
3	G	250	LEU	C-N	-5.52	1.25	1.33
3	C	171	TRP	C-O	-5.48	1.16	1.23
1	A	608	PHE	CA-C	5.46	1.60	1.52
1	E	35	GLN	CA-C	5.46	1.60	1.52
1	A	763	ARG	C-N	-5.41	1.25	1.33
1	E	685	THR	CA-CB	5.39	1.62	1.53
1	E	420	LEU	C-O	-5.36	1.16	1.24
1	A	529	LEU	N-CA	5.33	1.52	1.46
1	E	324	PRO	CB-CG	-5.32	1.23	1.49
1	A	337	TYR	CA-C	5.32	1.59	1.52
1	A	582	PRO	CA-C	5.29	1.59	1.52
2	B	193	HIS	C-N	-5.23	1.26	1.33
2	B	91	ILE	CA-CB	5.19	1.60	1.54
1	A	97	ARG	C-N	5.18	1.40	1.33
1	E	210	ILE	CA-CB	5.16	1.59	1.54
1	A	529	LEU	CA-C	5.11	1.59	1.52
1	E	595	GLN	CA-C	5.11	1.59	1.52
1	E	315	VAL	CA-CB	5.10	1.60	1.54
3	G	112	GLN	CA-C	5.04	1.58	1.52
1	A	692	CYS	CA-C	-5.01	1.46	1.52

All (438) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	171	THR	N-CA-C	23.79	139.41	111.82
1	E	323	LYS	O-C-N	-21.81	96.24	121.32
1	E	323	LYS	CA-C-N	19.34	144.02	119.84
1	E	323	LYS	C-N-CA	19.34	144.02	119.84
1	E	467	VAL	N-CA-C	18.26	129.53	110.36
3	G	114	ALA	N-CA-C	-18.19	91.46	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	44	GLY	N-CA-C	17.70	137.24	112.81
1	E	324	PRO	CA-N-CD	-16.35	89.11	112.00
1	A	401	PHE	N-CA-C	16.20	133.81	113.88
1	A	189	ILE	N-CA-C	-15.87	98.16	111.81
1	E	594	CYS	N-CA-C	15.69	128.47	111.36
2	B	169	GLN	N-CA-C	-15.01	89.64	110.35
3	G	225	LEU	N-CA-C	-14.51	92.68	112.12
1	E	659	LEU	N-CA-C	-14.28	90.64	110.35
1	E	189	ILE	N-CA-C	-14.17	98.27	111.45
1	E	323	LYS	C-N-CD	-13.97	67.71	125.00
1	E	582	PRO	N-CA-C	13.64	131.68	113.40
1	E	583	PHE	CA-C-N	13.55	131.53	122.18
1	E	583	PHE	C-N-CA	13.55	131.53	122.18
1	E	185	PHE	N-CA-C	-13.25	88.98	109.65
1	A	364	TYR	N-CA-C	13.14	127.07	111.82
3	C	114	ARG	N-CA-C	-13.01	95.87	113.18
1	E	324	PRO	N-CA-C	-12.56	86.59	112.47
2	B	46	TYR	N-CA-C	12.29	136.97	109.81
3	G	249	GLY	N-CA-C	12.26	142.23	113.18
1	A	608	PHE	N-CA-C	-12.23	97.61	112.54
1	A	659	LEU	N-CA-C	-12.22	95.04	110.19
2	F	16	CYS	N-CA-C	-12.22	93.27	110.50
1	A	583	PHE	CA-C-N	11.39	143.74	121.41
1	A	583	PHE	C-N-CA	11.39	143.74	121.41
1	A	109	GLU	N-CA-C	-11.34	95.50	110.24
3	G	171	ALA	N-CA-C	10.88	124.22	111.71
1	E	665	ASP	N-CA-C	10.85	125.11	110.35
1	A	592	LEU	N-CA-C	10.84	133.89	110.80
1	E	387	GLY	CA-C-O	10.69	139.17	120.57
2	B	72	THR	N-CA-C	-10.66	93.34	109.86
1	E	387	GLY	CA-C-N	-10.57	101.35	121.54
1	E	387	GLY	C-N-CA	-10.57	101.35	121.54
1	E	585	THR	CB-CA-C	10.57	131.45	110.42
3	G	193	LEU	CA-C-N	-10.49	109.57	120.38
3	G	193	LEU	C-N-CA	-10.49	109.57	120.38
2	B	44	GLY	N-CA-C	10.40	123.94	112.29
2	F	152	VAL	CB-CA-C	-10.24	98.86	111.97
2	F	64	PRO	N-CA-C	10.21	123.16	110.70
1	E	388	CYS	N-CA-C	10.17	132.46	110.80
1	A	433	LYS	N-CA-C	-10.15	95.44	110.46
1	A	644	ASP	CA-C-N	10.11	130.96	120.04
1	A	644	ASP	C-N-CA	10.11	130.96	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	680	VAL	CB-CA-C	-10.02	95.69	110.62
1	E	686	ALA	N-CA-C	10.02	132.14	110.80
2	B	1	MET	CA-C-N	-9.99	107.35	119.84
2	B	1	MET	C-N-CA	-9.99	107.35	119.84
1	E	583	PHE	N-CA-C	9.97	132.04	110.80
1	E	340	ASP	N-CA-C	9.91	123.11	111.71
1	A	213	ASP	N-CA-C	-9.73	94.37	109.25
1	E	184	VAL	N-CA-C	9.62	121.48	111.00
1	A	731	GLY	N-CA-C	9.54	122.52	111.36
1	E	608	PHE	N-CA-C	-9.46	100.85	111.82
1	A	401	PHE	CA-C-O	-9.36	108.66	119.24
1	A	477	ASP	N-CA-C	-9.36	94.08	108.96
1	A	683	LYS	CA-C-N	9.24	131.39	119.84
1	A	683	LYS	C-N-CA	9.24	131.39	119.84
1	E	736	VAL	N-CA-CB	-9.11	100.16	112.28
3	G	109	LYS	O-C-N	9.07	132.18	122.20
1	E	590	ILE	CB-CA-C	-9.05	99.69	110.91
1	E	240	SER	N-CA-CB	-9.04	95.95	110.51
1	E	685	THR	CA-C-N	9.02	138.78	121.54
1	E	685	THR	C-N-CA	9.02	138.78	121.54
3	G	18	ALA	N-CA-C	-9.02	102.40	113.41
2	B	152	VAL	CB-CA-C	-8.93	99.89	112.22
1	E	213	ASP	N-CA-C	-8.81	95.01	108.67
2	F	43	VAL	N-CA-C	-8.70	94.89	107.77
1	A	736	VAL	N-CA-CB	-8.70	101.04	112.26
1	E	594	CYS	O-C-N	-8.67	112.26	122.15
1	E	216	ASN	N-CA-C	8.66	121.59	111.02
3	C	113	GLN	N-CA-C	8.63	129.19	110.80
1	E	174	THR	N-CA-C	8.62	123.92	113.23
1	E	603	GLN	N-CA-C	8.61	128.84	109.81
1	A	193	GLU	CA-C-N	8.61	130.60	119.84
1	A	193	GLU	C-N-CA	8.61	130.60	119.84
2	F	16	CYS	CA-C-N	-8.56	107.38	122.62
2	F	16	CYS	C-N-CA	-8.56	107.38	122.62
3	C	195	PRO	N-CA-C	-8.50	101.49	110.58
1	A	340	ASP	N-CA-C	8.43	128.76	110.80
1	E	327	VAL	CB-CA-C	-8.43	97.20	110.69
1	E	678	GLY	CA-C-N	-8.42	110.73	119.83
1	E	678	GLY	C-N-CA	-8.42	110.73	119.83
1	A	327	VAL	CB-CA-C	-8.41	97.55	110.50
1	A	409	LYS	N-CA-C	8.38	122.80	112.23
2	F	29	VAL	CA-C-N	8.37	129.00	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	29	VAL	C-N-CA	8.37	129.00	120.38
1	A	691	ASP	CB-CA-C	-8.37	92.82	110.31
1	E	409	LYS	N-CA-C	8.31	123.23	113.18
3	G	207	PHE	CB-CA-C	-8.29	93.92	110.42
1	E	390	GLY	N-CA-C	-8.28	95.46	112.34
1	E	466	ASP	CA-C-N	8.28	131.27	120.60
1	E	466	ASP	C-N-CA	8.28	131.27	120.60
1	A	591	GLU	N-CA-C	-8.23	102.31	111.28
1	E	590	ILE	N-CA-CB	8.20	119.66	110.72
1	E	212	GLU	N-CA-C	-8.19	101.79	112.68
3	G	83	HIS	CA-C-N	8.17	130.06	119.84
3	G	83	HIS	C-N-CA	8.17	130.06	119.84
1	A	174	THR	N-CA-C	8.16	123.41	113.38
1	E	92	PRO	N-CA-C	-8.12	95.75	112.47
1	A	153	VAL	N-CA-C	8.06	120.12	111.58
1	E	593	TYR	N-CA-CB	8.05	124.09	110.49
1	E	96	LYS	N-CA-C	8.02	123.66	113.55
1	E	150	TYR	N-CA-C	-8.01	102.63	111.36
1	E	428	GLU	N-CA-C	8.00	127.49	109.81
3	G	166	LEU	N-CA-C	-7.97	104.53	112.97
3	C	226	LEU	N-CA-C	-7.89	103.78	113.41
1	E	288	GLU	N-CA-C	-7.89	103.49	113.43
1	E	428	GLU	CA-C-N	-7.87	110.00	119.84
1	E	428	GLU	C-N-CA	-7.87	110.00	119.84
1	E	595	GLN	N-CA-CB	-7.85	96.66	110.39
2	B	46	TYR	CB-CA-C	-7.84	94.72	110.17
1	A	328	LEU	CA-C-N	-7.79	112.36	120.38
1	A	328	LEU	C-N-CA	-7.79	112.36	120.38
2	F	46	TYR	N-CA-C	7.79	127.02	109.81
1	E	593	TYR	CB-CA-C	-7.75	95.00	110.42
1	E	593	TYR	N-CA-C	-7.73	94.34	110.80
1	A	582	PRO	N-CA-C	7.71	128.34	112.47
2	F	18	ALA	N-CA-C	7.70	119.68	111.28
3	G	248	GLN	N-CA-CB	-7.70	99.96	110.67
2	F	152	VAL	N-CA-CB	7.67	119.53	110.55
1	E	278	TYR	N-CA-C	-7.65	102.88	111.14
1	E	692	CYS	N-CA-C	7.61	120.48	109.14
1	E	606	PRO	N-CA-C	-7.59	96.83	112.47
1	A	467	VAL	CB-CA-C	-7.58	103.48	110.91
1	E	731	GLY	N-CA-C	7.56	131.09	113.18
1	E	592	LEU	N-CA-C	7.53	121.33	109.81
1	A	212	GLU	N-CA-C	-7.51	102.69	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	281	LYS	N-CA-C	7.51	122.74	113.50
1	E	187	ARG	CA-C-N	7.49	127.65	120.31
1	E	187	ARG	C-N-CA	7.49	127.65	120.31
3	C	136	ALA	N-CA-C	7.49	122.07	112.34
1	E	214	THR	N-CA-CB	-7.48	98.90	111.17
3	G	4	TYR	N-CA-C	-7.48	94.94	108.02
1	E	34	ALA	CA-C-N	7.47	135.81	121.54
1	E	34	ALA	C-N-CA	7.47	135.81	121.54
1	E	594	CYS	N-CA-CB	-7.46	99.12	110.16
1	E	323	LYS	CB-CA-C	7.46	124.86	110.17
1	A	628	VAL	N-CA-CB	-7.40	104.07	112.21
1	E	338	GLY	N-CA-C	7.38	125.56	115.30
1	A	648	GLU	N-CA-CB	-7.37	98.44	110.81
1	A	364	TYR	CA-C-N	7.36	135.22	121.97
1	A	364	TYR	C-N-CA	7.36	135.22	121.97
1	A	534	TYR	N-CA-C	-7.34	97.28	109.46
1	E	707	ARG	N-CA-C	7.33	120.14	111.71
2	B	46	TYR	CA-C-N	7.32	129.28	120.94
2	B	46	TYR	C-N-CA	7.32	129.28	120.94
1	E	323	LYS	CA-C-O	-7.28	110.19	120.16
1	E	337	TYR	N-CA-C	7.26	126.25	110.80
3	G	130	PRO	N-CA-C	-7.24	97.55	112.47
1	E	411	PHE	N-CA-C	7.23	119.24	111.36
1	A	232	VAL	N-CA-C	7.18	118.21	107.80
3	G	170	TRP	N-CA-C	7.17	119.96	111.71
3	C	6	GLY	N-CA-C	-7.15	99.21	112.37
1	A	365	ILE	N-CA-CB	7.15	123.03	111.23
1	E	710	HIS	N-CA-C	7.09	125.91	110.80
3	G	131	GLY	N-CA-C	-7.09	96.37	113.18
1	E	154	ASP	N-CA-C	7.08	121.92	113.28
1	A	281	LYS	N-CA-C	7.07	121.90	113.28
2	F	43	VAL	CA-C-N	-7.06	115.35	122.69
2	F	43	VAL	C-N-CA	-7.06	115.35	122.69
1	E	335	VAL	N-CA-CB	-7.04	99.62	111.23
2	B	71	PRO	N-CA-C	7.04	122.83	113.40
2	B	180	ALA	CA-C-N	7.03	126.86	119.05
2	B	180	ALA	C-N-CA	7.03	126.86	119.05
1	A	596	ARG	N-CA-C	-7.03	103.33	112.68
1	E	276	LYS	N-CA-C	7.01	119.00	111.36
2	B	64	PRO	N-CA-C	6.99	119.23	110.70
1	A	207	GLY	CA-C-O	6.99	126.83	119.00
1	E	297	THR	N-CA-CB	-6.99	101.58	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	588	GLY	CA-C-N	-6.96	112.90	122.30
1	E	588	GLY	C-N-CA	-6.96	112.90	122.30
1	E	207	GLY	N-CA-C	-6.95	99.14	110.95
1	E	734	LEU	N-CA-C	6.93	121.48	112.89
1	A	707	ARG	N-CA-C	6.87	119.61	111.71
1	A	649	VAL	CB-CA-C	-6.83	103.09	111.08
2	B	72	THR	N-CA-CB	-6.82	99.54	110.39
1	E	712	ARG	N-CA-C	6.77	119.97	109.07
1	E	431	PRO	N-CA-C	6.76	121.01	110.80
1	E	191	GLY	N-CA-C	6.71	120.29	112.50
1	A	601	GLY	CA-C-N	-6.69	112.30	122.81
1	A	601	GLY	C-N-CA	-6.69	112.30	122.81
3	C	250	GLY	N-CA-C	6.66	128.95	113.18
1	A	185	PHE	CA-C-N	-6.65	108.38	121.41
1	A	185	PHE	C-N-CA	-6.65	108.38	121.41
1	E	214	THR	CB-CA-C	6.64	121.82	111.13
1	A	663	GLU	N-CA-C	6.59	122.24	111.37
1	E	402	LYS	CA-C-N	-6.56	113.88	120.31
1	E	402	LYS	C-N-CA	-6.56	113.88	120.31
1	A	513	PHE	CB-CA-C	-6.50	109.08	116.63
1	E	152	PHE	N-CA-C	6.50	121.07	113.20
3	G	168	SER	N-CA-C	-6.50	100.20	109.62
1	E	433	LYS	N-CA-C	-6.50	99.13	109.59
3	C	116	LEU	N-CA-C	-6.48	105.51	113.41
1	A	427	GLY	N-CA-C	-6.47	106.31	115.30
1	E	690	LYS	CA-C-N	6.46	132.44	121.14
1	E	690	LYS	C-N-CA	6.46	132.44	121.14
1	A	570	PRO	O-C-N	-6.46	113.92	122.64
1	E	174	THR	N-CA-CB	-6.46	100.37	110.44
2	F	16	CYS	O-C-N	-6.44	115.26	122.86
1	A	219	LEU	N-CA-C	-6.44	104.19	111.14
1	E	388	CYS	CA-C-O	6.43	129.70	120.51
1	A	626	SER	N-CA-C	-6.43	100.30	109.62
1	E	594	CYS	CA-C-N	6.42	133.90	121.18
1	E	594	CYS	C-N-CA	6.42	133.90	121.18
2	B	4	TYR	N-CA-C	6.40	119.75	110.28
1	E	596	ARG	N-CA-C	-6.39	104.18	112.68
1	A	359	ARG	CA-C-N	-6.38	112.38	120.23
1	A	359	ARG	C-N-CA	-6.38	112.38	120.23
1	E	335	VAL	CB-CA-C	6.36	121.72	111.29
1	E	172	LEU	CA-CB-CG	-6.34	94.11	116.30
1	E	710	HIS	CA-C-N	-6.33	109.00	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	710	HIS	C-N-CA	-6.33	109.00	121.41
1	E	562	GLY	CA-C-N	6.33	131.19	122.77
1	E	562	GLY	C-N-CA	6.33	131.19	122.77
2	B	16	CYS	N-CA-C	-6.32	96.87	107.99
3	G	51	TYR	N-CA-C	-6.30	97.37	110.80
2	B	134	THR	CB-CA-C	-6.29	100.41	111.05
3	C	169	SER	CA-C-N	6.29	126.03	119.05
3	C	169	SER	C-N-CA	6.29	126.03	119.05
1	E	354	LEU	N-CA-C	-6.29	105.25	113.17
1	E	498	LYS	N-CA-C	-6.29	101.06	111.37
1	A	595	GLN	N-CA-C	6.28	120.94	113.16
1	A	411	PHE	N-CA-C	6.27	117.91	111.14
1	A	706	MET	N-CA-C	-6.27	96.19	107.98
1	A	476	ALA	N-CA-C	6.24	120.25	110.32
1	A	576	GLU	N-CA-C	6.23	118.07	111.28
3	G	42	ASP	N-CA-C	6.21	119.37	110.24
1	E	492	PHE	N-CA-C	6.20	119.03	110.35
2	F	117	THR	N-CA-CB	-6.20	100.98	111.27
1	E	585	THR	CA-CB-CG2	-6.19	99.97	110.50
1	A	371	LEU	N-CA-C	-6.18	97.50	108.13
1	A	692	CYS	N-CA-C	6.18	118.80	109.41
1	A	454	GLU	N-CA-C	-6.18	104.46	111.07
1	E	256	THR	N-CA-CB	-6.16	101.30	110.61
2	B	171	THR	N-CA-C	6.14	120.61	113.18
1	E	400	GLY	N-CA-C	-6.13	98.64	113.18
1	A	356	ASN	N-CA-C	6.13	120.76	113.28
1	E	585	THR	CA-C-O	-6.13	111.75	120.51
2	F	156	LEU	N-CA-C	-6.12	104.52	111.07
1	A	150	TYR	N-CA-C	-6.11	104.53	111.07
2	F	179	ASN	N-CA-C	6.10	123.80	110.80
1	E	428	GLU	CA-C-O	-6.10	111.81	120.16
1	A	690	LYS	CA-C-N	6.09	130.90	120.72
1	A	690	LYS	C-N-CA	6.09	130.90	120.72
3	G	70	ARG	N-CA-C	6.09	117.60	110.97
3	C	5	TYR	N-CA-C	-6.08	97.39	108.02
2	F	187	THR	N-CA-CB	-6.07	100.66	109.83
1	E	198	GLU	N-CA-C	6.07	118.69	111.71
2	F	4	TYR	N-CA-C	6.07	119.06	109.96
1	A	583	PHE	N-CA-C	6.06	123.72	110.80
3	G	109	LYS	N-CA-C	6.05	118.64	109.63
1	E	499	THR	CB-CA-C	-6.04	102.97	109.85
2	F	135	CYS	CA-C-N	6.04	125.75	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	135	CYS	C-N-CA	6.04	125.75	119.05
1	E	402	LYS	N-CA-C	6.04	117.50	109.83
1	A	488	ARG	N-CA-C	6.03	118.58	109.23
1	A	606	PRO	N-CA-C	-6.03	106.32	113.86
1	E	38	LYS	N-CA-C	-6.03	97.63	108.48
1	A	633	ARG	N-CA-C	6.02	123.61	110.80
2	F	111	GLY	N-CA-C	6.01	124.98	114.76
1	E	33	TYR	N-CA-C	6.00	120.44	113.18
1	E	93	ASP	N-CA-C	6.00	123.58	110.80
1	A	491	ASP	N-CA-C	-5.99	102.20	110.35
3	C	8	PRO	N-CA-C	-5.99	102.47	111.57
1	A	211	GLY	N-CA-C	-5.98	107.19	113.58
1	A	334	ASN	N-CA-C	5.97	120.18	112.41
2	F	83	VAL	N-CA-C	-5.97	99.82	108.36
1	E	239	PHE	CB-CA-C	-5.96	100.98	111.05
1	E	661	LEU	N-CA-C	5.93	119.14	109.59
3	G	154	THR	CB-CA-C	5.93	122.05	110.67
3	C	168	LYS	N-CA-C	5.92	120.09	112.86
1	E	594	CYS	CA-C-O	5.92	126.69	120.42
1	A	400	GLY	CA-C-N	-5.90	112.21	122.36
1	A	400	GLY	C-N-CA	-5.90	112.21	122.36
3	G	172	LEU	N-CA-C	5.90	117.38	111.07
1	E	339	ASP	N-CA-C	-5.89	103.43	111.56
1	E	651	ILE	CB-CA-C	-5.88	100.18	110.71
1	E	285	GLY	N-CA-C	5.87	124.01	115.32
2	F	186	LEU	CA-C-N	5.87	129.05	120.71
2	F	186	LEU	C-N-CA	5.87	129.05	120.71
1	E	324	PRO	N-CD-CG	-5.86	94.41	103.20
2	F	5	ALA	N-CA-C	5.86	117.98	109.07
1	E	294	LYS	N-CA-C	5.86	118.14	111.11
2	F	175	LEU	N-CA-C	-5.86	98.73	108.34
1	E	679	PRO	N-CA-C	5.85	120.04	111.03
1	E	297	THR	N-CA-C	5.84	118.36	110.29
1	E	193	GLU	N-CA-C	5.83	117.88	109.48
2	B	108	HIS	N-CA-C	-5.82	101.74	110.24
1	A	570	PRO	N-CA-C	5.82	124.45	112.47
1	E	757	LYS	N-CA-C	5.82	120.10	112.89
1	E	687	ARG	CB-CG-CD	-5.81	97.94	111.30
1	A	498	LYS	N-CA-C	-5.80	104.15	111.11
1	E	105	SER	CA-C-N	5.78	128.97	120.82
1	E	105	SER	C-N-CA	5.78	128.97	120.82
2	F	14	VAL	N-CA-C	-5.78	107.35	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	113	ARG	N-CA-C	5.78	123.10	110.80
1	A	680	VAL	CB-CA-C	-5.77	101.94	110.82
3	G	86	SER	N-CA-C	5.76	119.89	108.59
1	A	35	GLN	N-CA-C	-5.75	102.79	110.55
1	A	590	ILE	N-CA-C	5.75	116.40	110.36
1	A	252	ILE	N-CA-C	5.75	117.90	109.63
1	A	407	LYS	N-CA-C	5.72	119.07	111.75
2	F	29	VAL	N-CA-C	-5.72	103.34	108.95
1	E	706	MET	N-CA-C	-5.72	96.48	107.57
1	E	280	ALA	N-CA-C	5.71	118.24	111.33
3	G	162	LEU	N-CA-C	-5.68	104.78	110.97
1	A	327	VAL	N-CA-C	5.67	116.92	108.46
1	E	632	ALA	N-CA-C	5.67	119.94	113.19
1	A	417	ILE	N-CA-C	5.67	117.08	110.62
1	A	489	TYR	N-CA-C	-5.67	101.04	110.17
3	G	248	GLN	O-C-N	5.67	129.34	122.48
1	E	478	VAL	CA-C-N	5.66	132.68	122.43
1	E	478	VAL	C-N-CA	5.66	132.68	122.43
1	E	226	LEU	N-CA-C	-5.65	105.20	111.36
2	F	19	CYS	N-CA-C	-5.65	105.04	111.14
1	A	265	ILE	N-CA-C	-5.64	105.01	110.42
1	A	294	LYS	N-CA-C	5.64	117.88	111.11
1	E	193	GLU	CA-C-N	5.63	126.88	119.84
1	E	193	GLU	C-N-CA	5.63	126.88	119.84
1	E	421	ILE	N-CA-CB	-5.63	104.78	112.28
1	A	555	LEU	N-CA-C	5.63	117.09	111.07
3	C	225	ARG	N-CA-C	5.62	119.77	113.02
1	A	374	TYR	N-CA-C	-5.62	102.57	109.65
2	B	169	GLN	CA-C-N	-5.61	110.41	121.41
2	B	169	GLN	C-N-CA	-5.61	110.41	121.41
1	E	668	MET	N-CA-C	-5.61	100.57	109.59
1	E	69	GLU	N-CA-C	-5.59	102.61	110.50
2	F	160	GLU	N-CA-C	-5.58	105.20	112.23
1	E	583	PHE	N-CA-CB	-5.57	101.08	110.49
1	E	649	VAL	CB-CA-C	-5.56	104.01	110.91
1	A	231	LYS	CA-C-N	5.56	130.35	123.12
1	A	231	LYS	C-N-CA	5.56	130.35	123.12
1	A	569	LYS	N-CA-C	5.55	118.20	108.82
1	E	231	LYS	N-CA-CB	-5.54	101.37	110.52
2	F	105	ARG	N-CA-C	5.53	118.83	109.76
3	G	141	PRO	N-CA-C	5.51	121.97	113.75
3	G	78	LEU	N-CA-C	-5.51	105.37	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	397	GLU	N-CA-C	5.50	121.97	109.81
1	A	97	ARG	CA-C-N	-5.50	114.04	119.92
1	A	97	ARG	C-N-CA	-5.50	114.04	119.92
1	A	736	VAL	CB-CA-C	5.49	118.01	111.20
3	C	87	SER	N-CA-C	5.49	118.58	108.69
1	E	601	GLY	N-CA-C	5.48	126.17	113.18
1	A	97	ARG	N-CA-C	5.48	118.83	110.50
1	E	538	LYS	N-CA-C	5.46	117.31	111.36
1	E	584	GLY	CA-C-N	5.44	131.94	121.54
1	E	584	GLY	C-N-CA	5.44	131.94	121.54
1	A	194	PRO	N-CA-C	5.44	123.67	112.47
1	A	648	GLU	CB-CA-C	5.44	119.16	109.65
3	C	53	ALA	N-CA-C	-5.43	105.52	111.82
1	A	661	LEU	N-CA-C	5.42	117.80	109.07
1	E	629	HIS	N-CA-C	5.42	118.07	109.24
2	F	102	TYR	N-CA-C	5.42	121.74	113.61
1	A	257	ASP	N-CA-C	5.42	117.94	111.71
1	A	508	ALA	N-CA-C	-5.41	106.52	113.23
1	E	749	LEU	CA-C-N	-5.41	114.68	120.03
1	E	749	LEU	C-N-CA	-5.41	114.68	120.03
1	A	270	TYR	N-CA-C	5.40	119.13	112.54
2	F	86	ASP	N-CA-C	-5.40	98.98	108.69
3	C	20	LEU	N-CA-C	-5.38	105.33	111.14
1	A	254	PRO	N-CA-C	5.38	119.65	111.15
1	A	413	ARG	N-CA-C	5.38	119.95	113.17
1	A	583	PHE	CB-CA-C	-5.37	99.73	110.42
1	E	40	VAL	CB-CA-C	-5.37	103.86	111.38
1	E	190	GLY	N-CA-C	5.37	121.95	112.83
3	G	219	THR	N-CA-C	-5.37	105.99	112.54
1	E	271	GLU	N-CA-C	-5.36	106.42	113.17
2	B	27	ASN	N-CA-C	5.35	119.91	113.17
1	E	49	TRP	N-CA-C	-5.35	106.26	112.89
1	E	478	VAL	N-CA-C	-5.35	98.22	109.34
1	E	45	GLU	N-CA-C	-5.34	106.53	112.57
3	G	107	LEU	N-CA-C	-5.34	105.45	112.72
2	F	64	PRO	CA-C-N	-5.34	114.17	119.56
2	F	64	PRO	C-N-CA	-5.34	114.17	119.56
1	E	184	VAL	CB-CA-C	-5.33	105.10	112.24
1	A	246	ALA	N-CA-C	5.32	118.78	110.32
1	E	739	VAL	N-CA-CB	-5.31	101.98	111.92
1	E	693	VAL	CB-CA-C	5.31	119.28	110.30
1	E	35	GLN	CA-C-N	5.30	128.30	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	GLN	C-N-CA	5.30	128.30	120.82
1	E	580	ARG	N-CA-C	5.30	117.25	109.24
1	A	510	GLU	N-CA-C	5.28	117.37	110.08
1	A	336	TRP	N-CA-C	5.28	122.04	110.80
3	C	44	ALA	N-CA-C	5.25	117.75	111.71
1	A	428	GLU	CA-C-N	-5.25	113.28	119.84
1	A	428	GLU	C-N-CA	-5.25	113.28	119.84
1	E	478	VAL	CB-CA-C	5.25	119.90	111.29
1	A	167	LYS	CA-C-N	5.25	124.91	119.56
1	A	167	LYS	C-N-CA	5.25	124.91	119.56
3	C	51	LEU	CA-C-N	5.24	127.31	120.28
3	C	51	LEU	C-N-CA	5.24	127.31	120.28
1	A	542	GLU	CA-C-N	5.24	127.25	120.44
1	A	542	GLU	C-N-CA	5.24	127.25	120.44
1	A	111	LYS	N-CA-C	5.23	116.82	108.41
1	E	305	THR	N-CA-CB	-5.23	102.47	110.26
1	A	483	ALA	N-CA-C	-5.22	102.02	110.32
1	E	477	ASP	O-C-N	-5.22	115.31	122.46
3	C	47	ARG	N-CA-C	5.21	118.10	111.69
1	A	730	GLY	N-CA-C	5.21	125.54	113.18
1	E	610	PRO	N-CA-C	5.21	117.06	110.70
3	C	142	PRO	N-CA-C	5.20	121.35	113.81
1	A	271	GLU	N-CA-C	-5.19	106.63	113.17
2	B	32	GLY	N-CA-C	5.18	125.46	113.18
2	B	179	ASN	N-CA-C	5.18	118.35	111.30
1	A	686	ALA	N-CA-C	5.18	117.73	109.96
1	E	685	THR	N-CA-CB	-5.17	101.76	110.49
3	G	72	ARG	N-CA-C	-5.17	106.94	114.12
2	B	102	TYR	N-CA-C	5.17	120.22	112.94
1	E	194	PRO	N-CA-C	5.17	123.11	112.47
1	E	300	TRP	N-CA-C	-5.17	105.56	111.14
3	G	129	TYR	CA-C-N	-5.16	113.39	119.84
3	G	129	TYR	C-N-CA	-5.16	113.39	119.84
1	A	702	LYS	N-CA-C	-5.16	97.91	107.71
1	E	91	ASP	CA-C-N	-5.15	113.41	119.84
1	E	91	ASP	C-N-CA	-5.15	113.41	119.84
1	E	47	CYS	N-CA-C	-5.14	101.45	108.24
1	E	588	GLY	CA-C-O	5.13	124.56	120.30
1	A	407	LYS	CA-C-N	-5.12	114.52	122.30
1	A	407	LYS	C-N-CA	-5.12	114.52	122.30
1	E	231	LYS	CA-CB-CG	5.11	124.31	114.10
1	E	388	CYS	N-CA-CB	-5.10	101.88	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	ALA	N-CA-C	-5.09	101.37	108.54
2	B	54	ARG	CA-C-N	-5.07	114.51	119.99
2	B	54	ARG	C-N-CA	-5.07	114.51	119.99
1	E	185	PHE	CA-C-N	-5.07	111.47	121.41
1	E	185	PHE	C-N-CA	-5.07	111.47	121.41
1	E	585	THR	N-CA-C	-5.05	100.04	110.80
1	A	383	PRO	N-CA-C	5.04	119.24	111.57
1	A	274	TYR	N-CA-C	5.04	117.18	110.53
2	B	137	THR	N-CA-C	5.03	119.27	113.18
1	A	98	PRO	CA-N-CD	-5.02	104.98	112.00
1	A	166	ALA	N-CA-C	5.01	116.69	109.07
1	A	389	SER	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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	5896	0	5814	594	3
1	E	5896	0	5815	542	3
2	B	1475	0	1453	138	0
2	F	1475	0	1454	106	0
3	C	1948	0	2001	120	0
3	G	1948	0	2004	133	0
4	A	8	0	0	0	0
4	B	32	0	0	4	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	44	7	0
5	E	94	0	44	12	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	12	0	0	11	0
7	G	12	0	1	11	0
8	A	387	0	0	78	0
8	B	150	0	0	38	0
8	C	90	0	0	7	0
8	E	452	0	0	114	0
8	F	129	0	0	22	0
8	G	77	0	0	23	0
All	All	20217	0	18630	1592	3

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 42.

All (1592) 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)
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.48	1.45
1:E:324:PRO:CD	1:E:324:PRO:CG	1.78	1.45
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.24	1.44
2:F:135:CYS:CB	2:F:135:CYS:SG	2.06	1.43
1:A:186:GLY:HA3	1:A:583:PHE:C	1.45	1.40
1:E:605:LEU:H	1:E:605:LEU:CD2	1.28	1.39
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.24	1.34
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.59	1.32
1:A:582:PRO:HB2	8:A:2097:HOH:O	1.26	1.28
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.24	1.26
2:B:46:TYR:HB2	8:B:2032:HOH:O	1.33	1.26
1:A:604:PRO:O	1:A:606:PRO:HD2	1.37	1.23
1:E:477:ASP:O	1:E:478:VAL:HG23	1.32	1.22
1:E:605:LEU:HD23	1:E:605:LEU:N	1.42	1.22
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.53	1.21
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.36	1.20
1:A:601:GLY:HA2	8:A:2284:HOH:O	1.05	1.20
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.75	1.20
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.76	1.19
3:C:171:TRP:O	3:C:171:TRP:CE3	1.97	1.17
1:E:36:GLU:O	1:E:58:VAL:HG22	1.01	1.17
1:E:562:GLY:O	8:E:2316:HOH:O	1.59	1.16
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.43	1.16
1:A:337:TYR:O	1:A:340:ASP:OD2	1.59	1.16
1:A:395:ASP:O	1:A:399:GLU:HB2	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:O	1:A:53:ILE:HG13	1.45	1.15
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.56	1.15
1:E:477:ASP:O	1:E:478:VAL:CG2	1.95	1.15
1:A:583:PHE:CE2	1:A:588:GLY:N	2.16	1.14
1:E:36:GLU:O	1:E:58:VAL:CG2	1.96	1.14
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.44	1.14
1:A:584:GLY:HA2	8:A:2277:HOH:O	0.96	1.13
1:A:395:ASP:HA	1:A:399:GLU:CG	1.78	1.13
1:A:69:GLU:O	8:A:2034:HOH:O	1.65	1.12
1:A:284:VAL:O	1:A:590:ILE:HG22	1.47	1.12
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.24	1.12
2:B:134:THR:O	2:B:134:THR:HG23	1.47	1.12
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.51	1.11
1:E:607:VAL:HG12	1:E:607:VAL:O	1.46	1.10
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.34	1.09
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.75	1.09
1:E:607:VAL:O	1:E:607:VAL:CG1	1.97	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.15	1.09
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.82	1.09
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.21	1.09
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.82	1.09
1:A:601:GLY:CA	8:A:2284:HOH:O	1.68	1.09
1:A:604:PRO:O	1:A:606:PRO:CD	2.01	1.09
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.00	1.09
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.50	1.09
2:B:134:THR:O	2:B:134:THR:CG2	1.97	1.08
1:E:97:ARG:HG3	8:E:2194:HOH:O	1.52	1.08
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.37	1.07
1:E:605:LEU:CD2	1:E:605:LEU:N	1.92	1.07
1:A:632:ALA:O	1:A:635:GLN:HG2	1.56	1.06
1:A:467:VAL:HB	8:A:2230:HOH:O	1.55	1.06
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.52	1.06
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.89	1.06
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.52	1.06
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.72	1.05
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.39	1.04
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.05	1.04
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.17	1.04
1:E:763:ARG:HG2	8:E:2442:HOH:O	1.56	1.04
1:A:186:GLY:HA3	1:A:583:PHE:O	1.58	1.04
2:B:46:TYR:CD1	8:B:2032:HOH:O	2.09	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.41	1.03
1:E:95:LEU:HD12	1:E:466:ASP:O	1.57	1.03
1:E:626:SER:HB2	8:E:2349:HOH:O	1.56	1.03
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.38	1.02
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.41	1.02
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.38	1.02
3:C:22:PHE:O	3:C:239:ARG:NH1	1.91	1.02
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.87	1.02
1:A:165:ALA:O	1:A:415:THR:HG21	1.57	1.02
1:A:592:LEU:O	1:A:593:TYR:HB2	1.56	1.02
1:E:429:PRO:HD2	8:E:2259:HOH:O	1.57	1.02
1:A:685:THR:HB	2:B:42:GLU:OE2	1.60	1.01
1:E:413:ARG:HD3	8:E:2251:HOH:O	1.59	1.01
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.90	1.01
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.11	1.01
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.89	1.01
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.73	1.01
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.24	1.00
1:A:172:LEU:HD13	1:A:445:SER:O	1.61	1.00
1:A:186:GLY:CA	1:A:583:PHE:C	2.34	1.00
1:A:569:LYS:O	8:A:2272:HOH:O	1.79	1.00
1:E:47:CYS:HB2	8:E:2451:HOH:O	1.60	1.00
1:E:116:THR:CG2	1:E:119:GLU:H	1.75	1.00
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.24	1.00
1:E:598:LYS:HD2	8:E:2332:HOH:O	1.61	1.00
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.84	1.00
1:A:395:ASP:HA	1:A:399:GLU:HG3	1.00	1.00
1:E:224:LEU:HD12	8:E:2134:HOH:O	1.61	0.99
1:E:230:ALA:O	8:E:2140:HOH:O	1.77	0.99
1:E:323:LYS:HD3	1:E:354:LEU:HA	1.02	0.99
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.39	0.98
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.11	0.98
1:E:608:PHE:O	8:E:2337:HOH:O	1.80	0.98
1:A:763:ARG:HG2	8:A:2379:HOH:O	1.62	0.98
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.25	0.98
1:A:632:ALA:O	1:A:635:GLN:CG	2.11	0.97
3:C:130:TYR:OH	7:C:1252:PCI:O1	1.80	0.97
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.44	0.97
1:A:42:GLN:O	1:A:53:ILE:CG1	2.11	0.97
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.98	0.97
1:A:583:PHE:HE2	1:A:588:GLY:N	1.58	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:CE2	8:B:2031:HOH:O	2.17	0.97
1:A:170:VAL:O	1:A:175:ALA:HB2	1.62	0.97
2:B:192:VAL:HG21	8:B:2020:HOH:O	1.66	0.96
3:C:171:TRP:O	3:C:171:TRP:CD2	2.19	0.96
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.27	0.96
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.45	0.96
3:C:155:THR:HG22	3:C:239:ARG:HE	1.30	0.95
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.48	0.95
2:B:160:GLU:H	2:B:179:ASN:HD21	1.14	0.95
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.91	0.95
1:E:764:ARG:N	8:E:2446:HOH:O	1.99	0.95
1:A:585:THR:O	1:A:586:ALA:HB3	1.67	0.94
3:G:111:SER:HB3	8:G:2034:HOH:O	1.65	0.94
1:A:116:THR:HG22	1:A:119:GLU:H	1.25	0.94
1:E:590:ILE:HG13	8:E:2182:HOH:O	1.67	0.94
3:G:206:GLY:O	3:G:209:TYR:N	2.00	0.94
1:A:360:PRO:HD3	1:A:571:TRP:CE3	2.02	0.94
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.98	0.94
1:E:428:GLU:O	1:E:430:TYR:N	2.01	0.93
1:E:112:TYR:OH	1:E:474:MET:O	1.86	0.93
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.98	0.93
1:A:531:LEU:O	1:A:534:TYR:O	1.86	0.93
2:F:46:TYR:HB3	8:F:2035:HOH:O	1.67	0.93
1:A:345:MET:HE2	1:A:605:LEU:HD22	1.48	0.93
1:A:599:GLU:O	8:A:2283:HOH:O	1.87	0.92
1:E:349:TYR:OH	1:E:591:GLU:HA	1.69	0.92
1:A:580:ARG:CB	1:A:580:ARG:HH11	1.83	0.92
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.48	0.92
1:E:551:LEU:O	1:E:553:LEU:N	2.01	0.92
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.83	0.92
1:A:680:VAL:HG11	8:A:2313:HOH:O	1.69	0.92
2:B:46:TYR:CB	8:B:2032:HOH:O	2.00	0.92
1:E:533:GLN:H	1:E:533:GLN:HE21	1.16	0.92
1:A:434:GLY:HA2	1:A:461:LEU:O	1.70	0.91
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.52	0.91
1:A:335:VAL:CG1	1:A:732:ALA:O	2.19	0.91
1:A:608:PHE:O	1:A:608:PHE:CD1	2.23	0.91
1:A:729:SER:O	1:A:731:GLY:N	2.04	0.91
1:A:349:TYR:OH	1:A:591:GLU:O	1.89	0.91
2:B:72:THR:HG22	2:B:74:ALA:H	1.33	0.91
3:C:207:GLY:O	3:C:210:TYR:N	2.03	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ARG:HB2	8:A:2381:HOH:O	1.70	0.90
2:B:25:MET:HA	2:B:25:MET:HE2	1.52	0.90
1:E:92:PRO:O	1:E:94:ARG:N	2.04	0.90
1:E:604:PRO:O	1:E:606:PRO:HD3	1.71	0.90
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.07	0.90
1:A:116:THR:CG2	1:A:119:GLU:H	1.83	0.90
1:A:186:GLY:HA3	1:A:584:GLY:N	1.87	0.90
1:E:116:THR:HG23	1:E:119:GLU:H	1.36	0.90
1:E:297:THR:HG22	1:E:300:TRP:H	1.37	0.90
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.85	0.90
1:A:604:PRO:C	1:A:606:PRO:CD	2.46	0.89
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.06	0.89
1:A:397:GLU:HB3	1:A:398:PRO:CD	2.03	0.89
1:E:635:GLN:O	1:E:641:MET:CG	2.20	0.89
1:E:569:LYS:HD2	8:E:2322:HOH:O	1.70	0.89
1:E:635:GLN:O	1:E:641:MET:HG3	1.73	0.89
1:A:314:GLU:O	1:A:318:GLU:HG3	1.72	0.88
2:B:146:GLU:HG2	8:B:2110:HOH:O	1.73	0.88
1:E:95:LEU:CD1	1:E:466:ASP:O	2.20	0.88
2:F:160:GLU:H	2:F:179:ASN:HD21	1.19	0.88
3:G:154:THR:HG22	3:G:238:ARG:HE	1.36	0.88
1:A:607:VAL:HG12	1:A:607:VAL:O	1.73	0.88
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.55	0.88
1:E:209:HIS:HE1	1:E:625:ARG:H	1.21	0.88
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.04	0.88
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.89	0.87
3:C:140:ASN:H	3:C:140:ASN:HD22	1.22	0.87
1:E:606:PRO:O	1:E:608:PHE:N	2.06	0.87
1:E:493:VAL:HG13	8:E:2014:HOH:O	1.74	0.87
1:A:276:LYS:HA	8:A:2152:HOH:O	1.74	0.87
2:B:16:CYS:O	2:B:16:CYS:SG	2.32	0.87
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.88	0.87
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.75	0.87
3:C:128:LEU:HB3	8:C:2063:HOH:O	1.73	0.87
2:B:159:ALA:O	2:F:183:LYS:HE2	1.74	0.86
1:E:428:GLU:O	1:E:429:PRO:C	2.13	0.86
3:C:108:LEU:O	3:C:110:LYS:HG2	1.74	0.86
1:E:324:PRO:HD3	8:E:2170:HOH:O	1.73	0.86
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.38	0.86
1:E:562:GLY:C	8:E:2316:HOH:O	2.06	0.86
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.15	0.86
3:C:168:LYS:HE2	8:C:2065:HOH:O	1.74	0.86
1:E:605:LEU:N	1:E:605:LEU:HD22	1.90	0.86
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.90	0.85
3:G:139:ASN:H	3:G:139:ASN:HD22	1.24	0.85
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.58	0.85
1:A:335:VAL:O	1:A:733:GLY:HA2	1.75	0.85
1:E:614:PRO:HG2	8:E:2343:HOH:O	1.75	0.85
3:G:206:GLY:O	3:G:210:GLY:N	2.08	0.85
1:A:335:VAL:HG11	1:A:732:ALA:O	1.74	0.85
1:E:590:ILE:CG1	8:E:2182:HOH:O	2.23	0.85
1:A:604:PRO:C	1:A:606:PRO:HD3	2.01	0.85
1:E:323:LYS:CD	1:E:354:LEU:HA	1.98	0.85
1:E:301:ALA:O	1:E:305:THR:HB	1.77	0.85
2:B:25:MET:HA	2:B:25:MET:CE	2.07	0.84
1:E:608:PHE:O	1:E:608:PHE:CD1	2.30	0.84
1:E:608:PHE:CD1	1:E:608:PHE:C	2.55	0.84
1:A:400:GLY:HA3	8:A:2196:HOH:O	1.77	0.84
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.12	0.84
2:F:47:PRO:HD2	8:F:2035:HOH:O	1.75	0.84
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.16	0.84
1:A:601:GLY:N	8:A:2284:HOH:O	1.94	0.84
1:A:653:LYS:HG3	1:A:684:PRO:O	1.78	0.84
3:G:196:GLU:HG2	8:G:2056:HOH:O	1.76	0.84
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.08	0.84
2:B:117:THR:HG21	8:B:2095:HOH:O	1.78	0.84
1:A:42:GLN:NE2	1:A:485:TYR:O	2.11	0.83
1:E:498:LYS:HE2	8:E:2297:HOH:O	1.78	0.83
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.50	0.83
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.96	0.83
2:B:46:TYR:HD1	8:B:2032:HOH:O	1.50	0.83
1:E:305:THR:HG22	1:E:307:ILE:H	1.43	0.83
1:E:388:CYS:SG	1:E:413:ARG:NE	2.51	0.83
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.11	0.83
1:E:510:GLU:HG3	8:E:2301:HOH:O	1.77	0.83
2:F:146:GLU:HG2	8:F:2004:HOH:O	1.77	0.83
1:A:256:THR:HG21	1:A:305:THR:HA	1.61	0.83
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.93	0.83
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.79	0.82
3:C:53:ALA:O	3:C:57:ILE:HG13	1.78	0.82
2:F:72:THR:HG22	2:F:74:ALA:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.43	0.82
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.13	0.82
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.11	0.82
1:E:116:THR:HG22	1:E:119:GLU:CB	2.09	0.82
1:A:186:GLY:CA	1:A:583:PHE:O	2.28	0.82
2:B:46:TYR:HE2	8:B:2031:HOH:O	1.57	0.82
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.62	0.81
1:E:305:THR:CG2	1:E:307:ILE:H	1.93	0.81
1:E:685:THR:HG22	2:F:42:GLU:CD	2.04	0.81
1:A:591:GLU:O	1:A:592:LEU:HD12	1.80	0.81
1:E:283:THR:HG22	8:E:2181:HOH:O	1.78	0.81
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.46	0.81
1:E:81:ARG:HG2	1:E:628:VAL:O	1.80	0.81
1:A:429:PRO:O	1:A:430:TYR:CD2	2.33	0.81
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.35	0.81
1:A:740:ARG:NH1	8:A:2361:HOH:O	2.12	0.81
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.44	0.80
1:A:629:HIS:HA	1:A:634:THR:HG21	1.63	0.80
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.97	0.80
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.70	0.80
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.44	0.80
1:E:109:GLU:HG3	8:E:2066:HOH:O	1.80	0.80
1:E:89:THR:OG1	1:E:484:THR:HG21	1.82	0.80
1:A:413:ARG:H	1:A:413:ARG:CD	1.95	0.80
1:E:308:PRO:HB2	8:E:2198:HOH:O	1.82	0.80
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.62	0.80
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.03	0.80
1:A:686:ALA:HB3	8:A:2332:HOH:O	1.81	0.80
1:A:647:ASN:C	1:A:648:GLU:HG3	2.07	0.79
1:E:256:THR:HG21	1:E:305:THR:HA	1.62	0.79
3:C:64:LEU:HD22	7:C:1252:PCI:C4	2.12	0.79
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.64	0.79
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.97	0.79
8:B:2146:HOH:O	3:C:251:LEU:HD11	1.81	0.79
3:C:155:THR:CG2	3:C:239:ARG:HE	1.95	0.79
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.82	0.79
1:E:95:LEU:HD21	8:E:2278:HOH:O	1.82	0.79
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.42	0.79
1:A:70:ALA:O	8:A:2037:HOH:O	1.98	0.79
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.65	0.79
1:A:585:THR:O	1:A:586:ALA:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLY:H	1:A:595:GLN:HE22	1.31	0.79
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.45	0.78
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
3:G:206:GLY:O	3:G:207:PHE:C	2.26	0.78
1:E:469:PRO:O	1:E:706:MET:HG3	1.83	0.78
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.10	0.78
1:A:605:LEU:CD2	1:A:605:LEU:H	1.97	0.78
3:C:207:GLY:O	3:C:209:TRP:N	2.16	0.78
1:A:336:TRP:H	1:A:336:TRP:CD1	2.02	0.78
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.32	0.78
1:A:605:LEU:H	1:A:605:LEU:HD23	1.48	0.78
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.84	0.77
3:C:241:LEU:C	3:C:241:LEU:HD12	2.08	0.77
1:E:438:TYR:HD2	8:E:2094:HOH:O	1.66	0.77
3:G:111:SER:O	3:G:115:LEU:HD12	1.84	0.77
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.83	0.77
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.14	0.77
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.29	0.77
1:E:539:THR:HG23	1:E:542:GLU:H	1.49	0.77
2:B:160:GLU:H	2:B:179:ASN:ND2	1.81	0.77
1:E:109:GLU:CG	8:E:2066:HOH:O	2.31	0.77
1:E:277:GLU:O	1:E:281:LYS:HG2	1.84	0.77
2:F:1:MET:HA	8:F:2001:HOH:O	1.85	0.77
1:A:320:ALA:O	1:A:323:LYS:HG2	1.85	0.77
3:C:173:LEU:HG	3:C:173:LEU:O	1.84	0.77
1:E:311:VAL:HB	8:E:2198:HOH:O	1.84	0.77
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.67	0.76
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.20	0.76
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.98	0.76
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.49	0.76
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.66	0.76
1:E:95:LEU:HD11	8:E:2278:HOH:O	1.84	0.76
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.83	0.76
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.49	0.76
1:E:604:PRO:O	1:E:606:PRO:CD	2.33	0.76
1:A:677:GLU:O	1:A:678:GLY:O	2.03	0.76
3:C:155:THR:HG21	3:C:239:ARG:CG	2.16	0.76
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.16	0.76
1:E:297:THR:HG23	1:E:299:GLU:H	1.49	0.76
1:A:457:LYS:HA	8:A:2224:HOH:O	1.85	0.76
1:A:672:GLN:NE2	1:A:738:PHE:H	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:O	1:A:429:PRO:C	2.26	0.76
1:A:209:HIS:HE1	1:A:625:ARG:H	1.34	0.75
3:C:235:ALA:O	3:C:239:ARG:HG3	1.86	0.75
1:E:421:ILE:HG23	1:E:421:ILE:O	1.84	0.75
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.00	0.75
3:G:234:ALA:O	3:G:238:ARG:HG3	1.84	0.75
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.21	0.75
1:A:388:CYS:HA	1:A:593:TYR:OH	1.85	0.75
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.16	0.75
3:G:21:PHE:O	3:G:238:ARG:NH1	2.20	0.75
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.34	0.75
1:A:395:ASP:O	1:A:399:GLU:CB	2.28	0.75
3:C:64:LEU:HD22	7:C:1252:PCI:C3	2.16	0.75
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.68	0.75
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.22	0.74
3:C:140:ASN:H	3:C:140:ASN:ND2	1.80	0.74
2:F:117:THR:HG23	2:F:120:ALA:H	1.52	0.74
1:E:473:VAL:HG11	8:E:2278:HOH:O	1.87	0.74
1:E:671:ASN:C	1:E:671:ASN:HD22	1.95	0.74
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.67	0.74
1:A:232:VAL:H	1:A:247:HIS:HD2	1.32	0.74
1:A:170:VAL:O	1:A:175:ALA:CB	2.36	0.74
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.18	0.74
1:E:421:ILE:O	1:E:421:ILE:CG2	2.34	0.74
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.69	0.74
1:E:431:PRO:HD2	8:E:2262:HOH:O	1.88	0.74
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.84	0.74
1:E:477:ASP:C	1:E:478:VAL:HG23	2.13	0.74
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.88	0.74
1:A:604:PRO:C	1:A:606:PRO:HD2	2.10	0.73
2:B:16:CYS:O	2:B:18:ALA:N	2.19	0.73
1:E:297:THR:CG2	1:E:299:GLU:H	2.00	0.73
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.18	0.73
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.36	0.73
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.52	0.73
1:E:38:LYS:HG3	8:E:2021:HOH:O	1.88	0.73
3:G:107:LEU:O	3:G:109:LYS:N	2.20	0.73
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.71	0.73
1:A:395:ASP:C	1:A:399:GLU:HB2	2.13	0.73
1:A:285:GLY:O	1:A:590:ILE:HG23	1.88	0.73
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ARG:NH1	1:E:114:VAL:HG13	2.02	0.73
1:A:345:MET:HE2	1:A:605:LEU:CD2	2.19	0.73
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.18	0.73
1:E:605:LEU:H	1:E:605:LEU:HD23	0.57	0.73
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.71	0.73
1:A:390:GLY:N	1:A:595:GLN:HE22	1.87	0.73
2:B:6:MET:HE3	8:B:2045:HOH:O	1.88	0.73
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.69	0.73
3:G:139:ASN:H	3:G:139:ASN:ND2	1.87	0.73
1:A:427:GLY:O	1:A:428:GLU:O	2.05	0.73
1:A:629:HIS:CA	1:A:634:THR:HG21	2.19	0.72
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.68	0.72
3:G:63:LEU:HD13	7:G:1251:PCI:CL5	2.26	0.72
1:A:595:GLN:CG	1:A:595:GLN:O	2.37	0.72
1:A:519:TRP:NE1	1:A:540:ILE:HG12	2.03	0.72
3:C:145:ASN:C	3:C:145:ASN:HD22	1.95	0.72
3:C:171:TRP:O	3:C:172:ALA:HB2	1.89	0.72
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.70	0.72
1:A:510:GLU:HG3	8:A:2024:HOH:O	1.90	0.72
1:E:539:THR:HG22	1:E:542:GLU:CB	2.20	0.72
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.38	0.72
2:B:190:SER:HB3	3:C:252:GLY:N	2.03	0.72
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.70	0.72
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.70	0.72
1:A:467:VAL:HG13	8:A:2050:HOH:O	1.90	0.72
1:E:91:ASP:O	1:E:92:PRO:O	2.08	0.72
1:E:635:GLN:NE2	1:E:635:GLN:H	1.88	0.72
1:A:393:GLY:HA3	1:A:407:LYS:NZ	2.04	0.72
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.19	0.71
1:E:69:GLU:O	1:E:70:ALA:HB3	1.88	0.71
3:G:76:ILE:O	3:G:80:LEU:HG	1.90	0.71
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.71	0.71
1:A:653:LYS:HD2	1:A:686:ALA:H	1.53	0.71
1:E:116:THR:HG21	8:E:2072:HOH:O	1.90	0.71
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.72	0.71
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.21	0.71
1:A:608:PHE:CD1	1:A:608:PHE:C	2.64	0.71
3:C:108:LEU:O	3:C:110:LYS:CG	2.39	0.71
1:A:209:HIS:O	1:A:213:ASP:HB3	1.89	0.71
3:C:101:LEU:O	3:C:105:LEU:HD12	1.90	0.71
1:A:301:ALA:O	1:A:305:THR:HB	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:GLU:HB2	8:F:2021:HOH:O	1.91	0.71
1:A:605:LEU:HD23	1:A:605:LEU:N	2.06	0.71
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.56	0.71
1:E:232:VAL:H	1:E:247:HIS:CD2	2.09	0.71
1:A:595:GLN:O	1:A:595:GLN:HG3	1.89	0.70
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.73	0.70
1:E:209:HIS:HE1	1:E:625:ARG:N	1.89	0.70
1:E:478:VAL:HG23	8:E:2283:HOH:O	1.90	0.70
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.55	0.70
1:A:284:VAL:O	1:A:590:ILE:CG2	2.35	0.70
2:B:47:PRO:O	2:B:48:ASN:OD1	2.10	0.70
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.05	0.70
3:C:197:GLU:HG2	8:C:2074:HOH:O	1.89	0.70
1:E:232:VAL:H	1:E:247:HIS:HD2	1.40	0.70
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.06	0.70
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.72	0.70
1:A:382:GLU:HA	8:A:2188:HOH:O	1.90	0.70
1:A:729:SER:O	1:A:729:SER:OG	2.01	0.70
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.40	0.70
1:A:611:PRO:HB3	8:A:2139:HOH:O	1.90	0.70
1:E:465:ILE:O	1:E:466:ASP:HB3	1.90	0.70
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.30	0.70
1:A:592:LEU:O	1:A:593:TYR:CB	2.37	0.70
1:E:762:GLU:HB2	8:E:2445:HOH:O	1.90	0.70
1:A:89:THR:OG1	1:A:484:THR:HG21	1.92	0.69
1:A:367:GLN:HG3	8:A:2271:HOH:O	1.92	0.69
1:A:561:MET:O	1:A:563:THR:N	2.24	0.69
2:B:47:PRO:HD3	8:B:2034:HOH:O	1.92	0.69
1:E:69:GLU:O	1:E:70:ALA:CB	2.40	0.69
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.40	0.69
1:E:139:ALA:O	1:E:433:LYS:O	2.10	0.69
2:F:169:GLN:NE2	8:F:2107:HOH:O	2.25	0.69
1:A:152:PHE:O	1:A:157:PRO:HD3	1.91	0.69
1:A:632:ALA:O	1:A:635:GLN:HG3	1.92	0.69
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.92	0.69
1:E:118:GLU:HG3	8:E:2307:HOH:O	1.93	0.69
1:E:259:ALA:HB3	8:E:2196:HOH:O	1.92	0.69
1:E:577:LYS:HE2	8:E:2323:HOH:O	1.92	0.69
1:E:734:LEU:HD22	8:E:2419:HOH:O	1.91	0.69
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.58	0.69
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:ARG:HG2	8:F:2003:HOH:O	1.92	0.69
3:G:63:LEU:HD22	7:G:1251:PCI:C6	2.23	0.69
1:A:186:GLY:H	1:A:583:PHE:HA	1.58	0.69
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.28	0.69
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.92	0.69
1:E:438:TYR:CD2	8:E:2094:HOH:O	2.44	0.69
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.75	0.69
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.27	0.69
1:A:36:GLU:O	1:A:58:VAL:HG22	1.93	0.69
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.75	0.69
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.07	0.69
1:E:591:GLU:O	1:E:591:GLU:HG3	1.92	0.69
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.92	0.69
2:F:117:THR:HG21	8:F:2077:HOH:O	1.91	0.69
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.74	0.68
3:G:51:TYR:N	8:G:2015:HOH:O	2.26	0.68
1:A:483:ALA:HA	1:A:515:THR:CG2	2.23	0.68
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.59	0.68
2:B:46:TYR:CE2	8:B:2033:HOH:O	2.46	0.68
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.75	0.68
1:A:95:LEU:HD12	1:A:467:VAL:C	2.18	0.68
1:A:116:THR:HG22	1:A:119:GLU:N	2.06	0.68
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.76	0.68
1:E:71:ASN:HD22	1:E:74:SER:H	1.40	0.68
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.57	0.68
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.71	0.68
1:A:429:PRO:O	1:A:430:TYR:CG	2.46	0.68
3:G:115:LEU:HD13	8:G:2032:HOH:O	1.93	0.68
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.29	0.68
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.24	0.68
1:A:606:PRO:O	1:A:608:PHE:N	2.26	0.68
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.22	0.68
1:E:708:LEU:HA	8:E:2408:HOH:O	1.93	0.68
1:A:232:VAL:H	1:A:247:HIS:CD2	2.11	0.68
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.76	0.68
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.76	0.68
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.93	0.68
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.24	0.68
1:A:349:TYR:CE2	1:A:590:ILE:O	2.47	0.68
8:A:2015:HOH:O	2:B:25:MET:HE1	1.93	0.68
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.91	0.67
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.23	0.67
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.76	0.67
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.75	0.67
1:E:434:GLY:HA2	1:E:461:LEU:O	1.93	0.67
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.29	0.67
2:B:72:THR:HG21	2:B:89:LYS:O	1.94	0.67
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.77	0.67
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.54	0.67
2:F:72:THR:HG21	2:F:89:LYS:O	1.93	0.67
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.76	0.67
2:F:47:PRO:CD	8:F:2035:HOH:O	2.37	0.67
2:F:160:GLU:H	2:F:179:ASN:ND2	1.93	0.67
3:G:225:LEU:HB3	8:G:2068:HOH:O	1.93	0.67
1:A:305:THR:HG22	1:A:307:ILE:H	1.60	0.67
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.28	0.67
1:E:346:ALA:N	1:E:605:LEU:HD12	2.10	0.67
2:F:43:VAL:HG23	8:F:2121:HOH:O	1.95	0.67
1:A:293:VAL:HG13	1:A:293:VAL:O	1.94	0.66
1:A:400:GLY:CA	8:A:2196:HOH:O	2.37	0.66
1:E:465:ILE:O	1:E:466:ASP:CB	2.43	0.66
1:E:575:TRP:O	1:E:578:GLU:HB2	1.94	0.66
1:A:338:GLY:O	1:A:726:ASP:HA	1.95	0.66
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.77	0.66
1:E:253:LYS:O	1:E:256:THR:HB	1.94	0.66
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.43	0.66
1:A:330:PRO:HD2	8:A:2168:HOH:O	1.94	0.66
1:A:336:TRP:H	1:A:336:TRP:HD1	1.43	0.66
1:A:413:ARG:H	1:A:413:ARG:HD2	1.59	0.66
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.25	0.66
1:A:335:VAL:HG13	1:A:732:ALA:C	2.20	0.66
2:B:46:TYR:O	8:B:2029:HOH:O	2.14	0.66
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.61	0.66
1:E:589:LYS:NZ	8:E:2326:HOH:O	2.27	0.66
1:A:685:THR:HB	2:B:42:GLU:CD	2.20	0.66
1:E:311:VAL:CB	8:E:2198:HOH:O	2.42	0.66
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.76	0.66
1:E:642:GLU:OE2	2:F:32:GLY:N	2.24	0.66
3:G:207:PHE:HE2	3:G:211:LEU:CD1	2.00	0.66
1:A:37:VAL:HG12	1:A:38:LYS:N	2.10	0.66
1:A:195:ILE:HA	1:A:362:GLY:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:HIS:O	2:B:125:LYS:HE2	1.96	0.66
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.61	0.66
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.20	0.66
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.94	0.66
1:E:424:MET:HE2	1:E:455:ALA:CB	2.24	0.66
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.78	0.66
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.77	0.66
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.78	0.66
1:E:551:LEU:O	1:E:553:LEU:HB2	1.96	0.66
1:A:305:THR:O	1:A:306:GLU:HB2	1.95	0.66
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.76	0.66
1:E:686:ALA:HB1	8:E:2386:HOH:O	1.95	0.66
1:A:71:ASN:HD22	1:A:74:SER:H	1.41	0.65
1:A:134:LYS:HE2	8:A:2079:HOH:O	1.95	0.65
1:A:642:GLU:OE2	2:B:31:PRO:O	2.14	0.65
3:C:222:TRP:CG	3:C:223:GLN:N	2.59	0.65
3:C:241:LEU:C	3:C:241:LEU:CD1	2.68	0.65
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.92	0.65
1:E:470:GLN:HG2	1:E:706:MET:SD	2.36	0.65
1:E:632:ALA:O	1:E:635:GLN:NE2	2.29	0.65
3:G:63:LEU:CD1	7:G:1251:PCI:CL5	2.81	0.65
1:E:391:PRO:O	1:E:413:ARG:HG2	1.96	0.65
1:E:490:ASP:O	8:E:2290:HOH:O	2.14	0.65
1:E:608:PHE:C	8:E:2337:HOH:O	2.30	0.65
1:E:720:GLN:HB3	8:E:2419:HOH:O	1.96	0.65
1:A:95:LEU:HD11	1:A:468:LEU:O	1.95	0.65
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.23	0.65
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.27	0.65
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.78	0.65
2:F:78:THR:HG21	8:F:2059:HOH:O	1.96	0.65
2:B:44:GLY:O	2:B:49:LEU:HD13	1.97	0.65
2:F:117:THR:HG22	2:F:119:CYS:H	1.60	0.65
1:A:139:ALA:O	1:A:433:LYS:O	2.14	0.65
1:A:672:GLN:HE22	1:A:738:PHE:H	1.42	0.65
2:B:78:THR:HG21	8:B:2068:HOH:O	1.97	0.65
2:F:88:LYS:O	3:G:74:THR:HG22	1.96	0.65
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.78	0.64
2:F:45:GLU:HB2	8:F:2028:HOH:O	1.96	0.64
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.28	0.64
1:A:495:VAL:HG13	8:A:2020:HOH:O	1.96	0.64
1:A:755:LEU:O	1:A:758:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.78	0.64
3:G:63:LEU:HD22	7:G:1251:PCI:C5	2.27	0.64
1:A:127:LYS:HE2	8:A:2228:HOH:O	1.98	0.64
1:A:152:PHE:O	1:A:157:PRO:CD	2.46	0.64
3:G:150:LEU:O	3:G:154:THR:HB	1.98	0.64
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.58	0.64
2:F:78:THR:HG22	2:F:80:ASP:H	1.61	0.64
3:G:196:GLU:CD	3:G:196:GLU:H	2.04	0.64
1:A:387:GLY:O	1:A:593:TYR:CE1	2.51	0.64
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.26	0.64
1:E:539:THR:CG2	1:E:542:GLU:H	2.10	0.64
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.63	0.64
1:A:647:ASN:H	1:A:647:ASN:HD22	1.45	0.64
2:B:142:PHE:C	2:B:152:VAL:HG22	2.22	0.64
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.97	0.64
2:B:44:GLY:O	2:B:49:LEU:CD1	2.45	0.64
2:B:134:THR:O	2:B:134:THR:HG22	1.92	0.64
1:E:591:GLU:CD	1:E:604:PRO:CB	2.61	0.64
3:G:206:GLY:O	3:G:209:TYR:CA	2.45	0.64
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.80	0.64
1:A:604:PRO:O	1:A:606:PRO:HD3	1.92	0.64
1:E:267:VAL:HG22	8:E:2200:HOH:O	1.97	0.64
1:E:588:GLY:HA3	8:E:2178:HOH:O	1.97	0.64
1:A:391:PRO:O	1:A:413:ARG:HB3	1.98	0.63
1:A:561:MET:HE1	1:A:564:LEU:HD12	1.79	0.63
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.12	0.63
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.81	0.63
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.32	0.63
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.31	0.63
1:E:597:PHE:HB3	8:E:2327:HOH:O	1.97	0.63
3:C:222:TRP:CG	3:C:223:GLN:H	2.15	0.63
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.28	0.63
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.81	0.63
8:E:2386:HOH:O	2:F:49:LEU:HD11	1.99	0.63
1:A:99:LEU:O	1:A:478:VAL:HA	1.99	0.63
1:A:581:LEU:HD11	8:A:2274:HOH:O	1.98	0.63
1:A:583:PHE:CE2	1:A:587:SER:C	2.76	0.63
2:B:57:GLN:O	2:B:58:CYS:C	2.41	0.63
3:C:47:ARG:NH1	3:C:107:TYR:O	2.31	0.63
2:B:117:THR:HG22	2:B:119:CYS:N	2.13	0.63
3:C:207:GLY:O	3:C:208:PHE:C	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:CD	8:B:2034:HOH:O	2.46	0.63
1:E:282:TYR:O	1:E:587:SER:HB3	1.98	0.63
1:A:581:LEU:CD1	8:A:2274:HOH:O	2.46	0.63
1:A:635:GLN:O	1:A:709:ALA:HB2	1.98	0.63
3:C:197:GLU:CD	3:C:197:GLU:H	2.06	0.63
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.33	0.63
1:E:318:GLU:O	1:E:322:HIS:HD2	1.82	0.63
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.34	0.62
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.98	0.62
2:F:193:HIS:HB2	8:F:2129:HOH:O	1.98	0.62
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.63	0.62
1:A:314:GLU:HG2	8:A:2165:HOH:O	1.98	0.62
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.80	0.62
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.47	0.62
1:A:293:VAL:O	1:A:293:VAL:CG1	2.46	0.62
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.30	0.62
1:E:708:LEU:O	1:E:712:ARG:HD2	2.00	0.62
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.64	0.62
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.32	0.62
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.78	0.62
1:E:511:PRO:CB	1:E:515:THR:HG22	2.25	0.62
2:B:117:THR:HB	8:B:2010:HOH:O	1.99	0.62
1:E:474:MET:HE3	8:E:2069:HOH:O	1.99	0.62
1:E:672:GLN:NE2	1:E:738:PHE:H	1.97	0.62
1:E:740:ARG:NH1	8:E:2428:HOH:O	2.32	0.62
1:A:609:THR:O	1:A:610:PRO:C	2.43	0.62
1:A:428:GLU:O	1:A:430:TYR:N	2.33	0.62
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.82	0.62
1:E:418:GLN:H	1:E:418:GLN:NE2	1.97	0.62
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.65	0.62
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.80	0.62
2:B:192:VAL:HG12	2:B:193:HIS:N	2.15	0.61
1:E:297:THR:HG21	8:E:2087:HOH:O	2.00	0.61
1:E:604:PRO:C	1:E:606:PRO:HD3	2.25	0.61
1:E:639:VAL:HG21	2:F:25:MET:HE1	1.81	0.61
3:G:105:LEU:HG	8:G:2032:HOH:O	1.98	0.61
1:E:495:VAL:CG2	8:E:2299:HOH:O	2.48	0.61
1:E:569:LYS:CD	8:E:2322:HOH:O	2.38	0.61
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.30	0.61
3:G:206:GLY:C	3:G:209:TYR:H	2.07	0.61
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:105:LEU:HB3	8:G:2011:HOH:O	2.00	0.61
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.16	0.61
1:A:413:ARG:H	1:A:413:ARG:NE	1.97	0.61
1:A:653:LYS:CG	1:A:684:PRO:O	2.48	0.61
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.30	0.61
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.23	0.61
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.83	0.61
1:A:335:VAL:HG13	1:A:732:ALA:O	1.97	0.61
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.35	0.61
1:E:116:THR:HG22	1:E:119:GLU:H	1.56	0.61
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.83	0.61
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.83	0.61
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.83	0.61
1:E:606:PRO:CD	1:E:607:VAL:H	2.12	0.60
1:A:428:GLU:O	1:A:430:TYR:O	2.19	0.60
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.83	0.60
1:A:630:THR:H	1:A:634:THR:HG21	1.66	0.60
1:E:607:VAL:O	1:E:607:VAL:HG13	1.97	0.60
2:F:194:HIS:N	8:F:2128:HOH:O	2.33	0.60
1:A:594:CYS:O	1:A:598:LYS:HG3	2.01	0.60
1:E:647:ASN:HD21	1:E:714:ALA:H	1.48	0.60
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.16	0.60
3:C:171:TRP:O	3:C:172:ALA:CB	2.48	0.60
1:E:479:ILE:O	1:E:480:LEU:HD23	2.02	0.60
2:F:43:VAL:CG2	8:F:2121:HOH:O	2.50	0.60
1:A:631:PHE:O	1:A:698:GLY:HA3	2.01	0.60
1:A:658:ARG:C	1:A:659:LEU:O	2.37	0.60
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.20	0.60
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.36	0.60
1:E:108:GLY:HA3	8:E:2064:HOH:O	2.01	0.60
1:A:186:GLY:C	1:A:583:PHE:O	2.44	0.60
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.84	0.60
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.54	0.60
1:A:109:GLU:OE2	1:A:111:LYS:HE2	2.01	0.60
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.83	0.60
1:A:120:ALA:HB3	8:A:2068:HOH:O	2.01	0.60
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.37	0.60
1:A:204:VAL:HB	1:A:328:LEU:HG	1.84	0.59
1:A:319:MET:CE	1:A:328:LEU:HD11	2.31	0.59
1:A:427:GLY:O	1:A:430:TYR:O	2.19	0.59
1:A:382:GLU:HB3	8:A:2189:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:648:GLU:OE2	2.20	0.59
2:B:88:LYS:O	3:C:75:THR:HG22	2.01	0.59
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.84	0.59
2:B:117:THR:CG2	2:B:120:ALA:H	2.15	0.59
3:C:155:THR:CG2	3:C:239:ARG:NE	2.65	0.59
1:A:256:THR:CG2	1:A:305:THR:HA	2.30	0.59
1:A:582:PRO:C	8:A:2097:HOH:O	2.44	0.59
2:B:3:ARG:HG2	8:B:2001:HOH:O	2.02	0.59
1:E:551:LEU:O	1:E:552:GLY:C	2.46	0.59
1:A:42:GLN:O	1:A:53:ILE:HG12	2.02	0.59
1:A:534:TYR:O	1:A:535:PHE:HB2	2.02	0.59
1:A:558:MET:HE2	1:A:558:MET:HA	1.83	0.59
1:A:607:VAL:O	1:A:607:VAL:CG1	2.46	0.59
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.98	0.59
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.32	0.59
1:E:642:GLU:HG3	8:E:2436:HOH:O	2.02	0.59
1:E:591:GLU:O	1:E:603:GLN:NE2	2.36	0.59
1:E:658:ARG:C	1:E:659:LEU:O	2.35	0.59
1:A:710:HIS:O	8:A:2346:HOH:O	2.17	0.59
1:E:209:HIS:CE1	1:E:625:ARG:H	2.12	0.59
1:E:418:GLN:H	1:E:418:GLN:HE21	1.49	0.59
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.27	0.59
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.32	0.59
2:B:166:ARG:HH22	3:C:249:GLN:NE2	2.00	0.59
1:E:81:ARG:HE	1:E:214:THR:HG22	1.67	0.59
3:G:189:TYR:O	3:G:192:THR:HB	2.03	0.59
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.84	0.58
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.50	0.58
8:B:2028:HOH:O	3:C:2:ALA:HB1	2.02	0.58
1:A:540:ILE:O	1:A:544:LEU:HG	2.03	0.58
1:A:558:MET:CE	1:A:561:MET:SD	2.91	0.58
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.38	0.58
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.85	0.58
1:A:107:ARG:HG2	1:A:475:TRP:O	2.02	0.58
1:A:277:GLU:HB3	1:A:281:LYS:HZ3	1.68	0.58
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.51	0.58
1:E:671:ASN:ND2	1:E:673:ASP:H	2.01	0.58
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.51	0.58
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.84	0.58
2:B:36:LEU:HD11	8:B:2104:HOH:O	2.03	0.58
1:E:647:ASN:H	1:E:647:ASN:HD22	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HB2	8:A:2005:HOH:O	2.03	0.58
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.84	0.58
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.86	0.58
1:E:483:ALA:N	1:E:516:LYS:O	2.25	0.58
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.28	0.58
1:A:37:VAL:HG13	1:A:57:ALA:O	2.04	0.58
1:A:471:GLU:O	1:A:471:GLU:HG2	2.04	0.58
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.85	0.58
1:A:345:MET:HE3	1:A:592:LEU:CD1	2.33	0.58
3:C:207:GLY:C	3:C:209:TRP:N	2.61	0.58
1:A:426:THR:HG23	8:A:2052:HOH:O	2.03	0.58
1:A:483:ALA:HA	1:A:515:THR:HG21	1.86	0.57
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.16	0.57
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.99	0.57
3:C:128:LEU:HD22	8:C:2063:HOH:O	2.04	0.57
3:C:171:TRP:O	3:C:171:TRP:CG	2.57	0.57
1:E:204:VAL:HG21	1:E:319:MET:HE2	1.85	0.57
1:E:204:VAL:HB	1:E:328:LEU:HG	1.86	0.57
1:E:386:GLY:O	1:E:388:CYS:SG	2.48	0.57
1:E:549:GLN:HG3	8:E:2313:HOH:O	2.04	0.57
3:C:239:ARG:NH2	8:C:2084:HOH:O	2.35	0.57
1:E:77:ARG:NE	8:E:2046:HOH:O	2.37	0.57
1:E:129:LEU:O	1:E:133:GLU:HG2	2.03	0.57
1:E:279:VAL:O	1:E:283:THR:HB	2.03	0.57
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.86	0.57
3:G:115:LEU:HB3	8:G:2032:HOH:O	2.04	0.57
3:C:140:ASN:HD22	3:C:140:ASN:N	1.99	0.57
1:E:116:THR:CG2	1:E:119:GLU:N	2.57	0.57
1:E:686:ALA:CB	8:E:2386:HOH:O	2.52	0.57
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.37	0.57
1:A:427:GLY:C	1:A:428:GLU:O	2.48	0.57
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.87	0.57
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.86	0.57
1:E:590:ILE:HB	8:E:2182:HOH:O	2.04	0.57
3:G:220:PHE:HD1	8:G:2064:HOH:O	1.87	0.57
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.51	0.57
3:C:17:THR:CG2	3:C:67:GLU:CG	2.75	0.57
3:C:89:ILE:HD12	7:C:1252:PCI:C6	2.34	0.57
1:E:311:VAL:CG2	8:E:2198:HOH:O	2.52	0.57
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.87	0.57
1:A:558:MET:HE2	1:A:561:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.87	0.57
3:C:112:SER:O	3:C:113:GLN:HG2	2.05	0.57
1:E:724:LYS:HG2	8:E:2424:HOH:O	2.04	0.57
1:A:379:LEU:O	1:A:380:PRO:C	2.48	0.57
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.04	0.57
1:A:636:ASN:HB2	1:A:706:MET:HE2	1.87	0.57
1:E:590:ILE:O	1:E:592:LEU:HG	2.05	0.57
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.55	0.57
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.53	0.56
3:G:207:PHE:C	3:G:207:PHE:CD2	2.82	0.56
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.40	0.56
1:E:320:ALA:O	1:E:323:LYS:HB2	2.05	0.56
3:G:240:LEU:C	3:G:240:LEU:HD12	2.30	0.56
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.37	0.56
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.14	0.56
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.41	0.56
1:A:678:GLY:HA3	8:A:2330:HOH:O	2.05	0.56
2:B:57:GLN:NE2	8:B:2045:HOH:O	2.38	0.56
1:A:81:ARG:HE	1:A:214:THR:HG22	1.69	0.56
1:E:632:ALA:C	1:E:635:GLN:NE2	2.63	0.56
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.86	0.56
1:A:384:ALA:N	8:A:2190:HOH:O	2.30	0.56
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.40	0.56
1:E:186:GLY:HA3	1:E:584:GLY:N	2.21	0.56
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.87	0.56
1:A:367:GLN:O	1:A:500:PRO:HG3	2.05	0.56
1:E:396:HIS:CE1	1:E:404:ARG:H	2.24	0.56
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.88	0.56
3:G:49:THR:HG21	8:G:2011:HOH:O	2.04	0.56
2:B:114:SER:O	2:B:115:LYS:HB3	2.06	0.56
1:E:91:ASP:C	1:E:92:PRO:O	2.49	0.56
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.88	0.56
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.88	0.56
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.88	0.56
1:E:470:GLN:NE2	8:E:2279:HOH:O	2.39	0.56
1:E:109:GLU:HG2	8:E:2066:HOH:O	2.01	0.55
1:A:630:THR:N	1:A:634:THR:HG21	2.22	0.55
1:E:474:MET:HE2	1:E:705:LEU:CD1	2.36	0.55
2:B:121:HIS:O	2:B:125:LYS:CE	2.53	0.55
1:E:286:PHE:CB	8:E:2182:HOH:O	2.54	0.55
1:A:151:TRP:O	1:A:156:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.21	0.55
1:A:193:GLU:HG2	8:A:2120:HOH:O	2.07	0.55
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.36	0.55
1:A:295:ASP:HB2	8:A:2160:HOH:O	2.06	0.55
1:A:607:VAL:HG13	1:A:609:THR:CB	2.36	0.55
2:F:44:GLY:O	2:F:45:GLU:HB2	2.06	0.55
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.55	0.55
3:C:67:GLU:O	3:C:67:GLU:HG2	2.07	0.55
3:C:130:TYR:CZ	7:C:1252:PCI:O1	2.60	0.55
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.40	0.55
2:F:72:THR:HG22	2:F:74:ALA:N	2.17	0.55
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.37	0.55
1:A:428:GLU:OE2	1:A:428:GLU:HA	2.01	0.55
1:A:483:ALA:CA	1:A:515:THR:HG23	2.37	0.55
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.07	0.55
1:E:684:PRO:O	1:E:685:THR:C	2.48	0.55
1:E:208:HIS:HE1	1:E:218:GLN:NE2	2.04	0.55
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.90	0.55
1:E:607:VAL:HG23	8:E:2148:HOH:O	2.07	0.55
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.06	0.55
2:F:41:ARG:CD	2:F:187:THR:HG23	2.31	0.55
1:A:422:GLU:HB2	8:A:2206:HOH:O	2.06	0.55
1:E:346:ALA:H	1:E:605:LEU:HD12	1.71	0.55
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.89	0.55
3:G:207:PHE:O	3:G:211:LEU:N	2.40	0.55
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.89	0.54
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.14	0.54
1:A:285:GLY:C	1:A:590:ILE:HG23	2.32	0.54
1:A:467:VAL:CG2	8:A:2230:HOH:O	2.55	0.54
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.42	0.54
1:E:568:GLY:O	1:E:570:PRO:HD3	2.07	0.54
3:G:154:THR:HG22	3:G:238:ARG:NE	2.15	0.54
1:E:635:GLN:NE2	1:E:635:GLN:N	2.53	0.54
3:G:63:LEU:CD2	7:G:1251:PCI:C1	2.85	0.54
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.37	0.54
1:E:671:ASN:C	1:E:671:ASN:ND2	2.64	0.54
1:A:358:GLY:O	1:A:571:TRP:HA	2.07	0.54
1:A:421:ILE:HG22	1:A:421:ILE:O	2.06	0.54
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.88	0.54
1:E:99:LEU:O	1:E:478:VAL:HA	2.08	0.54
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:MET:CB	1:E:605:LEU:HD13	2.37	0.54
1:E:359:ARG:HD3	8:E:2101:HOH:O	2.07	0.54
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.08	0.54
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.42	0.54
2:B:140:ARG:NH2	8:B:2045:HOH:O	2.40	0.54
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.43	0.54
1:A:336:TRP:O	1:A:735:ARG:HB2	2.07	0.54
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.90	0.54
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.90	0.54
1:E:81:ARG:HE	1:E:214:THR:CG2	2.20	0.54
3:G:70:ARG:HG2	3:G:71:PHE:H	1.72	0.54
2:B:192:VAL:HG12	2:B:193:HIS:H	1.72	0.54
1:A:73:LYS:HZ1	1:A:192:HIS:CD2	2.25	0.54
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.72	0.54
3:C:145:ASN:C	3:C:145:ASN:ND2	2.61	0.54
1:E:586:ALA:HB3	8:E:2326:HOH:O	2.07	0.54
3:G:66:GLU:O	3:G:66:GLU:HG2	2.08	0.54
1:A:118:GLU:H	1:A:118:GLU:CD	2.15	0.54
1:A:152:PHE:O	1:A:157:PRO:CG	2.56	0.54
1:E:286:PHE:C	1:E:288:GLU:H	2.14	0.54
1:E:497:HIS:O	1:E:498:LYS:C	2.50	0.54
3:G:222:GLN:C	8:G:2068:HOH:O	2.51	0.54
1:A:320:ALA:O	1:A:323:LYS:CG	2.55	0.54
1:E:81:ARG:NE	1:E:214:THR:HG22	2.22	0.54
1:E:391:PRO:HG2	1:E:392:SER:H	1.72	0.54
1:A:36:GLU:O	1:A:36:GLU:HG2	2.08	0.53
1:A:429:PRO:C	1:A:430:TYR:CD2	2.85	0.53
2:B:72:THR:CG2	2:B:74:ALA:H	2.14	0.53
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.38	0.53
1:A:415:THR:HG22	8:A:2204:HOH:O	2.09	0.53
1:E:273:LEU:O	1:E:323:LYS:NZ	2.32	0.53
2:B:117:THR:HG22	2:B:119:CYS:H	1.74	0.53
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.89	0.53
3:G:221:TRP:HD1	8:G:2033:HOH:O	1.91	0.53
1:A:536:PRO:HG2	1:A:537:TRP:H	1.74	0.53
1:A:583:PHE:CZ	1:A:587:SER:HA	2.44	0.53
1:A:635:GLN:C	1:A:709:ALA:HB2	2.33	0.53
1:E:186:GLY:H	1:E:583:PHE:HA	1.73	0.53
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.91	0.53
1:A:525:LEU:O	1:A:529:LEU:HG	2.08	0.53
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:H	1:E:423:PRO:HD2	1.73	0.53
1:E:635:GLN:O	1:E:641:MET:HG2	2.04	0.53
1:A:535:PHE:N	1:A:536:PRO:CD	2.71	0.53
1:A:388:CYS:O	1:A:391:PRO:HD3	2.09	0.53
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.37	0.53
2:F:46:TYR:CD1	2:F:46:TYR:C	2.85	0.53
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.57	0.53
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.18	0.53
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.08	0.53
1:E:37:VAL:HA	1:E:57:ALA:O	2.09	0.53
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.90	0.53
1:E:622:LEU:HD22	8:E:2426:HOH:O	2.08	0.53
1:A:134:LYS:CE	8:A:2079:HOH:O	2.54	0.53
1:A:457:LYS:HD3	8:A:2223:HOH:O	2.09	0.53
1:A:647:ASN:HD21	1:A:714:ALA:H	1.57	0.53
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.41	0.53
1:A:468:LEU:HD13	1:A:706:MET:HE3	1.90	0.53
1:E:336:TRP:O	1:E:340:ASP:OD1	2.27	0.53
1:E:632:ALA:C	1:E:635:GLN:HE22	2.17	0.53
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.07	0.53
1:A:81:ARG:HE	1:A:214:THR:CG2	2.23	0.52
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.44	0.52
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.39	0.52
1:A:413:ARG:HD2	1:A:413:ARG:N	2.23	0.52
1:A:708:LEU:HD23	1:A:708:LEU:N	2.24	0.52
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.39	0.52
1:E:69:GLU:HA	8:E:2039:HOH:O	2.08	0.52
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.91	0.52
1:A:671:ASN:HD21	1:A:675:VAL:H	1.58	0.52
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.09	0.52
1:E:755:LEU:O	1:E:758:ARG:HD3	2.09	0.52
2:B:32:GLY:N	8:B:2011:HOH:O	2.40	0.52
2:B:183:LYS:HE3	8:B:2143:HOH:O	2.09	0.52
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.45	0.52
8:E:2168:HOH:O	2:F:46:TYR:HB2	2.09	0.52
3:G:129:TYR:OH	7:G:1251:PCI:O1	2.27	0.52
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.92	0.52
1:A:113:ARG:NH2	8:A:2066:HOH:O	2.42	0.52
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.90	0.52
2:B:25:MET:HE2	2:B:25:MET:CA	2.34	0.52
8:B:2075:HOH:O	3:C:82:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:GLU:HG2	8:E:2274:HOH:O	2.09	0.52
3:G:144:ASN:C	3:G:144:ASN:HD22	2.16	0.52
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.40	0.52
1:A:572:LEU:HD22	8:A:2274:HOH:O	2.09	0.52
3:C:140:ASN:O	3:C:142:PRO:HD3	2.09	0.52
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.91	0.52
1:E:635:GLN:H	1:E:635:GLN:HE21	1.57	0.52
3:G:225:LEU:CB	8:G:2068:HOH:O	2.56	0.52
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.40	0.52
1:E:621:LEU:HD22	1:E:622:LEU:O	2.09	0.52
3:G:63:LEU:CD2	7:G:1251:PCI:C6	2.88	0.52
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.44	0.52
2:F:115:LYS:HG3	2:F:116:CYS:O	2.10	0.52
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.07	0.52
1:A:285:GLY:C	1:A:590:ILE:CG2	2.83	0.52
1:A:345:MET:CE	1:A:592:LEU:HD11	2.38	0.52
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.90	0.52
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.44	0.52
1:A:239:PHE:O	1:A:687:ARG:HD2	2.10	0.52
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.35	0.52
1:A:647:ASN:C	1:A:648:GLU:CG	2.81	0.52
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.08	0.52
1:E:41:TYR:HE1	1:E:560:GLY:O	1.93	0.52
3:G:206:GLY:CA	3:G:209:TYR:CB	2.88	0.52
1:A:454:GLU:HG2	8:A:2102:HOH:O	2.10	0.51
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.93	0.51
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.57	0.51
3:C:140:ASN:ND2	3:C:140:ASN:N	2.55	0.51
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.25	0.51
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.75	0.51
3:G:172:LEU:O	3:G:176:ARG:HG3	2.11	0.51
1:A:337:TYR:O	1:A:340:ASP:CG	2.45	0.51
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.92	0.51
2:B:117:THR:O	2:B:117:THR:HG23	2.11	0.51
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.38	0.51
1:E:512:LEU:O	1:E:515:THR:HB	2.11	0.51
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.75	0.51
1:E:474:MET:HE2	1:E:705:LEU:HD11	1.92	0.51
1:E:606:PRO:CG	1:E:607:VAL:N	2.73	0.51
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.28	0.51
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.94	0.51
1:E:606:PRO:HG2	1:E:607:VAL:N	2.26	0.51
3:G:139:ASN:HD22	3:G:139:ASN:N	2.02	0.51
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.93	0.51
1:A:232:VAL:N	1:A:247:HIS:HD2	2.04	0.51
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.91	0.51
2:B:57:GLN:CD	8:B:2045:HOH:O	2.54	0.51
3:C:17:THR:HG22	3:C:18:ASN:N	2.26	0.51
1:E:225:ALA:O	1:E:230:ALA:HB3	2.11	0.51
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.93	0.51
1:A:336:TRP:CD1	1:A:336:TRP:N	2.69	0.51
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.40	0.51
1:A:592:LEU:C	1:A:592:LEU:HD13	2.35	0.51
2:B:160:GLU:N	2:B:179:ASN:HD21	1.97	0.51
3:C:68:SER:O	3:C:71:ARG:HB3	2.11	0.51
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.92	0.51
3:G:40:LYS:HG3	3:G:40:LYS:O	2.11	0.51
1:A:390:GLY:H	1:A:595:GLN:NE2	2.05	0.51
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.11	0.51
2:B:155:ALA:HB1	8:B:2113:HOH:O	2.11	0.51
3:C:174:PHE:H	3:C:175:PRO:HD2	1.76	0.51
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.93	0.51
1:A:585:THR:O	1:A:585:THR:HG22	2.10	0.50
1:E:201:ARG:HD3	8:E:2124:HOH:O	2.10	0.50
1:A:69:GLU:C	8:A:2034:HOH:O	2.35	0.50
2:F:190:SER:O	2:F:194:HIS:N	2.43	0.50
1:A:183:TRP:HB3	1:A:592:LEU:O	2.11	0.50
1:A:214:THR:HG23	1:A:214:THR:O	2.11	0.50
1:A:483:ALA:HA	1:A:515:THR:HG23	1.90	0.50
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.58	0.50
2:B:46:TYR:CD2	8:B:2033:HOH:O	2.64	0.50
1:E:701:HIS:O	1:E:710:HIS:O	2.28	0.50
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.20	0.50
3:C:21:HIS:CD2	3:C:21:HIS:C	2.90	0.50
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.40	0.50
1:A:654:GLU:HG3	8:A:2319:HOH:O	2.11	0.50
8:A:2041:HOH:O	2:B:133:GLU:HG3	2.12	0.50
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.42	0.50
3:G:132:LEU:O	3:G:136:VAL:HB	2.12	0.50
1:A:548:LEU:C	1:A:553:LEU:O	2.55	0.50
1:A:558:MET:HE1	1:A:561:MET:SD	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:THR:O	3:C:54:LEU:HG	2.11	0.50
3:C:151:LEU:O	3:C:155:THR:HB	2.12	0.50
1:A:554:ASP:OD2	1:A:554:ASP:N	2.45	0.50
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.11	0.50
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.46	0.50
1:E:630:THR:HG23	8:E:2451:HOH:O	2.11	0.50
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.10	0.50
1:A:428:GLU:CB	1:A:429:PRO:CD	2.87	0.50
1:E:345:MET:CB	1:E:605:LEU:CD1	2.90	0.50
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.94	0.50
1:A:599:GLU:HB2	8:A:2280:HOH:O	2.12	0.50
1:E:256:THR:CG2	1:E:305:THR:HA	2.36	0.50
1:E:311:VAL:HG23	8:E:2198:HOH:O	2.10	0.50
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.47	0.49
2:F:78:THR:CG2	2:F:79:LYS:N	2.76	0.49
2:B:36:LEU:CD1	8:B:2104:HOH:O	2.60	0.49
2:B:47:PRO:CG	8:B:2034:HOH:O	2.60	0.49
3:G:63:LEU:HD21	7:G:1251:PCI:C1	2.42	0.49
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.94	0.49
1:A:592:LEU:O	1:A:592:LEU:HD13	2.12	0.49
1:E:160:TRP:O	1:E:160:TRP:CG	2.65	0.49
1:E:576:GLU:C	1:E:578:GLU:H	2.20	0.49
1:E:93:ASP:O	1:E:469:PRO:HD3	2.12	0.49
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.76	0.49
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.47	0.49
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.94	0.49
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.12	0.49
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.94	0.49
1:E:623:TYR:HA	1:E:695:ILE:O	2.12	0.49
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.60	0.49
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.94	0.49
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.94	0.49
3:G:227:PRO:O	3:G:231:LEU:HB2	2.12	0.49
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.20	0.49
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.12	0.49
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.11	0.49
1:A:276:LYS:CA	8:A:2152:HOH:O	2.47	0.49
1:A:449:VAL:O	1:A:453:LYS:HG3	2.12	0.49
2:B:117:THR:CG2	2:B:117:THR:O	2.58	0.49
8:B:2081:HOH:O	3:C:251:LEU:HD11	2.12	0.49
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.48	0.49
1:E:305:THR:HG23	1:E:307:ILE:H	1.75	0.49
1:E:620:ARG:HB3	8:E:2392:HOH:O	2.12	0.49
2:F:172:ARG:N	2:F:173:PRO:HD3	2.28	0.49
3:G:70:ARG:HG2	3:G:71:PHE:N	2.27	0.49
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.13	0.49
1:E:116:THR:HG23	1:E:119:GLU:N	2.16	0.49
1:E:724:LYS:CG	8:E:2424:HOH:O	2.61	0.49
3:G:63:LEU:HD22	7:G:1251:PCI:C1	2.43	0.49
3:G:17:ASN:O	3:G:21:PHE:HD1	1.95	0.49
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.13	0.48
1:E:112:TYR:CZ	1:E:474:MET:O	2.65	0.48
1:E:247:HIS:CE1	8:E:2149:HOH:O	2.66	0.48
1:E:335:VAL:HG13	1:E:732:ALA:O	2.13	0.48
1:E:601:GLY:HA2	8:E:2334:HOH:O	2.13	0.48
2:F:16:CYS:SG	2:F:16:CYS:O	2.71	0.48
2:F:88:LYS:O	3:G:74:THR:CG2	2.60	0.48
1:A:209:HIS:CE1	1:A:625:ARG:H	2.23	0.48
1:A:310:GLN:HG3	8:A:2164:HOH:O	2.13	0.48
3:C:21:HIS:CE1	3:C:64:LEU:CD2	2.97	0.48
1:A:37:VAL:CG1	1:A:38:LYS:N	2.75	0.48
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.79	0.48
2:B:55:PRO:HB2	8:B:2104:HOH:O	2.12	0.48
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.49	0.48
1:E:336:TRP:O	1:E:338:GLY:N	2.47	0.48
1:E:495:VAL:HG21	8:E:2299:HOH:O	2.12	0.48
3:G:70:ARG:CG	3:G:71:PHE:N	2.76	0.48
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.95	0.48
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.14	0.48
1:E:149:ASP:CB	8:E:2094:HOH:O	2.61	0.48
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.42	0.48
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.07	0.48
1:A:116:THR:HG23	1:A:118:GLU:N	2.29	0.48
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.49	0.48
1:A:605:LEU:N	1:A:606:PRO:CD	2.73	0.48
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.35	0.48
1:E:397:GLU:HB3	8:E:2242:HOH:O	2.13	0.48
1:E:469:PRO:O	1:E:706:MET:CG	2.59	0.48
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.12	0.48
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.96	0.48
1:A:132:ARG:CD	8:A:2077:HOH:O	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:N	1:A:195:ILE:HD12	2.27	0.48
1:A:305:THR:CG2	1:A:307:ILE:HB	2.43	0.48
1:A:512:LEU:O	1:A:515:THR:HB	2.13	0.48
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.96	0.48
1:E:214:THR:HG21	1:E:627:PRO:O	2.12	0.48
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.43	0.48
3:G:52:ALA:O	3:G:56:ILE:HG13	2.14	0.48
3:G:100:LEU:HB3	8:G:2031:HOH:O	2.14	0.48
3:G:139:ASN:ND2	8:G:2041:HOH:O	2.46	0.48
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.96	0.48
1:A:284:VAL:HG12	1:A:285:GLY:N	2.28	0.48
1:A:483:ALA:CA	1:A:515:THR:CG2	2.90	0.48
1:A:623:TYR:HA	1:A:695:ILE:O	2.13	0.48
1:A:761:ASP:C	1:A:763:ARG:H	2.21	0.48
1:E:591:GLU:O	1:E:591:GLU:CG	2.60	0.48
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.96	0.48
3:C:64:LEU:HD21	7:C:1252:PCI:C1	2.44	0.48
1:E:323:LYS:HD3	1:E:354:LEU:C	2.39	0.48
3:G:107:LEU:C	3:G:109:LYS:H	2.20	0.48
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.43	0.48
1:A:107:ARG:HB2	8:A:2224:HOH:O	2.13	0.48
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.27	0.48
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.96	0.48
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.66	0.48
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.27	0.48
1:E:677:GLU:O	1:E:678:GLY:O	2.31	0.48
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.27	0.47
3:C:208:PHE:C	3:C:208:PHE:CD2	2.90	0.47
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.07	0.47
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.30	0.47
1:E:397:GLU:CB	1:E:398:PRO:CD	2.85	0.47
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.49	0.47
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.43	0.47
3:C:222:TRP:CD1	3:C:222:TRP:C	2.91	0.47
1:E:302:GLU:O	1:E:302:GLU:HG2	2.14	0.47
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.29	0.47
1:E:426:THR:C	1:E:428:GLU:N	2.72	0.47
1:E:647:ASN:HD22	1:E:647:ASN:N	2.07	0.47
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.48	0.47
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.19	0.47
2:B:46:TYR:HE2	8:B:2033:HOH:O	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:THR:HG22	2:B:80:ASP:H	1.80	0.47
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.96	0.47
1:A:533:GLN:HG2	1:A:534:TYR:N	2.28	0.47
1:A:575:TRP:O	1:A:580:ARG:HG2	2.15	0.47
1:A:85:ALA:HA	8:A:2044:HOH:O	2.13	0.47
2:B:191:GLU:HG3	8:B:2144:HOH:O	2.14	0.47
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.41	0.47
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.29	0.47
1:E:606:PRO:CG	1:E:607:VAL:H	2.27	0.47
2:F:63:ASN:HB2	8:F:2110:HOH:O	2.13	0.47
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.95	0.47
1:A:534:TYR:O	1:A:535:PHE:CB	2.63	0.47
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.97	0.47
3:C:64:LEU:CD2	7:C:1252:PCI:C4	2.89	0.47
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.95	0.47
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.68	0.47
1:A:548:LEU:O	1:A:553:LEU:O	2.33	0.47
1:E:275:ASP:N	1:E:323:LYS:HE3	2.29	0.47
1:E:346:ALA:N	1:E:605:LEU:CD1	2.76	0.47
1:E:683:LYS:HE2	1:E:685:THR:HB	1.95	0.47
1:A:555:LEU:O	1:A:559:LYS:HG3	2.14	0.47
1:A:647:ASN:HD22	1:A:647:ASN:N	2.07	0.47
1:E:672:GLN:NE2	1:E:672:GLN:H	2.13	0.47
3:G:86:SER:O	3:G:87:PRO:C	2.55	0.47
1:A:295:ASP:O	1:A:297:THR:HG22	2.15	0.47
1:A:591:GLU:O	1:A:592:LEU:CD1	2.58	0.47
1:A:671:ASN:ND2	1:A:675:VAL:H	2.12	0.47
1:E:48:PHE:CZ	1:E:145:HIS:CE1	3.03	0.47
1:E:428:GLU:O	1:E:430:TYR:CA	2.62	0.47
1:A:391:PRO:O	1:A:413:ARG:CB	2.63	0.47
1:E:287:GLU:OE1	1:E:287:GLU:N	2.48	0.47
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.50	0.47
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.50	0.47
1:A:193:GLU:CG	8:A:2120:HOH:O	2.62	0.46
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.97	0.46
1:E:606:PRO:CD	1:E:607:VAL:N	2.78	0.46
1:E:609:THR:HG23	8:E:2338:HOH:O	2.15	0.46
3:G:208:TRP:HA	3:G:208:TRP:HE3	1.80	0.46
1:A:42:GLN:OE1	1:A:506:THR:N	2.48	0.46
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.40	0.46
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:CG2	1:A:307:ILE:H	2.25	0.46
8:B:2078:HOH:O	7:C:1252:PCI:CL3	2.58	0.46
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.97	0.46
3:C:155:THR:CG2	3:C:239:ARG:CG	2.89	0.46
3:C:229:TRP:O	3:C:233:LEU:HG	2.14	0.46
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.54	0.46
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.40	0.46
1:E:186:GLY:HA3	1:E:583:PHE:C	2.41	0.46
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.62	0.46
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.97	0.46
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.55	0.46
3:G:63:LEU:HD11	7:G:1251:PCI:CL5	2.51	0.46
1:A:194:PRO:O	1:A:363:PHE:HA	2.15	0.46
1:A:686:ALA:CB	8:A:2332:HOH:O	2.50	0.46
2:F:27:ASN:O	2:F:28:GLU:C	2.58	0.46
3:G:46:ARG:CG	8:G:2014:HOH:O	2.64	0.46
3:G:240:LEU:C	3:G:240:LEU:CD1	2.88	0.46
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.15	0.46
3:C:108:LEU:O	3:C:109:GLY:C	2.59	0.46
1:E:308:PRO:CB	8:E:2198:HOH:O	2.51	0.46
2:F:117:THR:HG22	2:F:119:CYS:N	2.27	0.46
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.45	0.46
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.97	0.46
1:A:256:THR:HG23	1:A:256:THR:O	2.14	0.46
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.15	0.46
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.56	0.46
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.56	0.46
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.43	0.46
3:C:171:TRP:O	3:C:171:TRP:HE3	1.81	0.46
3:C:185:LEU:O	3:C:189:LEU:HG	2.15	0.46
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.44	0.46
1:E:169:SER:O	1:E:174:THR:HB	2.15	0.46
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.96	0.46
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.96	0.46
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.96	0.46
1:A:183:TRP:HE1	1:A:413:ARG:NH2	2.08	0.46
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.98	0.46
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.48	0.46
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.78	0.46
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.98	0.46
3:C:222:TRP:CD1	3:C:223:GLN:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.98	0.46
1:E:620:ARG:O	1:E:620:ARG:CG	2.63	0.46
2:F:147:ASP:O	2:F:150:SER:HB2	2.15	0.46
3:G:91:GLY:O	3:G:95:LEU:HD12	2.15	0.46
1:A:341:THR:OG1	1:A:729:SER:HB3	2.15	0.46
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.40	0.46
1:A:124:ILE:O	1:A:128:MET:HG3	2.16	0.46
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.45	0.46
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.97	0.46
2:F:166:ARG:HD2	8:F:2105:HOH:O	2.16	0.46
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.48	0.46
1:E:48:PHE:CE1	1:E:145:HIS:CE1	3.04	0.46
1:E:107:ARG:O	1:E:108:GLY:C	2.56	0.46
1:A:605:LEU:CD2	1:A:605:LEU:N	2.67	0.46
1:E:39:SER:OG	1:E:56:HIS:ND1	2.39	0.46
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.49	0.46
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.27	0.46
1:E:708:LEU:HD22	8:E:2408:HOH:O	2.15	0.46
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.08	0.46
2:F:55:PRO:CG	4:F:1194:SF4:S2	3.02	0.46
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.98	0.46
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.97	0.46
1:A:116:THR:HG22	1:A:119:GLU:CB	2.41	0.45
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.98	0.45
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.50	0.45
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.66	0.45
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.61	0.45
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.97	0.45
1:E:647:ASN:H	1:E:647:ASN:ND2	2.15	0.45
2:F:117:THR:HG23	2:F:117:THR:O	2.15	0.45
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.99	0.45
2:B:88:LYS:O	3:C:75:THR:CG2	2.64	0.45
1:E:95:LEU:CD1	8:E:2278:HOH:O	2.56	0.45
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.81	0.45
1:A:122:ASP:HB2	8:A:2070:HOH:O	2.15	0.45
1:A:279:VAL:HA	1:A:283:THR:HB	1.99	0.45
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.57	0.45
1:E:256:THR:HG23	8:E:2196:HOH:O	2.16	0.45
1:E:397:GLU:CB	8:E:2242:HOH:O	2.64	0.45
2:F:72:THR:HG21	2:F:89:LYS:C	2.40	0.45
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.31	0.45
1:A:284:VAL:HB	1:A:589:LYS:HA	1.99	0.45
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.52	0.45
1:E:149:ASP:HA	8:E:2094:HOH:O	2.16	0.45
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.98	0.45
1:E:447:PRO:HB3	8:E:2419:HOH:O	2.16	0.45
1:E:484:THR:HB	1:E:487:GLU:OE1	2.16	0.45
8:E:2134:HOH:O	2:F:138:TYR:CE1	2.70	0.45
2:F:16:CYS:O	4:F:1194:SF4:S3	2.75	0.45
2:F:44:GLY:HA3	8:F:2025:HOH:O	2.16	0.45
1:A:77:ARG:NH2	8:A:2041:HOH:O	2.39	0.45
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.51	0.45
1:E:113:ARG:HB3	8:E:2044:HOH:O	2.17	0.45
1:A:170:VAL:HG12	1:A:171:SER:N	2.31	0.45
1:A:702:LYS:HG3	8:A:2234:HOH:O	2.16	0.45
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.31	0.45
1:E:622:LEU:HB2	1:E:693:VAL:O	2.17	0.45
2:F:125:LYS:HE2	8:F:2078:HOH:O	2.17	0.45
1:A:583:PHE:CZ	1:A:587:SER:CA	2.99	0.45
3:C:64:LEU:HD21	7:C:1252:PCI:C6	2.46	0.45
1:E:112:TYR:OH	1:E:476:ALA:O	2.35	0.45
1:E:116:THR:HG22	1:E:119:GLU:N	2.27	0.45
1:E:533:GLN:HE21	1:E:533:GLN:N	1.98	0.45
1:E:638:TRP:O	1:E:642:GLU:HB2	2.17	0.45
1:A:116:THR:HG23	1:A:118:GLU:H	1.81	0.45
1:A:422:GLU:N	1:A:423:PRO:HD2	2.31	0.45
1:A:499:THR:HB	1:A:565:VAL:CG1	2.47	0.45
1:A:586:ALA:O	1:A:587:SER:CB	2.64	0.45
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.44	0.45
1:E:730:GLY:HA3	8:E:2252:HOH:O	2.16	0.45
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.49	0.45
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.52	0.45
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.99	0.45
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.99	0.45
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.17	0.45
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.28	0.45
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.47	0.45
1:E:239:PHE:O	1:E:687:ARG:HD2	2.17	0.45
3:G:148:ALA:HA	8:G:2047:HOH:O	2.17	0.45
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.17	0.45
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:NE	1:A:214:THR:HG22	2.32	0.44
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.99	0.44
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.98	0.44
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.99	0.44
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.99	0.44
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.84	0.44
2:F:117:THR:HB	8:F:2012:HOH:O	2.15	0.44
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.42	0.44
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.47	0.44
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.99	0.44
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.25	0.44
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.31	0.44
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.73	0.44
3:C:228:PRO:O	3:C:232:LEU:HD12	2.18	0.44
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.82	0.44
8:F:2029:HOH:O	3:G:250:LEU:HD12	2.16	0.44
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.47	0.44
1:A:42:GLN:OE1	1:A:506:THR:O	2.35	0.44
1:A:207:GLY:O	5:A:1766:MGD:PB	2.75	0.44
2:B:190:SER:CB	3:C:252:GLY:N	2.77	0.44
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.47	0.44
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.47	0.44
1:A:477:ASP:C	1:A:478:VAL:HG23	2.43	0.44
2:B:81:GLY:O	2:B:174:LYS:NZ	2.46	0.44
1:E:504:LEU:HD22	1:E:505:ARG:N	2.33	0.44
1:E:734:LEU:CD2	8:E:2419:HOH:O	2.59	0.44
2:F:190:SER:N	3:G:251:GLY:N	2.65	0.44
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.98	0.44
1:A:647:ASN:H	1:A:647:ASN:ND2	2.12	0.44
3:C:173:LEU:O	3:C:173:LEU:CG	2.62	0.44
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.99	0.44
1:E:470:GLN:O	1:E:471:GLU:C	2.59	0.44
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.99	0.44
2:B:25:MET:CE	2:B:25:MET:CA	2.87	0.44
1:E:201:ARG:CD	8:E:2124:HOH:O	2.65	0.44
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.99	0.44
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.47	0.44
2:F:107:LEU:HD21	3:G:68:PRO:HG2	2.00	0.44
2:B:25:MET:HA	2:B:25:MET:HE3	1.97	0.44
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.53	0.44
1:E:297:THR:HG22	1:E:299:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.95	0.44
1:E:647:ASN:C	1:E:648:GLU:HG3	2.43	0.44
3:G:206:GLY:O	3:G:209:TYR:CB	2.66	0.44
1:A:349:TYR:HH	1:A:591:GLU:C	2.10	0.44
1:A:677:GLU:C	1:A:678:GLY:O	2.61	0.44
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.65	0.44
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.86	0.44
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.51	0.44
1:E:591:GLU:O	1:E:603:GLN:CD	2.60	0.44
1:A:65:VAL:HG13	1:A:78:LEU:HD21	2.00	0.43
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.57	0.43
2:B:52:GLU:OE2	2:B:187:THR:HB	2.18	0.43
1:E:204:VAL:HG21	1:E:319:MET:CE	2.47	0.43
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.99	0.43
1:E:315:VAL:HG12	1:E:319:MET:CE	2.44	0.43
3:G:112:GLN:N	8:G:2034:HOH:O	2.50	0.43
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.53	0.43
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.48	0.43
1:E:158:ALA:HB1	1:E:381:LEU:O	2.17	0.43
1:E:499:THR:HA	1:E:567:ARG:O	2.19	0.43
1:E:575:TRP:HB3	1:E:580:ARG:O	2.18	0.43
1:E:708:LEU:HD22	1:E:755:LEU:HB3	2.00	0.43
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.99	0.43
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.71	0.43
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.18	0.43
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.98	0.43
1:A:186:GLY:N	1:A:583:PHE:HA	2.27	0.43
2:B:166:ARG:HG2	8:B:2146:HOH:O	2.19	0.43
3:C:133:LEU:O	3:C:137:VAL:HG22	2.18	0.43
3:C:153:PRO:HB3	8:C:2063:HOH:O	2.17	0.43
1:A:113:ARG:NE	8:A:2066:HOH:O	2.52	0.43
1:A:166:ALA:CB	1:A:415:THR:CG2	2.95	0.43
1:A:482:GLU:HG2	1:A:483:ALA:H	1.84	0.43
1:A:587:SER:O	1:A:589:LYS:HE2	2.18	0.43
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.50	0.43
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.48	0.43
1:E:630:THR:HA	5:E:1766:MGD:C17	2.47	0.43
3:G:207:PHE:HB3	3:G:208:TRP:H	1.42	0.43
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.48	0.43
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.48	0.43
1:A:651:ILE:HG23	1:A:693:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:HA	2:B:140:ARG:HG3	2.01	0.43
1:E:247:HIS:CD2	1:E:247:HIS:N	2.85	0.43
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.59	0.43
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.49	0.43
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.80	0.43
1:A:671:ASN:C	1:A:671:ASN:HD22	2.26	0.43
3:C:64:LEU:CD2	7:C:1252:PCI:C5	2.96	0.43
1:E:488:ARG:HG3	8:E:2288:HOH:O	2.18	0.43
1:A:743:LYS:HG3	8:A:2365:HOH:O	2.18	0.43
2:B:168:GLU:C	2:B:169:GLN:O	2.50	0.43
3:C:172:ALA:HA	3:C:175:PRO:CG	2.37	0.43
1:E:630:THR:HA	5:E:1766:MGD:N18	2.34	0.43
1:E:761:ASP:C	1:E:763:ARG:H	2.25	0.43
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.74	0.43
1:A:158:ALA:HB1	1:A:381:LEU:O	2.18	0.43
1:A:319:MET:CE	1:A:328:LEU:CD1	2.97	0.43
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.67	0.43
1:A:721:THR:OG1	8:A:2354:HOH:O	2.21	0.43
3:C:125:LEU:HD23	3:C:125:LEU:HA	1.95	0.43
1:E:583:PHE:CD2	1:E:583:PHE:N	2.81	0.43
1:E:746:ARG:HH11	1:E:746:ARG:CG	2.30	0.43
3:G:65:ALA:O	3:G:70:ARG:NH1	2.52	0.43
1:A:418:GLN:H	1:A:418:GLN:HG3	1.49	0.43
1:E:285:GLY:HA3	1:E:592:LEU:HD11	2.01	0.43
1:E:388:CYS:O	1:E:389:SER:C	2.61	0.43
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.81	0.43
3:G:165:LEU:C	3:G:167:LYS:H	2.26	0.43
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.48	0.43
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.54	0.43
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.49	0.43
3:C:155:THR:CG2	3:C:239:ARG:CD	2.97	0.43
1:E:123:HIS:CE1	8:E:2080:HOH:O	2.72	0.43
1:E:293:VAL:O	1:E:293:VAL:HG13	2.18	0.43
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.18	0.43
1:E:627:PRO:CB	2:F:16:CYS:HA	2.49	0.43
2:F:175:LEU:HD12	2:F:175:LEU:C	2.43	0.43
1:A:506:THR:CG2	8:A:2248:HOH:O	2.66	0.42
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.83	0.42
2:B:159:ALA:O	2:F:183:LYS:CE	2.59	0.42
2:B:164:VAL:HG22	2:B:173:PRO:HB2	2.00	0.42
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:HIS:CD2	1:A:266:HIS:C	2.97	0.42
1:A:635:GLN:HG2	1:A:635:GLN:H	1.38	0.42
2:B:192:VAL:CG1	2:B:193:HIS:H	2.32	0.42
3:C:21:HIS:ND1	3:C:64:LEU:CG	2.80	0.42
1:E:540:ILE:O	1:E:544:LEU:HG	2.19	0.42
1:E:604:PRO:C	1:E:605:LEU:CD2	2.80	0.42
2:F:59:LEU:O	2:F:60:HIS:C	2.62	0.42
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.34	0.42
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.54	0.42
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.49	0.42
1:A:39:SER:C	8:A:2005:HOH:O	2.62	0.42
1:A:90:TYR:OH	1:A:509:HIS:HE1	2.01	0.42
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.94	0.42
2:B:41:ARG:CD	2:B:187:THR:HG23	2.46	0.42
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.49	0.42
3:C:130:TYR:CE1	7:C:1252:PCI:O1	2.72	0.42
1:E:30:ALA:N	1:E:31:PRO:CD	2.82	0.42
1:E:275:ASP:C	1:E:275:ASP:OD1	2.62	0.42
1:E:289:LEU:HD12	1:E:590:ILE:HG21	2.00	0.42
1:E:384:ALA:HB1	8:E:2240:HOH:O	2.20	0.42
1:E:591:GLU:O	1:E:603:GLN:HG2	2.18	0.42
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.49	0.42
1:A:129:LEU:O	1:A:133:GLU:HG2	2.20	0.42
1:A:349:TYR:OH	1:A:592:LEU:HG	2.19	0.42
1:A:483:ALA:CB	1:A:515:THR:CG2	2.97	0.42
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.83	0.42
1:A:589:LYS:O	1:A:592:LEU:CA	2.67	0.42
2:B:117:THR:HG23	2:B:120:ALA:H	1.84	0.42
8:B:2081:HOH:O	3:C:251:LEU:CD1	2.66	0.42
1:E:325:ARG:NH1	8:E:2214:HOH:O	2.34	0.42
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.55	0.42
1:E:622:LEU:O	1:E:623:TYR:HB3	2.19	0.42
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.64	0.42
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.20	0.42
1:A:541:GLU:O	1:A:545:GLU:HG2	2.19	0.42
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.85	0.42
3:C:17:THR:HG21	8:C:2014:HOH:O	2.18	0.42
3:C:174:PHE:N	3:C:175:PRO:HD2	2.35	0.42
1:E:50:ARG:HD2	8:E:2014:HOH:O	2.18	0.42
1:E:371:LEU:HD12	1:E:494:LEU:HD21	2.02	0.42
1:E:590:ILE:HG22	1:E:591:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:630:THR:H	1:E:634:THR:HG21	1.84	0.42
3:G:154:THR:CG2	3:G:238:ARG:CG	2.97	0.42
3:G:206:GLY:O	3:G:209:TYR:C	2.63	0.42
1:A:447:PRO:HD3	8:A:2216:HOH:O	2.19	0.42
1:E:622:LEU:HD23	1:E:622:LEU:HA	1.92	0.42
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.68	0.42
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.55	0.42
1:A:66:GLU:HG3	8:A:2040:HOH:O	2.20	0.42
2:B:57:GLN:O	2:B:59:LEU:HD23	2.20	0.42
2:B:72:THR:CG2	2:B:73:GLY:N	2.80	0.42
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.49	0.42
1:E:391:PRO:C	1:E:413:ARG:CG	2.93	0.42
1:E:501:PHE:HB3	1:E:565:VAL:HG13	2.01	0.42
2:F:117:THR:CG2	2:F:119:CYS:N	2.82	0.42
1:A:561:MET:O	1:A:563:THR:O	2.38	0.42
3:C:143:LEU:HD23	3:C:198:ALA:HB1	2.02	0.42
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.50	0.42
3:C:215:LEU:O	3:C:216:LEU:C	2.62	0.42
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.20	0.42
1:E:523:ARG:HH11	1:E:523:ARG:HG2	1.85	0.42
1:A:457:LYS:HD2	8:A:2224:HOH:O	2.20	0.42
1:A:589:LYS:H	1:A:589:LYS:HG2	1.60	0.42
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.19	0.42
1:E:592:LEU:HA	1:E:603:GLN:HE21	0.64	0.42
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.67	0.42
1:A:225:ALA:C	1:A:230:ALA:HB3	2.45	0.41
1:A:494:LEU:HD22	1:A:502:ILE:HG12	2.01	0.41
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.66	0.41
2:B:169:GLN:NE2	8:B:2129:HOH:O	2.37	0.41
1:E:53:ILE:HG22	1:E:78:LEU:HD11	2.02	0.41
1:E:288:GLU:HG3	8:E:2186:HOH:O	2.20	0.41
1:E:369:PRO:HG2	1:E:494:LEU:HB3	2.02	0.41
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.50	0.41
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.73	0.41
1:A:712:ARG:NH2	8:A:2348:HOH:O	2.52	0.41
3:C:193:THR:O	3:C:193:THR:HG23	2.20	0.41
1:E:106:GLN:NE2	8:E:2062:HOH:O	2.53	0.41
1:E:494:LEU:HD23	1:E:502:ILE:HG23	2.02	0.41
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.80	0.41
1:E:670:VAL:HB	1:E:740:ARG:HG3	2.01	0.41
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:HA	1:A:564:LEU:O	2.20	0.41
1:E:95:LEU:CD2	8:E:2278:HOH:O	2.52	0.41
1:E:201:ARG:NH2	1:E:228:ASN:O	2.43	0.41
3:G:19:LEU:HD23	3:G:19:LEU:O	2.20	0.41
3:G:73:PHE:HA	8:G:2022:HOH:O	2.21	0.41
1:A:113:ARG:CZ	8:A:2066:HOH:O	2.69	0.41
1:A:122:ASP:CB	8:A:2070:HOH:O	2.68	0.41
1:A:241:THR:HG21	2:B:14:VAL:HB	2.02	0.41
1:A:626:SER:HB2	1:A:696:VAL:HG11	2.02	0.41
2:B:157:LYS:HD3	8:F:2039:HOH:O	2.20	0.41
3:C:227:ALA:HB3	3:C:228:PRO:HD3	2.03	0.41
1:E:604:PRO:O	1:E:606:PRO:HD2	2.18	0.41
2:F:122:ARG:HG2	2:F:127:LYS:HE3	2.03	0.41
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.35	0.41
3:G:63:LEU:HD22	7:G:1251:PCI:C4	2.51	0.41
3:G:208:TRP:O	3:G:212:PHE:CD2	2.73	0.41
1:A:462:TYR:OH	1:A:472:HIS:O	2.31	0.41
2:B:135:CYS:HA	2:B:136:PRO:HD3	1.88	0.41
2:B:192:VAL:CG1	2:B:193:HIS:N	2.81	0.41
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.86	0.41
1:E:314:GLU:HG3	8:E:2202:HOH:O	2.19	0.41
1:E:335:VAL:O	1:E:335:VAL:CG1	2.68	0.41
1:E:345:MET:HB3	1:E:605:LEU:HD11	2.02	0.41
1:E:422:GLU:N	1:E:423:PRO:CD	2.83	0.41
1:E:497:HIS:HB3	1:E:499:THR:O	2.20	0.41
1:E:649:VAL:HG13	1:E:695:ILE:HG23	2.01	0.41
1:E:753:THR:HG22	1:E:757:LYS:HE3	2.01	0.41
2:F:19:CYS:HB2	2:F:131:CYS:HB2	2.02	0.41
3:G:223:GLU:N	8:G:2068:HOH:O	2.52	0.41
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.35	0.41
1:A:722:ARG:NE	8:A:2356:HOH:O	2.54	0.41
1:E:292:HIS:HD2	8:E:2085:HOH:O	2.02	0.41
1:E:606:PRO:HG2	1:E:607:VAL:H	1.85	0.41
2:F:78:THR:HG23	2:F:79:LYS:N	2.35	0.41
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.68	0.41
1:A:248:ARG:HB3	8:A:2136:HOH:O	2.20	0.41
1:A:395:ASP:CA	1:A:399:GLU:CG	2.68	0.41
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.51	0.41
1:A:538:LYS:HE2	1:A:538:LYS:N	2.35	0.41
1:E:101:ARG:HB2	1:E:477:ASP:HA	2.03	0.41
1:E:193:GLU:CD	1:E:193:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:THR:HG22	1:E:300:TRP:N	2.17	0.41
3:G:144:ASN:C	3:G:144:ASN:ND2	2.78	0.41
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.56	0.41
1:A:423:PRO:HB2	1:A:432:ILE:HD12	2.02	0.41
1:E:60:ASN:ND2	8:E:2022:HOH:O	2.52	0.41
1:E:283:THR:HG23	1:E:590:ILE:HG13	2.03	0.41
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.61	0.41
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.55	0.41
1:E:346:ALA:HB2	1:E:605:LEU:HD12	2.02	0.41
3:G:32:LEU:HD12	3:G:120:LEU:HD12	2.03	0.41
3:G:170:TRP:CE3	3:G:171:ALA:N	2.89	0.41
1:A:319:MET:HE1	1:A:328:LEU:CD1	2.49	0.41
1:A:422:GLU:N	1:A:423:PRO:CD	2.84	0.41
1:A:435:LEU:O	1:A:462:TYR:HA	2.21	0.41
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.35	0.41
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.51	0.41
1:E:630:THR:O	1:E:631:PHE:O	2.38	0.41
3:G:150:LEU:HD23	3:G:150:LEU:HA	1.87	0.41
3:C:76:HIS:O	3:C:79:LEU:HB2	2.21	0.40
1:E:576:GLU:C	1:E:578:GLU:N	2.77	0.40
1:E:621:LEU:HD22	1:E:622:LEU:N	2.36	0.40
1:A:389:SER:CA	1:A:595:GLN:HE22	2.35	0.40
1:A:588:GLY:HA3	8:A:2156:HOH:O	2.21	0.40
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.22	0.40
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.51	0.40
1:E:422:GLU:N	1:E:423:PRO:HD2	2.35	0.40
1:E:427:GLY:O	1:E:428:GLU:O	2.39	0.40
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.86	0.40
1:A:108:GLY:C	1:A:109:GLU:O	2.62	0.40
1:A:232:VAL:N	1:A:247:HIS:CD2	2.84	0.40
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.79	0.40
1:A:558:MET:HA	1:A:558:MET:CE	2.46	0.40
1:A:642:GLU:OE2	2:B:31:PRO:C	2.65	0.40
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.35	0.40
3:C:71:ARG:HG2	3:C:72:PHE:N	2.36	0.40
1:E:233:VAL:HG13	1:E:248:ARG:HB2	2.03	0.40
1:E:474:MET:HE2	1:E:705:LEU:HD12	2.04	0.40
1:E:647:ASN:C	1:E:648:GLU:CG	2.95	0.40
3:G:47:ARG:O	3:G:50:LEU:O	2.39	0.40
2:B:117:THR:HG22	2:B:119:CYS:CA	2.51	0.40
2:B:143:GLY:N	2:B:152:VAL:CG2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.56	0.40
3:C:166:LEU:C	3:C:168:LYS:H	2.29	0.40
3:C:207:GLY:C	3:C:209:TRP:H	2.28	0.40
1:E:422:GLU:HG3	8:E:2107:HOH:O	2.20	0.40
1:A:258:THR:HB	1:A:608:PHE:HA	2.03	0.40
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.52	0.40
1:E:650:TRP:HB2	1:E:694:TYR:HB3	2.03	0.40
1:E:650:TRP:O	1:E:693:VAL:HG22	2.21	0.40
5:E:1766:MGD:H8	8:E:2426:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.63	0.57
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.75	0.45
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	733/765 (96%)	653 (89%)	46 (6%)	34 (5%)	2	2
1	E	733/765 (96%)	635 (87%)	63 (9%)	35 (5%)	2	2
2	B	192/195 (98%)	177 (92%)	12 (6%)	3 (2%)	7	14
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	5	9
3	C	249/253 (98%)	232 (93%)	12 (5%)	5 (2%)	6	10
3	G	249/253 (98%)	221 (89%)	21 (8%)	7 (3%)	4	6
All	All	2348/2426 (97%)	2097 (89%)	163 (7%)	88 (4%)	2	3

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	324	PRO
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	552	GLY
1	E	567	ARG
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	113	ARG
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO

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Mol	Chain	Res	Type
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	389	SER
1	E	429	PRO
1	E	466	ASP
1	E	469	PRO
1	E	471	GLU
1	E	513	PHE
1	E	570	PRO
1	E	627	PRO
2	F	45	GLU
2	F	178	LEU
1	A	478	VAL
2	B	115	LYS
1	E	478	VAL
1	E	763	ARG
3	G	38	HIS
1	A	387	GLY
3	C	113	GLN
1	E	70	ALA
1	E	710	HIS
1	A	610	PRO
1	A	684	PRO
1	E	610	PRO
1	A	584	GLY
1	A	609	THR

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Mol	Chain	Res	Type
1	E	434	GLY
1	A	194	PRO
1	E	604	PRO
1	E	609	THR

5.3.2 Protein sidechains ⓘ

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	610/632 (96%)	491 (80%)	119 (20%)	1	2
1	E	610/632 (96%)	495 (81%)	115 (19%)	1	3
2	B	162/163 (99%)	140 (86%)	22 (14%)	3	8
2	F	162/163 (99%)	142 (88%)	20 (12%)	4	10
3	C	185/187 (99%)	160 (86%)	25 (14%)	4	8
3	G	185/187 (99%)	163 (88%)	22 (12%)	5	11
All	All	1914/1964 (98%)	1591 (83%)	323 (17%)	2	4

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	ILE
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	167	LYS
1	A	170	VAL
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	193	GLU
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	250	LEU
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	289	LEU
1	A	293	VAL
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	371	LEU
1	A	372	GLU
1	A	378	PRO
1	A	379	LEU
1	A	382	GLU
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	433	LYS
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS

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Mol	Chain	Res	Type
1	A	465	ILE
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	504	LEU
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	531	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	540	ILE
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	581	LEU
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	599	GLU
1	A	603	GLN
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN

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Mol	Chain	Res	Type
1	A	648	GLU
1	A	649	VAL
1	A	651	ILE
1	A	663	GLU
1	A	667	VAL
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	693	VAL
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	24	LYS
2	B	25	MET
2	B	39	ARG
2	B	41	ARG
2	B	45	GLU
2	B	54	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	145	LEU
2	B	152	VAL
2	B	164	VAL
2	B	166	ARG
2	B	175	LEU

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Mol	Chain	Res	Type
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	21	HIS
3	C	40	LEU
3	C	57	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	79	LEU
3	C	105	LEU
3	C	110	LYS
3	C	130	TYR
3	C	140	ASN
3	C	145	ASN
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	197	GLU
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	102	VAL
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	189	ILE
1	E	193	GLU
1	E	208	HIS
1	E	213	ASP

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Mol	Chain	Res	Type
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	284	VAL
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	314	GLU
1	E	323	LYS
1	E	327	VAL
1	E	335	VAL
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	457	LYS
1	E	466	ASP
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU

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Mol	Chain	Res	Type
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	589	LYS
1	E	590	ILE
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	612	GLU
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	628	VAL
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	663	GLU
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR

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Mol	Chain	Res	Type
1	E	691	ASP
1	E	693	VAL
1	E	696	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	741	LEU
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	68	PRO
2	F	69	VAL
2	F	72	THR
2	F	78	THR
2	F	80	ASP
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	166	ARG
2	F	171	THR
2	F	175	LEU
2	F	187	THR
2	F	191	GLU
3	G	10	GLN
3	G	17	ASN
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR

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Mol	Chain	Res	Type
3	G	88	ILE
3	G	109	LYS
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	123	HIS
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	472	HIS
1	A	509	HIS
1	A	533	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	35	ASN
2	B	48	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	11	GLN
3	C	21	HIS
3	C	84	HIS
3	C	140	ASN
3	C	145	ASN
3	C	249	GLN
1	E	35	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	192	HIS
1	E	209	HIS
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	441	ASN
1	E	470	GLN
1	E	472	HIS
1	E	509	HIS
1	E	533	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	169	GLN
2	F	179	ASN

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Mol	Chain	Res	Type
3	G	10	GLN
3	G	38	HIS
3	G	83	HIS
3	G	137	ASN
3	G	139	ASN
3	G	200	HIS
3	G	248	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	$\# Z > 2$
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
4	SF4	B	1197	2	0,12,12	-	-	-		
7	PCI	G	1251	-	12,12,12	1.11	0	18,18,18	1.01	1 (5%)
4	SF4	F	1197	2	0,12,12	-	-	-		
5	MGD	E	1765	6	47,52,52	2.08	13 (27%)	58,81,81	3.13	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	A	1766	6	47,52,52	1.97	13 (27%)	58,81,81	2.98	21 (36%)
4	SF4	F	1196	2	0,12,12	-	-	-		
4	SF4	F	1194	2	0,12,12	-	-	-		
4	SF4	F	1195	2	0,12,12	-	-	-		
5	MGD	A	1765	6	47,52,52	1.90	12 (25%)	58,81,81	3.00	19 (32%)
4	SF4	B	1195	2	0,12,12	-	-	-		
5	MGD	E	1766	6	47,52,52	2.20	14 (29%)	58,81,81	2.62	19 (32%)
7	PCI	C	1252	-	12,12,12	1.19	1 (8%)	18,18,18	1.15	3 (16%)
4	SF4	E	1764	1	0,12,12	-	-	-		
4	SF4	B	1194	2	0,12,12	-	-	-		

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
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
7	PCI	G	1251	-	-	-	0/1/1/1
4	SF4	F	1197	2	-	-	0/6/5/5
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	F	1196	2	-	-	0/6/5/5
5	MGD	A	1765	6	-	5/22/66/66	0/6/6/6
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	F	1195	2	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6
7	PCI	C	1252	-	-	-	0/1/1/1
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	B	1194	2	-	-	0/6/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C21-N22	-7.54	1.27	1.35
5	A	1765	MGD	C23-C14	-6.66	1.48	1.53
5	E	1765	MGD	C16-C21	5.67	1.48	1.38
5	A	1766	MGD	C14-N15	-5.22	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C16-C21	4.54	1.46	1.38
5	A	1765	MGD	C16-C21	4.48	1.46	1.38
5	A	1766	MGD	C23-C14	-4.45	1.50	1.53
5	E	1765	MGD	C5-N7	-4.32	1.30	1.39
5	E	1765	MGD	PB-O3B	4.29	1.64	1.59
5	A	1766	MGD	C16-C21	4.15	1.45	1.38
5	E	1766	MGD	C5-C4	4.13	1.50	1.38
5	E	1766	MGD	C14-N15	-4.12	1.41	1.46
5	A	1766	MGD	C21-N22	-4.11	1.31	1.35
5	E	1765	MGD	C23-C14	-4.09	1.50	1.53
5	E	1765	MGD	C10-C11	-3.85	1.46	1.51
5	E	1765	MGD	PA-O3B	3.83	1.63	1.59
5	E	1766	MGD	C23-C14	-3.74	1.50	1.53
5	A	1766	MGD	O11-C23	3.52	1.48	1.43
5	E	1765	MGD	C8-N9	-3.45	1.29	1.37
5	A	1766	MGD	C6-N1	-3.42	1.32	1.38
5	A	1765	MGD	C5-C4	3.41	1.48	1.38
5	E	1766	MGD	C5-N7	-3.37	1.32	1.39
5	A	1766	MGD	C5-C4	3.32	1.47	1.38
5	E	1766	MGD	O3'-C3'	3.25	1.51	1.43
5	E	1765	MGD	C5-C4	3.23	1.47	1.38
5	E	1766	MGD	C19-N18	-3.23	1.29	1.37
5	A	1765	MGD	C17-N18	-3.19	1.32	1.38
5	A	1765	MGD	C21-N22	-3.01	1.32	1.35
5	E	1766	MGD	C19-N19	-2.95	1.27	1.34
5	E	1766	MGD	C16-N15	-2.90	1.31	1.37
5	E	1766	MGD	C6-N1	-2.78	1.33	1.38
5	A	1765	MGD	C10-C11	-2.66	1.48	1.51
5	A	1765	MGD	C5-N7	-2.65	1.33	1.39
5	A	1766	MGD	PB-O2B	-2.60	1.43	1.55
5	A	1766	MGD	C16-C17	2.56	1.49	1.41
5	E	1765	MGD	C19-N18	-2.47	1.31	1.37
5	A	1765	MGD	C21-N20	-2.43	1.32	1.36
5	A	1766	MGD	PA-O2A	-2.38	1.44	1.55
5	E	1766	MGD	PA-O3B	2.37	1.62	1.59
5	E	1765	MGD	C2-N1	-2.35	1.31	1.37
5	E	1765	MGD	C3'-C4'	-2.34	1.47	1.53
5	A	1765	MGD	C4-N9	-2.32	1.32	1.38
5	E	1765	MGD	C17-N18	-2.31	1.34	1.38
5	E	1766	MGD	O4'-C4'	-2.29	1.39	1.45
5	A	1766	MGD	C10-C11	-2.28	1.48	1.51
5	A	1765	MGD	O6-C6	2.23	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C8-N9	-2.22	1.32	1.37
5	E	1765	MGD	C4-N9	-2.18	1.32	1.38
5	A	1765	MGD	C23-N22	-2.17	1.41	1.45
5	E	1766	MGD	C19-N20	2.10	1.38	1.33
5	A	1766	MGD	C5-N7	-2.07	1.34	1.39
5	A	1766	MGD	C23-N22	-2.07	1.41	1.45
7	C	1252	PCI	C4-C3	2.03	1.44	1.39

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	O11-C23-C14	13.65	118.07	108.96
5	A	1765	MGD	O11-C23-C14	12.34	117.19	108.96
5	E	1765	MGD	O11-C23-N22	-10.87	98.74	108.61
5	E	1766	MGD	O11-C23-C14	10.20	115.77	108.96
5	E	1765	MGD	C23-C14-N15	9.09	116.80	107.87
5	A	1765	MGD	C23-C14-N15	7.86	115.58	107.87
5	E	1765	MGD	O11-C23-C14	-7.49	103.97	108.96
5	E	1766	MGD	C5-C4-N3	-7.11	117.08	128.39
5	A	1765	MGD	C5-C4-N3	-7.10	117.09	128.39
5	A	1765	MGD	C2-N3-C4	7.07	124.47	112.30
5	E	1765	MGD	C5-C4-N3	-6.80	117.57	128.39
5	E	1765	MGD	C2-N3-C4	6.37	123.27	112.30
5	A	1766	MGD	C5-C4-N3	-6.23	118.47	128.39
5	E	1765	MGD	C19-N20-C21	6.00	123.95	113.36
5	E	1766	MGD	O17-C17-C16	-5.61	113.74	127.26
5	A	1765	MGD	C19-N20-C21	5.54	123.14	113.36
5	E	1766	MGD	C23-C14-N15	5.19	112.97	107.87
5	E	1765	MGD	C6-C5-N7	5.12	139.60	130.29
5	A	1766	MGD	C2-N3-C4	5.07	121.04	112.30
5	A	1766	MGD	O4'-C1'-N9	5.02	119.74	108.36
5	A	1766	MGD	N9-C4-N3	5.02	136.00	125.95
5	A	1766	MGD	C23-C14-N15	4.82	112.61	107.87
5	E	1766	MGD	C2-N3-C4	4.63	120.27	112.30
5	A	1766	MGD	O11-C23-N22	4.61	112.78	108.61
5	E	1766	MGD	N9-C4-N3	4.45	134.84	125.95
5	A	1766	MGD	O3B-PB-O1B	-4.42	97.40	110.70
5	A	1765	MGD	N9-C4-N3	4.34	134.64	125.95
5	E	1765	MGD	C4-C5-N7	-4.26	103.92	110.67
5	E	1766	MGD	C19-N20-C21	4.11	120.61	113.36
5	A	1765	MGD	C17-C16-N15	3.93	126.98	116.27
5	E	1765	MGD	N9-C4-N3	3.88	133.71	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1765	MGD	C6-C5-N7	3.85	137.30	130.29
5	A	1766	MGD	C19-N18-C17	-3.72	118.36	125.11
5	A	1765	MGD	C4-C5-N7	-3.68	104.84	110.67
5	E	1766	MGD	C16-C17-N18	3.58	121.97	112.13
5	E	1765	MGD	C17-C16-N15	3.54	125.91	116.27
5	A	1766	MGD	O6-C6-C5	-3.46	117.39	126.53
5	A	1765	MGD	O2B-PB-O3B	3.45	116.60	107.27
5	E	1766	MGD	O4'-C1'-N9	3.39	116.05	108.36
5	A	1766	MGD	O2B-PB-O3B	3.29	116.16	107.27
5	A	1766	MGD	O17-C17-C16	-3.27	119.38	127.26
5	A	1766	MGD	C17-C16-N15	3.23	125.08	116.27
5	A	1765	MGD	N2-C2-N1	3.19	123.50	116.76
5	E	1765	MGD	C16-C17-N18	3.12	120.70	112.13
5	E	1766	MGD	O2A-PA-O1A	3.00	126.39	112.44
5	A	1765	MGD	O17-C17-C16	-2.89	120.29	127.26
5	E	1766	MGD	O11-C23-N22	-2.85	106.02	108.61
5	E	1765	MGD	O2A-PA-O3B	-2.79	99.72	107.27
5	A	1766	MGD	O5'-C5'-C4'	-2.78	99.52	108.99
5	A	1765	MGD	O3B-PA-O1A	-2.76	102.39	110.70
5	A	1765	MGD	O4'-C4'-C5'	-2.74	100.57	109.33
5	A	1766	MGD	C16-C17-N18	2.73	119.61	112.13
5	E	1765	MGD	O3'-C3'-C4'	-2.72	103.28	111.08
7	C	1252	PCI	C1-C2-C3	-2.71	118.87	121.16
5	E	1766	MGD	C19-N18-C17	-2.68	120.26	125.11
5	E	1766	MGD	O3'-C3'-C4'	2.64	118.67	111.08
5	E	1766	MGD	C2-N1-C6	-2.61	120.38	125.11
5	A	1765	MGD	N19-C19-N18	2.59	122.22	116.76
5	A	1766	MGD	C6-C5-N7	2.57	134.96	130.29
5	E	1765	MGD	C8-N7-C5	2.54	108.78	104.26
5	A	1765	MGD	O3B-PB-O1B	-2.53	103.10	110.70
5	E	1765	MGD	O2B-PB-O1B	2.52	124.19	112.44
5	A	1765	MGD	O4'-C1'-C2'	-2.52	101.22	106.62
5	E	1766	MGD	C4-C5-N7	-2.52	106.67	110.67
5	E	1765	MGD	O17-C17-C16	-2.52	121.19	127.26
5	E	1766	MGD	O6-C6-C5	-2.51	119.90	126.53
5	E	1765	MGD	O3B-PB-O1B	-2.48	103.25	110.70
5	A	1766	MGD	C19-N20-C21	2.41	117.62	113.36
5	E	1765	MGD	O6-C6-C5	-2.35	120.32	126.53
5	E	1765	MGD	O2A-PA-O1A	2.30	123.13	112.44
5	A	1766	MGD	O4'-C4'-C5'	-2.26	102.09	109.33
7	G	1251	PCI	C1-C2-C3	-2.26	119.25	121.16
7	C	1252	PCI	C6-C1-C2	2.24	120.18	117.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	C5-C6-N1	2.24	118.94	113.25
7	C	1252	PCI	C1-C6-CL5	2.20	120.75	118.09
5	E	1766	MGD	O17-C17-N18	2.19	124.23	120.11
5	E	1766	MGD	C6-C5-N7	2.19	134.27	130.29
5	E	1765	MGD	O2B-PB-O3B	-2.19	101.36	107.27
5	E	1765	MGD	C19-N18-C17	-2.18	121.15	125.11
5	A	1765	MGD	C16-C17-N18	2.16	118.07	112.13
5	A	1765	MGD	C2'-C1'-N9	2.14	119.20	113.25
5	E	1765	MGD	N2-C2-N1	2.13	121.25	116.76
5	A	1766	MGD	C2'-C1'-N9	2.11	119.13	113.25
5	E	1766	MGD	C4'-O4'-C1'	-2.07	104.91	109.47
5	A	1766	MGD	N18-C19-N20	2.03	127.03	123.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
5	A	1765	MGD	C5'-O5'-PB-O3B
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	PA-O3B-PB-O1B

There are no ring outliers.

13 monomers are involved in 52 short contacts:

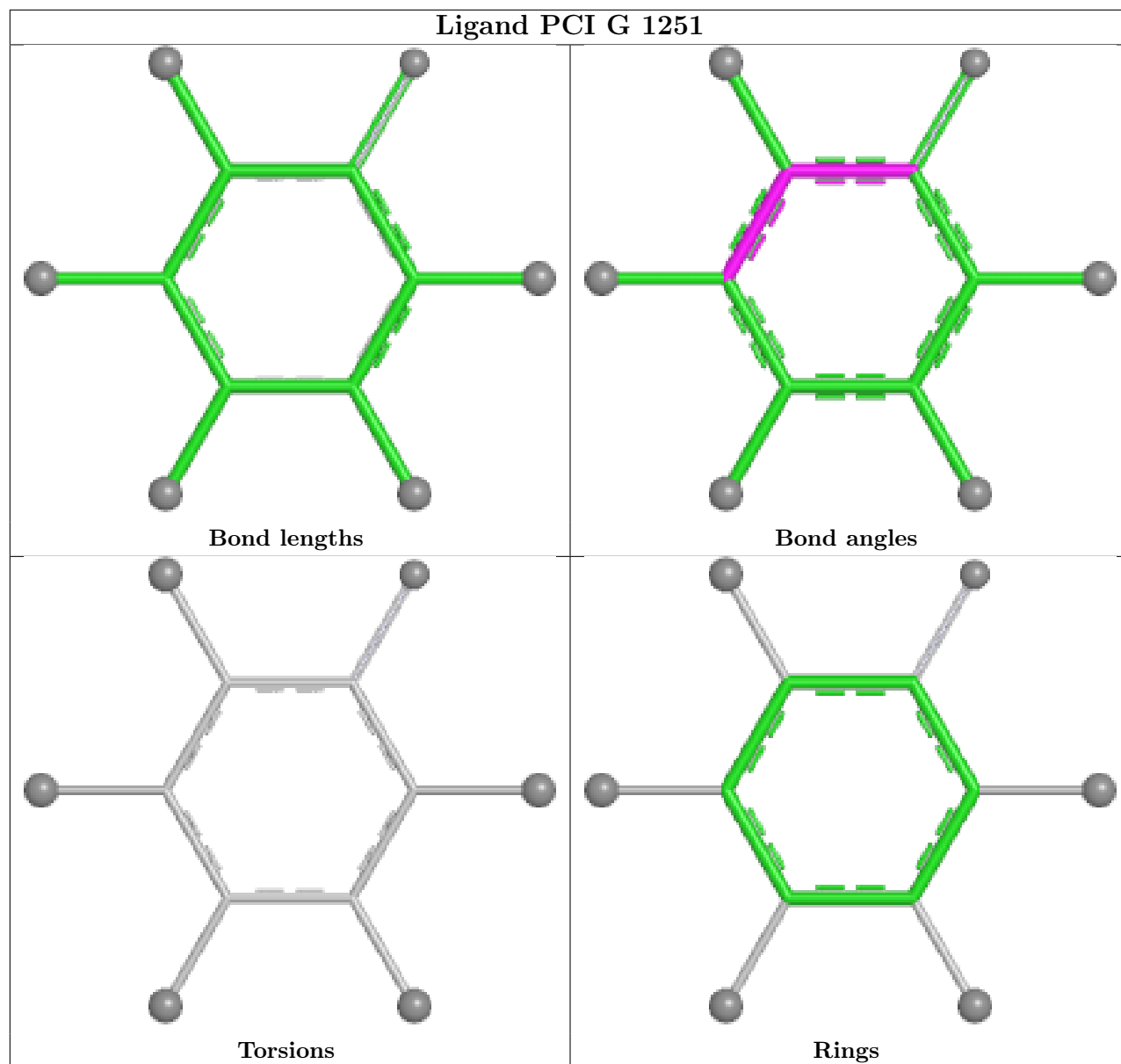
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1196	SF4	2	0
7	G	1251	PCI	11	0
5	E	1765	MGD	5	0
5	A	1766	MGD	3	0
4	F	1196	SF4	1	0
4	F	1194	SF4	3	0
4	F	1195	SF4	2	0
5	A	1765	MGD	4	0
4	B	1195	SF4	1	0
5	E	1766	MGD	7	0

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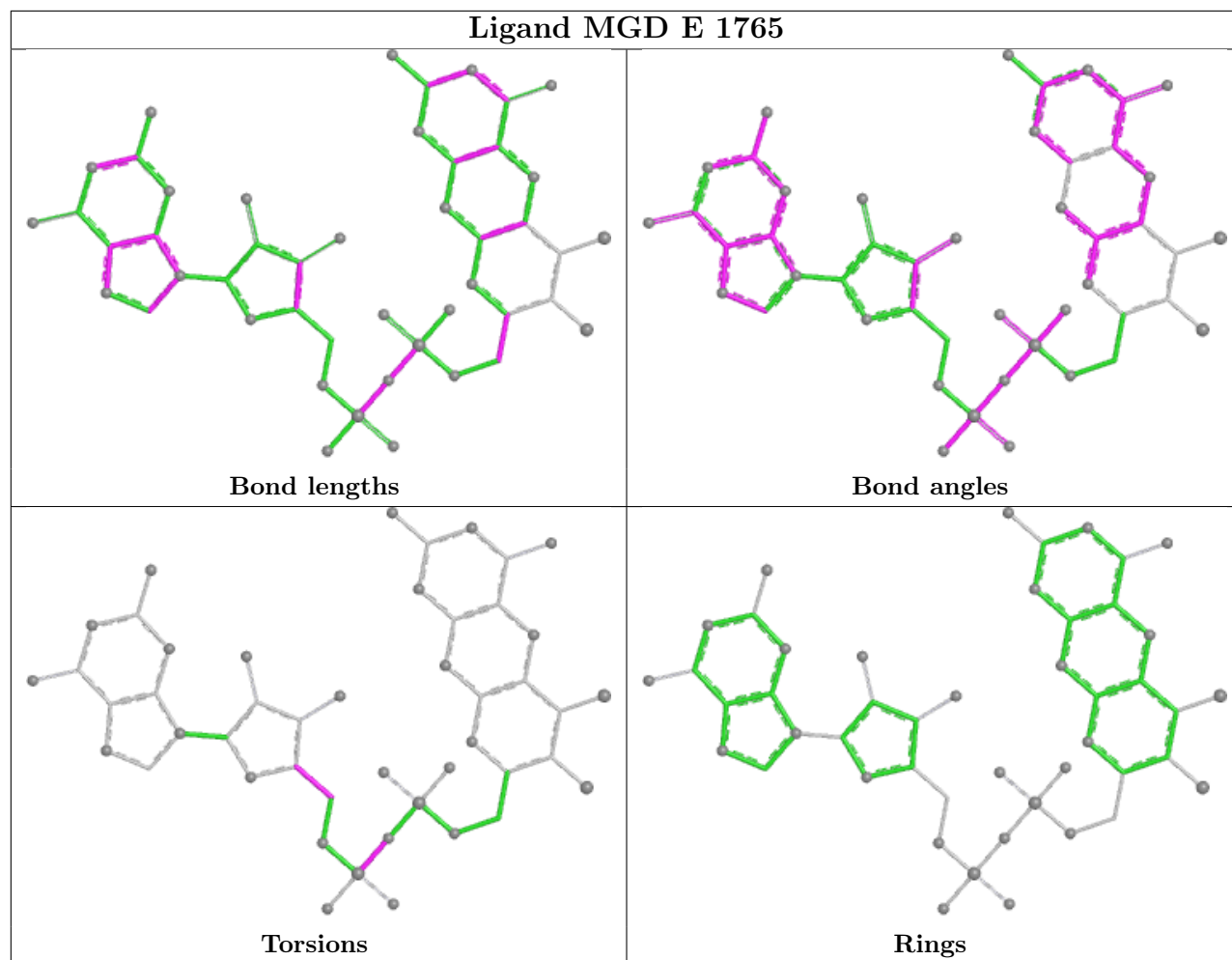
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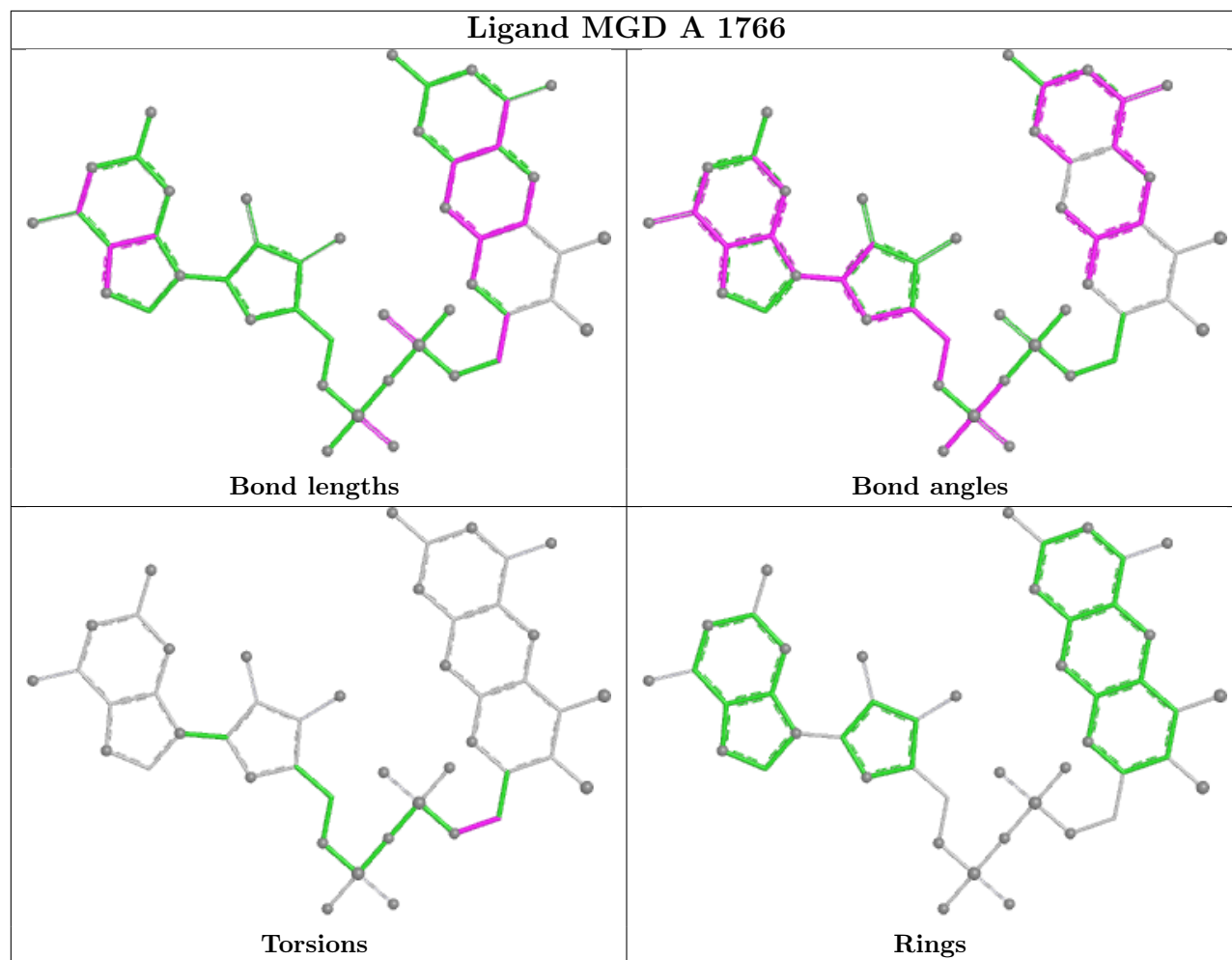
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1252	PCI	11	0
4	E	1764	SF4	1	0
4	B	1194	SF4	1	0

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 than 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.

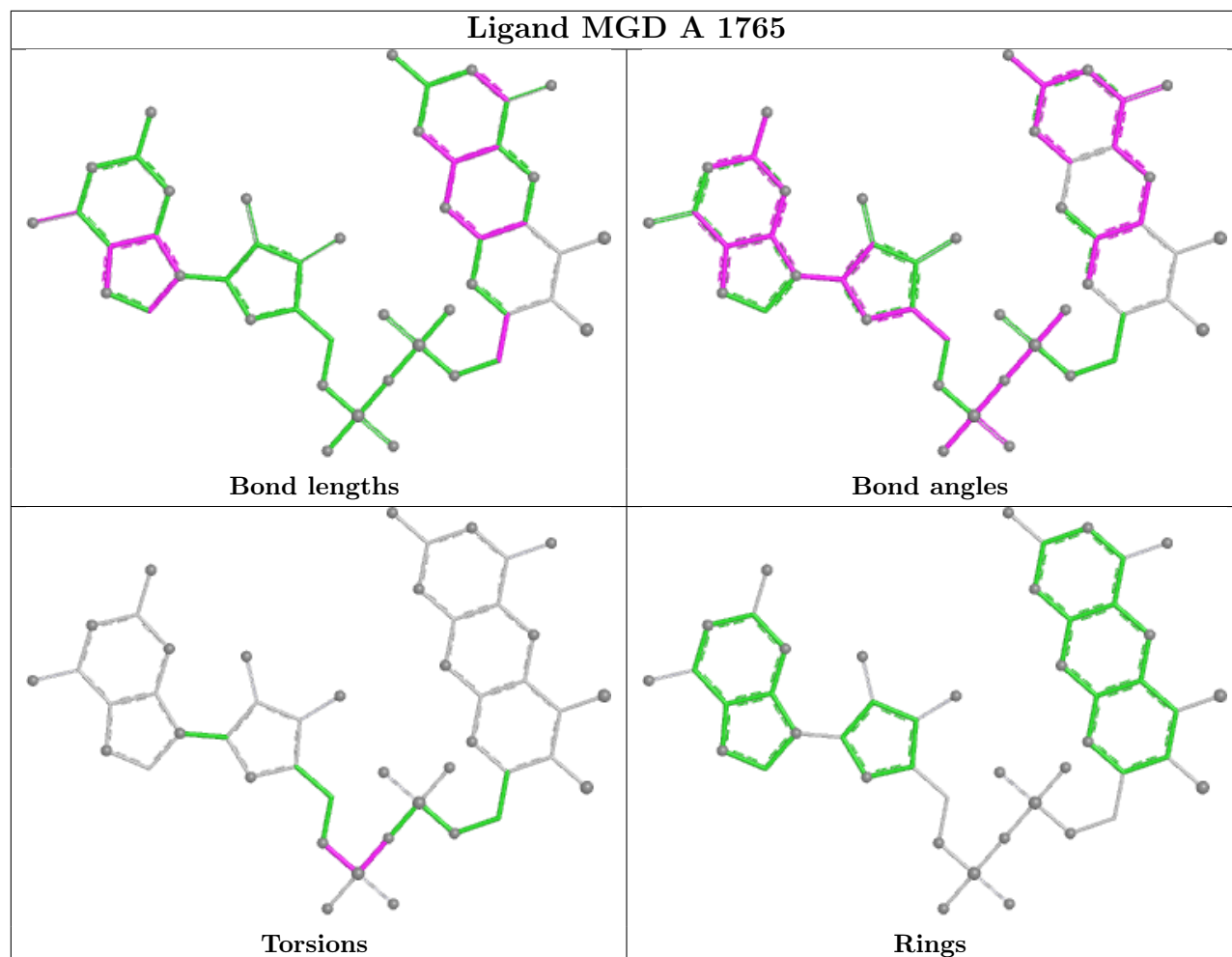


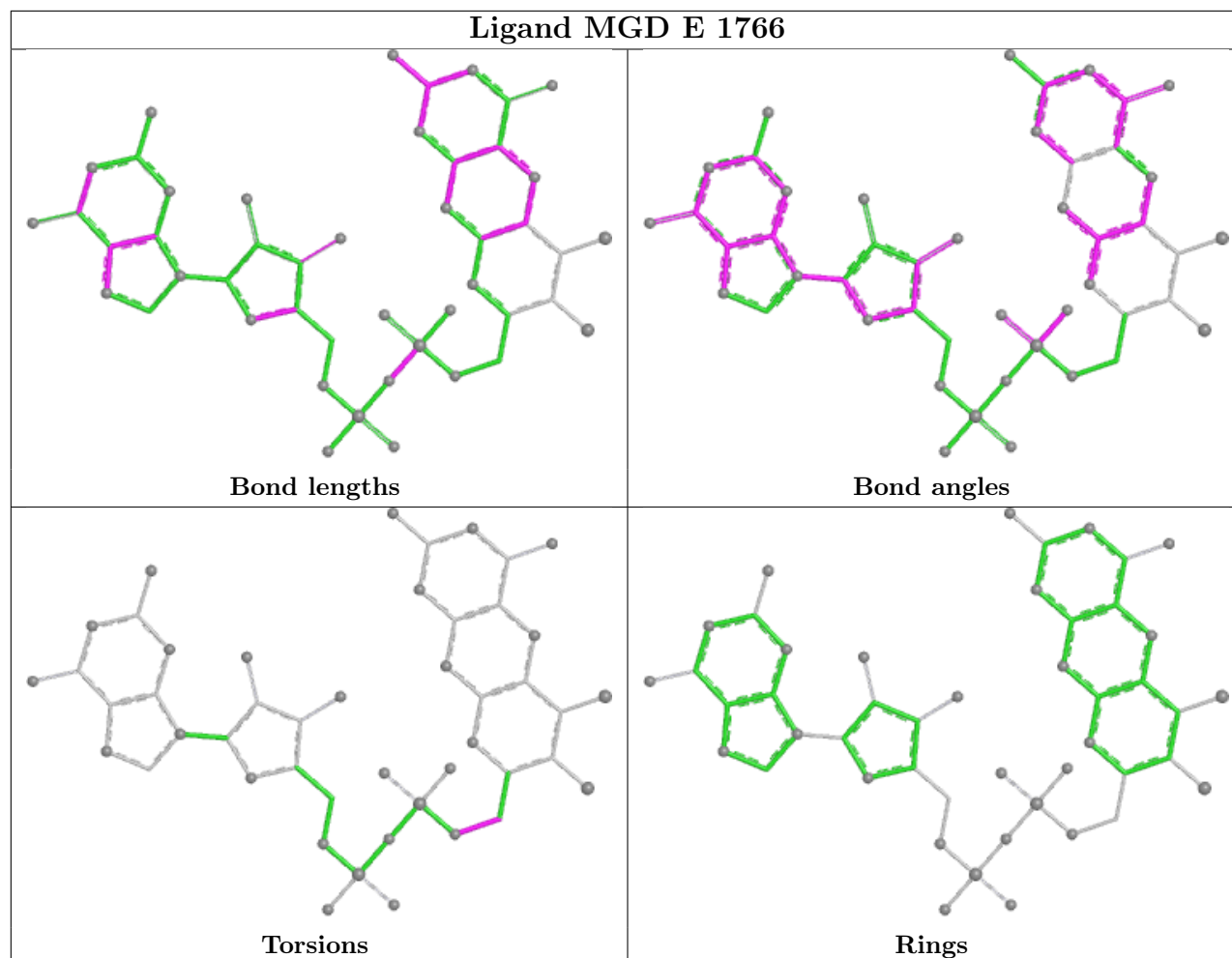
Ligand MGD E 1765

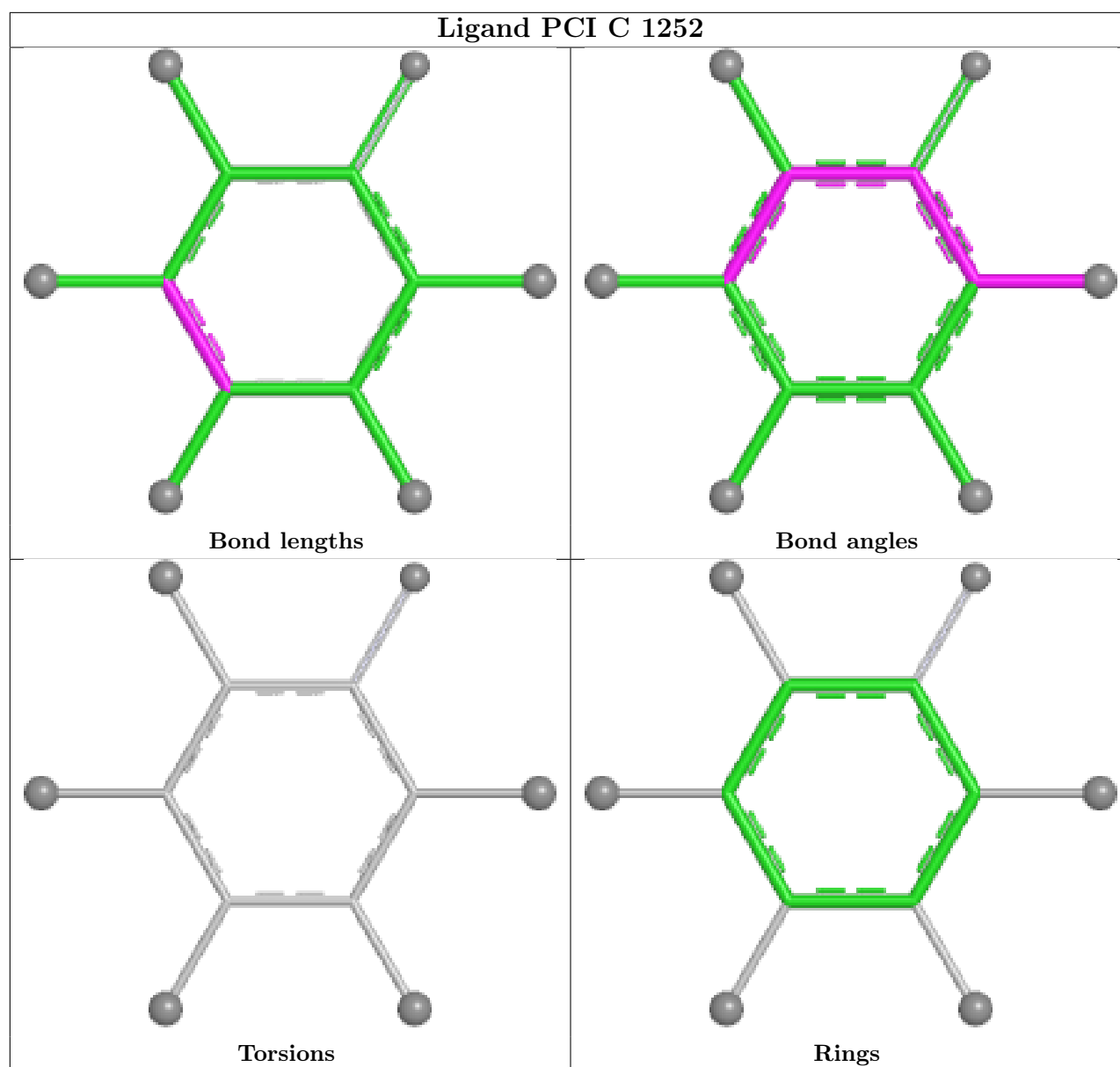




Ligand MGD A 1765







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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	735/765 (96%)	2.07	311 (42%) 0 0	27, 53, 85, 139	0
1	E	735/765 (96%)	1.68	229 (31%) 1 1	27, 52, 83, 141	0
2	B	194/195 (99%)	1.58	60 (30%) 1 1	29, 46, 70, 94	0
2	F	194/195 (99%)	1.85	77 (39%) 1 0	34, 51, 72, 93	0
3	C	251/253 (99%)	2.29	134 (53%) 0 0	35, 59, 85, 103	0
3	G	251/253 (99%)	2.80	165 (65%) 0 0	37, 68, 97, 111	0
All	All	2360/2426 (97%)	1.99	976 (41%) 0 0	27, 54, 86, 141	0

All (976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	252	GLY	19.7
3	G	251	GLY	17.4
1	A	764	ARG	14.9
1	A	607	VAL	13.3
1	A	583	PHE	11.0
1	A	586	ALA	9.7
3	C	111	GLY	9.7
1	A	606	PRO	9.5
1	A	362	GLY	9.5
1	E	592	LEU	9.1
1	A	592	LEU	8.7
1	E	600	ALA	8.6
1	E	607	VAL	8.4
1	E	398	PRO	8.0
1	E	764	ARG	7.5
3	G	63	LEU	7.4
3	G	49	THR	7.1
1	A	401	PHE	7.1
1	A	585	THR	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	605	LEU	7.0
3	G	69	ALA	7.0
2	F	1	MET	6.9
1	A	285	GLY	6.9
1	E	396	HIS	6.8
1	A	591	GLU	6.8
3	G	62	ILE	6.7
3	C	75	THR	6.5
1	E	584	GLY	6.4
3	G	76	ILE	6.3
2	B	1	MET	6.2
1	A	385	ALA	6.0
1	E	599	GLU	6.0
1	E	468	LEU	6.0
1	E	323	LYS	6.0
1	A	608	PHE	6.0
1	A	284	VAL	5.9
1	E	593	TYR	5.9
3	C	223	GLN	5.9
1	A	590	ILE	5.9
1	E	30	ALA	5.9
1	E	384	ALA	5.9
1	E	393	GLY	5.9
3	G	221	TRP	5.8
1	A	632	ALA	5.8
1	A	207	GLY	5.8
1	E	590	ILE	5.8
1	A	384	ALA	5.8
1	E	397	GLU	5.8
1	E	469	PRO	5.7
1	A	685	THR	5.7
1	E	394	GLY	5.7
3	G	28	GLY	5.7
3	C	68	SER	5.7
3	G	27	ALA	5.7
1	A	42	GLN	5.7
3	C	226	LEU	5.7
1	E	591	GLU	5.7
1	A	584	GLY	5.7
3	G	171	ALA	5.6
1	A	391	PRO	5.6
2	F	194	HIS	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	570	PRO	5.6
3	C	222	TRP	5.5
3	C	114	ARG	5.5
1	E	582	PRO	5.5
3	C	69	PRO	5.5
1	E	608	PHE	5.4
3	G	207	PHE	5.4
1	E	392	SER	5.4
1	A	515	THR	5.4
1	A	603	GLN	5.3
2	B	44	GLY	5.3
1	E	401	PHE	5.3
3	C	63	ILE	5.3
1	A	386	GLY	5.3
1	E	391	PRO	5.3
2	F	2	PRO	5.3
1	E	595	GLN	5.3
1	E	597	PHE	5.2
3	G	45	ALA	5.2
3	G	206	GLY	5.2
2	F	71	PRO	5.2
3	G	55	LEU	5.2
2	B	46	TYR	5.2
1	E	596	ARG	5.1
1	A	398	PRO	5.1
1	A	361	GLY	5.1
3	G	36	LEU	5.1
3	G	66	GLU	5.1
1	A	597	PHE	5.1
1	E	385	ALA	5.1
3	C	95	GLY	5.0
1	E	508	ALA	5.0
1	A	548	LEU	5.0
3	C	64	LEU	5.0
1	A	686	ALA	5.0
1	A	364	TYR	5.0
1	A	40	VAL	5.0
3	G	39	LEU	5.0
3	G	101	THR	5.0
3	G	116	ALA	4.9
1	A	55	ALA	4.9
1	E	685	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	606	PRO	4.9
1	A	596	ARG	4.8
3	G	68	PRO	4.8
1	E	585	THR	4.8
1	A	537	TRP	4.8
1	E	478	VAL	4.8
2	F	68	PRO	4.8
1	A	535	PHE	4.8
3	C	208	PHE	4.8
3	G	64	TRP	4.8
3	C	224	GLU	4.8
1	A	63	TYR	4.8
1	E	603	GLN	4.7
3	G	78	LEU	4.7
1	E	383	PRO	4.7
1	E	470	GLN	4.7
1	E	628	VAL	4.7
1	A	730	GLY	4.7
3	C	115	ALA	4.7
1	A	395	ASP	4.7
1	E	113	ARG	4.6
1	A	270	TYR	4.6
3	G	59	ASP	4.6
1	E	568	GLY	4.6
1	A	57	ALA	4.6
1	E	579	GLY	4.6
1	E	36	GLU	4.6
3	G	104	LEU	4.6
3	G	174	PRO	4.5
3	G	53	LEU	4.5
1	A	526	GLY	4.5
3	G	77	TRP	4.5
3	G	117	TRP	4.5
1	E	467	VAL	4.5
1	E	389	SER	4.5
3	G	10	GLN	4.5
1	A	30	ALA	4.5
3	C	108	LEU	4.5
2	B	4	TYR	4.5
1	A	117	TRP	4.5
1	A	389	SER	4.5
3	G	178	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	342	TYR	4.4
3	G	65	ALA	4.4
1	E	387	GLY	4.4
2	F	113	VAL	4.4
2	F	193	HIS	4.4
3	C	70	ALA	4.4
3	C	172	ALA	4.4
1	A	582	PRO	4.4
1	E	567	ARG	4.4
3	G	113	ARG	4.4
3	G	1	ALA	4.4
1	E	622	LEU	4.4
1	A	293	VAL	4.4
1	E	537	TRP	4.4
1	A	394	GLY	4.3
3	C	26	GLY	4.3
1	E	605	LEU	4.3
1	E	632	ALA	4.3
3	G	163	ALA	4.3
1	A	387	GLY	4.3
3	C	71	ARG	4.3
3	G	170	TRP	4.3
1	A	561	MET	4.3
2	B	115	LYS	4.3
1	E	34	ALA	4.3
1	E	594	CYS	4.3
1	A	396	HIS	4.3
1	E	730	GLY	4.3
1	A	43	ILE	4.3
1	A	335	VAL	4.3
1	A	569	LYS	4.3
1	A	571	TRP	4.2
1	A	678	GLY	4.2
1	E	390	GLY	4.2
3	G	109	LYS	4.2
3	G	48	TYR	4.2
1	A	76	GLY	4.2
1	E	386	GLY	4.2
2	F	170	GLY	4.2
3	C	78	TRP	4.2
2	F	74	ALA	4.2
1	E	588	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	G	102	GLY	4.2
1	E	581	LEU	4.2
3	G	34	ALA	4.2
1	A	595	GLN	4.2
1	E	574	ASP	4.2
1	A	95	LEU	4.2
1	A	544	LEU	4.2
1	E	381	LEU	4.2
3	C	174	PHE	4.2
3	G	160	LEU	4.2
2	B	193	HIS	4.2
3	G	67	SER	4.1
1	A	102	VAL	4.1
1	E	575	TRP	4.1
3	C	206	ALA	4.1
3	G	35	ALA	4.1
3	G	33	LEU	4.1
3	G	107	LEU	4.1
3	G	99	PHE	4.1
3	C	112	SER	4.1
3	G	42	ASP	4.1
1	A	337	TYR	4.1
1	A	421	ILE	4.1
1	A	594	CYS	4.1
3	G	162	LEU	4.1
3	C	65	TRP	4.1
3	G	129	TYR	4.1
2	B	72	THR	4.1
3	C	37	LEU	4.1
2	F	95	ALA	4.0
3	G	17	ASN	4.0
1	A	589	LYS	4.0
2	B	123	LEU	4.0
2	B	124	GLU	4.0
1	A	587	SER	4.0
3	G	23	LEU	4.0
1	A	547	ARG	4.0
3	G	226	ALA	4.0
1	A	400	GLY	4.0
1	A	540	ILE	4.0
3	G	88	ILE	4.0
3	G	74	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	429	PRO	4.0
1	A	289	LEU	3.9
3	C	40	LEU	3.9
3	G	58	LEU	3.9
3	G	157	VAL	3.9
1	A	36	GLU	3.9
1	A	349	TYR	3.9
1	A	593	TYR	3.9
1	E	286	PHE	3.9
1	A	365	ILE	3.9
2	B	134	THR	3.9
3	G	93	TRP	3.9
1	A	230	ALA	3.9
2	B	145	LEU	3.9
2	F	123	LEU	3.9
3	C	173	LEU	3.9
2	B	79	LYS	3.9
1	A	32	TRP	3.9
3	G	30	VAL	3.9
1	A	430	TYR	3.9
1	A	534	TYR	3.9
2	F	92	ALA	3.9
3	C	113	GLN	3.9
1	A	48	PHE	3.8
3	G	118	ALA	3.8
3	G	122	PHE	3.8
1	E	400	GLY	3.8
3	G	60	LEU	3.8
1	A	729	SER	3.8
2	B	85	VAL	3.8
3	C	94	TRP	3.8
3	G	89	TRP	3.8
2	F	44	GLY	3.8
3	C	79	LEU	3.8
1	A	501	PHE	3.8
3	C	66	ALA	3.8
3	C	74	PHE	3.8
3	G	110	GLY	3.8
1	E	133	GLU	3.8
2	F	84	LEU	3.8
2	F	91	ILE	3.8
3	C	67	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
3	G	119	LEU	3.8
1	E	39	SER	3.7
1	E	495	VAL	3.7
3	G	224	ARG	3.7
1	A	159	ALA	3.7
1	A	286	PHE	3.7
1	A	553	LEU	3.7
3	G	106	TYR	3.7
3	G	175	LEU	3.7
1	A	392	SER	3.7
3	C	169	SER	3.7
1	E	55	ALA	3.7
1	A	507	PRO	3.7
1	A	64	LYS	3.7
2	B	127	LYS	3.7
1	A	563	THR	3.7
2	F	85	VAL	3.7
3	G	111	SER	3.7
3	G	75	HIS	3.7
3	C	221	PHE	3.7
3	C	77	ILE	3.7
3	G	95	LEU	3.7
1	A	506	THR	3.7
3	G	125	VAL	3.7
3	C	250	GLY	3.7
3	G	220	PHE	3.7
1	E	572	LEU	3.7
3	G	250	LEU	3.7
3	G	169	PRO	3.7
1	A	296	PHE	3.6
1	E	67	GLY	3.6
2	B	81	GLY	3.6
1	A	38	LYS	3.6
2	B	125	LYS	3.6
2	B	16	CYS	3.6
1	A	371	LEU	3.6
1	A	390	GLY	3.6
1	E	583	PHE	3.6
3	G	100	LEU	3.6
3	G	161	GLY	3.6
1	A	604	PRO	3.6
1	A	283	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	117	THR	3.6
3	C	118	TRP	3.6
2	F	79	LYS	3.6
3	G	155	ALA	3.6
3	G	61	PHE	3.6
1	A	663	GLU	3.6
1	A	538	LYS	3.6
3	G	22	VAL	3.6
3	G	47	ARG	3.6
3	G	32	LEU	3.6
1	E	421	ILE	3.6
1	E	498	LYS	3.5
1	A	374	TYR	3.5
1	E	580	ARG	3.5
1	E	586	ALA	3.5
3	C	46	ALA	3.5
3	G	56	ILE	3.5
2	F	117	THR	3.5
1	A	34	ALA	3.5
3	C	56	LEU	3.5
1	A	602	HIS	3.5
1	E	287	GLU	3.5
1	A	388	CYS	3.5
3	C	107	TYR	3.5
1	A	186	GLY	3.5
3	C	119	ALA	3.5
3	G	91	GLY	3.5
1	A	546	THR	3.5
1	A	549	GLN	3.5
1	A	531	LEU	3.5
1	A	67	GLY	3.5
1	A	518	GLY	3.5
2	F	112	TYR	3.5
1	A	467	VAL	3.4
3	C	59	LEU	3.4
3	C	105	LEU	3.4
1	E	601	GLY	3.4
1	A	70	ALA	3.4
1	A	397	GLU	3.4
3	G	166	LEU	3.4
2	F	136	PRO	3.4
3	G	114	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	114	SER	3.4
3	G	38	HIS	3.4
3	G	73	PHE	3.4
1	E	395	ASP	3.4
1	E	32	TRP	3.4
1	E	531	LEU	3.4
3	G	50	LEU	3.4
1	A	369	PRO	3.4
3	C	109	GLY	3.4
3	G	52	ALA	3.4
1	A	277	GLU	3.4
1	E	66	GLU	3.4
1	E	578	GLU	3.4
2	B	142	PHE	3.4
1	E	569	LYS	3.4
1	A	493	VAL	3.4
1	A	486	LEU	3.3
1	E	298	PRO	3.3
1	A	588	GLY	3.3
3	G	223	GLU	3.3
2	B	138	TYR	3.3
1	A	339	ASP	3.3
1	A	298	PRO	3.3
1	A	684	PRO	3.3
1	A	568	GLY	3.3
2	B	110	ALA	3.3
1	A	431	PRO	3.3
2	F	107	LEU	3.3
1	E	37	VAL	3.3
1	A	288	GLU	3.3
1	A	484	THR	3.3
1	E	285	GLY	3.3
2	B	73	GLY	3.3
2	F	111	GLY	3.3
3	G	44	GLU	3.3
3	C	53	ALA	3.3
1	E	577	LYS	3.3
3	G	82	PHE	3.3
1	A	692	CYS	3.3
1	E	525	LEU	3.3
2	F	133	GLU	3.3
2	F	192	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	508	ALA	3.3
3	G	159	ALA	3.3
1	E	635	GLN	3.2
1	A	527	LEU	3.2
1	E	555	LEU	3.2
1	E	564	LEU	3.2
2	F	16	CYS	3.2
3	C	96	LEU	3.2
2	B	194	HIS	3.2
1	A	62	VAL	3.2
1	A	634	THR	3.2
2	B	120	ALA	3.2
3	C	80	PHE	3.2
1	A	33	TYR	3.2
1	A	558	MET	3.2
2	F	70	CYS	3.2
1	A	54	VAL	3.2
1	A	125	ALA	3.2
3	G	13	TRP	3.2
1	E	407	LYS	3.2
3	C	110	LYS	3.2
1	E	70	ALA	3.2
3	G	18	ALA	3.2
3	G	164	ALA	3.2
1	E	151	TRP	3.2
1	E	541	GLU	3.2
3	C	41	LYS	3.2
3	G	37	LEU	3.2
1	E	489	TYR	3.2
1	A	393	GLY	3.2
1	A	601	GLY	3.2
3	G	25	GLY	3.2
1	A	465	ILE	3.2
3	C	227	ALA	3.1
3	G	21	PHE	3.1
1	A	490	ASP	3.1
3	C	61	LEU	3.1
3	G	225	LEU	3.1
1	A	267	VAL	3.1
2	B	128	VAL	3.1
1	A	502	ILE	3.1
1	E	117	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	604	PRO	3.1
3	C	60	ASP	3.1
1	A	504	LEU	3.1
1	A	555	LEU	3.1
1	E	512	LEU	3.1
3	G	97	LEU	3.1
1	E	284	VAL	3.1
3	C	29	GLY	3.1
1	A	485	TYR	3.1
3	C	2	ALA	3.1
3	C	62	PHE	3.1
3	G	26	LEU	3.1
3	G	168	SER	3.1
1	A	495	VAL	3.1
1	A	505	ARG	3.1
1	A	530	GLY	3.1
1	A	282	TYR	3.1
3	G	222	GLN	3.1
1	A	577	LYS	3.1
3	G	57	ALA	3.1
1	A	128	MET	3.1
1	A	536	PRO	3.1
1	A	295	ASP	3.1
3	C	54	LEU	3.1
3	C	163	LEU	3.1
2	B	114	SER	3.1
1	E	519	TRP	3.1
1	E	355	GLY	3.1
3	G	108	GLY	3.1
1	A	434	GLY	3.0
3	G	41	GLY	3.0
1	A	65	VAL	3.0
1	E	283	THR	3.0
2	B	74	ALA	3.0
1	E	31	PRO	3.0
1	A	129	LEU	3.0
1	E	388	CYS	3.0
1	E	413	ARG	3.0
1	A	294	LYS	3.0
1	A	58	VAL	3.0
2	F	72	THR	3.0
2	B	121	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	581	LEU	3.0
3	G	165	LEU	3.0
1	A	598	LYS	3.0
1	E	310	GLN	3.0
3	C	86	THR	3.0
3	C	165	ALA	3.0
3	G	115	LEU	3.0
1	E	565	VAL	2.9
1	A	116	THR	2.9
1	E	630	THR	2.9
3	C	182	ALA	2.9
1	A	380	PRO	2.9
2	F	4	TYR	2.9
2	F	138	TYR	2.9
3	G	105	LEU	2.9
3	C	117	ALA	2.9
1	A	151	TRP	2.9
1	A	520	TRP	2.9
3	G	124	LEU	2.9
1	A	492	PHE	2.9
2	B	146	GLU	2.9
2	B	135	CYS	2.9
1	A	609	THR	2.9
3	C	220	THR	2.9
2	F	104	ALA	2.9
2	B	49	LEU	2.9
3	C	166	LEU	2.9
1	A	49	TRP	2.9
1	A	543	TYR	2.9
1	E	535	PHE	2.9
1	E	549	GLN	2.9
1	E	362	GLY	2.9
3	C	207	GLY	2.9
2	F	83	VAL	2.9
1	E	402	LYS	2.9
1	A	383	PRO	2.9
1	A	41	TYR	2.9
1	A	370	TYR	2.9
3	C	49	TYR	2.9
1	E	678	GLY	2.9
1	A	509	HIS	2.8
1	E	62	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	89	THR	2.8
1	A	610	PRO	2.8
1	A	461	LEU	2.8
3	C	27	LEU	2.8
1	A	183	TRP	2.8
1	E	561	MET	2.8
1	E	513	PHE	2.8
1	E	573	GLU	2.8
1	E	63	TYR	2.8
1	A	488	ARG	2.8
3	G	40	LYS	2.8
3	G	249	GLY	2.8
3	C	82	SER	2.8
3	C	44	ALA	2.8
3	C	101	LEU	2.8
1	E	466	ASP	2.8
1	A	363	PHE	2.8
1	E	296	PHE	2.8
3	G	15	TRP	2.8
3	G	79	PHE	2.8
1	A	156	LEU	2.8
1	A	273	LEU	2.8
1	A	468	LEU	2.8
1	A	494	LEU	2.8
1	A	512	LEU	2.8
1	E	280	ALA	2.8
1	E	289	LEU	2.8
2	F	82	LEU	2.8
3	G	120	LEU	2.8
3	G	112	GLN	2.8
3	G	151	PHE	2.8
1	A	358	GLY	2.8
2	F	32	GLY	2.8
1	A	184	VAL	2.8
1	A	120	ALA	2.8
2	B	84	LEU	2.8
3	C	241	LEU	2.8
3	G	158	LEU	2.8
1	A	510	GLU	2.8
1	E	490	ASP	2.8
2	B	170	GLY	2.7
1	A	189	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	380	PRO	2.7
1	E	500	PRO	2.7
3	C	178	VAL	2.7
1	E	268	LEU	2.7
3	G	126	ALA	2.7
1	E	292	HIS	2.7
1	E	602	HIS	2.7
3	G	14	HIS	2.7
1	A	432	ILE	2.7
1	A	728	ILE	2.7
1	E	324	PRO	2.7
1	A	68	TYR	2.7
1	A	262	LEU	2.7
1	A	459	LEU	2.7
3	G	215	LEU	2.7
1	A	496	ALA	2.7
2	F	110	ALA	2.7
1	E	50	ARG	2.7
1	A	541	GLU	2.7
1	E	288	GLU	2.7
2	F	96	CYS	2.7
1	E	48	PHE	2.7
1	E	570	PRO	2.7
1	A	279	VAL	2.7
1	A	300	TRP	2.7
1	A	575	TRP	2.7
1	E	520	TRP	2.7
1	E	662	LYS	2.7
3	C	51	LEU	2.7
3	C	116	LEU	2.7
3	C	168	LYS	2.7
3	G	156	LEU	2.7
1	A	50	ARG	2.7
1	E	120	ALA	2.7
1	E	763	ARG	2.7
3	G	229	ALA	2.7
1	A	542	GLU	2.7
1	E	760	PHE	2.7
2	B	136	PRO	2.7
1	A	550	SER	2.7
1	E	504	LEU	2.7
2	B	188	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	33	TYR	2.7
1	A	519	TRP	2.7
1	A	557	THR	2.7
2	F	149	GLU	2.7
3	C	91	TRP	2.7
2	F	86	ASP	2.6
3	C	219	GLY	2.6
3	G	94	GLY	2.6
1	A	53	ILE	2.6
2	B	58	CYS	2.6
2	B	65	PRO	2.6
2	F	97	ILE	2.6
1	A	94	ARG	2.6
3	C	73	ARG	2.6
1	A	172	LEU	2.6
1	A	529	LEU	2.6
3	G	123	SER	2.6
1	A	301	ALA	2.6
1	A	476	ALA	2.6
1	E	291	ALA	2.6
2	B	112	TYR	2.6
2	F	78	THR	2.6
3	G	92	ALA	2.6
3	G	103	GLY	2.6
1	E	429	PRO	2.6
3	G	227	PRO	2.6
1	A	708	LEU	2.6
3	G	172	LEU	2.6
1	A	66	GLU	2.6
1	A	487	GLU	2.6
1	E	293	VAL	2.6
1	E	382	GLU	2.6
1	E	563	THR	2.6
2	F	120	ALA	2.6
3	C	160	ALA	2.6
3	G	90	TRP	2.6
3	G	96	GLY	2.6
1	E	540	ILE	2.6
3	C	225	ARG	2.6
1	A	155	PHE	2.6
3	C	33	LEU	2.6
3	G	132	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	214	LEU	2.6
3	G	231	LEU	2.6
1	E	40	VAL	2.6
1	E	125	ALA	2.6
3	G	205	ALA	2.6
1	A	266	HIS	2.6
1	E	64	LYS	2.6
1	A	61	ARG	2.6
1	E	434	GLY	2.6
2	F	87	PRO	2.6
3	C	103	GLY	2.6
3	G	218	GLY	2.6
1	A	651	ILE	2.6
1	A	152	PHE	2.6
1	A	381	LEU	2.6
2	F	145	LEU	2.6
1	E	279	VAL	2.6
2	F	99	ALA	2.6
3	G	133	ALA	2.6
1	A	290	LYS	2.6
2	F	148	PRO	2.5
3	C	228	PRO	2.5
1	E	54	VAL	2.5
1	A	373	LYS	2.5
1	A	305	THR	2.5
3	C	50	THR	2.5
3	G	176	ARG	2.5
1	A	274	TYR	2.5
1	A	118	GLU	2.5
3	C	251	LEU	2.5
1	A	114	VAL	2.5
1	A	402	LYS	2.5
1	E	65	VAL	2.5
3	G	242	VAL	2.5
3	C	198	ALA	2.5
1	E	484	THR	2.5
1	A	746	ARG	2.5
2	B	100	CYS	2.5
2	B	119	CYS	2.5
1	A	511	PRO	2.5
3	C	52	TYR	2.5
1	E	338	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	358	GLY	2.5
1	E	562	GLY	2.5
1	A	599	GLU	2.5
1	A	224	LEU	2.5
3	C	215	LEU	2.5
1	A	533	GLN	2.5
1	A	523	ARG	2.5
1	E	301	ALA	2.5
1	E	557	THR	2.5
3	G	154	THR	2.5
2	F	131	CYS	2.5
1	E	536	PRO	2.5
2	B	2	PRO	2.5
2	F	76	TYR	2.5
1	A	96	LYS	2.5
1	A	572	LEU	2.5
1	E	527	LEU	2.5
3	C	171	TRP	2.5
1	A	748	ARG	2.5
1	E	515	THR	2.5
1	A	69	GLU	2.4
1	A	552	GLY	2.4
2	B	191	GLU	2.4
1	A	357	TYR	2.4
1	A	491	ASP	2.4
3	G	51	TYR	2.4
1	E	553	LEU	2.4
3	C	167	LEU	2.4
3	G	173	PHE	2.4
1	A	97	ARG	2.4
3	G	239	ALA	2.4
1	E	634	THR	2.4
1	E	711	GLY	2.4
2	F	119	CYS	2.4
1	E	551	LEU	2.4
3	C	128	LEU	2.4
3	C	83	PHE	2.4
3	G	43	ALA	2.4
1	E	375	PRO	2.4
1	E	729	SER	2.4
1	A	281	LYS	2.4
1	E	457	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	47	CYS	2.4
1	E	53	ILE	2.4
2	F	93	CYS	2.4
1	A	420	LEU	2.4
1	E	220	GLN	2.4
3	C	176	LEU	2.4
1	A	567	ARG	2.4
2	F	121	HIS	2.4
1	E	282	TYR	2.4
1	A	513	PHE	2.4
2	F	118	PHE	2.4
1	E	706	MET	2.4
3	C	55	MET	2.4
1	A	656	ALA	2.4
1	E	57	ALA	2.4
1	E	571	TRP	2.4
1	A	31	PRO	2.4
1	A	399	GLU	2.4
1	E	663	GLU	2.4
2	F	81	GLY	2.4
1	A	307	ILE	2.4
1	A	376	LEU	2.4
1	A	554	ASP	2.4
1	E	752	LEU	2.4
3	C	232	LEU	2.4
3	G	19	LEU	2.4
2	F	90	CYS	2.4
1	A	150	TYR	2.4
2	B	192	VAL	2.4
1	A	516	LYS	2.4
1	A	522	ALA	2.4
3	G	167	LYS	2.4
3	G	235	ALA	2.4
1	A	539	THR	2.3
1	E	183	TRP	2.4
1	E	539	THR	2.3
1	E	530	GLY	2.3
1	E	560	GLY	2.3
2	B	77	GLN	2.3
1	A	272	ASP	2.3
3	C	218	LEU	2.3
3	G	54	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	760	PHE	2.3
1	E	462	TYR	2.3
2	F	67	VAL	2.3
2	B	27	ASN	2.3
1	A	576	GLU	2.3
1	E	399	GLU	2.3
1	A	415	THR	2.3
3	G	210	GLY	2.3
1	E	367	GLN	2.3
1	A	725	LEU	2.3
2	F	125	LYS	2.3
2	F	46	TYR	2.3
1	A	287	GLU	2.3
1	A	416	ALA	2.3
1	E	405	ALA	2.3
2	B	7	ALA	2.3
1	E	546	THR	2.3
2	B	137	THR	2.3
1	A	59	GLY	2.3
1	E	186	GLY	2.3
2	B	75	SER	2.3
1	A	78	LEU	2.3
2	B	82	LEU	2.3
3	C	121	LEU	2.3
3	C	179	LEU	2.3
1	E	370	TYR	2.3
2	F	69	VAL	2.3
2	F	128	VAL	2.3
1	A	464	ALA	2.3
1	E	412	ALA	2.3
2	B	104	ALA	2.3
3	C	127	ALA	2.3
3	G	181	ALA	2.3
1	A	132	ARG	2.3
2	F	3	ARG	2.3
3	C	15	HIS	2.3
3	G	98	GLY	2.3
1	A	425	ILE	2.3
3	G	185	LEU	2.3
3	G	213	LEU	2.3
1	E	589	LYS	2.3
2	F	142	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	511	PRO	2.3
2	F	105	ARG	2.3
2	F	135	CYS	2.3
3	C	190	TYR	2.3
3	G	8	ASN	2.2
3	G	70	ARG	2.3
3	G	152	PRO	2.3
1	A	304	HIS	2.2
1	E	56	HIS	2.2
1	E	76	GLY	2.2
3	C	76	HIS	2.2
1	E	544	LEU	2.2
1	E	728	ILE	2.2
3	C	233	LEU	2.2
3	G	153	LEU	2.2
1	A	761	ASP	2.2
3	C	229	TRP	2.2
3	C	45	GLU	2.2
1	E	411	PHE	2.2
3	G	71	PHE	2.2
1	A	412	ALA	2.2
3	C	187	ALA	2.2
3	C	230	ALA	2.2
3	G	31	ALA	2.2
3	C	130	TYR	2.2
1	A	292	HIS	2.2
1	E	116	THR	2.2
1	E	516	LYS	2.2
2	B	89	LYS	2.2
1	A	119	GLU	2.2
1	A	75	ARG	2.2
1	A	37	VAL	2.2
1	A	92	PRO	2.2
2	F	29	VAL	2.2
3	C	234	ALA	2.2
1	A	35	GLN	2.2
1	E	274	TYR	2.2
2	B	139	CYS	2.2
2	F	106	TYR	2.2
1	A	711	GLY	2.2
3	C	159	LEU	2.2
3	C	200	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	203	LEU	2.2
3	C	212	LEU	2.2
3	G	127	LEU	2.2
1	A	124	ILE	2.2
1	A	39	SER	2.2
1	E	550	SER	2.2
2	B	151	PRO	2.2
2	F	173	PRO	2.2
3	C	72	PHE	2.2
3	C	25	VAL	2.2
1	A	291	ALA	2.2
1	A	600	ALA	2.2
1	E	686	ALA	2.2
1	E	756	ALA	2.2
3	C	32	ALA	2.2
3	C	149	ALA	2.2
1	A	211	GLY	2.2
1	E	374	TYR	2.2
2	F	178	LEU	2.2
3	C	216	LEU	2.2
2	B	8	ILE	2.2
1	E	77	ARG	2.2
2	B	118	PHE	2.2
3	C	100	PHE	2.2
1	A	56	HIS	2.1
3	C	93	ALA	2.1
1	A	456	LEU	2.1
1	A	660	GLY	2.1
1	E	297	THR	2.1
2	B	126	GLY	2.1
1	A	573	GLU	2.1
1	E	523	ARG	2.1
1	E	295	ASP	2.1
1	A	247	HIS	2.1
1	A	497	HIS	2.1
1	E	58	VAL	2.1
1	E	493	VAL	2.1
1	E	35	GLN	2.1
1	E	558	MET	2.1
2	F	108	HIS	2.1
1	A	321	ALA	2.1
2	B	5	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	19	ALA	2.1
2	F	35	ASN	2.1
1	A	135	TYR	2.1
1	A	489	TYR	2.1
1	A	532	GLU	2.1
1	A	633	ARG	2.1
1	E	545	GLU	2.1
2	F	191	GLU	2.1
1	A	74	SER	2.1
1	E	587	SER	2.1
1	E	373	LYS	2.1
1	E	72	PRO	2.1
2	F	151	PRO	2.1
3	C	170	PRO	2.1
3	C	123	PHE	2.1
1	A	366	ALA	2.1
1	A	255	GLY	2.1
1	A	187	ARG	2.1
1	A	545	GLU	2.1
2	B	76	TYR	2.1
1	A	181	SER	2.1
1	A	759	PRO	2.1
1	E	759	PRO	2.1
2	B	6	MET	2.1
1	A	503	GLN	2.1
1	A	232	VAL	2.1
3	C	22	PHE	2.1
1	A	455	ALA	2.1
2	F	155	ALA	2.1
3	C	36	ALA	2.1
1	E	640	LEU	2.1
3	C	161	LEU	2.1
1	A	190	GLY	2.1
1	E	52	GLY	2.1
1	E	104	GLY	2.1
1	E	103	GLU	2.1
1	E	576	GLU	2.1
2	F	88	LYS	2.1
3	G	209	TYR	2.1
1	A	162	SER	2.1
3	G	87	PRO	2.1
1	A	478	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	152	PHE	2.0
2	F	98	ALA	2.0
1	A	121	LEU	2.0
1	E	99	LEU	2.0
1	E	224	LEU	2.0
1	E	621	LEU	2.0
3	C	125	LEU	2.0
3	C	192	LEU	2.0
3	G	217	LEU	2.0
1	A	109	GLU	2.0
2	F	124	GLU	2.0
1	E	281	LYS	2.0
1	E	41	TYR	2.0
1	A	240	SER	2.0
3	G	130	PRO	2.0
1	E	247	HIS	2.0
2	B	105	ARG	2.0
2	F	14	VAL	2.0
3	C	122	VAL	2.0
3	C	213	PHE	2.0
1	A	314	GLU	2.0
3	G	211	LEU	2.0
1	A	338	GLY	2.0
1	A	560	GLY	2.0
1	E	598	LYS	2.0
3	C	211	GLY	2.0
3	C	102	THR	2.0
3	C	209	TRP	2.0
1	E	196	ASP	2.0
2	F	30	PRO	2.0
1	A	462	TYR	2.0
1	E	509	HIS	2.0
2	F	150	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

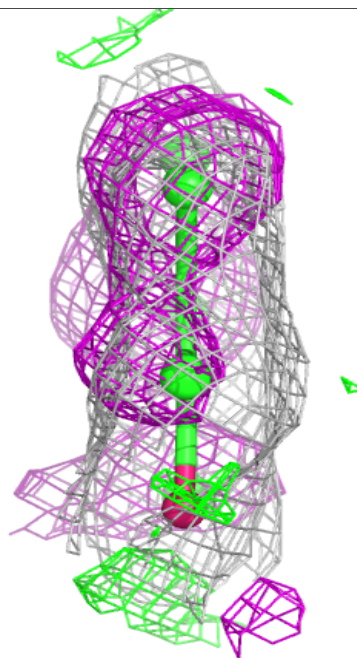
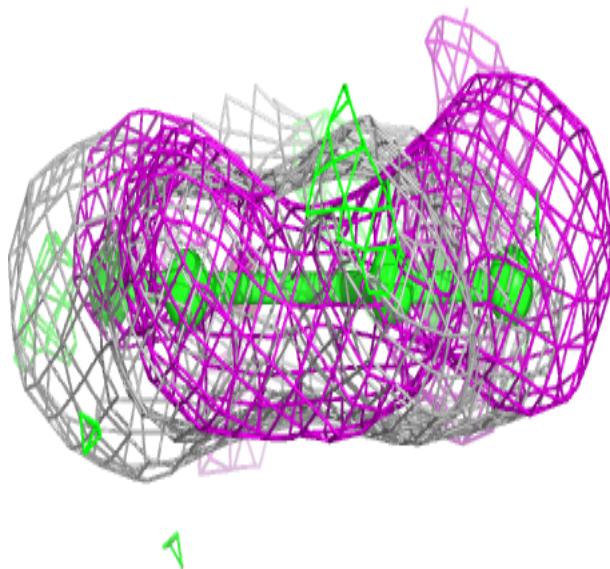
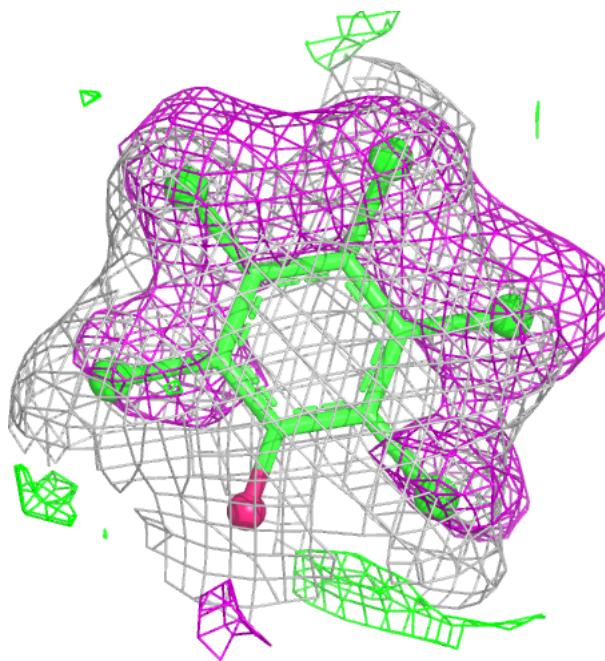
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PCI	G	1251	12/12	0.79	0.14	48,49,50,50	0
4	SF4	B	1194	8/8	0.83	0.14	70,71,72,73	0
4	SF4	F	1194	8/8	0.85	0.13	75,78,79,81	0
4	SF4	B	1196	8/8	0.85	0.16	47,53,56,58	0
7	PCI	C	1252	12/12	0.90	0.23	34,37,38,41	0
4	SF4	F	1196	8/8	0.91	0.11	42,45,47,48	0
5	MGD	A	1765	47/47	0.93	0.12	33,42,44,45	0
4	SF4	B	1195	8/8	0.93	0.09	47,50,52,53	0
4	SF4	F	1197	8/8	0.93	0.10	49,51,53,55	0
5	MGD	A	1766	47/47	0.94	0.11	29,36,41,42	0
5	MGD	E	1766	47/47	0.95	0.10	25,34,40,42	0
4	SF4	F	1195	8/8	0.95	0.07	38,43,44,44	0
5	MGD	E	1765	47/47	0.95	0.10	35,41,46,48	0
4	SF4	A	1764	8/8	0.96	0.07	35,41,42,44	0
6	MO	A	1767	1/1	0.97	0.06	42,42,42,42	0
4	SF4	B	1197	8/8	0.97	0.06	39,40,43,45	0
4	SF4	E	1764	8/8	0.97	0.07	37,42,46,46	0
6	MO	E	1767	1/1	0.99	0.03	32,32,32,32	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.

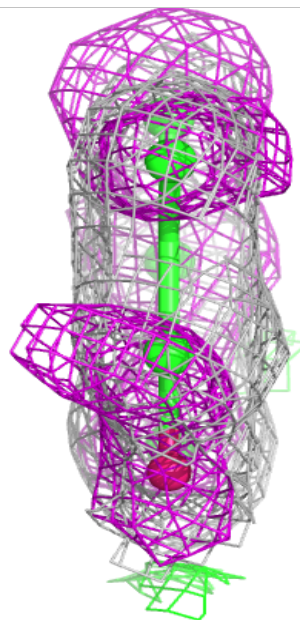
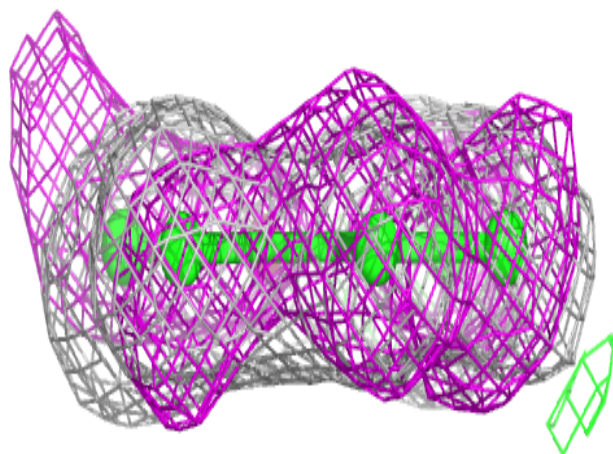
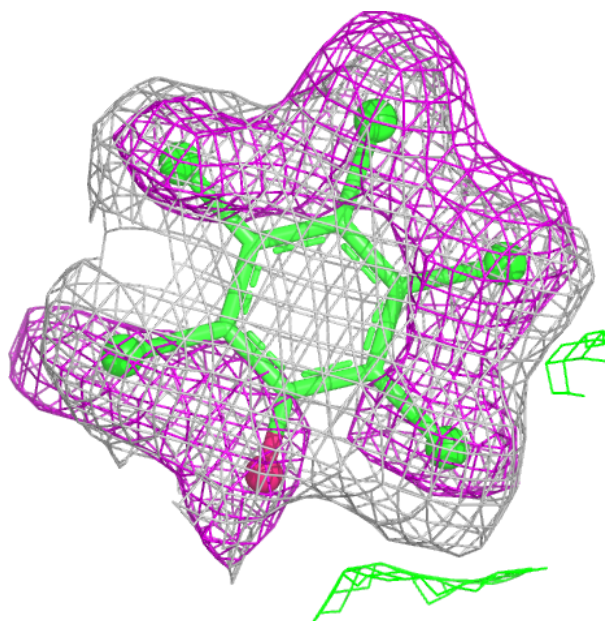
Electron density around PCI G 1251:

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



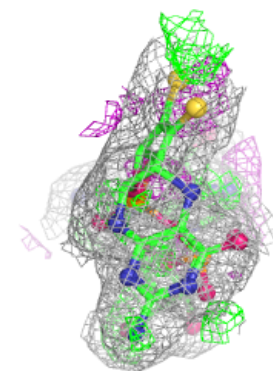
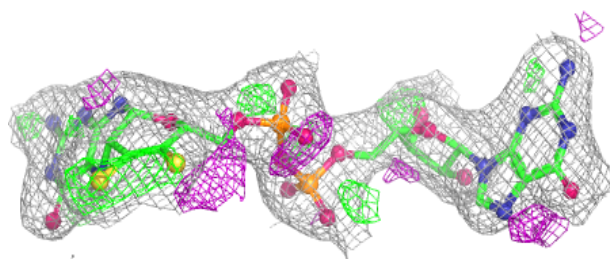
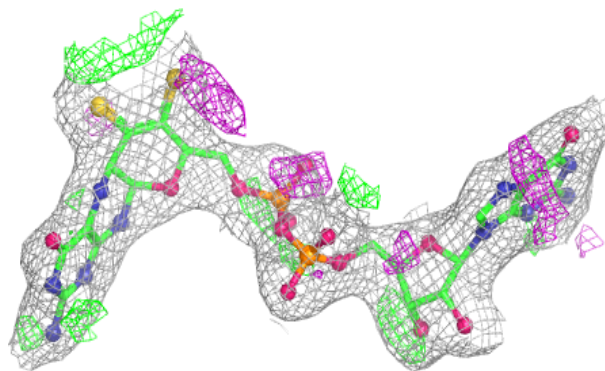
Electron density around PCI C 1252:

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

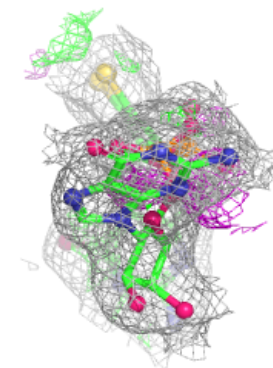
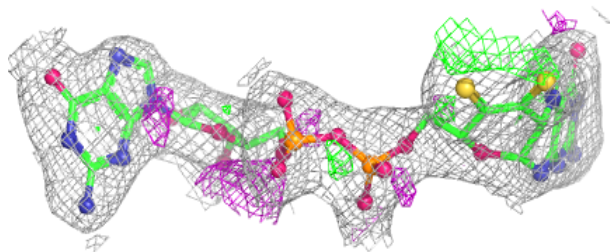
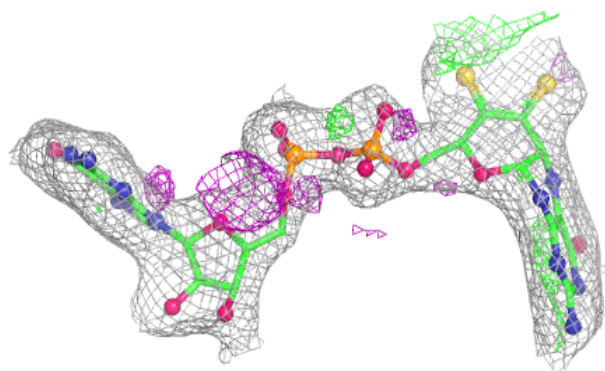


Electron density around MGD A 1765:

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

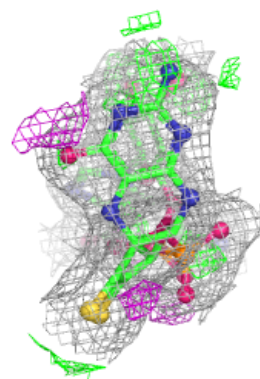
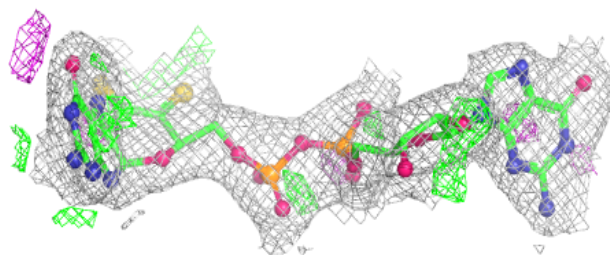
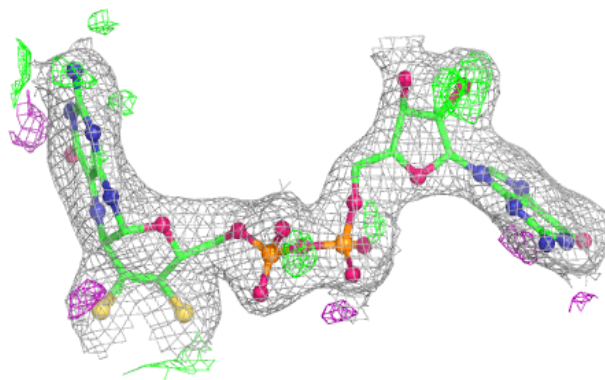
**Electron density around MGD A 1766:**

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

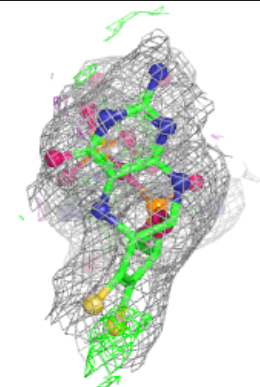
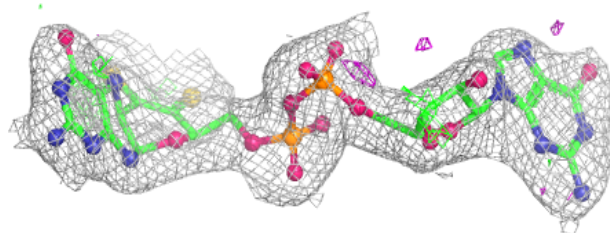
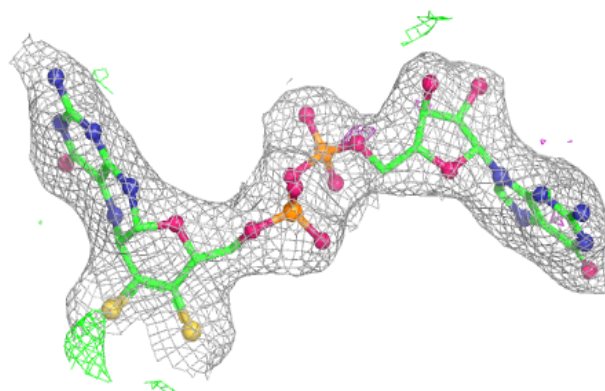


Electron density around MGD E 1766:

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

**Electron density around MGD E 1765:**

$2mF_o-DF_c$ (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.