Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 04:01 PM EDT

PDB ID	:	4HHH
Title	:	Structure of Pisum sativum Rubisco
Authors	:	Loewen, P.C.; Didychuk, A.L.; Switala, J.; Loewen, M.C.
Deposited on	:	2012-10-09
Resolution	:	2.20 Å(reported)

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

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

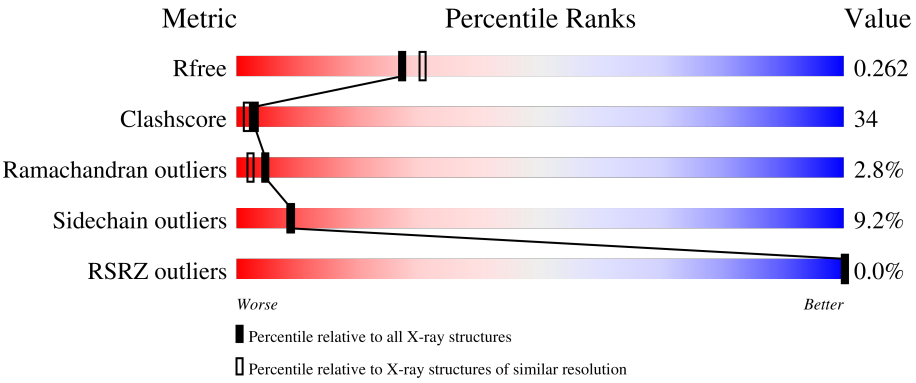
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	475	45% 43% 7%
1	B	475	42% 43% 10%
1	C	475	43% 44% 9%
1	D	475	44% 44% 8%
2	S	123	50% 35% 11%

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Mol	Chain	Length	Quality of chain
2	T	123	38% 52% 10%
2	U	123	41% 45% 14%
2	V	123	% 43% 44% 12%

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
3	RUB	B	501	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19680 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.

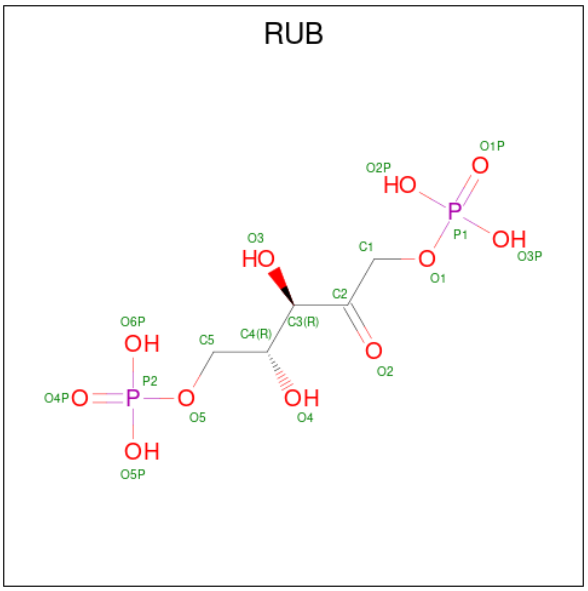
- Molecule 1 is a protein called Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	11	0
			3648	2332	634	664	18			
1	B	458	Total	C	N	O	S	0	13	0
			3653	2340	635	660	18			
1	C	458	Total	C	N	O	S	0	12	0
			3662	2338	644	662	18			
1	D	458	Total	C	N	O	S	0	9	0
			3647	2323	643	663	18			

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	2	0
			1049	694	172	178	5			
2	T	123	Total	C	N	O	S	0	3	0
			1056	698	175	178	5			
2	U	123	Total	C	N	O	S	0	2	0
			1047	690	172	180	5			
2	V	123	Total	C	N	O	S	0	3	0
			1057	697	175	180	5			

- Molecule 3 is RIBULOSE-1,5-DIPHOSPHATE (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 18 5 11 2	0	0
3	B	1	Total C O P 18 5 11 2	0	0
3	C	1	Total C O P 18 5 11 2	0	0
3	D	1	Total C O P 18 5 11 2	0	0

- Molecule 4 is water.

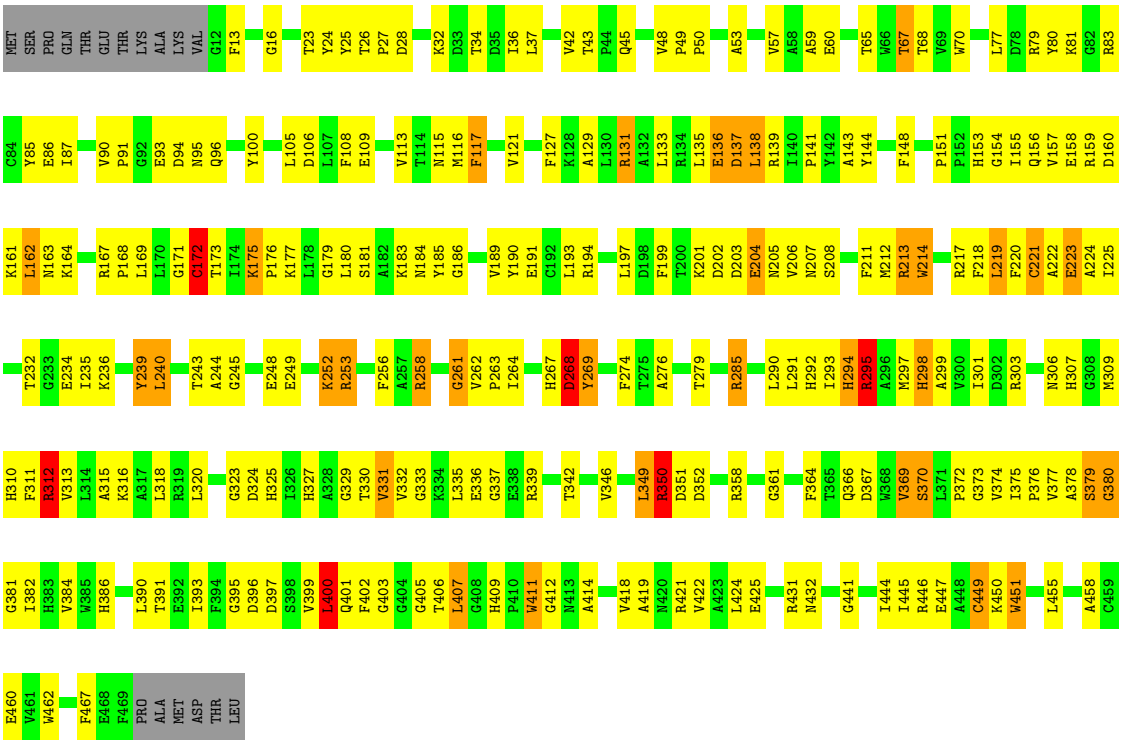
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	161	Total O 161 161	0	0
4	B	175	Total O 175 175	0	0
4	C	137	Total O 137 137	0	0
4	D	147	Total O 147 147	0	0
4	S	49	Total O 49 49	0	0
4	T	50	Total O 50 50	0	0
4	U	30	Total O 30 30	0	0
4	V	40	Total O 40 40	0	0

3 Residue-property plots (i)

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

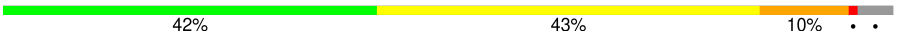
• Molecule 1: Ribulose bisphosphate carboxylase large chain

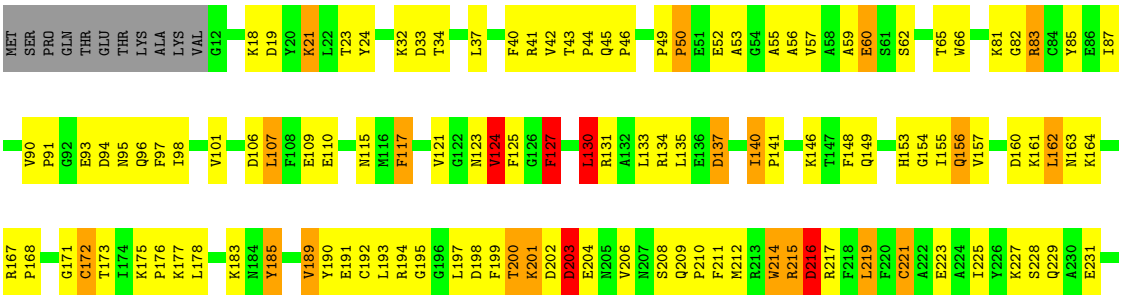
Chain A:

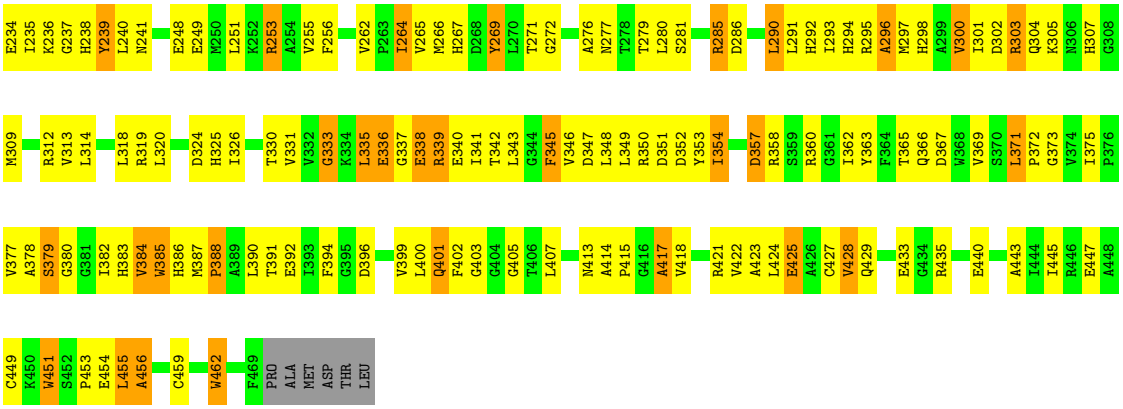


• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain B:

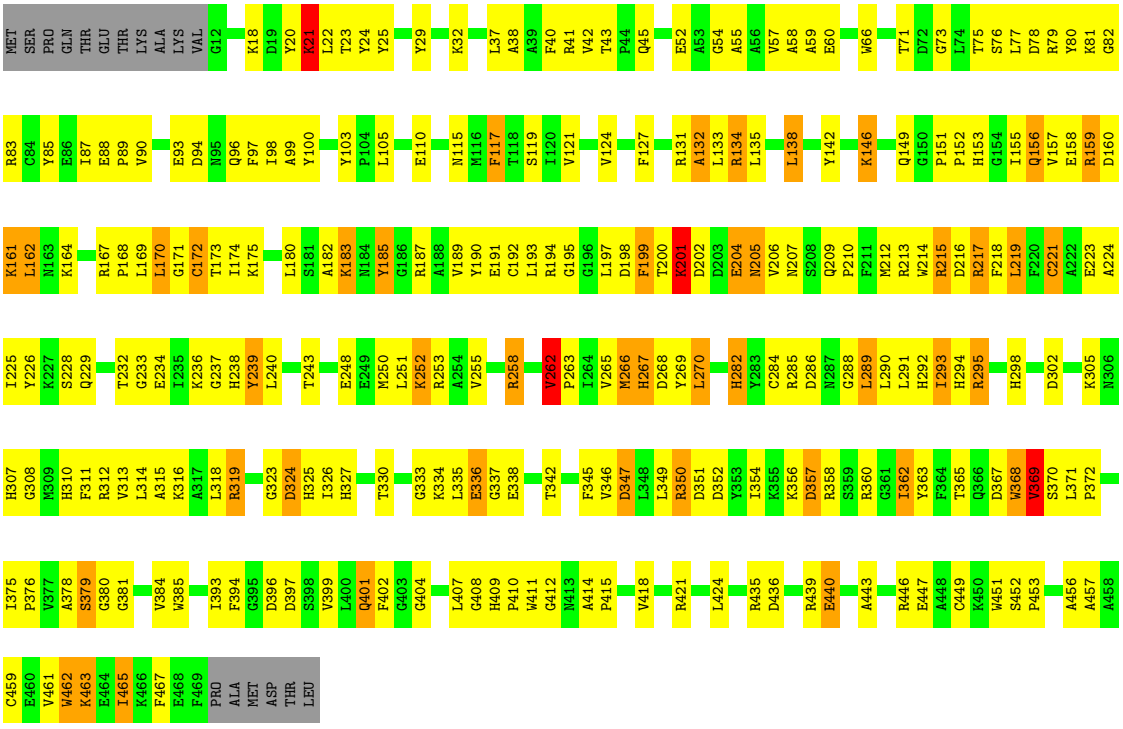






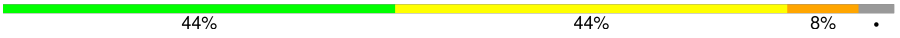
• Molecule 1: Ribulose bisphosphate carboxylase large chain

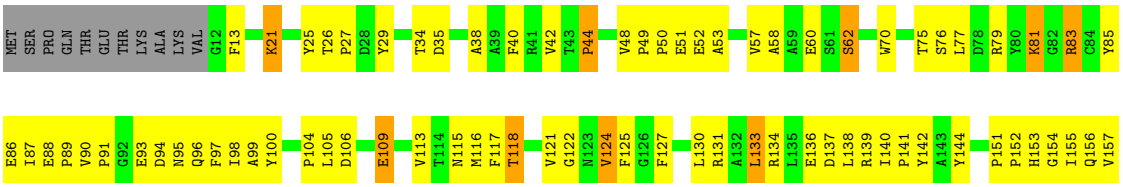
Chain C:

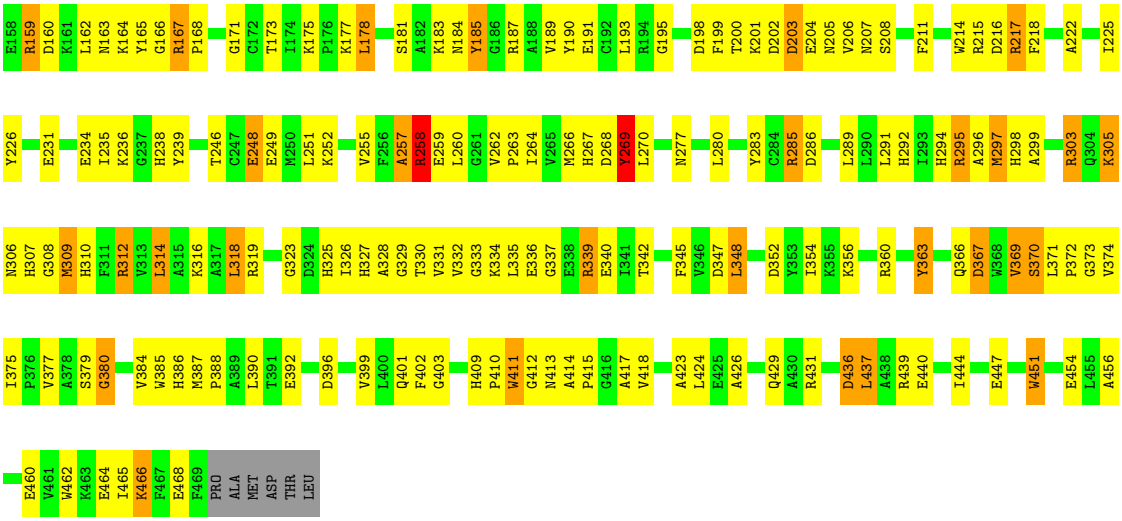


• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain D:

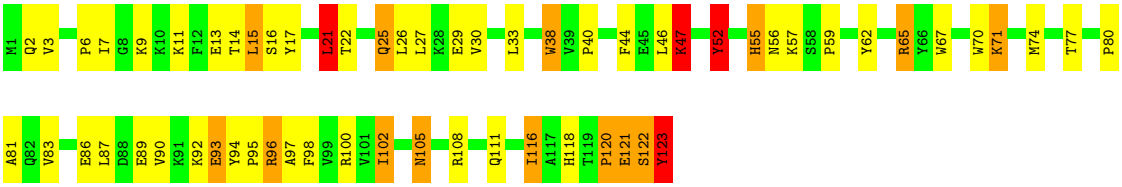






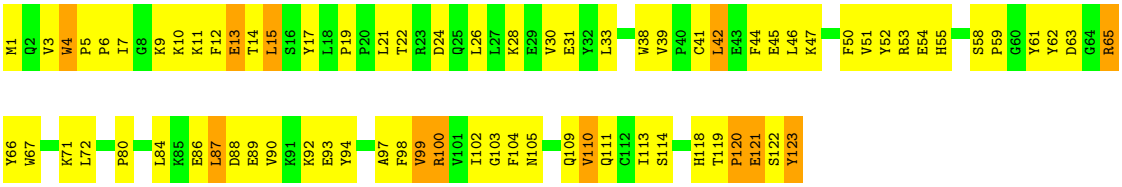
• Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain S:



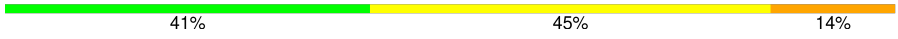
• Molecule 2: Ribulose bisphosphate carboxylase small chain

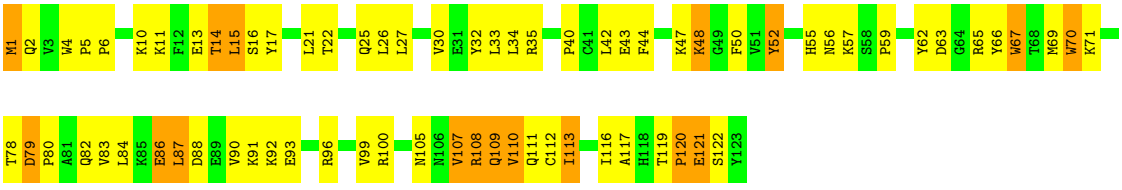
Chain T:



• Molecule 2: Ribulose bisphosphate carboxylase small chain

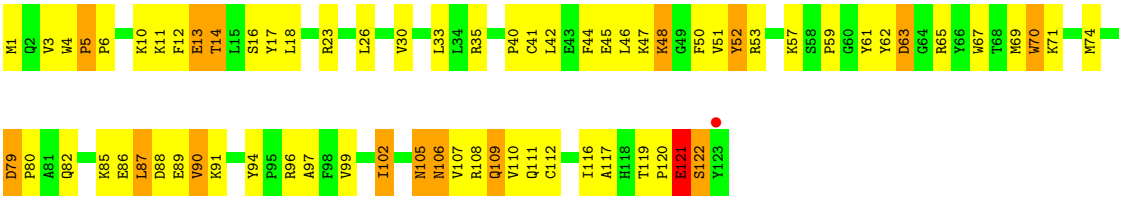
Chain U:





• Molecule 2: Ribulose bisphosphate carboxylase small chain

Chain V:


M1
Q2
V3
W4
P5
P6
K10
K11
F12
E13
T14
L15
S16
Y17
L18
R23
L26
V30
L33
L34
R35
P40
C41
L42
E43
F44
E45
L46
K47
K48
G49
F50
V51
Y52
R53
K57
S58
P59
G60
Y61
Y62
D63
G64
R65
Y66
W67
T68
M69
W70
K71
M74
D79
P80
A81
Q82
K85
E86
L87
D88
E89
V90
K91
Y94
P95
R96
A97
F98
V99
I102
N105
N106
V107
R108
Q109
V110
Q111
C112
I116
A117
H118
T119
P120
E121
S122
Y123

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	109.79Å 109.95Å 201.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.95 – 2.20 48.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (109.95-2.20) 93.1 (48.20-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.279 0.198 , 0.262	Depositor DCC
R_{free} test set	5831 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	10.4	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 3.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.349 for k,h,-l	Xtriage
Reported twinning fraction	0.580 for H, K, L 0.420 for K, H, -L	Depositor
Outliers	0 of 116024 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	19680	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RUB

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	1.15	9/3765 (0.2%)	1.35	33/5104 (0.6%)
1	B	1.15	4/3783 (0.1%)	1.35	31/5128 (0.6%)
1	C	1.01	6/3790 (0.2%)	1.19	24/5135 (0.5%)
1	D	1.03	8/3758 (0.2%)	1.27	25/5090 (0.5%)
2	S	0.95	3/1089 (0.3%)	1.07	3/1474 (0.2%)
2	T	0.94	1/1099 (0.1%)	1.02	1/1487 (0.1%)
2	U	0.81	3/1087 (0.3%)	0.90	0/1472
2	V	0.84	2/1100 (0.2%)	0.94	3/1489 (0.2%)
All	All	1.04	36/19471 (0.2%)	1.23	120/26379 (0.5%)

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	A	0	1
1	C	0	3
2	S	0	1
2	V	0	1
All	All	0	6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TRP	NE1-CE2	-6.74	1.28	1.37
1	A	373	GLY	N-CA	6.64	1.56	1.46
1	C	204	GLU	CD-OE2	6.45	1.32	1.25
1	D	70	TRP	CD2-CE2	6.11	1.48	1.41
1	D	411	TRP	CD2-CE2	6.07	1.48	1.41
1	D	248	GLU	CD-OE2	6.01	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	38	TRP	CD2-CE2	5.93	1.48	1.41
1	B	214	TRP	CD2-CE2	5.86	1.48	1.41
1	C	66	TRP	CD2-CE2	5.83	1.48	1.41
1	C	368	TRP	CD2-CE2	5.57	1.48	1.41
1	A	70	TRP	CD2-CE2	5.57	1.48	1.41
2	U	4	TRP	CD2-CE2	5.56	1.48	1.41
1	C	411	TRP	CD2-CE2	5.51	1.48	1.41
1	A	214	TRP	CG-CD2	5.50	1.53	1.43
1	A	451	TRP	CD2-CE2	5.46	1.47	1.41
2	T	4	TRP	CD2-CE2	5.41	1.47	1.41
1	D	109	GLU	CD-OE1	-5.40	1.19	1.25
1	D	385	TRP	CD2-CE2	5.39	1.47	1.41
2	V	70	TRP	CD2-CE2	5.36	1.47	1.41
1	B	385	TRP	CD2-CE2	5.33	1.47	1.41
1	A	411	TRP	CD2-CE2	5.33	1.47	1.41
2	V	67	TRP	CD2-CE2	5.31	1.47	1.41
1	D	451	TRP	CD2-CE2	5.28	1.47	1.41
1	D	462	TRP	CD2-CE2	5.28	1.47	1.41
1	B	462	TRP	CD2-CE2	5.25	1.47	1.41
1	B	391	THR	CB-CG2	-5.22	1.35	1.52
2	S	52	TYR	CZ-OH	5.20	1.46	1.37
2	S	55	HIS	CB-CG	5.19	1.59	1.50
1	D	283	TYR	CE1-CZ	5.17	1.45	1.38
2	U	67	TRP	CD2-CE2	5.13	1.47	1.41
2	U	70	TRP	CD2-CE2	5.13	1.47	1.41
1	C	226	TYR	CE1-CZ	5.09	1.45	1.38
1	C	103	TYR	CB-CG	5.06	1.59	1.51
1	A	462	TRP	CD2-CE2	5.03	1.47	1.41
1	A	261	GLY	N-CA	5.03	1.53	1.46
1	A	204	GLU	CD-OE2	5.02	1.31	1.25

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	D	367	ASP	CB-CG-OD2	9.96	127.27	118.30
1	D	295	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	253	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	160	ASP	CB-CG-OD2	8.97	126.38	118.30
1	B	130	LEU	CA-CB-CG	8.97	135.93	115.30
1	D	295	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	286	ASP	CB-CG-OD1	8.93	126.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	367	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	B	286	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	D	35	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	A	202	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	A	367	ASP	CB-CG-OD1	8.32	125.79	118.30
1	D	339	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	367	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	D	268	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	D	268	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	202	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	217	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	213	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	131	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	258	ARG	CG-CD-NE	-7.59	95.87	111.80
1	A	203	ASP	CB-CG-OD1	7.57	125.12	118.30
2	V	63	ASP	CB-CG-OD1	-7.55	111.51	118.30
1	B	253	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	135	LEU	CB-CG-CD1	7.43	123.62	111.00
2	V	33	LEU	CA-CB-CG	7.36	132.24	115.30
1	A	213	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	324	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	352	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	240	LEU	CB-CG-CD1	7.22	123.27	111.00
1	A	350	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	253	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	B	290	LEU	CB-CG-CD1	-7.05	99.01	111.00
1	D	269	TYR	CB-CG-CD1	6.98	125.19	121.00
1	C	138	LEU	CA-CB-CG	6.79	130.91	115.30
2	S	123	TYR	CA-CB-CG	6.66	126.05	113.40
1	C	319	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	D	303	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	253	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	206	VAL	CB-CA-C	-6.56	98.94	111.40
1	D	269	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	C	289	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	221	CYS	CA-CB-SG	-6.40	102.48	114.00
1	A	358	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	339	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	268	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	B	396	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	314	LEU	CA-CB-CG	6.20	129.57	115.30
1	B	335	LEU	CA-CB-CG	6.14	129.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	137	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	D	159	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	138	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	B	303	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	295	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	357	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	214	TRP	CD1-CG-CD2	-5.83	101.63	106.30
1	D	133	LEU	CB-CG-CD2	5.83	120.92	111.00
2	S	65	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	T	53	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	194	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	C	170	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	C	219	LEU	CA-CB-CG	5.68	128.38	115.30
1	B	239	TYR	CB-CG-CD1	5.67	124.40	121.00
2	S	21	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	417	ALA	CB-CA-C	-5.64	101.64	110.10
1	A	349	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	A	172	CYS	CA-CB-SG	5.62	124.12	114.00
1	A	268	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	219	LEU	CB-CG-CD1	5.62	120.55	111.00
1	D	363	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	C	224	ALA	N-CA-CB	-5.56	102.31	110.10
1	C	215	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	291	LEU	CB-CG-CD1	5.56	120.45	111.00
1	D	139	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	135	LEU	CA-CB-CG	-5.52	102.61	115.30
1	D	260	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	D	314	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	371	LEU	CA-CB-CG	-5.46	102.73	115.30
1	D	260	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	400	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	A	312	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	262	VAL	N-CA-CB	-5.40	99.62	111.50
1	D	130	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	B	117	PHE	CB-CG-CD1	5.39	124.57	120.80
1	D	285	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	312[A]	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	312[B]	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	140[A]	ILE	C-N-CD	5.35	139.64	128.40
1	B	140[B]	ILE	C-N-CD	5.35	139.64	128.40
1	C	266	MET	CA-CB-CG	5.31	122.33	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	TRP	CD1-NE1-CE2	5.30	113.77	109.00
1	A	303	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	C	162	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	B	239	TYR	N-CA-CB	5.28	120.10	110.60
1	C	250	MET	CA-CB-CG	5.26	122.24	113.30
1	C	146	LYS	N-CA-C	5.25	125.17	111.00
1	B	300	VAL	CA-CB-CG2	5.21	118.71	110.90
1	B	221	CYS	CA-CB-SG	5.19	123.34	114.00
1	C	347	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	C	270	LEU	CB-CG-CD1	5.13	119.72	111.00
1	C	138	LEU	CB-CG-CD2	5.13	119.72	111.00
1	A	303	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	162	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	C	221	CYS	CA-CB-SG	-5.09	104.83	114.00
1	D	77	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	117	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	C	350	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	V	53	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	348	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	267	HIS	CB-CA-C	-5.06	100.28	110.40
1	C	285	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	203	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	172	CYS	CA-CB-SG	-5.03	104.95	114.00
1	B	352	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	107	LEU	CB-CA-C	-5.01	100.69	110.20
1	D	142	TYR	N-CA-C	5.00	124.51	111.00
1	B	189	VAL	CA-CB-CG1	5.00	118.40	110.90
1	C	295	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	PHE	Peptide
1	C	195	GLY	Peptide
1	C	199	PHE	Peptide
1	C	93	GLU	Peptide
2	S	47	LYS	Peptide
2	V	121	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3648	0	3615	263	2
1	B	3653	0	3642	270	1
1	C	3662	0	3632	268	1
1	D	3647	0	3601	248	3
2	S	1049	0	1065	75	1
2	T	1056	0	1076	83	1
2	U	1047	0	1057	75	1
2	V	1057	0	1071	83	0
3	A	18	0	8	4	0
3	B	18	0	8	4	0
3	C	18	0	8	4	0
3	D	18	0	8	1	0
4	A	161	0	0	28	1
4	B	175	0	0	31	1
4	C	137	0	0	29	1
4	D	147	0	0	30	0
4	S	49	0	0	8	0
4	T	50	0	0	3	0
4	U	30	0	0	3	0
4	V	40	0	0	6	0
All	All	19680	0	18791	1296	7

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 34.

All (1296) 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:C:201:LYS:NZ	1:C:294:HIS:NE2	1.70	1.35
1:C:201:LYS:HE3	1:C:202:ASP:O	1.40	1.16
1:D:201:LYS:NZ	1:D:294:HIS:NE2	1.98	1.11
1:A:60:GLU:HG3	1:A:127:PHE:HZ	1.04	1.09
1:A:409:HIS:HD2	1:A:458:ALA:HB2	1.16	1.08
1:C:75:THR:HG22	1:C:76:SER:H	1.11	1.08
1:A:252:LYS:NZ	1:D:286:ASP:OD1	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:46:LEU:HD23	2:T:97:ALA:HB2	1.37	1.07
1:A:60:GLU:HG3	1:A:127:PHE:CZ	1.89	1.07
1:A:131:ARG:HD2	4:A:694:HOH:O	1.52	1.07
1:C:21:LYS:HE2	1:C:52:GLU:HB2	1.32	1.07
1:D:124:VAL:HG12	1:D:127:PHE:HE2	1.14	1.06
1:A:409:HIS:CD2	1:A:458:ALA:HB2	1.91	1.05
1:A:173:THR:O	1:A:175:LYS:HE2	1.58	1.04
1:D:178:LEU:HD21	1:D:205:ASN:HB3	1.35	1.04
1:A:323:GLY:O	1:A:374:VAL:HG22	1.57	1.02
1:D:124:VAL:HG12	1:D:127:PHE:CE2	1.96	1.00
1:D:60:GLU:HG3	1:D:127:PHE:CZ	1.96	0.99
1:B:133:LEU:H	1:B:307:HIS:HD2	1.00	0.99
1:B:56:ALA:HB1	1:B:127:PHE:CE2	1.99	0.97
1:C:346:VAL:HG13	1:C:376:PRO:HG3	1.45	0.97
1:D:234:GLU:OE1	4:D:667:HOH:O	1.84	0.96
2:U:121:GLU:N	2:U:122:SER:HA	1.80	0.96
1:C:251:LEU:O	1:C:255:VAL:HG23	1.66	0.94
1:A:113:VAL:HG11	1:A:274:PHE:CD1	2.03	0.93
1:C:45:GLN:NE2	1:C:131:ARG:HG2	1.83	0.93
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.07	0.93
1:C:88:GLU:O	1:C:97:PHE:HB2	1.69	0.93
1:A:264:ILE:HG13	1:A:290:LEU:HB2	1.50	0.93
1:B:237:GLY:HA3	1:B:264[A]:ILE:HD11	1.50	0.93
2:U:105:ASN:OD1	2:U:108:ARG:HG3	1.68	0.92
1:D:60:GLU:HG3	1:D:127:PHE:CE1	2.04	0.92
1:A:201:LYS:HB3	1:A:239:TYR:CD2	2.04	0.92
1:B:208:SER:HB2	1:B:214:TRP:HB3	1.50	0.91
1:B:354:ILE:HD12	1:B:354:ILE:N	1.85	0.91
1:C:367:ASP:OD2	4:C:732:HOH:O	1.87	0.91
1:A:85:TYR:CZ	1:A:100:TYR:HB3	2.06	0.90
1:C:171:GLY:HA3	1:C:401:GLN:HE21	1.34	0.90
1:D:121:VAL:HG11	1:D:309[A]:MET:SD	2.09	0.90
1:D:251:LEU:O	1:D:255:VAL:HG23	1.70	0.90
2:T:102[B]:ILE:HG21	2:T:111:GLN:HG2	1.51	0.90
1:B:23:THR:HG23	1:B:24:TYR:CE2	2.07	0.89
1:C:153:HIS:CE1	4:C:610:HOH:O	2.26	0.89
1:C:189:VAL:O	1:C:193:LEU:HD12	1.71	0.89
2:V:41:CYS:HB3	2:V:102:ILE:HG22	1.55	0.89
2:S:67:TRP:CZ3	2:S:100:ARG:HG3	2.08	0.88
2:V:51:VAL:HG23	4:V:213:HOH:O	1.73	0.88
1:A:168:PRO:HG3	1:A:396:ASP:HA	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:THR:HG22	1:C:76:SER:N	1.87	0.88
1:C:352:ASP:HA	4:C:645:HOH:O	1.72	0.88
1:D:178:LEU:CD2	1:D:205:ASN:HB3	2.03	0.88
1:D:124:VAL:HA	1:D:127:PHE:CE2	2.08	0.87
1:A:96:GLN:NE2	1:A:306:ASN:OD1	2.06	0.87
2:S:62:TYR:O	2:S:65:ARG:HD2	1.75	0.87
2:V:40:PRO:HG2	2:V:74:MET:HB2	1.55	0.87
1:C:115:ASN:HB2	4:C:615:HOH:O	1.75	0.86
1:B:372:PRO:HA	4:B:772:HOH:O	1.75	0.86
1:C:232:THR:HG22	4:U:215:HOH:O	1.74	0.86
1:D:252:LYS:HG2	4:D:651:HOH:O	1.76	0.86
1:C:85:TYR:CZ	1:C:100:TYR:HB3	2.10	0.86
1:A:60:GLU:CG	1:A:127:PHE:HZ	1.88	0.86
1:B:56:ALA:HB1	1:B:127:PHE:CZ	2.10	0.86
1:C:117:PHE:O	1:C:121:VAL:HG22	1.75	0.86
1:B:133:LEU:H	1:B:307:HIS:CD2	1.92	0.85
1:B:23:THR:HG23	1:B:24:TYR:CD2	2.10	0.85
1:A:264:ILE:HG13	1:A:290:LEU:CB	2.07	0.85
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.94	0.85
1:A:297:MET:HG2	1:A:297:MET:O	1.75	0.85
1:C:42:VAL:HG22	1:C:133:LEU:CD1	2.07	0.85
1:D:173:THR:HA	1:D:201:LYS:HG2	1.59	0.84
1:B:285:ARG:O	1:B:285:ARG:HG3	1.77	0.84
1:C:75:THR:CG2	1:C:76:SER:H	1.88	0.84
1:B:201:LYS:HB2	1:B:239:TYR:CD2	2.13	0.84
1:B:57:VAL:HA	1:B:124[A]:VAL:HG21	1.58	0.84
2:V:87:LEU:HD22	2:V:91:LYS:HE3	1.60	0.84
1:B:110:GLU:OE1	1:B:110:GLU:N	2.10	0.83
1:D:75:THR:HG22	1:D:76:SER:H	1.44	0.83
1:A:179:GLY:O	2:V:109:GLN:NE2	2.11	0.83
1:B:123:ASN:OD1	4:B:716:HOH:O	1.96	0.82
1:D:124:VAL:CG1	1:D:127:PHE:HE2	1.92	0.82
1:C:25:TYR:HB2	1:C:55:ALA:HB2	1.60	0.82
1:D:294:HIS:CE1	1:D:327:HIS:NE2	2.47	0.82
1:B:309[B]:MET:HE2	1:B:314:LEU:HD21	1.62	0.82
1:B:309[B]:MET:CE	1:B:314:LEU:HD21	2.10	0.82
1:B:333:GLY:HA3	1:B:380:GLY:O	1.79	0.82
1:C:172:CYS:HB2	1:C:402:PHE:O	1.79	0.82
1:C:42:VAL:HG22	1:C:133:LEU:HD12	1.60	0.81
1:D:347:ASP:OD1	4:D:646:HOH:O	1.97	0.81
1:C:318:LEU:HG	1:C:326:ILE:HD12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:96:ARG:HD3	2:V:121:GLU:HG2	1.63	0.81
1:C:201:LYS:NZ	1:C:294:HIS:CD2	2.48	0.80
1:D:48:VAL:CG1	1:D:53:ALA:HB2	2.12	0.80
1:D:60:GLU:HB2	1:D:127:PHE:HZ	1.46	0.80
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.63	0.80
1:D:97:PHE:HE1	1:D:99:ALA:HB2	1.44	0.80
2:S:70:TRP:HZ2	2:S:89:GLU:HG2	1.45	0.80
1:A:234:GLU:HG2	2:S:13:GLU:OE2	1.81	0.80
1:A:346:VAL:O	1:A:350:ARG:HB2	1.82	0.80
1:A:377:VAL:HG22	1:A:399:VAL:HB	1.65	0.79
2:U:32:TYR:HD1	2:U:35:ARG:HH21	1.27	0.79
1:A:291:LEU:N	1:A:324:ASP:OD2	2.16	0.79
1:D:49:PRO:HB2	1:D:52:GLU:HB3	1.64	0.79
1:C:435:ARG:HH11	1:C:440:GLU:HG2	1.48	0.79
1:D:285:ARG:NH1	4:D:669:HOH:O	2.09	0.79
1:D:340:GLU:OE1	4:D:712:HOH:O	2.00	0.79
1:D:173:THR:OG1	1:D:201:LYS:HD3	1.83	0.78
1:C:286:ASP:OD1	1:D:252:LYS:NZ	2.15	0.78
1:D:306[A]:ASN:ND2	4:D:728:HOH:O	2.15	0.78
1:A:201:LYS:HD2	1:A:239:TYR:CD2	2.19	0.78
1:C:20:TYR:O	1:C:22:LEU:N	2.16	0.78
1:D:60:GLU:CB	1:D:127:PHE:HZ	1.97	0.78
2:T:102[B]:ILE:CG2	2:T:111:GLN:HG2	2.13	0.78
1:A:131:ARG:CD	4:A:694:HOH:O	2.19	0.77
1:B:353:TYR:O	4:B:707:HOH:O	2.02	0.77
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.19	0.77
1:C:173:THR:HG23	1:C:201:LYS:HE2	1.66	0.77
1:B:90:VAL:HB	1:B:96:GLN:O	1.84	0.77
1:D:294:HIS:CE1	1:D:327:HIS:CE1	2.73	0.77
1:C:81:LYS:O	1:C:83[A]:ARG:NH1	2.18	0.76
1:C:21:LYS:CE	1:C:52:GLU:HB2	2.12	0.76
2:T:31:GLU:HG3	2:T:80:PRO:HG3	1.65	0.76
1:B:229:GLN:HE22	2:T:62:TYR:HE1	1.31	0.76
1:D:60:GLU:CG	1:D:127:PHE:HZ	1.99	0.76
1:A:421:ARG:O	1:A:425:GLU:HG3	1.85	0.76
1:B:216:ASP:O	1:B:219[A]:LEU:HD12	1.85	0.76
2:U:86:GLU:O	2:U:90:VAL:HG23	1.84	0.76
1:B:325:HIS:CE1	1:B:399:VAL:HG21	2.21	0.75
1:B:330:THR:CG2	1:B:379:SER:H	1.99	0.75
1:D:294:HIS:HE1	1:D:327:HIS:CE1	2.04	0.75
1:B:56:ALA:CB	1:B:127:PHE:HE2	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:THR:OG1	1:C:96:GLN:NE2	2.17	0.75
1:D:347:ASP:OD2	1:D:360[A]:ARG:NH1	2.16	0.75
1:B:300:VAL:HB	1:B:301:ILE:HD12	1.70	0.74
1:D:60:GLU:CG	1:D:127:PHE:CZ	2.70	0.74
1:A:351:ASP:OD2	4:A:731:HOH:O	2.05	0.74
1:D:113:VAL:O	1:D:116:MET:HB3	1.87	0.74
1:D:377:VAL:HG22	1:D:399:VAL:HB	1.69	0.74
2:V:87:LEU:CD2	2:V:91:LYS:HE3	2.18	0.74
1:A:298:HIS:CD2	1:A:299:ALA:H	2.05	0.74
1:D:85:TYR:CZ	1:D:100:TYR:HB3	2.23	0.74
1:D:164:LYS:NZ	1:D:235:ILE:O	2.20	0.74
1:D:329:GLY:HA3	4:D:734:HOH:O	1.87	0.74
2:U:108:ARG:HH11	2:U:108:ARG:HB3	1.51	0.74
1:B:330:THR:HG22	1:B:379:SER:H	1.53	0.74
2:U:71:LYS:HD3	2:V:1:MET:HB2	1.70	0.73
1:B:56:ALA:CB	1:B:127:PHE:CE2	2.70	0.73
2:T:5:PRO:HG2	2:T:9:LYS:HE3	1.71	0.73
1:A:316:LYS:HZ3	1:A:366:GLN:HE21	1.34	0.73
1:C:229:GLN:NE2	4:C:691:HOH:O	2.21	0.73
1:A:136[B]:GLU:O	1:A:137:ASP:HB2	1.86	0.73
1:D:190:TYR:OH	1:D:231:GLU:OE1	2.05	0.73
1:D:134[A]:ARG:NE	1:D:136:GLU:OE1	2.21	0.73
2:U:87:LEU:HD11	2:U:117:ALA:HB1	1.71	0.72
1:A:37:LEU:HB2	1:A:139:ARG:HB3	1.71	0.72
1:C:174:ILE:HD11	1:C:189:VAL:HG22	1.71	0.72
2:T:52:TYR:O	2:T:63:ASP:HB2	1.88	0.72
1:A:153:HIS:HB3	1:A:157:VAL:CG1	2.20	0.72
1:C:88:GLU:O	1:C:97:PHE:CB	2.37	0.72
1:D:431:ARG:HB2	1:D:437:LEU:HD22	1.71	0.72
1:B:330:THR:HG22	1:B:379:SER:N	2.05	0.72
1:B:133:LEU:N	1:B:307:HIS:HD2	1.81	0.71
2:V:13:GLU:OE2	4:V:212:HOH:O	2.07	0.71
1:B:87:ILE:HG23	1:B:97:PHE:CD1	2.26	0.71
1:B:269:TYR:CD1	1:B:318:LEU:HD23	2.24	0.71
1:C:25:TYR:CB	1:C:55:ALA:HB2	2.20	0.71
1:D:167:ARG:NH2	2:V:13:GLU:OE1	2.23	0.71
1:C:159[B]:ARG:NH1	1:C:397:ASP:OD1	2.23	0.71
1:C:385:TRP:NE1	1:C:463:LYS:HA	2.05	0.71
1:B:140[A]:ILE:H	1:B:366:GLN:HE22	1.37	0.71
1:A:315:ALA:HB1	1:A:349:LEU:HD21	1.72	0.71
1:B:140[B]:ILE:H	1:B:366:GLN:HE22	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:HG3	1:C:127:PHE:HZ	1.55	0.71
1:C:199:PHE:HB3	1:C:239:TYR:CE1	2.25	0.71
1:D:133:LEU:H	1:D:307:HIS:HD2	1.36	0.71
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.55	0.71
2:S:47:LYS:NZ	2:S:47:LYS:HB3	2.05	0.71
2:S:70:TRP:CZ2	2:S:89:GLU:HG2	2.25	0.71
1:A:330:THR:HG22	1:A:379:SER:H	1.56	0.71
1:C:88:GLU:OE2	1:C:358:ARG:NH2	2.21	0.71
1:D:328:ALA:O	4:D:734:HOH:O	2.07	0.71
1:D:379:SER:O	4:D:730:HOH:O	2.08	0.71
2:T:33:LEU:HB2	2:T:113:ILE:HD11	1.72	0.71
1:C:199:PHE:HB3	1:C:239:TYR:HE1	1.55	0.70
1:B:177:LYS:NZ	1:B:203:ASP:OD2	2.24	0.70
1:C:40:PHE:HB3	1:C:133:LEU:HD11	1.73	0.70
1:D:267:HIS:HD2	1:D:277:ASN:OD1	1.74	0.70
2:S:95:PRO:O	2:S:118:HIS:HE1	1.75	0.70
2:V:96:ARG:HA	2:V:120:PRO:HB3	1.73	0.70
1:A:243:THR:OG1	1:A:267:HIS:HA	1.92	0.70
1:A:205:ASN:OD1	4:A:749:HOH:O	2.08	0.70
2:U:25:GLN:OE1	4:U:221:HOH:O	2.10	0.70
1:C:443:ALA:O	1:C:447:GLU:HG3	1.92	0.70
2:S:100:ARG:NH2	4:S:210:HOH:O	2.23	0.70
1:A:113:VAL:HG11	1:A:274:PHE:CE1	2.26	0.70
1:C:325:HIS:CE1	1:C:399:VAL:HG21	2.26	0.70
1:C:350:ARG:NH2	1:C:394:PHE:O	2.24	0.70
1:D:117:PHE:O	1:D:121:VAL:HG22	1.91	0.70
1:B:23:THR:HG22	4:B:665:HOH:O	1.91	0.69
1:D:42:VAL:HB	1:D:97:PHE:CE2	2.27	0.69
2:V:35[A]:ARG:HG3	2:V:35[A]:ARG:HH11	1.57	0.69
1:D:48:VAL:HG11	1:D:53:ALA:HB2	1.75	0.69
1:C:240:LEU:HD12	1:C:262:VAL:HG11	1.74	0.69
1:A:36:ILE:HD12	1:A:108:PHE:CE2	2.28	0.69
1:D:40:PHE:HB3	1:D:133:LEU:HD11	1.73	0.69
1:B:304:GLN:OE1	4:B:708:HOH:O	2.10	0.69
1:A:232:THR:HG22	4:S:227:HOH:O	1.92	0.69
1:A:168:PRO:HD2	1:A:424:LEU:HD11	1.75	0.69
1:A:184:ASN:ND2	2:V:109:GLN:OE1	2.26	0.69
1:B:57:VAL:HA	1:B:124[A]:VAL:CG2	2.22	0.69
1:A:193:LEU:O	1:A:236:LYS:HE3	1.93	0.68
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.28	0.68
2:S:52:TYR:N	2:S:52:TYR:CD2	2.60	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:O	1:A:175:LYS:CE	2.38	0.68
1:B:292:HIS:HE1	1:B:377:VAL:HG21	1.58	0.68
1:D:201:LYS:CE	1:D:294:HIS:NE2	2.55	0.68
1:D:456:ALA:O	1:D:460:GLU:HG3	1.93	0.68
1:A:36:ILE:HG12	1:A:141:PRO:HD3	1.75	0.68
1:B:296:ALA:O	1:B:297:MET:CB	2.41	0.68
1:D:217:ARG:NH1	4:D:601:HOH:O	2.26	0.68
2:T:94:TYR:OH	4:T:228:HOH:O	1.79	0.68
1:C:174:ILE:CD1	1:C:238:HIS:HE1	2.07	0.68
1:D:44:PRO:HD3	1:D:95:ASN:O	1.94	0.68
2:T:39:VAL:O	2:T:103:GLY:HA2	1.93	0.68
1:A:342:THR:O	1:A:346:VAL:HG23	1.94	0.68
1:C:135:LEU:HD23	1:C:313:VAL:HG11	1.75	0.67
1:D:178:LEU:HD11	1:D:205:ASN:HD22	1.59	0.67
1:C:204:GLU:HG2	1:C:205:ASN:OD1	1.94	0.67
1:D:226:TYR:HB3	2:U:55:HIS:CD2	2.29	0.67
2:S:70:TRP:CD2	2:S:90:VAL:HG22	2.30	0.67
1:C:131:ARG:O	1:C:132:ALA:HB2	1.93	0.67
1:B:385:TRP:CZ2	1:B:459:CYS:HB3	2.29	0.67
2:V:108:ARG:O	2:V:109:GLN:HB2	1.93	0.67
2:T:61:TYR:C	2:T:61:TYR:CD2	2.67	0.67
1:C:29:TYR:OH	1:C:32:LYS:HE2	1.95	0.67
1:A:450:LYS:HB2	1:A:451:TRP:CD1	2.30	0.67
2:S:46[A]:LEU:HD12	2:T:6:PRO:HG2	1.76	0.67
2:V:10:LYS:HB3	2:V:50:PHE:CZ	2.30	0.67
1:C:153:HIS:HE1	4:C:610:HOH:O	1.70	0.67
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.78	0.67
1:C:24:TYR:CD1	1:C:59:ALA:HA	2.30	0.67
3:C:501:RUB:O4P	4:C:703:HOH:O	2.12	0.67
2:U:121:GLU:H	2:U:122:SER:HA	1.56	0.67
1:B:358:ARG:N	4:B:767:HOH:O	2.23	0.66
1:D:195:GLY:O	1:D:418:VAL:CG2	2.42	0.66
1:C:371:LEU:HG	1:C:372:PRO:HD2	1.77	0.66
1:D:124:VAL:HA	1:D:127:PHE:CD2	2.31	0.66
2:T:89:GLU:HA	2:T:92:LYS:HE2	1.77	0.66
1:B:208:SER:HB3	1:B:253:ARG:HH22	1.61	0.66
1:B:414:ALA:HB3	1:B:415:PRO:HD2	1.78	0.66
1:C:201:LYS:CE	1:C:202:ASP:O	2.32	0.66
1:C:385:TRP:HE1	1:C:463:LYS:HA	1.58	0.66
1:D:234:GLU:OE2	2:V:13:GLU:N	2.27	0.66
1:D:266:MET:HE1	1:D:294:HIS:HD2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLY:CA	1:B:264[A]:ILE:HD11	2.25	0.66
1:C:187:ARG:HH22	2:T:111:GLN:NE2	1.94	0.66
1:B:160:ASP:OD1	4:B:647:HOH:O	2.13	0.66
1:B:201:LYS:HD2	1:B:239:TYR:CE2	2.31	0.66
2:U:88:ASP:O	2:U:92:LYS:HG3	1.96	0.66
2:U:119:THR:HB	2:U:120:PRO:CD	2.26	0.66
2:T:54:GLU:OE1	2:T:55:HIS:NE2	2.29	0.66
1:A:201:LYS:HD2	1:A:239:TYR:CE2	2.31	0.65
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.31	0.65
1:B:202:ASP:HB3	1:B:206:VAL:HB	1.77	0.65
1:B:383:HIS:HE1	1:B:385:TRP:HB2	1.59	0.65
1:C:169:LEU:HB2	1:C:399:VAL:HG22	1.77	0.65
1:D:177:LYS:HG2	1:D:203:ASP:OD2	1.96	0.65
1:A:148:PHE:CD1	1:A:320:LEU:HB3	2.31	0.65
1:C:266:MET:HG3	1:C:292:HIS:HD2	1.61	0.65
2:V:71:LYS:NZ	2:V:86:GLU:OE1	2.28	0.65
1:B:338:GLU:O	1:B:342:THR:OG1	2.12	0.65
2:V:11:LYS:HG3	2:V:17:TYR:CE2	2.30	0.65
1:C:171:GLY:HA3	1:C:401:GLN:NE2	2.10	0.65
1:D:141:PRO:HA	4:D:631:HOH:O	1.97	0.65
2:T:15:LEU:HD13	2:T:21:LEU:HD21	1.78	0.65
2:V:40:PRO:HG2	2:V:74:MET:CB	2.25	0.65
1:B:414:ALA:HB3	1:B:415:PRO:CD	2.27	0.65
2:T:47:LYS:NZ	4:T:217:HOH:O	2.28	0.65
1:A:133:LEU:H	1:A:307:HIS:HD2	1.44	0.65
1:B:125:PHE:HB2	4:B:673:HOH:O	1.96	0.65
2:S:21:LEU:H	2:S:21:LEU:CD1	2.10	0.65
2:V:30:VAL:HG12	2:V:80:PRO:HB3	1.79	0.65
1:B:109:GLU:H	1:B:115:ASN:ND2	1.94	0.65
1:A:421:ARG:O	1:A:425:GLU:CG	2.45	0.65
1:A:350:ARG:HD2	4:A:656:HOH:O	1.97	0.65
1:A:316:LYS:NZ	1:A:366:GLN:HE21	1.95	0.64
1:C:155:ILE:HG12	1:C:375:ILE:HG13	1.78	0.64
1:C:190:TYR:CE1	1:C:194:ARG:HD2	2.31	0.64
1:B:240:LEU:O	1:B:265:VAL:CG2	2.45	0.64
1:C:168:PRO:HD2	1:C:424:LEU:HD11	1.79	0.64
1:D:42:VAL:HB	1:D:97:PHE:CZ	2.33	0.64
1:B:347:ASP:HB3	1:B:351:ASP:OD2	1.98	0.64
2:S:27:LEU:CD1	2:S:80:PRO:HB2	2.28	0.64
2:V:69:MET:O	4:V:209:HOH:O	2.14	0.64
2:V:87:LEU:O	2:V:90:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:O	1:A:449:CYS:HB2	1.98	0.64
1:C:239:TYR:CD1	1:C:239:TYR:N	2.66	0.64
1:A:154:GLY:HA3	1:A:372:PRO:HB3	1.80	0.64
1:B:342:THR:HG23	1:B:345:PHE:CZ	2.33	0.64
1:C:239:TYR:N	1:C:239:TYR:HD1	1.94	0.64
1:D:323:GLY:O	1:D:374:VAL:HG22	1.97	0.64
1:A:36:ILE:HD12	1:A:108:PHE:CD2	2.33	0.64
1:A:264:ILE:HG22	4:A:630:HOH:O	1.98	0.64
1:C:185:TYR:O	1:C:189:VAL:HG23	1.97	0.64
1:C:295:ARG:O	1:C:298:HIS:HB3	1.98	0.64
1:D:121:VAL:HG11	1:D:309[B]:MET:CE	2.28	0.64
1:B:387:MET:N	1:B:388:PRO:HD3	2.12	0.64
2:U:62:TYR:O	2:U:65:ARG:HD2	1.98	0.64
1:B:309[B]:MET:CE	1:B:314:LEU:CD2	2.76	0.63
1:C:378:ALA:HB2	1:C:394:PHE:CZ	2.33	0.63
1:A:269:TYR:CD1	1:A:318:LEU:HD23	2.33	0.63
1:C:258:ARG:NH1	4:C:694:HOH:O	2.31	0.63
1:A:225:ILE:HD13	1:A:262:VAL:HG22	1.81	0.63
1:C:218:PHE:CZ	1:C:240:LEU:HB3	2.33	0.63
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.79	0.63
1:D:48:VAL:HG12	1:D:53:ALA:HB2	1.79	0.63
1:D:208:SER:HB2	1:D:214:TRP:HB3	1.79	0.63
1:A:153:HIS:HB3	1:A:157:VAL:HG12	1.79	0.63
2:S:120:PRO:O	2:S:121:GLU:HG2	1.99	0.63
2:S:70:TRP:CE2	2:S:90:VAL:HG22	2.34	0.63
1:B:292:HIS:HA	1:B:325:HIS:HB2	1.80	0.63
1:C:221:CYS:O	1:C:225:ILE:HG13	1.99	0.63
1:D:97:PHE:CE1	1:D:99:ALA:HB2	2.32	0.63
1:C:201:LYS:HZ1	1:C:294:HIS:CD2	2.08	0.63
1:C:209:GLN:HB3	1:C:210:PRO:HD2	1.81	0.63
1:A:171:GLY:O	1:A:401:GLN:HA	1.98	0.62
1:C:379:SER:HB2	1:C:401:GLN:HB3	1.81	0.62
1:D:356:LYS:HD2	1:D:363:TYR:O	1.99	0.62
1:B:161:LYS:O	2:T:65[A]:ARG:NE	2.31	0.62
1:A:386:HIS:O	1:A:390:LEU:HG	2.00	0.62
1:B:421:ARG:O	1:B:425:GLU:HG3	1.98	0.62
1:B:429:GLN:O	1:B:433:GLU:HG3	1.99	0.62
2:U:44:PHE:HZ	2:V:3:VAL:HG11	1.64	0.62
1:B:209:GLN:HB2	1:B:211:PHE:CE2	2.34	0.62
1:B:248:GLU:N	1:B:248:GLU:OE1	2.32	0.62
1:C:310:HIS:ND1	1:C:311:PHE:N	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134[A]:ARG:HB2	1:D:307:HIS:HA	1.82	0.62
2:U:70:TRP:HE1	2:U:86:GLU:HG3	1.64	0.62
1:D:266:MET:CE	1:D:294:HIS:HD2	2.12	0.62
1:C:23:THR:O	1:C:81:LYS:HE3	1.99	0.62
1:D:133:LEU:H	1:D:307:HIS:CD2	2.17	0.62
2:U:32:TYR:HD1	2:U:35:ARG:NH2	1.97	0.62
1:A:219[B]:LEU:HG	1:A:256:PHE:HZ	1.65	0.61
1:B:326:ILE:HG21	1:B:349:LEU:HD22	1.82	0.61
1:A:243:THR:HG1	1:A:267:HIS:HA	1.62	0.61
1:C:233:GLY:O	4:C:725:HOH:O	2.15	0.61
1:A:349:LEU:HD11	4:A:760:HOH:O	1.99	0.61
1:C:180:LEU:HB2	4:C:626:HOH:O	1.99	0.61
1:A:186:GLY:HA2	1:A:189:VAL:HB	1.82	0.61
1:C:346:VAL:HG13	1:C:376:PRO:CG	2.25	0.61
1:D:89:PRO:HB3	4:D:743:HOH:O	1.99	0.61
2:S:14:THR:O	4:S:224:HOH:O	2.16	0.61
2:U:52:TYR:CZ	2:U:63:ASP:HB3	2.35	0.61
1:A:43:THR:HG22	1:A:131:ARG:HD3	1.82	0.61
1:A:175:LYS:HA	1:A:176:PRO:C	2.21	0.61
1:B:45:GLN:HB3	1:B:46:PRO:CD	2.30	0.61
1:D:352:ASP:OD1	4:D:608:HOH:O	2.16	0.61
1:D:246:THR:HG21	4:D:630:HOH:O	1.99	0.61
1:B:292:HIS:CE1	1:B:377:VAL:HG21	2.36	0.61
1:B:353:TYR:C	1:B:354:ILE:HD12	2.21	0.61
2:S:55:HIS:HB3	4:S:242:HOH:O	2.00	0.61
2:S:62:TYR:C	2:S:65:ARG:HD2	2.21	0.61
1:A:414:ALA:O	1:A:418:VAL:HG23	2.01	0.60
1:B:414:ALA:O	1:B:417:ALA:HB3	2.01	0.60
1:A:138:LEU:HD12	1:A:313:VAL:HG13	1.82	0.60
1:A:151:PRO:HD2	1:A:372:PRO:HD2	1.83	0.60
1:A:396:ASP:OD1	1:A:431:ARG:NH1	2.32	0.60
1:B:214:TRP:CD1	1:B:253:ARG:NH2	2.67	0.60
1:D:436:ASP:O	1:D:440:GLU:HG3	2.01	0.60
2:V:96:ARG:CA	2:V:120:PRO:HB3	2.30	0.60
1:B:90:VAL:HG23	1:B:97:PHE:HA	1.82	0.60
1:C:319:ARG:NH2	4:C:645:HOH:O	2.31	0.60
1:B:240:LEU:O	1:B:265:VAL:HG22	2.01	0.60
1:C:381:GLY:O	1:C:467:PHE:HE2	1.83	0.60
1:D:160:ASP:OD1	1:D:165:TYR:OH	2.15	0.60
1:D:181:SER:OG	1:D:184:ASN:HB2	2.01	0.60
1:D:316:LYS:CE	1:D:348:LEU:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLN:CB	1:B:211:PHE:CE2	2.85	0.60
1:D:354:ILE:N	1:D:354:ILE:HD12	2.16	0.60
1:B:453:PRO:HD2	1:B:454:GLU:OE1	2.01	0.60
1:C:167:ARG:HH22	1:C:198:ASP:CG	2.04	0.60
1:C:193:LEU:HD22	1:C:236:LYS:HB3	1.83	0.60
1:B:379:SER:HB2	1:B:401:GLN:HB3	1.83	0.60
1:A:330:THR:HG21	1:A:380:GLY:N	2.15	0.60
1:B:173:THR:HA	1:B:201:LYS:HG2	1.84	0.60
1:C:218:PHE:CD2	1:C:240:LEU:HD22	2.37	0.60
1:A:384[A]:VAL:HG11	1:A:455:LEU:HD11	1.83	0.60
1:B:342:THR:HA	1:B:345:PHE:CZ	2.36	0.60
1:D:124:VAL:CA	1:D:127:PHE:CE2	2.85	0.60
1:A:117:PHE:O	1:A:121:VAL:HG22	2.01	0.60
1:A:329:GLY:HA3	4:A:721:HOH:O	2.02	0.60
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.84	0.60
1:A:249:GLU:O	1:A:253:ARG:HG3	2.02	0.59
1:B:271:THR:O	1:B:272:GLY:C	2.39	0.59
1:D:167:ARG:HD3	2:V:14:THR:HG23	1.84	0.59
2:U:33:LEU:HD22	2:U:40:PRO:HG3	1.84	0.59
1:A:167:ARG:NE	4:A:740:HOH:O	2.30	0.59
1:A:294:HIS:CE1	3:A:501:RUB:H4	2.37	0.59
1:C:237:GLY:HA2	1:C:263:PRO:HG3	1.83	0.59
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.84	0.59
2:U:108:ARG:HB3	2:U:108:ARG:NH1	2.18	0.59
1:A:162:LEU:O	1:A:235:ILE:HD12	2.02	0.59
1:C:334:LYS:HG3	1:C:335:LEU:HD12	1.84	0.59
2:T:46:LEU:HD21	2:T:94:TYR:HB3	1.84	0.59
1:A:244:ALA:HA	4:A:607:HOH:O	2.03	0.59
1:A:335:LEU:HB3	4:A:682:HOH:O	2.02	0.59
1:B:345:PHE:HA	1:B:348:LEU:HD12	1.84	0.59
1:C:234:GLU:HG2	2:U:13:GLU:OE2	2.02	0.59
1:C:291:LEU:O	1:C:324:ASP:HB2	2.02	0.59
2:U:44:PHE:HE1	2:V:6:PRO:HG3	1.66	0.59
1:A:370[A]:SER:HB2	1:B:210:PRO:HB3	1.84	0.59
1:B:18[B]:LYS:CB	1:B:18[B]:LYS:NZ	2.65	0.59
1:B:354:ILE:N	1:B:354:ILE:CD1	2.59	0.59
1:D:140:ILE:HG23	1:D:144:TYR:HD2	1.68	0.59
1:D:171:GLY:HA2	1:D:199:PHE:O	2.03	0.59
1:D:178:LEU:HD21	1:D:205:ASN:CB	2.22	0.59
1:D:222:ALA:HA	1:D:225:ILE:HD12	1.84	0.59
1:A:295:ARG:CZ	1:A:298:HIS:CE1	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:HB3	4:B:672:HOH:O	2.02	0.59
1:C:40:PHE:CD1	1:C:133:LEU:HD21	2.38	0.59
2:T:97:ALA:O	2:T:118:HIS:HD2	1.86	0.59
1:A:181:SER:OG	1:A:184:ASN:HB2	2.03	0.59
1:B:267:HIS:HB2	1:B:280:LEU:CD2	2.33	0.59
1:C:37:LEU:O	1:C:138:LEU:HA	2.02	0.59
2:S:52:TYR:N	2:S:52:TYR:HD2	2.00	0.59
2:V:47:LYS:HB3	2:V:47:LYS:HZ2	1.67	0.59
1:A:168:PRO:CG	1:A:396:ASP:HA	2.32	0.59
1:B:32:LYS:C	1:B:34:THR:H	2.06	0.59
1:A:411:TRP:CZ3	2:S:2:GLN:HG3	2.38	0.59
1:C:290:LEU:HA	1:C:324:ASP:OD2	2.02	0.59
1:D:115:ASN:ND2	4:D:675:HOH:O	2.36	0.59
1:A:450:LYS:HB2	1:A:451:TRP:NE1	2.16	0.58
1:B:262:VAL:HB	4:B:645:HOH:O	2.03	0.58
1:D:310:HIS:CE1	1:D:312:ARG:NH2	2.71	0.58
1:B:339:ARG:O	1:B:343:LEU:N	2.34	0.58
2:U:70:TRP:CD2	2:U:90:VAL:HG22	2.37	0.58
2:V:105:ASN:HD22	2:V:106:ASN:N	2.01	0.58
1:C:78:ASP:O	1:C:83[A]:ARG:NH2	2.36	0.58
1:D:60:GLU:HB2	1:D:127:PHE:CZ	2.33	0.58
1:D:75:THR:HG22	1:D:76:SER:N	2.16	0.58
1:D:181:SER:HG	1:D:184:ASN:HB2	1.69	0.58
2:U:99:VAL:O	2:U:116:ILE:HD12	2.04	0.58
1:B:201:LYS:HD2	1:B:239:TYR:HE2	1.68	0.58
1:C:132:ALA:HA	1:C:307:HIS:HD2	1.68	0.58
2:U:108:ARG:NH2	2:U:112:CYS:SG	2.77	0.58
1:B:350:ARG:NH2	1:B:394:PHE:O	2.36	0.58
1:B:330:THR:CG2	1:B:379:SER:N	2.64	0.58
1:C:151:PRO:HD2	1:C:372:PRO:HD2	1.85	0.58
2:T:26:LEU:O	2:T:30:VAL:HG23	2.04	0.57
1:B:318:LEU:HG	1:B:326:ILE:HD12	1.85	0.57
2:S:27:LEU:HD12	2:S:80:PRO:HB2	1.84	0.57
1:A:86:GLU:HB3	1:A:100:TYR:CD2	2.39	0.57
1:B:301:ILE:C	4:B:614:HOH:O	2.42	0.57
1:C:90:VAL:O	4:C:646:HOH:O	2.18	0.57
1:C:201:LYS:HZ2	1:C:294:HIS:CD2	2.19	0.57
1:D:411:TRP:O	1:D:415:PRO:HG2	2.04	0.57
1:A:201:LYS:HB3	1:A:239:TYR:CG	2.39	0.57
1:A:403:GLY:O	1:A:407:LEU:HD12	2.03	0.57
1:B:298:HIS:NE2	4:B:682:HOH:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:HG23	4:D:655:HOH:O	2.03	0.57
1:A:158:GLU:HG2	1:A:162:LEU:HD11	1.85	0.57
1:B:135:LEU:HB3	1:B:309[A]:MET:HG3	1.86	0.57
1:C:190:TYR:CZ	1:C:194:ARG:HD2	2.39	0.57
1:A:276:ALA:O	1:A:279[A]:THR:OG1	2.22	0.57
1:D:195:GLY:O	1:D:418:VAL:HG22	2.04	0.57
1:D:335:LEU:HB2	4:D:619:HOH:O	2.05	0.57
1:B:382:ILE:HD12	1:B:402:PHE:CE1	2.40	0.57
1:D:195:GLY:O	1:D:418:VAL:HG23	2.03	0.57
1:A:264:ILE:CG1	1:A:290:LEU:HB2	2.32	0.57
1:B:18[B]:LYS:HZ2	1:B:18[B]:LYS:HB2	1.69	0.57
1:C:157:VAL:HG11	1:D:216:ASP:OD2	2.04	0.56
1:C:159[A]:ARG:HG3	1:C:164:LYS:O	2.04	0.56
2:S:9:LYS:HB2	4:S:203:HOH:O	2.03	0.56
1:B:41:ARG:O	4:B:628:HOH:O	2.17	0.56
1:B:237:GLY:HA3	1:B:264[A]:ILE:CD1	2.31	0.56
1:C:157:VAL:O	1:C:161:LYS:HG3	2.05	0.56
1:D:191:GLU:HB3	1:D:413:ASN:HB2	1.86	0.56
2:S:44:PHE:HA	2:S:98:PHE:O	2.05	0.56
1:A:221:CYS:O	1:A:225:ILE:HG13	2.06	0.56
1:C:158:GLU:HG3	1:C:162:LEU:HD11	1.87	0.56
2:S:95:PRO:O	2:S:118:HIS:CE1	2.58	0.56
1:D:187:ARG:HH22	2:U:111:GLN:NE2	2.03	0.56
1:D:316:LYS:HE2	1:D:348:LEU:HD13	1.87	0.56
1:D:249:GLU:HG3	4:D:614:HOH:O	2.04	0.56
1:A:290:LEU:HA	1:A:324:ASP:OD2	2.06	0.56
1:B:42:VAL:HG13	1:B:130:LEU:CD2	2.36	0.56
1:A:37:LEU:HB2	1:A:139:ARG:CB	2.34	0.56
1:A:161:LYS:NZ	1:B:219[A]:LEU:HD21	2.20	0.56
1:A:168:PRO:HG2	1:A:391:THR:HG23	1.88	0.56
1:D:117:PHE:O	1:D:121:VAL:CG2	2.54	0.56
1:A:412:GLY:HA2	4:A:645:HOH:O	2.06	0.56
1:B:231:GLU:OE2	4:B:680:HOH:O	2.18	0.56
4:B:603:HOH:O	1:C:215:ARG:HB2	2.05	0.56
1:C:255:VAL:HG21	4:C:719:HOH:O	2.05	0.56
1:A:201:LYS:NZ	1:A:294:HIS:CD2	2.75	0.55
1:B:117:PHE:O	1:B:121:VAL:HG22	2.06	0.55
1:B:384:VAL:HG21	1:B:455:LEU:CD1	2.35	0.55
2:T:46:LEU:HD12	2:U:6:PRO:HG2	1.88	0.55
2:T:113:ILE:HG22	4:T:215:HOH:O	2.05	0.55
2:U:70:TRP:NE1	2:U:86:GLU:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:108:ARG:HH12	2:U:110:VAL:CG2	2.19	0.55
2:U:121:GLU:N	2:U:122:SER:CA	2.63	0.55
1:B:339:ARG:HB2	4:B:723:HOH:O	2.06	0.55
1:C:380:GLY:HA2	3:C:501:RUB:H11	1.86	0.55
1:A:379:SER:HB2	1:A:401:GLN:HB3	1.88	0.55
1:B:164:LYS:HE3	1:B:198:ASP:HB3	1.88	0.55
2:U:52:TYR:N	2:U:52:TYR:CD2	2.71	0.55
1:C:54:GLY:O	1:C:57:VAL:HB	2.06	0.55
1:C:199:PHE:CB	1:C:239:TYR:HE1	2.19	0.55
2:T:93:GLU:HG3	2:T:94:TYR:CD2	2.41	0.55
1:B:253:ARG:NH1	4:B:627:HOH:O	2.39	0.55
1:C:266:MET:HG3	1:C:292:HIS:CD2	2.40	0.55
1:D:195:GLY:HA3	1:D:417:ALA:HB3	1.86	0.55
2:U:10:LYS:O	2:U:11:LYS:HD3	2.06	0.55
1:D:177:LYS:NZ	1:D:203:ASP:OD2	2.29	0.55
1:D:269:TYR:CD1	1:D:318:LEU:HD23	2.41	0.55
2:T:22:THR:O	2:T:26:LEU:HD12	2.07	0.55
1:A:155:ILE:HG12	1:A:375:ILE:HG13	1.88	0.55
1:B:217:ARG:O	1:B:221:CYS:HB2	2.07	0.55
1:C:124[A]:VAL:HG12	1:C:133:LEU:HD22	1.88	0.55
1:C:347:ASP:O	1:C:351:ASP:HB2	2.06	0.55
2:U:47:LYS:HZ3	2:U:48:LYS:HD2	1.72	0.55
1:A:37:LEU:HB3	1:A:364:PHE:CE1	2.42	0.55
1:A:298:HIS:CD2	1:A:299:ALA:N	2.75	0.55
1:B:337:GLY:HA2	4:B:739:HOH:O	2.05	0.55
1:C:356:LYS:HE3	1:C:363:TYR:O	2.07	0.55
2:S:30:VAL:CG2	2:S:83:VAL:HG11	2.36	0.55
2:T:46:LEU:CD2	2:T:97:ALA:HB2	2.25	0.55
2:V:102:ILE:HG12	2:V:111:GLN:OE1	2.07	0.55
1:C:330:THR:HG22	1:C:379:SER:H	1.72	0.54
1:D:51:GLU:HA	1:D:87:ILE:HD11	1.88	0.54
1:D:60:GLU:HG3	1:D:127:PHE:HE1	1.68	0.54
2:T:5:PRO:HB2	2:T:9:LYS:HG3	1.88	0.54
1:B:234:GLU:OE2	2:T:13:GLU:N	2.40	0.54
1:C:170:LEU:HD11	1:C:421:ARG:HA	1.89	0.54
1:D:388:PRO:HB3	1:D:437:LEU:HD12	1.88	0.54
1:A:219[B]:LEU:HD22	2:V:61:TYR:HB2	1.90	0.54
1:C:88:GLU:HB3	1:C:98:ILE:HB	1.89	0.54
1:D:292:HIS:CD2	1:D:325:HIS:HB2	2.42	0.54
2:T:15:LEU:CD1	2:T:21:LEU:HD21	2.36	0.54
2:T:38:TRP:HA	2:T:104:PHE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:HG2	1:C:368:TRP:CZ3	2.43	0.54
1:C:456:ALA:HA	1:C:459:CYS:HB2	1.88	0.54
1:D:151:PRO:HB3	1:D:323:GLY:O	2.08	0.54
1:D:466:LYS:HD3	1:D:468:GLU:HB2	1.90	0.54
1:B:291:LEU:O	1:B:324:ASP:N	2.33	0.54
1:C:75:THR:CG2	1:C:76:SER:N	2.58	0.54
1:B:156:GLN:HG3	2:T:110:VAL:HG13	1.89	0.54
1:B:435:ARG:NH2	1:B:447:GLU:OE1	2.36	0.54
1:C:45:GLN:NE2	1:C:131:ARG:CG	2.65	0.54
1:D:21:LYS:HB2	1:D:21:LYS:NZ	2.21	0.54
2:U:21:LEU:HB2	2:U:26:LEU:HG	1.90	0.54
1:A:169:LEU:HB2	1:A:399:VAL:HG22	1.90	0.54
1:C:462[B]:TRP:HZ3	4:C:622:HOH:O	1.90	0.54
1:B:160:ASP:HB3	1:C:183:LYS:HG3	1.89	0.54
1:D:164:LYS:HE3	1:D:198:ASP:HB3	1.89	0.54
1:A:258:ARG:HD3	2:S:59:PRO:HG2	1.89	0.54
1:B:291:LEU:O	1:B:324:ASP:HB2	2.07	0.54
1:C:174:ILE:HD11	1:C:189:VAL:CG2	2.38	0.54
1:A:79:ARG:HD3	1:A:80:TYR:CZ	2.43	0.53
1:A:269:TYR:CE1	1:A:318:LEU:HB2	2.43	0.53
1:B:365:THR:HB	4:B:676:HOH:O	2.07	0.53
1:D:403:GLY:HA3	3:D:501:RUB:O2P	2.07	0.53
2:S:9:LYS:O	2:S:11:LYS:HG2	2.08	0.53
1:A:330:THR:OG1	1:A:333:GLY:HA3	2.09	0.53
1:B:40:PHE:HB3	1:B:133:LEU:HD11	1.90	0.53
1:B:167:ARG:HG2	2:T:14:THR:OG1	2.08	0.53
1:B:296:ALA:O	1:B:297:MET:HB3	2.07	0.53
1:C:234:GLU:CG	2:U:13:GLU:OE2	2.56	0.53
2:V:10:LYS:HB3	2:V:50:PHE:CE1	2.42	0.53
1:A:16:GLY:C	1:A:67:THR:HG22	2.28	0.53
1:A:48:VAL:CG1	1:A:53:ALA:HB2	2.39	0.53
1:A:201:LYS:CB	1:A:239:TYR:CD2	2.86	0.53
2:U:43:GLU:OE1	2:U:100:ARG:NH1	2.39	0.53
2:V:45:GLU:HG2	2:V:48:LYS:O	2.08	0.53
1:C:158:GLU:CG	1:C:162:LEU:HD11	2.38	0.53
1:D:105:LEU:HB3	4:D:747:HOH:O	2.08	0.53
1:D:292:HIS:HD2	1:D:325:HIS:HB2	1.72	0.53
1:A:219[B]:LEU:CD2	2:V:61:TYR:HD1	2.22	0.53
1:B:65:THR:OG1	1:B:66:TRP:N	2.34	0.53
1:A:85:TYR:HB2	4:A:648:HOH:O	2.08	0.53
1:B:24:TYR:HB2	1:B:55:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.43	0.53
1:B:237:GLY:CA	1:B:264[A]:ILE:CD1	2.87	0.53
2:T:87:LEU:C	2:T:87:LEU:HD23	2.29	0.53
2:U:10:LYS:HD2	2:U:50:PHE:CE2	2.44	0.53
2:U:113:ILE:HG12	4:U:210:HOH:O	2.07	0.53
1:B:24:TYR:CG	1:B:59:ALA:HB2	2.43	0.53
1:D:49:PRO:HB2	1:D:52:GLU:CB	2.36	0.53
2:T:102[B]:ILE:HG22	2:T:103:GLY:N	2.23	0.53
1:B:43:THR:O	1:B:131:ARG:HB2	2.09	0.53
1:A:219[B]:LEU:HD22	2:V:61:TYR:HD1	1.74	0.53
1:B:191:GLU:HB3	1:B:413:ASN:HB2	1.91	0.53
1:C:60:GLU:CG	1:C:127:PHE:HZ	2.22	0.53
1:C:180:LEU:HA	2:T:109:GLN:HE22	1.74	0.53
1:D:104:PRO:HA	4:D:657:HOH:O	2.08	0.53
2:V:105:ASN:ND2	2:V:107:VAL:H	2.07	0.53
1:A:285:ARG:NH2	4:A:698:HOH:O	2.41	0.52
1:C:206:VAL:HG12	1:C:217:ARG:CZ	2.40	0.52
1:D:267:HIS:CD2	1:D:277:ASN:OD1	2.61	0.52
1:A:211:PHE:CD1	1:A:212:MET:HB3	2.44	0.52
1:D:42:VAL:O	1:D:96:GLN:HA	2.09	0.52
1:D:201:LYS:CB	1:D:239:TYR:CD2	2.92	0.52
1:A:172:CYS:HB3	1:A:197:LEU:HD13	1.92	0.52
1:B:41:ARG:NH1	1:B:96:GLN:OE1	2.41	0.52
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.44	0.52
1:C:174:ILE:HD13	1:C:185:TYR:CE2	2.44	0.52
1:D:162:LEU:HB3	1:D:164:LYS:HG3	1.91	0.52
2:S:30:VAL:HG21	2:S:83:VAL:HG11	1.90	0.52
1:C:159[B]:ARG:CZ	1:C:397:ASP:OD1	2.58	0.52
1:C:243:THR:HG23	1:C:267:HIS:CE1	2.45	0.52
2:U:11:LYS:HG3	2:U:17:TYR:CE2	2.45	0.52
2:V:62:TYR:O	2:V:65:ARG:HD2	2.10	0.52
1:A:155:ILE:HD11	1:A:350:ARG:HG2	1.91	0.52
1:A:201:LYS:CB	1:A:239:TYR:HB2	2.40	0.52
1:A:245:GLY:N	4:A:607:HOH:O	2.43	0.52
1:B:60:GLU:OE1	1:B:123:ASN:HB2	2.09	0.52
1:B:135:LEU:HB3	1:B:309[B]:MET:HG2	1.91	0.52
1:D:303:ARG:HG2	1:D:303:ARG:HH11	1.74	0.52
1:C:174:ILE:HD12	1:C:238:HIS:HE1	1.75	0.52
1:D:319[A]:ARG:NH2	1:D:371:LEU:O	2.42	0.52
1:D:339:ARG:NH2	1:D:392:GLU:OE2	2.43	0.52
2:U:21:LEU:HD23	2:U:25:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:HG2	4:A:749:HOH:O	2.09	0.52
1:B:195:GLY:HA3	1:B:414:ALA:O	2.09	0.52
1:B:240:LEU:O	1:B:265:VAL:HG23	2.10	0.52
1:C:153:HIS:HA	4:C:606:HOH:O	2.10	0.52
1:C:223:GLU:OE2	2:T:65[B]:ARG:HB2	2.10	0.52
1:D:201:LYS:HB2	1:D:239:TYR:CD2	2.45	0.52
2:T:71:LYS:HG2	2:U:1:MET:HG3	1.92	0.52
2:U:22:THR:OG1	2:U:25:GLN:HG3	2.09	0.52
1:B:168:PRO:HG2	1:B:424:LEU:HD11	1.93	0.51
1:B:295:ARG:O	1:B:298:HIS:HB3	2.10	0.51
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.91	0.51
1:B:346:VAL:CG1	1:B:350:ARG:CZ	2.87	0.51
1:C:318:LEU:CG	1:C:326:ILE:HD12	2.34	0.51
1:D:193:LEU:HB3	1:D:236:LYS:HD2	1.92	0.51
1:A:201:LYS:HZ2	1:A:294:HIS:CD2	2.28	0.51
1:A:208:SER:HB2	1:A:214:TRP:HB3	1.91	0.51
1:B:201:LYS:HB2	1:B:239:TYR:HD2	1.72	0.51
1:D:266:MET:HE1	1:D:294:HIS:CD2	2.45	0.51
1:A:193:LEU:O	1:A:236:LYS:CE	2.59	0.51
1:A:298:HIS:O	1:A:301:ILE:N	2.42	0.51
1:C:79:ARG:HB3	1:C:80:TYR:CD2	2.45	0.51
1:C:79:ARG:HB3	1:C:80:TYR:HD2	1.76	0.51
1:C:200:THR:O	1:C:201:LYS:HB3	2.08	0.51
1:C:369:VAL:O	1:C:370[A]:SER:OG	2.24	0.51
1:D:90:VAL:HG12	1:D:91:PRO:O	2.11	0.51
2:T:99:VAL:HG23	2:T:118:HIS:HB3	1.92	0.51
1:A:381:GLY:O	1:A:467:PHE:HE2	1.94	0.51
1:B:373:GLY:N	4:B:772:HOH:O	2.43	0.51
1:C:134[B]:ARG:HA	1:C:308:GLY:O	2.11	0.51
1:C:175:LYS:O	1:C:407:LEU:HD22	2.10	0.51
1:C:294:HIS:HE1	3:C:501:RUB:O4	1.94	0.51
2:T:93:GLU:OE1	2:T:94:TYR:CE2	2.63	0.51
1:A:32[B]:LYS:HE3	1:A:34:THR:OG1	2.11	0.51
1:B:167:ARG:CZ	4:B:695:HOH:O	2.58	0.51
1:C:187:ARG:HH22	2:T:111:GLN:HE22	1.57	0.51
1:D:298:HIS:NE2	4:D:717:HOH:O	2.34	0.51
1:D:330:THR:OG1	1:D:333:GLY:HA3	2.11	0.51
1:A:45:GLN:HA	1:A:45:GLN:OE1	2.11	0.51
1:B:414:ALA:CB	1:B:415:PRO:CD	2.88	0.51
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.14	0.51
1:A:421:ARG:NE	1:A:425:GLU:OE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:PRO:HA	1:D:396:ASP:O	2.11	0.51
1:D:316:LYS:HE3	1:D:348:LEU:HD13	1.93	0.51
2:T:14:THR:O	2:T:15:LEU:HB2	2.11	0.51
1:D:60:GLU:CB	1:D:127:PHE:CZ	2.88	0.51
2:S:7:ILE:HG22	2:V:46:LEU:HD13	1.91	0.51
1:B:379:SER:OG	3:B:501:RUB:O3	2.29	0.50
1:C:171:GLY:C	1:C:401:GLN:HG3	2.32	0.50
1:C:182:ALA:CB	1:C:216:ASP:HB3	2.41	0.50
1:D:267:HIS:HB2	1:D:280:LEU:CD2	2.42	0.50
2:V:80:PRO:HD3	4:V:222:HOH:O	2.11	0.50
1:C:435:ARG:NH1	1:C:440:GLU:HG2	2.22	0.50
1:A:327:HIS:ND1	3:A:501:RUB:O5P	2.37	0.50
1:B:90:VAL:CG2	1:B:97:PHE:HA	2.40	0.50
1:C:24:TYR:O	1:C:55:ALA:HA	2.11	0.50
4:C:613:HOH:O	2:T:71:LYS:HA	2.11	0.50
2:S:93:GLU:HB3	2:S:94:TYR:CD2	2.46	0.50
1:C:149:GLN:HE22	1:C:282:HIS:HA	1.76	0.50
1:A:219[A]:LEU:HD23	1:A:220:PHE:CE2	2.46	0.50
1:A:331:VAL:N	4:A:632:HOH:O	2.45	0.50
1:B:162:LEU:O	1:B:163:ASN:CB	2.59	0.50
1:B:193:LEU:O	1:B:236:LYS:NZ	2.34	0.50
1:B:414:ALA:O	1:B:418:VAL:HG23	2.11	0.50
1:C:368:TRP:O	1:C:369:VAL:C	2.50	0.50
1:D:294:HIS:CE1	4:D:745:HOH:O	2.64	0.50
2:T:66:TYR:O	2:T:67:TRP:HD1	1.94	0.50
1:A:36:ILE:CG1	1:A:141:PRO:HD3	2.39	0.50
1:C:131:ARG:O	1:C:132:ALA:CB	2.60	0.50
1:C:239:TYR:HD2	1:C:292:HIS:CD2	2.29	0.50
1:D:26:THR:OG1	1:D:29:TYR:HB2	2.11	0.50
1:D:466:LYS:C	1:D:466:LYS:HD2	2.32	0.50
2:U:55:HIS:O	2:V:57:LYS:HE2	2.12	0.50
2:V:120:PRO:O	2:V:122:SER:N	2.45	0.50
1:A:252:LYS:NZ	1:D:286:ASP:CG	2.61	0.50
1:A:419:ALA:HB1	1:A:455:LEU:HA	1.93	0.50
1:D:109:GLU:H	1:D:115:ASN:ND2	2.10	0.50
2:S:46[A]:LEU:HD21	2:S:97:ALA:HB2	1.93	0.50
1:C:446:ARG:O	1:C:449:CYS:HB2	2.11	0.50
2:S:7:ILE:CG2	2:V:46:LEU:HD13	2.42	0.50
1:C:60:GLU:HB2	1:C:127:PHE:HZ	1.77	0.50
1:C:199:PHE:CG	1:C:239:TYR:HE1	2.30	0.50
1:D:263:PRO:HA	4:V:203:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:70:TRP:HZ2	2:V:89:GLU:HG2	1.75	0.50
1:A:297:MET:O	1:A:297:MET:CG	2.53	0.49
1:B:251:LEU:O	1:B:255:VAL:HG23	2.12	0.49
1:B:290:LEU:HA	1:B:324:ASP:OD2	2.12	0.49
1:B:371:LEU:HG	1:B:372:PRO:HD2	1.95	0.49
1:A:48:VAL:HG12	1:A:53:ALA:HB2	1.93	0.49
1:B:134:ARG:HD2	4:B:701:HOH:O	2.11	0.49
1:B:223:GLU:OE1	2:S:65:ARG:HD3	2.12	0.49
1:B:339:ARG:HE	1:B:343:LEU:HD11	1.77	0.49
1:C:97:PHE:HE1	1:C:99:ALA:HB2	1.77	0.49
1:D:151:PRO:HD2	1:D:372:PRO:HD2	1.93	0.49
1:D:264:ILE:CD1	1:D:325:HIS:HE1	2.25	0.49
2:S:21:LEU:HB3	2:S:25:GLN:HB2	1.94	0.49
2:V:70:TRP:CE3	2:V:90:VAL:HG23	2.47	0.49
1:A:85:TYR:CE2	1:A:100:TYR:HB3	2.47	0.49
1:C:134[A]:ARG:HA	1:C:308:GLY:O	2.11	0.49
1:D:88:GLU:HB3	1:D:98[B]:ILE:HB	1.94	0.49
1:D:396:ASP:CG	1:D:431:ARG:HH12	2.15	0.49
2:T:12:PHE:O	2:T:13:GLU:HB2	2.13	0.49
2:U:44:PHE:CZ	2:V:3:VAL:HG11	2.46	0.49
2:V:11:LYS:HG3	2:V:17:TYR:CZ	2.47	0.49
2:V:46:LEU:HD11	2:V:94:TYR:CD1	2.48	0.49
2:V:96:ARG:HD2	2:V:120:PRO:HB2	1.94	0.49
1:B:56:ALA:HB3	1:B:127:PHE:HE2	1.76	0.49
1:D:75:THR:CG2	1:D:76:SER:H	2.22	0.49
2:T:11:LYS:HG3	2:T:17:TYR:CZ	2.46	0.49
1:B:342:THR:HG23	1:B:345:PHE:CE2	2.47	0.49
1:C:451:TRP:HH2	2:U:17:TYR:O	1.96	0.49
2:T:100:ARG:HD2	2:T:114:SER:OG	2.13	0.49
2:U:99:VAL:HG12	2:U:117:ALA:HB3	1.95	0.49
2:V:87:LEU:HD22	2:V:91:LYS:CE	2.38	0.49
1:A:261:GLY:O	4:A:624:HOH:O	2.20	0.49
1:A:384[A]:VAL:CG1	1:A:455:LEU:HD11	2.42	0.49
1:B:21:LYS:HB3	1:B:52:GLU:OE1	2.12	0.49
1:B:50:PRO:HA	1:B:97:PHE:CZ	2.48	0.49
2:T:44:PHE:HB3	2:T:99:VAL:HG13	1.93	0.49
2:T:45:GLU:O	2:T:98:PHE:HD2	1.95	0.49
2:V:47:LYS:HB3	2:V:47:LYS:NZ	2.27	0.49
2:V:90:VAL:CG1	2:V:91:LYS:N	2.74	0.49
1:B:32:LYS:C	1:B:34:THR:N	2.66	0.49
1:B:177:LYS:HZ2	1:B:203:ASP:CG	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HG3	1:B:303:ARG:O	2.12	0.49
1:C:164:LYS:HB3	4:C:707:HOH:O	2.12	0.49
1:C:167:ARG:HG2	2:U:14[A]:THR:HG23	1.93	0.49
1:D:380:GLY:HA3	4:D:619:HOH:O	2.12	0.49
2:S:70:TRP:NE1	2:S:71:LYS:HD2	2.27	0.49
1:A:159:ARG:HG2	1:A:159:ARG:NH1	2.25	0.49
1:B:293:ILE:N	1:B:325:HIS:O	2.45	0.49
1:C:262:VAL:HG13	4:C:611:HOH:O	2.13	0.49
2:S:46[A]:LEU:CD2	2:S:97:ALA:HB2	2.42	0.49
1:A:191:GLU:HA	1:A:194:ARG:HD3	1.95	0.49
1:B:45:GLN:HB3	1:B:46:PRO:HD3	1.94	0.49
1:B:387:MET:N	1:B:388:PRO:CD	2.76	0.49
2:S:3:VAL:HG21	2:V:70:TRP:CZ3	2.48	0.49
1:A:109:GLU:OE1	4:A:619:HOH:O	2.20	0.48
1:C:239:TYR:CD2	1:C:292:HIS:CG	3.01	0.48
1:D:134[B]:ARG:HB2	1:D:307:HIS:HA	1.94	0.48
1:C:157:VAL:O	1:C:161:LYS:CG	2.60	0.48
1:C:172:CYS:CB	1:C:402:PHE:O	2.56	0.48
1:C:237:GLY:CA	1:C:263:PRO:HG3	2.43	0.48
1:D:89:PRO:HA	1:D:97:PHE:CB	2.43	0.48
2:S:21:LEU:CD1	2:S:21:LEU:N	2.76	0.48
2:V:3:VAL:O	2:V:5:PRO:HD3	2.12	0.48
1:A:295:ARG:NE	1:A:298:HIS:CE1	2.81	0.48
1:B:23:THR:CG2	1:B:24:TYR:CE2	2.89	0.48
1:D:125:PHE:N	1:D:125:PHE:CD2	2.82	0.48
1:D:330:THR:OG1	1:D:333:GLY:N	2.47	0.48
1:D:367:ASP:OD2	1:D:369:VAL:HG13	2.13	0.48
2:T:102[A]:ILE:HG22	2:T:114:SER:HB2	1.96	0.48
1:A:155:ILE:CD1	1:A:350:ARG:HG2	2.43	0.48
1:D:263:PRO:HG2	1:D:264:ILE:HG22	1.96	0.48
1:C:200:THR:O	1:C:239:TYR:CD1	2.66	0.48
1:D:118:THR:O	1:D:122:GLY:HA3	2.14	0.48
1:D:329:GLY:CA	4:D:734:HOH:O	2.55	0.48
2:U:107:VAL:O	2:U:109:GLN:N	2.47	0.48
1:A:168:PRO:HG3	1:A:396:ASP:CA	2.37	0.48
1:B:449:CYS:SG	1:B:456:ALA:HA	2.54	0.48
1:C:158:GLU:OE1	1:C:325:HIS:NE2	2.35	0.48
2:T:120:PRO:HG2	2:T:123:TYR:HD1	1.78	0.48
2:U:96:ARG:HH21	2:U:121:GLU:H	1.60	0.48
1:A:225:ILE:CD1	1:A:262:VAL:HG22	2.43	0.48
1:C:330:THR:CG2	1:C:379:SER:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:14:THR:HG22	2:S:15:LEU:HG	1.95	0.48
2:T:119:THR:HB	2:T:123:TYR:CE1	2.49	0.48
1:A:411:TRP:CH2	2:S:2:GLN:HG3	2.48	0.48
1:C:159[A]:ARG:NH2	1:C:396:ASP:O	2.44	0.48
1:D:201:LYS:HE3	1:D:294:HIS:NE2	2.26	0.48
2:S:21:LEU:H	2:S:21:LEU:HD12	1.77	0.48
2:U:87:LEU:O	2:U:91:LYS:HB2	2.13	0.48
1:D:325:HIS:HD2	1:D:375:ILE:HB	1.79	0.48
1:D:366:GLN:NE2	1:D:367:ASP:O	2.46	0.48
1:D:418:VAL:HG21	2:V:4:TRP:CE2	2.49	0.48
2:U:52:TYR:H	2:U:52:TYR:HD2	1.61	0.48
1:A:234:GLU:O	1:A:236:LYS:HG2	2.14	0.48
1:B:372:PRO:CA	4:B:772:HOH:O	2.47	0.48
1:C:38:ALA:HB1	1:C:135:LEU:HD11	1.95	0.48
1:D:168:PRO:HG2	1:D:424:LEU:HD11	1.95	0.48
1:D:454:GLU:H	1:D:454:GLU:CD	2.17	0.48
2:S:74:MET:HB3	2:S:77:THR:OG1	2.14	0.48
2:V:96:ARG:HD2	2:V:120:PRO:CB	2.44	0.48
1:B:172:CYS:SG	1:B:403:GLY:HA2	2.54	0.47
1:C:71:THR:C	1:C:73:GLY:N	2.67	0.47
1:C:156:GLN:HB2	4:C:709:HOH:O	2.14	0.47
1:C:316:LYS:HG2	1:C:368:TRP:HZ2	1.79	0.47
1:C:342:THR:HA	1:C:345:PHE:CE2	2.49	0.47
1:D:34:THR:O	1:D:105:LEU:HD13	2.14	0.47
1:D:310:HIS:NE2	1:D:312:ARG:NH2	2.62	0.47
2:U:105:ASN:O	2:U:109:GLN:HA	2.14	0.47
1:A:425:GLU:OE1	2:S:15:LEU:CA	2.63	0.47
1:B:336:GLU:HA	4:B:687:HOH:O	2.14	0.47
1:B:385:TRP:CE2	1:B:459:CYS:HB3	2.49	0.47
1:C:372:PRO:HG3	4:D:602:HOH:O	2.14	0.47
1:D:178:LEU:HD11	1:D:205:ASN:ND2	2.29	0.47
1:D:201:LYS:HZ1	1:D:294:HIS:CD2	2.14	0.47
2:S:15:LEU:HB2	4:S:224:HOH:O	2.14	0.47
2:T:65[A]:ARG:HB2	2:T:65[A]:ARG:HH11	1.78	0.47
2:U:119:THR:HB	2:U:120:PRO:HD3	1.95	0.47
1:B:340:GLU:O	1:B:343:LEU:HB2	2.14	0.47
1:C:293:ILE:CG1	1:C:325:HIS:O	2.62	0.47
1:C:336:GLU:OE2	1:C:337:GLY:N	2.47	0.47
1:D:444:ILE:O	1:D:447:GLU:HB2	2.13	0.47
2:V:23:ARG:NH2	2:V:88:ASP:OD2	2.47	0.47
2:V:47:LYS:HE3	2:V:48:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:CB	1:B:363:TYR:HB2	2.44	0.47
1:B:149:GLN:OE1	1:B:281:SER:OG	2.32	0.47
1:C:253:ARG:NH1	4:C:617:HOH:O	2.45	0.47
1:A:23:THR:O	1:A:81:LYS:NZ	2.35	0.47
1:B:267:HIS:HE1	4:B:609:HOH:O	1.96	0.47
1:C:262:VAL:HA	1:C:263:PRO:HD2	1.63	0.47
1:C:310:HIS:CD2	1:C:312:ARG:CZ	2.98	0.47
1:C:325:HIS:HE1	1:C:399:VAL:HG21	1.73	0.47
1:D:159:ARG:HG2	1:D:159:ARG:HH11	1.80	0.47
2:T:10:LYS:HB3	2:T:50:PHE:CE1	2.50	0.47
1:B:157:VAL:HG23	4:B:606:HOH:O	2.14	0.47
1:A:86:GLU:HB3	1:A:100:TYR:HD2	1.79	0.47
1:A:148:PHE:CG	1:A:320:LEU:HB3	2.50	0.47
1:A:162:LEU:O	1:A:163:ASN:CB	2.62	0.47
1:A:239:TYR:N	1:A:239:TYR:CD1	2.81	0.47
1:A:390:LEU:HB3	1:A:400:LEU:HD22	1.96	0.47
1:B:348:LEU:HD11	1:B:362[B]:ILE:HD12	1.96	0.47
1:B:383:HIS:CD2	1:B:462:TRP:HB3	2.50	0.47
1:C:295:ARG:HG2	1:C:327:HIS:HB2	1.97	0.47
1:C:338:GLU:HA	4:C:643:HOH:O	2.13	0.47
1:D:13:PHE:HA	4:D:721:HOH:O	2.13	0.47
1:D:57:VAL:HA	1:D:124:VAL:HG11	1.97	0.47
2:S:27:LEU:HD11	2:S:80:PRO:HB2	1.97	0.47
2:S:62:TYR:HB2	2:S:65:ARG:NE	2.28	0.47
2:T:42:LEU:HD22	2:T:90:VAL:HG11	1.97	0.47
1:A:156:GLN:HG2	1:A:157:VAL:N	2.28	0.47
1:B:195:GLY:O	1:B:418:VAL:HG22	2.14	0.47
1:C:167:ARG:NH2	1:C:198:ASP:OD2	2.48	0.47
1:C:289:LEU:HD23	2:U:59:PRO:HB3	1.96	0.47
1:C:350:ARG:HD2	4:C:628:HOH:O	2.14	0.47
2:S:44:PHE:O	2:S:67:TRP:HB3	2.14	0.47
2:U:108:ARG:O	2:U:109:GLN:C	2.53	0.47
1:A:109:GLU:N	1:A:115:ASN:OD1	2.32	0.47
1:B:378:ALA:O	1:B:379:SER:HB2	2.15	0.47
1:C:60:GLU:CB	1:C:127:PHE:HZ	2.28	0.47
1:C:142:TYR:O	1:C:146:LYS:HG2	2.15	0.47
1:C:291:LEU:N	1:C:324:ASP:OD2	2.41	0.47
1:C:293:ILE:HG12	1:C:325:HIS:O	2.15	0.47
2:S:70:TRP:CZ3	2:T:3:VAL:HG21	2.50	0.47
2:V:62:TYR:HB2	2:V:65:ARG:HD2	1.96	0.47
2:V:90:VAL:CG1	2:V:99:VAL:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HA	1:A:95:ASN:H	1.80	0.47
1:A:183:LYS:NZ	1:D:163:ASN:OD1	2.48	0.47
1:B:295:ARG:HG3	1:B:298:HIS:CD2	2.49	0.47
1:B:340:GLU:O	1:B:360:ARG:HG2	2.15	0.47
1:C:357:ASP:OD2	1:C:360:ARG:HD2	2.14	0.47
1:D:201:LYS:HB3	1:D:239:TYR:CD2	2.50	0.47
1:D:409:HIS:CD2	1:D:410:PRO:HD2	2.50	0.47
2:T:119:THR:HB	2:T:123:TYR:HE1	1.80	0.47
1:C:269:TYR:CD1	1:C:318:LEU:HD23	2.50	0.46
1:C:457:ALA:O	1:C:461:VAL:HG23	2.15	0.46
2:V:119:THR:HB	2:V:120:PRO:CD	2.45	0.46
1:A:34:THR:O	1:A:105:LEU:HD13	2.16	0.46
1:A:158:GLU:OE2	1:A:375:ILE:HD12	2.14	0.46
1:A:176:PRO:HD2	1:A:180:LEU:HG	1.96	0.46
1:A:225:ILE:CD1	1:A:262:VAL:CG2	2.93	0.46
1:A:264:ILE:HG13	1:A:290:LEU:HB3	1.91	0.46
1:A:447:GLU:HA	1:A:450:LYS:HE3	1.95	0.46
1:B:93:GLU:HB2	1:B:96:GLN:HB3	1.96	0.46
2:S:6:PRO:HG3	2:V:44:PHE:CE1	2.50	0.46
2:S:56:ASN:ND2	4:S:206:HOH:O	2.47	0.46
1:A:330:THR:CG2	1:A:379:SER:C	2.83	0.46
1:B:94:ASP:HA	1:B:95:ASN:HA	1.57	0.46
1:B:133:LEU:O	1:B:307:HIS:HA	2.14	0.46
1:C:213:ARG:O	1:C:216:ASP:HB2	2.16	0.46
1:D:134[B]:ARG:HG3	1:D:308:GLY:H	1.80	0.46
1:D:402:PHE:N	1:D:402:PHE:CD2	2.84	0.46
2:V:108:ARG:O	2:V:109:GLN:CB	2.61	0.46
1:A:158:GLU:OE1	1:A:325:HIS:NE2	2.49	0.46
1:A:193:LEU:HB3	1:A:236:LYS:HD2	1.96	0.46
1:C:378:ALA:O	1:C:379:SER:CB	2.63	0.46
2:S:89:GLU:HA	2:S:92:LYS:HD2	1.97	0.46
1:A:262:VAL:HG13	1:A:263:PRO:HD2	1.97	0.46
1:B:24:TYR:CE1	1:B:81:LYS:HB2	2.51	0.46
1:D:168:PRO:HD3	1:D:396:ASP:OD1	2.14	0.46
2:T:86:GLU:O	2:T:90:VAL:HG12	2.15	0.46
1:A:13:PHE:HE1	1:A:68:THR:HG22	1.81	0.46
1:A:214:TRP:O	1:A:217:ARG:N	2.48	0.46
1:B:335:LEU:HD13	4:B:683:HOH:O	2.16	0.46
1:B:384:VAL:N	4:B:644:HOH:O	2.49	0.46
1:D:137:ASP:OD2	1:D:138:LEU:N	2.47	0.46
1:D:193:LEU:HD13	1:D:236:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ASP:OD2	1:D:439:ARG:HB2	2.16	0.46
2:U:120:PRO:HB2	2:U:122:SER:HA	1.97	0.46
1:A:262:VAL:HG12	1:A:264:ILE:H	1.80	0.46
1:B:87:ILE:HG23	1:B:97:PHE:HD1	1.77	0.46
1:B:235:ILE:HD11	2:T:51[B]:VAL:HG11	1.98	0.46
1:C:58:ALA:HB1	1:C:82:GLY:O	2.16	0.46
1:C:284:CYS:HB3	1:C:289:LEU:O	2.16	0.46
1:D:319[A]:ARG:HG3	1:D:374:VAL:HG23	1.98	0.46
1:C:200:THR:O	1:C:201:LYS:CB	2.64	0.46
1:D:134[A]:ARG:HD3	1:D:305:LYS:O	2.16	0.46
2:U:47:LYS:HZ3	2:U:48:LYS:CD	2.29	0.46
2:V:13:GLU:HB3	2:V:14:THR:H	1.61	0.46
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.50	0.46
1:A:306:ASN:HB2	4:A:678:HOH:O	2.16	0.46
1:B:342:THR:HA	1:B:345:PHE:CE1	2.51	0.46
1:D:97:PHE:CD1	1:D:97:PHE:C	2.90	0.46
1:D:140:ILE:CG2	1:D:144:TYR:HD2	2.29	0.46
1:D:200:THR:OG1	1:D:238:HIS:CD2	2.65	0.46
2:T:31:GLU:CG	2:T:80:PRO:HG3	2.40	0.46
2:T:61:TYR:HD2	2:T:61:TYR:O	1.99	0.46
2:U:67:TRP:CZ3	2:U:100:ARG:HG3	2.51	0.46
1:A:201:LYS:NZ	1:A:294:HIS:HD2	2.14	0.45
1:B:157:VAL:HG11	1:C:216:ASP:OD2	2.16	0.45
1:B:451:TRP:CE3	2:T:19:PRO:HG3	2.50	0.45
1:D:124:VAL:CB	1:D:127:PHE:HE2	2.29	0.45
2:S:21:LEU:N	2:S:21:LEU:HD12	2.30	0.45
2:U:56:ASN:OD1	2:U:57:LYS:N	2.48	0.45
1:A:16:GLY:N	4:A:631:HOH:O	2.42	0.45
1:A:133:LEU:N	1:A:307:HIS:HD2	2.11	0.45
1:A:406:THR:O	1:A:406:THR:HG22	2.16	0.45
1:B:360:ARG:NH2	4:B:689:HOH:O	2.45	0.45
1:C:174:ILE:HD11	1:C:238:HIS:HE1	1.81	0.45
1:D:305:LYS:H	1:D:305:LYS:HG2	1.49	0.45
2:U:52:TYR:N	2:U:52:TYR:HD2	2.14	0.45
1:A:90:VAL:HG13	1:A:91:PRO:HD2	1.99	0.45
1:A:295:ARG:HG2	1:A:327:HIS:HB2	1.97	0.45
1:A:441:GLY:O	1:A:445:ILE:HG12	2.15	0.45
1:B:171:GLY:HA2	1:B:199:PHE:O	2.16	0.45
1:B:338:GLU:OE2	1:B:339:ARG:N	2.49	0.45
1:C:40:PHE:HD1	1:C:133:LEU:HD21	1.79	0.45
1:C:209:GLN:HB3	1:C:210:PRO:CD	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:MET:SD	1:C:217:ARG:HD3	2.56	0.45
1:D:162:LEU:HD13	1:D:164:LYS:HE2	1.98	0.45
2:S:6:PRO:HG2	2:V:46:LEU:HD12	1.97	0.45
1:A:204:GLU:HG2	1:A:205:ASN:OD1	2.16	0.45
1:A:381:GLY:O	1:A:467:PHE:CE2	2.70	0.45
1:B:156:GLN:HG2	1:B:157:VAL:N	2.30	0.45
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.72	0.45
1:B:382:ILE:HD12	1:B:402:PHE:CZ	2.52	0.45
1:D:166:GLY:HA2	2:V:112:CYS:O	2.16	0.45
1:D:295:ARG:O	1:D:296:ALA:C	2.54	0.45
1:D:371:LEU:HG	1:D:372:PRO:HD2	1.99	0.45
1:C:45:GLN:HE22	1:C:131:ARG:HG2	1.74	0.45
2:T:61:TYR:CD2	2:T:61:TYR:O	2.69	0.45
1:A:127:PHE:C	1:A:129:ALA:N	2.70	0.45
1:A:222:ALA:C	1:A:224:ALA:N	2.70	0.45
1:A:243:THR:HG21	1:A:268:ASP:OD2	2.16	0.45
1:A:339:ARG:NH1	1:A:393:ILE:HG12	2.32	0.45
1:B:175:LYS:HB3	1:B:176:PRO:HA	1.99	0.45
1:D:184:ASN:ND2	2:U:109:GLN:OE1	2.44	0.45
2:S:33:LEU:HD23	2:S:38:TRP:HB2	1.98	0.45
2:S:40:PRO:HG2	2:S:74:MET:HB2	1.98	0.45
1:C:97:PHE:CE1	1:C:99:ALA:HB2	2.52	0.45
1:C:248:GLU:O	1:C:252:LYS:HB2	2.17	0.45
1:C:315:ALA:HB1	1:C:349:LEU:HD11	1.98	0.45
2:S:30:VAL:CG1	2:S:83:VAL:HG21	2.47	0.45
2:S:67:TRP:CE3	2:S:100:ARG:HG3	2.48	0.45
2:V:16:SER:HB3	4:V:224:HOH:O	2.16	0.45
2:V:94:TYR:HB3	2:V:97:ALA:HB2	1.99	0.45
1:A:232:THR:HG21	4:S:204:HOH:O	2.16	0.45
1:B:44:PRO:O	1:B:131:ARG:HG3	2.17	0.45
1:C:371:LEU:HG	1:C:372:PRO:CD	2.47	0.45
1:B:32:LYS:O	1:B:34:THR:N	2.50	0.45
1:B:34:THR:O	1:B:141:PRO:HG3	2.17	0.45
1:B:60:GLU:HB3	1:B:124[B]:VAL:HG12	1.98	0.45
1:B:208:SER:HB3	1:B:253:ARG:NH2	2.29	0.45
1:D:57:VAL:HA	1:D:124:VAL:CG1	2.47	0.45
1:A:201:LYS:HZ1	1:A:294:HIS:HD2	1.64	0.44
1:A:293:ILE:HG13	1:A:318:LEU:HD11	1.99	0.44
1:C:160:ASP:OD2	4:C:660:HOH:O	2.21	0.44
1:C:294:HIS:CE1	3:C:501:RUB:O4	2.69	0.44
1:C:436:ASP:O	1:C:440:GLU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:SER:HA	1:C:453:PRO:HD3	1.65	0.44
1:D:386:HIS:O	1:D:390:LEU:HG	2.16	0.44
1:A:262:VAL:CG1	4:A:630:HOH:O	2.65	0.44
1:A:378:ALA:O	1:A:379:SER:HB2	2.17	0.44
1:B:382:ILE:HA	1:B:386:HIS:ND1	2.32	0.44
1:C:191:GLU:OE1	1:C:194:ARG:NH1	2.50	0.44
2:U:44:PHE:O	2:U:67:TRP:HB3	2.16	0.44
2:V:52:TYR:O	2:V:63:ASP:N	2.50	0.44
1:A:127:PHE:C	1:A:129:ALA:H	2.19	0.44
1:A:451:TRP:CD1	1:A:451:TRP:N	2.80	0.44
1:B:90:VAL:HG22	1:B:98:ILE:HD12	2.00	0.44
1:B:225:ILE:HD11	1:B:238:HIS:HB3	2.00	0.44
1:B:335:LEU:HD12	3:B:501:RUB:O4P	2.17	0.44
1:B:357:ASP:HB3	1:B:362[A]:ILE:HD12	1.99	0.44
1:C:243:THR:OG1	1:C:267:HIS:HA	2.17	0.44
2:T:54:GLU:HG2	2:T:55:HIS:CD2	2.52	0.44
1:A:45:GLN:HB2	1:A:48:VAL:HG21	1.99	0.44
1:A:377:VAL:HG11	1:A:401:GLN:NE2	2.33	0.44
1:B:42:VAL:O	1:B:96:GLN:HA	2.17	0.44
1:B:109:GLU:H	1:B:115:ASN:HD22	1.63	0.44
1:B:249:GLU:O	1:B:253:ARG:HG3	2.17	0.44
2:T:42:LEU:HD23	2:T:99:VAL:HG12	1.99	0.44
2:T:58:SER:HB2	2:T:59:PRO:HD3	1.99	0.44
2:U:108:ARG:NH1	2:U:108:ARG:CB	2.81	0.44
2:V:51:VAL:O	2:V:51:VAL:HG12	2.18	0.44
1:A:116:MET:O	1:A:116:MET:HG2	2.17	0.44
1:B:123:ASN:O	1:B:125:PHE:N	2.51	0.44
1:B:155:ILE:HG12	1:B:375:ILE:HG13	1.99	0.44
1:D:25:TYR:CD2	1:D:27:PRO:HD3	2.52	0.44
1:A:42:VAL:HG22	1:A:133:LEU:CD1	2.48	0.44
1:A:50:PRO:HB3	1:A:87:ILE:HD13	1.99	0.44
1:B:83:ARG:O	1:B:101:VAL:HA	2.18	0.44
1:B:443:ALA:C	1:B:445:ILE:N	2.68	0.44
1:C:409:HIS:ND1	1:C:415:PRO:HB2	2.32	0.44
1:A:374:VAL:O	1:A:376:PRO:HD3	2.18	0.44
1:A:441:GLY:HA2	1:A:444:ILE:HD12	2.00	0.44
1:B:146:LYS:HD3	1:B:369[A]:VAL:HG13	2.00	0.44
1:B:177:LYS:NZ	1:B:203:ASP:CG	2.71	0.44
1:D:178:LEU:HB3	1:D:211:PHE:CZ	2.53	0.44
2:U:30:VAL:HG11	2:U:83:VAL:HB	1.98	0.44
2:V:23:ARG:NH1	2:V:23:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:47:LYS:HE3	2:V:48:LYS:HZ1	1.83	0.44
1:A:158:GLU:HG3	1:A:290:LEU:CD2	2.48	0.44
4:B:655:HOH:O	2:T:113:ILE:CG2	2.65	0.44
1:D:257:ALA:O	1:D:258:ARG:C	2.55	0.44
2:S:3:VAL:HG21	2:V:70:TRP:CE3	2.52	0.44
2:S:62:TYR:HB2	2:S:65:ARG:CD	2.47	0.44
2:S:70:TRP:CE3	2:T:3:VAL:HG21	2.51	0.44
1:A:336:GLU:CD	1:A:337:GLY:H	2.20	0.44
1:B:53:ALA:O	1:B:57:VAL:HG23	2.18	0.44
1:B:148:PHE:HD1	1:B:320:LEU:O	2.01	0.44
1:B:402:PHE:HB3	1:B:405:GLY:HA3	1.99	0.44
1:D:387:MET:O	1:D:387:MET:HG3	2.17	0.44
2:T:52:TYR:CD2	2:T:52:TYR:N	2.85	0.44
1:C:412:GLY:HA2	2:T:72:LEU:HD21	1.99	0.43
1:D:429:GLN:OE1	2:V:18:LEU:HD13	2.17	0.43
2:T:41:CYS:O	2:T:102[A]:ILE:HG12	2.18	0.43
2:U:44:PHE:CE1	2:V:6:PRO:HG3	2.50	0.43
2:V:99:VAL:O	2:V:116:ILE:HD12	2.18	0.43
1:A:201:LYS:HD3	1:A:401:GLN:OE1	2.18	0.43
1:B:90:VAL:HG13	1:B:91:PRO:HD2	1.98	0.43
1:C:305:LYS:HB2	4:C:722:HOH:O	2.18	0.43
1:D:202:ASP:OD1	1:D:238:HIS:CE1	2.55	0.43
1:D:270:LEU:HD11	1:D:314:LEU:HD13	1.99	0.43
2:S:13:GLU:O	2:S:14:THR:C	2.56	0.43
2:T:11:LYS:HG3	2:T:17:TYR:CE2	2.53	0.43
1:A:204:GLU:CG	4:A:749:HOH:O	2.66	0.43
1:B:49:PRO:HA	1:B:50:PRO:HD2	1.83	0.43
1:B:148:PHE:CE1	1:B:320:LEU:HB3	2.54	0.43
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.74	0.43
1:C:385:TRP:HZ2	1:C:459:CYS:O	2.01	0.43
1:D:202:ASP:HB3	1:D:206:VAL:HB	2.00	0.43
1:D:294:HIS:ND1	4:D:745:HOH:O	2.35	0.43
1:D:412:GLY:O	1:D:415:PRO:HD2	2.19	0.43
2:V:12:PHE:CZ	2:V:50:PHE:CZ	3.06	0.43
1:C:269:TYR:CE1	1:C:318:LEU:HB2	2.53	0.43
1:C:404:GLY:O	1:C:408:GLY:N	2.51	0.43
1:D:203:ASP:C	1:D:205:ASN:N	2.72	0.43
2:U:119:THR:CB	2:U:120:PRO:CD	2.94	0.43
1:A:36:ILE:CG2	1:A:138:LEU:HD22	2.49	0.43
1:A:158:GLU:HG3	1:A:290:LEU:HD22	1.99	0.43
1:A:190:TYR:CZ	1:A:194:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ASN:O	1:A:217:ARG:NH2	2.37	0.43
2:U:27:LEU:HA	2:U:84:LEU:HD11	2.00	0.43
1:A:113:VAL:CG1	1:A:274:PHE:CD1	2.90	0.43
1:B:387:MET:HA	1:B:390:LEU:HD12	2.01	0.43
1:C:199:PHE:CB	1:C:239:TYR:CE1	2.98	0.43
1:C:414:ALA:O	1:C:418:VAL:HG23	2.19	0.43
1:A:395:GLY:C	1:A:397:ASP:H	2.21	0.43
1:B:204:GLU:HA	1:B:266:MET:HE1	2.01	0.43
1:B:454:GLU:H	1:B:454:GLU:CD	2.21	0.43
1:C:251:LEU:HD23	1:C:251:LEU:HA	1.66	0.43
1:D:173:THR:HG1	1:D:201:LYS:HD3	1.80	0.43
2:S:122:SER:C	2:S:123:TYR:HD1	2.21	0.43
2:T:121:GLU:HG3	2:T:122:SER:N	2.32	0.43
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.81	0.43
1:B:93:GLU:H	1:B:93:GLU:HG2	1.61	0.43
1:C:88:GLU:HA	1:C:89:PRO:HD3	1.90	0.43
1:C:239:TYR:HD1	1:C:239:TYR:H	1.57	0.43
1:C:354:ILE:HG22	1:C:362:ILE:HD13	2.00	0.43
1:D:121:VAL:HG11	1:D:309[B]:MET:HE1	2.01	0.43
1:D:296:ALA:O	1:D:297:MET:CB	2.67	0.43
1:A:221:CYS:O	1:A:225:ILE:N	2.42	0.43
1:C:105:LEU:HB2	4:C:683:HOH:O	2.18	0.43
1:C:153:HIS:HE1	1:C:288:GLY:HA2	1.83	0.43
1:C:409:HIS:HA	1:C:410:PRO:HD2	1.67	0.43
1:D:318:LEU:HG	1:D:326:ILE:HD12	2.01	0.43
1:A:219[B]:LEU:HD22	2:V:61:TYR:CD1	2.54	0.43
1:B:154:GLY:HA3	1:B:372:PRO:HB3	2.01	0.43
1:C:151:PRO:HA	1:C:323:GLY:H	1.82	0.43
1:A:86:GLU:HB3	1:A:100:TYR:HB2	1.99	0.42
1:B:18[B]:LYS:NZ	1:B:18[B]:LYS:HB3	2.33	0.42
1:B:424:LEU:O	1:B:428:VAL:HG23	2.19	0.42
1:D:138:LEU:O	1:D:316:LYS:NZ	2.48	0.42
1:A:292:HIS:CD2	1:A:325:HIS:HB2	2.54	0.42
1:C:117:PHE:HD1	1:C:117:PHE:HA	1.59	0.42
1:D:58:ALA:O	1:D:62:SER:OG	2.36	0.42
1:D:201:LYS:HB2	1:D:239:TYR:HD2	1.84	0.42
1:D:412:GLY:C	1:D:415:PRO:HD2	2.39	0.42
2:S:86:GLU:O	2:S:89:GLU:HB3	2.19	0.42
2:S:96:ARG:HD2	2:S:120:PRO:HB3	2.00	0.42
1:A:53:ALA:O	1:A:57:VAL:HG23	2.19	0.42
1:A:158:GLU:OE2	1:A:375:ILE:CD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASN:ND2	2:S:29:GLU:OE2	2.51	0.42
1:A:151:PRO:HG2	1:A:372:PRO:HB2	2.02	0.42
1:A:349:LEU:CD1	4:A:760:HOH:O	2.65	0.42
1:C:268:ASP:HB3	4:C:612:HOH:O	2.19	0.42
1:C:378:ALA:O	1:C:379:SER:HB2	2.19	0.42
1:A:25:TYR:CE2	1:A:27:PRO:HD3	2.55	0.42
1:A:201:LYS:HE3	1:A:292:HIS:CE1	2.54	0.42
1:A:422:VAL:HG22	2:S:17:TYR:HB3	2.02	0.42
1:B:241:ASN:HA	1:B:266:MET:HB3	2.02	0.42
1:B:367:ASP:OD1	4:B:774:HOH:O	2.20	0.42
1:C:88:GLU:O	1:C:97:PHE:CA	2.67	0.42
1:C:214:TRP:CG	1:C:215:ARG:N	2.87	0.42
1:D:113:VAL:O	1:D:116:MET:CB	2.65	0.42
2:T:93:GLU:OE1	2:T:94:TYR:HE2	2.02	0.42
2:T:120:PRO:HB2	2:T:121:GLU:H	1.63	0.42
1:A:361:GLY:HA2	4:A:711:HOH:O	2.18	0.42
1:B:56:ALA:HB1	1:B:127:PHE:HZ	1.79	0.42
1:B:200:THR:O	1:B:201:LYS:HB3	2.20	0.42
1:C:393:ILE:HG22	1:C:394:PHE:N	2.34	0.42
2:T:71:LYS:NZ	2:T:86:GLU:OE2	2.46	0.42
1:A:137:ASP:OD1	1:A:138:LEU:N	2.53	0.42
1:A:291:LEU:H	1:A:324:ASP:CG	2.19	0.42
1:B:37:LEU:HD22	1:B:85:TYR:HE2	1.84	0.42
1:B:216:ASP:HA	1:B:219[A]:LEU:HD11	2.01	0.42
1:B:423:ALA:HB2	1:B:455:LEU:HD13	2.02	0.42
1:C:90:VAL:HB	1:C:96:GLN:HB3	2.01	0.42
1:C:214:TRP:O	1:C:216:ASP:N	2.53	0.42
1:D:211:PHE:CD1	1:D:211:PHE:C	2.93	0.42
1:D:340:GLU:CD	4:D:712:HOH:O	2.53	0.42
2:S:105:ASN:OD1	2:S:108:ARG:HB2	2.20	0.42
1:A:85:TYR:CE2	1:A:100:TYR:C	2.93	0.42
1:A:310:HIS:CE1	1:A:312:ARG:NH1	2.88	0.42
1:B:383:HIS:HB2	1:B:384:VAL:H	1.70	0.42
1:D:218:PHE:HD1	1:D:218:PHE:H	1.67	0.42
1:D:289:LEU:HD23	2:V:59:PRO:HB3	2.02	0.42
1:A:24:TYR:CE1	1:A:59:ALA:HA	2.54	0.42
1:A:180:LEU:HD22	1:A:184:ASN:HB3	2.02	0.42
1:B:185:TYR:O	1:B:189:VAL:HG23	2.19	0.42
1:B:330:THR:HG23	1:B:379:SER:H	1.77	0.42
1:B:215:ARG:HG2	1:B:256:PHE:CE2	2.55	0.42
1:C:45:GLN:HE21	1:C:131:ARG:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:VAL:HG11	1:D:309[B]:MET:HE3	1.95	0.42
1:A:172:CYS:HB2	1:A:402:PHE:O	2.20	0.41
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.77	0.41
1:B:135:LEU:HG	1:B:313:VAL:HG21	2.02	0.41
1:C:24:TYR:CG	1:C:59:ALA:HB2	2.55	0.41
1:C:180:LEU:O	1:C:212:MET:CE	2.68	0.41
1:D:248:GLU:OE1	4:D:726:HOH:O	2.22	0.41
1:A:193:LEU:HD22	1:A:236:LYS:HD2	2.02	0.41
1:B:341:ILE:HD13	1:B:341:ILE:HG21	1.76	0.41
1:B:347:ASP:CB	1:B:351:ASP:OD2	2.66	0.41
1:B:424:LEU:O	1:B:427:CYS:HB2	2.20	0.41
2:V:79[B]:ASP:HA	2:V:80:PRO:HD3	1.85	0.41
1:A:222:ALA:C	1:A:224:ALA:H	2.24	0.41
1:A:395:GLY:C	1:A:397:ASP:N	2.74	0.41
1:B:309[B]:MET:HB3	1:B:309[B]:MET:HE3	1.82	0.41
1:C:119[A]:SER:HB3	4:C:656:HOH:O	2.20	0.41
1:D:40:PHE:O	1:D:98[A]:ILE:HA	2.19	0.41
1:D:181:SER:HG	1:D:184:ASN:HD22	1.67	0.41
2:T:89:GLU:HG3	2:T:92:LYS:NZ	2.35	0.41
1:A:49:PRO:HA	1:A:50:PRO:HD2	1.86	0.41
1:A:244:ALA:C	4:A:607:HOH:O	2.58	0.41
1:A:267:HIS:CD2	1:A:269:TYR:HA	2.55	0.41
1:B:309[B]:MET:HE1	1:B:314:LEU:CD2	2.49	0.41
1:C:461:VAL:HG12	1:C:462[B]:TRP:CD1	2.55	0.41
1:D:140:ILE:HG22	1:D:144:TYR:HB3	2.02	0.41
2:U:42:LEU:HD21	2:U:87:LEU:HA	2.02	0.41
2:U:69:MET:HE2	2:U:69:MET:HB2	1.87	0.41
1:A:83:ARG:NH2	4:A:750:HOH:O	2.22	0.41
1:A:425:GLU:OE1	2:S:15:LEU:HA	2.21	0.41
1:B:294:HIS:CE1	3:B:501:RUB:HO4	2.36	0.41
1:B:422:VAL:HG22	2:T:17:TYR:HB3	2.01	0.41
1:C:133:LEU:H	1:C:307:HIS:CD2	2.38	0.41
1:D:154:GLY:HA2	1:D:373:GLY:O	2.19	0.41
1:D:200:THR:CB	1:D:238:HIS:HD2	2.32	0.41
2:S:22:THR:N	2:S:25:GLN:HG3	2.35	0.41
2:T:22:THR:C	2:T:26:LEU:HD12	2.40	0.41
2:U:15:LEU:O	2:U:17:TYR:N	2.53	0.41
2:U:108:ARG:NH1	2:U:110:VAL:CG2	2.84	0.41
1:A:213:ARG:HD3	1:A:213:ARG:HA	1.84	0.41
1:A:295:ARG:CZ	1:A:298:HIS:HE1	2.33	0.41
1:B:37:LEU:HD22	1:B:85:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309[B]:MET:HE2	1:B:309[B]:MET:HB2	1.69	0.41
1:C:71:THR:C	1:C:73:GLY:H	2.22	0.41
1:C:151:PRO:HB3	1:C:323:GLY:O	2.19	0.41
1:C:201:LYS:HB2	1:C:239:TYR:CG	2.56	0.41
1:C:302:ASP:HA	4:C:658:HOH:O	2.20	0.41
1:C:342:THR:HG23	1:C:345:PHE:CZ	2.56	0.41
1:C:404:GLY:O	1:C:408:GLY:HA3	2.20	0.41
1:A:143:ALA:CB	4:A:627:HOH:O	2.68	0.41
1:A:295:ARG:HG3	3:A:501:RUB:O6P	2.21	0.41
1:C:87:ILE:HG23	1:C:97:PHE:CD1	2.56	0.41
1:C:465:ILE:HA	1:C:465:ILE:HD13	1.76	0.41
1:D:306[B]:ASN:OD1	1:D:307:HIS:N	2.53	0.41
1:A:294:HIS:HE1	3:A:501:RUB:H4	1.83	0.41
1:B:400:LEU:HD12	1:B:424:LEU:HD13	2.02	0.41
1:D:342:THR:HA	1:D:345:PHE:CE1	2.54	0.41
2:T:38:TRP:CD1	2:T:105:ASN:HB2	2.56	0.41
2:T:104:PHE:CE1	2:T:111:GLN:HG3	2.55	0.41
2:V:52:TYR:N	2:V:52:TYR:CD2	2.89	0.41
1:A:201:LYS:HD2	1:A:239:TYR:HD2	1.76	0.41
1:A:223:GLU:HG2	1:A:223:GLU:O	2.20	0.41
1:A:248:GLU:OE1	1:A:248:GLU:N	2.52	0.41
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.81	0.41
1:B:265:VAL:HG22	1:B:266:MET:H	1.85	0.41
1:C:190:TYR:HD1	1:C:228:SER:HB3	1.84	0.41
1:D:38:ALA:O	1:D:100:TYR:HA	2.21	0.41
1:D:49:PRO:HA	1:D:50:PRO:HD3	1.83	0.41
1:D:151:PRO:HA	1:D:152:PRO:HD3	1.89	0.41
1:D:214:TRP:CG	1:D:215:ARG:N	2.89	0.41
1:D:218:PHE:CD1	1:D:218:PHE:N	2.89	0.41
1:D:269:TYR:OH	1:D:314:LEU:O	2.30	0.41
1:D:409:HIS:HD2	1:D:411:TRP:H	1.69	0.41
1:D:465:ILE:N	1:D:465:ILE:HD13	2.36	0.41
2:S:120:PRO:HB2	2:S:121:GLU:H	1.62	0.41
2:T:4:TRP:HA	2:T:5:PRO:HD3	1.86	0.41
2:U:70:TRP:CE3	2:U:90:VAL:HG22	2.56	0.41
2:U:107:VAL:C	2:U:109:GLN:H	2.23	0.41
2:V:23:ARG:HG2	2:V:23:ARG:HH11	1.86	0.41
1:A:218:PHE:CD2	1:A:240:LEU:HD22	2.56	0.41
1:B:153:HIS:HD2	1:B:290:LEU:HA	1.86	0.41
1:B:346:VAL:O	1:B:350:ARG:HB2	2.20	0.41
1:C:214:TRP:C	1:C:216:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LEU:CD1	1:C:326:ILE:HD12	2.51	0.41
1:D:185:TYR:O	1:D:189:VAL:HG23	2.21	0.41
1:D:299:ALA:CB	4:D:684:HOH:O	2.68	0.41
1:D:319[B]:ARG:HG3	1:D:374:VAL:HG23	2.02	0.41
1:D:423:ALA:O	1:D:426:ALA:HB3	2.20	0.41
2:V:35[A]:ARG:HG3	2:V:35[A]:ARG:NH1	2.30	0.41
1:B:18[B]:LYS:HB3	1:B:18[B]:LYS:HZ3	1.86	0.40
1:B:435:ARG:HH22	1:B:447:GLU:CD	2.22	0.40
1:C:330:THR:OG1	1:C:333:GLY:HA3	2.21	0.40
1:D:138:LEU:HA	1:D:138:LEU:HD23	1.68	0.40
1:D:336:GLU:HG3	1:D:337:GLY:N	2.35	0.40
1:D:414:ALA:N	1:D:415:PRO:CD	2.84	0.40
2:S:14:THR:O	2:S:15:LEU:HB2	2.20	0.40
1:B:269:TYR:CE1	1:B:318:LEU:HD23	2.55	0.40
1:C:40:PHE:HB3	1:C:133:LEU:CD1	2.49	0.40
1:D:81:LYS:HG3	1:D:83:ARG:HG3	2.04	0.40
2:T:24:ASP:O	2:T:28:LYS:HG3	2.21	0.40
1:A:26:THR:C	1:A:28:ASP:H	2.25	0.40
1:A:162:LEU:O	1:A:163:ASN:HB3	2.22	0.40
1:A:177:LYS:HB3	1:A:177:LYS:HE3	1.75	0.40
1:A:298:HIS:CG	1:A:299:ALA:N	2.90	0.40
1:B:148:PHE:CD1	1:B:320:LEU:HB3	2.57	0.40
1:B:157:VAL:HG23	1:B:157:VAL:H	1.55	0.40
1:B:294:HIS:CE1	3:B:501:RUB:O4	2.75	0.40
1:C:119[B]:SER:HB2	4:C:656:HOH:O	2.20	0.40
1:D:326:ILE:HG22	1:D:374:VAL:CG1	2.51	0.40
2:S:27:LEU:HD12	2:S:80:PRO:CB	2.51	0.40
2:S:116:ILE:HD12	2:S:116:ILE:HA	1.88	0.40
1:B:24:TYR:HE1	1:B:81:LYS:HB2	1.84	0.40
1:B:155:ILE:HD13	1:B:155:ILE:HG21	1.90	0.40
1:B:201:LYS:HD2	1:B:239:TYR:CD2	2.56	0.40
1:C:157:VAL:H	1:C:157:VAL:HG23	1.69	0.40
1:D:203:ASP:O	1:D:205:ASN:N	2.54	0.40
1:D:330:THR:OG1	1:D:333:GLY:CA	2.69	0.40
2:S:102:ILE:HG23	2:S:111:GLN:HG2	2.02	0.40
2:T:87:LEU:HD23	2:T:88:ASP:N	2.37	0.40
2:U:79:ASP:HA	2:U:80:PRO:HD2	1.88	0.40
2:V:26[B]:LEU:HD21	2:V:117:ALA:HB1	2.03	0.40
2:V:82:GLN:O	2:V:85:LYS:HB3	2.21	0.40
1:A:162:LEU:HB2	1:A:164:LYS:HG3	2.02	0.40
1:A:301:ILE:HG22	1:A:309[A]:MET:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:SER:HB2	1:B:82:GLY:H	1.86	0.40
1:B:276:ALA:O	1:B:279:THR:HB	2.22	0.40
1:C:20:TYR:C	1:C:22:LEU:H	2.24	0.40
1:C:334:LYS:CG	1:C:335:LEU:HD12	2.50	0.40
1:D:183:LYS:O	2:U:66:TYR:OH	2.24	0.40

All (7) 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)
2:S:105:ASN:O	4:A:727:HOH:O[2_555]	1.92	0.28
1:D:207:ASN:ND2	4:C:615:HOH:O[2_555]	1.94	0.26
1:D:75:THR:OG1	2:T:109:GLN:NE2[2_555]	2.00	0.20
1:A:106:ASP:OD2	1:A:370[B]:SER:OG[2_555]	2.05	0.15
1:A:65:THR:CG2	4:B:728:HOH:O[2_555]	2.07	0.13
1:B:106:ASP:OD2	1:D:370:SER:OG[2_555]	2.13	0.07
1:C:75:THR:OG1	2:U:109:GLN:NE2[2_555]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	467/475 (98%)	405 (87%)	51 (11%)	11 (2%)	6	3
1	B	469/475 (99%)	404 (86%)	48 (10%)	17 (4%)	3	1
1	C	468/475 (98%)	411 (88%)	47 (10%)	10 (2%)	7	4
1	D	465/475 (98%)	408 (88%)	47 (10%)	10 (2%)	6	4
2	S	123/123 (100%)	105 (85%)	12 (10%)	6 (5%)	2	1
2	T	124/123 (101%)	109 (88%)	12 (10%)	3 (2%)	6	3
2	U	123/123 (100%)	97 (79%)	20 (16%)	6 (5%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	V	124/123 (101%)	111 (90%)	9 (7%)	4 (3%)	4 2
All	All	2363/2392 (99%)	2050 (87%)	246 (10%)	67 (3%)	5 2

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	SER
1	B	212	MET
1	C	21	LYS
2	S	120	PRO
2	T	120	PRO
2	U	108	ARG
2	U	109	GLN
2	U	120	PRO
1	A	311	PHE
1	A	405	GLY
1	B	33	ASP
1	B	331	VAL
1	B	333	GLY
1	B	388	PRO
1	B	425	GLU
1	C	132	ALA
1	C	369	VAL
1	C	379	SER
1	D	106	ASP
2	S	15	LEU
2	S	16	SER
2	T	15	LEU
2	V	121	GLU
1	A	137	ASP
1	A	239	TYR
1	B	50	PRO
1	B	127	PHE
1	B	156	GLN
1	B	216	ASP
1	B	296	ALA
1	B	379	SER
1	C	110	GLU
1	D	297	MET
2	U	16	SER
2	V	122	SER
1	A	223	GLU

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Mol	Chain	Res	Type
1	B	455	LEU
1	C	201	LYS
1	C	207	ASN
2	S	81	ALA
2	T	13	GLU
1	A	94	ASP
1	A	331	VAL
1	B	124[A]	VAL
1	B	124[B]	VAL
1	B	456	ALA
1	C	357	ASP
1	C	463	LYS
1	D	21	LYS
1	D	204	GLU
1	D	258	ARG
1	D	331	VAL
2	S	71	LYS
2	S	121	GLU
2	U	15	LEU
2	V	13	GLU
1	D	124	VAL
1	D	257	ALA
1	B	428	VAL
1	D	380	GLY
2	U	107	VAL
1	A	369[A]	VAL
1	A	369[B]	VAL
1	A	380	GLY
2	V	5	PRO
1	D	369	VAL
1	C	362	ILE

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/385 (99%)	353 (93%)	28 (7%)	14 15
1	B	383/385 (100%)	348 (91%)	35 (9%)	9 9
1	C	382/385 (99%)	347 (91%)	35 (9%)	9 9
1	D	379/385 (98%)	341 (90%)	38 (10%)	7 7
2	S	115/113 (102%)	101 (88%)	14 (12%)	5 4
2	T	116/113 (103%)	104 (90%)	12 (10%)	7 6
2	U	115/113 (102%)	98 (85%)	17 (15%)	3 2
2	V	116/113 (103%)	103 (89%)	13 (11%)	6 5
All	All	1987/1992 (100%)	1795 (90%)	192 (10%)	9 7

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	117	PHE
1	A	136[A]	GLU
1	A	136[B]	GLU
1	A	144	TYR
1	A	162	LEU
1	A	172	CYS
1	A	175	LYS
1	A	185	TYR
1	A	219[A]	LEU
1	A	219[B]	LEU
1	A	252	LYS
1	A	268	ASP
1	A	269	TYR
1	A	285	ARG
1	A	294	HIS
1	A	295	ARG
1	A	298	HIS
1	A	312	ARG
1	A	332	VAL
1	A	350	ARG
1	A	370[A]	SER
1	A	370[B]	SER
1	A	382	ILE

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Mol	Chain	Res	Type
1	A	400	LEU
1	A	407	LEU
1	A	449	CYS
1	A	460	GLU
1	B	19	ASP
1	B	21	LYS
1	B	60	GLU
1	B	83	ARG
1	B	107	LEU
1	B	124[A]	VAL
1	B	124[B]	VAL
1	B	127	PHE
1	B	130	LEU
1	B	183	LYS
1	B	185	TYR
1	B	200	THR
1	B	201	LYS
1	B	203	ASP
1	B	215	ARG
1	B	219[A]	LEU
1	B	219[B]	LEU
1	B	228	SER
1	B	264[A]	ILE
1	B	264[B]	ILE
1	B	269	TYR
1	B	285	ARG
1	B	305	LYS
1	B	319	ARG
1	B	336	GLU
1	B	338	GLU
1	B	339	ARG
1	B	345	PHE
1	B	354	ILE
1	B	384	VAL
1	B	392	GLU
1	B	401	GLN
1	B	407	LEU
1	B	440	GLU
1	B	451	TRP
1	C	18	LYS
1	C	21	LYS
1	C	77	LEU

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Mol	Chain	Res	Type
1	C	94	ASP
1	C	117	PHE
1	C	134[A]	ARG
1	C	134[B]	ARG
1	C	156	GLN
1	C	159[A]	ARG
1	C	159[B]	ARG
1	C	161	LYS
1	C	172	CYS
1	C	183	LYS
1	C	185	TYR
1	C	201	LYS
1	C	205	ASN
1	C	219	LEU
1	C	239	TYR
1	C	252	LYS
1	C	258	ARG
1	C	262	VAL
1	C	265	VAL
1	C	282	HIS
1	C	293	ILE
1	C	336	GLU
1	C	365[A]	THR
1	C	365[B]	THR
1	C	369	VAL
1	C	384	VAL
1	C	401	GLN
1	C	439	ARG
1	C	440	GLU
1	C	462[A]	TRP
1	C	462[B]	TRP
1	C	465	ILE
1	D	44	PRO
1	D	62	SER
1	D	79	ARG
1	D	81	LYS
1	D	83	ARG
1	D	86	GLU
1	D	93	GLU
1	D	94	ASP
1	D	118	THR
1	D	131	ARG

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Mol	Chain	Res	Type
1	D	153	HIS
1	D	155	ILE
1	D	156	GLN
1	D	167	ARG
1	D	175	LYS
1	D	178	LEU
1	D	185	TYR
1	D	203	ASP
1	D	217	ARG
1	D	258	ARG
1	D	259	GLU
1	D	262	VAL
1	D	269	TYR
1	D	305	LYS
1	D	309[A]	MET
1	D	309[B]	MET
1	D	312	ARG
1	D	318	LEU
1	D	332	VAL
1	D	334	LYS
1	D	370	SER
1	D	384	VAL
1	D	401	GLN
1	D	436	ASP
1	D	437	LEU
1	D	451	TRP
1	D	464	GLU
1	D	466	LYS
2	S	21	LEU
2	S	25	GLN
2	S	26	LEU
2	S	47	LYS
2	S	52	TYR
2	S	57	LYS
2	S	87	LEU
2	S	93	GLU
2	S	96	ARG
2	S	102	ILE
2	S	105	ASN
2	S	116	ILE
2	S	122	SER
2	S	123	TYR

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Mol	Chain	Res	Type
2	T	1	MET
2	T	7	ILE
2	T	42	LEU
2	T	65[A]	ARG
2	T	65[B]	ARG
2	T	84	LEU
2	T	87	LEU
2	T	99	VAL
2	T	100	ARG
2	T	110	VAL
2	T	121	GLU
2	T	123	TYR
2	U	1	MET
2	U	2	GLN
2	U	5	PRO
2	U	14[A]	THR
2	U	14[B]	THR
2	U	34	LEU
2	U	48	LYS
2	U	52	TYR
2	U	78	THR
2	U	79	ASP
2	U	82	GLN
2	U	86	GLU
2	U	87	LEU
2	U	93	GLU
2	U	110	VAL
2	U	113	ILE
2	U	121	GLU
2	V	14	THR
2	V	42	LEU
2	V	48	LYS
2	V	52	TYR
2	V	79[A]	ASP
2	V	79[B]	ASP
2	V	87	LEU
2	V	90	VAL
2	V	102	ILE
2	V	105	ASN
2	V	106	ASN
2	V	109	GLN
2	V	110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	207	ASN
1	A	229	GLN
1	A	267	HIS
1	A	292	HIS
1	A	294	HIS
1	A	298	HIS
1	A	304	GLN
1	A	307	HIS
1	A	366	GLN
1	A	401	GLN
1	B	115	ASN
1	B	153	HIS
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	307	HIS
1	B	366	GLN
1	B	442	ASN
1	C	45	GLN
1	C	96	GLN
1	C	115	ASN
1	C	149	GLN
1	C	153	HIS
1	C	267	HIS
1	C	307	HIS
1	C	401	GLN
1	D	30	GLN
1	D	96	GLN
1	D	115	ASN
1	D	156	GLN
1	D	184	ASN
1	D	205	ASN
1	D	238	HIS
1	D	267	HIS
1	D	292	HIS
1	D	307	HIS
1	D	383	HIS
1	D	401	GLN
2	S	118	HIS
2	T	109	GLN

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Mol	Chain	Res	Type
2	T	111	GLN
2	U	2	GLN
2	U	25	GLN
2	U	55	HIS
2	U	111	GLN
2	U	118	HIS
2	V	105	ASN
2	V	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	RUB	D	501	-	17,17,17	1.07	0	17,25,25	1.84	5 (29%)
3	RUB	A	501	-	17,17,17	1.22	2 (11%)	17,25,25	2.05	7 (41%)
3	RUB	C	501	-	17,17,17	0.80	0	17,25,25	2.22	9 (52%)
3	RUB	B	501	-	17,17,17	1.61	4 (23%)	17,25,25	2.27	5 (29%)

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
3	RUB	D	501	-	-	10/20/20/20	-
3	RUB	A	501	-	-	14/20/20/20	-
3	RUB	C	501	-	-	7/20/20/20	-
3	RUB	B	501	-	-	16/20/20/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	RUB	O2-C2	3.65	1.27	1.21
3	B	501	RUB	P2-O5	2.75	1.69	1.60
3	A	501	RUB	O3-C3	2.67	1.47	1.42
3	B	501	RUB	O3-C3	2.47	1.47	1.42
3	A	501	RUB	C5-C4	2.42	1.55	1.51
3	B	501	RUB	O1-C1	2.25	1.45	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	RUB	O2P-P1-O1P	4.72	129.23	110.83
3	B	501	RUB	O5P-P2-O5	-4.01	96.20	106.67
3	D	501	RUB	O5-P2-O4P	-3.87	95.98	106.44
3	B	501	RUB	O6P-P2-O5	3.65	116.18	106.67
3	C	501	RUB	O5P-P2-O5	-3.53	97.46	106.67
3	A	501	RUB	O5-P2-O4P	3.51	115.94	106.44
3	D	501	RUB	O6P-P2-O5	3.51	115.81	106.67
3	A	501	RUB	O5-C5-C4	3.46	118.61	109.36
3	C	501	RUB	O5-P2-O4P	3.39	115.60	106.44
3	C	501	RUB	O4-C4-C3	3.32	114.50	109.67
3	B	501	RUB	O2-C2-C1	3.22	126.86	120.44
3	C	501	RUB	O6P-P2-O5P	3.16	119.67	107.80
3	C	501	RUB	O4-C4-C5	-3.16	103.01	109.99
3	A	501	RUB	O2P-P1-O1	-2.87	99.19	106.67
3	C	501	RUB	O3P-P1-O1P	2.66	121.21	110.83
3	D	501	RUB	O5P-P2-O4P	2.66	121.20	110.83
3	C	501	RUB	O2-C2-C1	-2.53	115.39	120.44
3	A	501	RUB	O3P-P1-O1P	2.46	120.42	110.83
3	A	501	RUB	O5P-P2-O5	-2.45	100.29	106.67
3	B	501	RUB	O1-P1-O1P	-2.43	99.88	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	RUB	O3P-P1-O2P	2.40	116.80	107.80
3	D	501	RUB	O1-P1-O1P	-2.32	100.16	106.44
3	D	501	RUB	O5-C5-C4	2.20	115.24	109.36
3	A	501	RUB	O1-P1-O1P	-2.14	100.66	106.44
3	C	501	RUB	O3P-P1-O2P	2.08	115.59	107.80
3	C	501	RUB	O3P-P1-O1	-2.02	101.41	106.67

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	RUB	O1-C1-C2-C3
3	A	501	RUB	O1-C1-C2-O2
3	A	501	RUB	O2-C2-C3-O3
3	A	501	RUB	C2-C3-C4-C5
3	A	501	RUB	C2-C3-C4-O4
3	A	501	RUB	O3-C3-C4-C5
3	A	501	RUB	O3-C3-C4-O4
3	A	501	RUB	C1-O1-P1-O2P
3	A	501	RUB	C1-O1-P1-O3P
3	A	501	RUB	C5-O5-P2-O6P
3	B	501	RUB	O1-C1-C2-C3
3	B	501	RUB	O1-C1-C2-O2
3	B	501	RUB	C1-C2-C3-C4
3	B	501	RUB	O2-C2-C3-C4
3	B	501	RUB	O2-C2-C3-O3
3	B	501	RUB	C2-C3-C4-C5
3	B	501	RUB	C2-C3-C4-O4
3	B	501	RUB	O3-C3-C4-C5
3	B	501	RUB	O3-C3-C4-O4
3	B	501	RUB	C1-O1-P1-O2P
3	B	501	RUB	C1-O1-P1-O3P
3	C	501	RUB	O1-C1-C2-C3
3	C	501	RUB	O1-C1-C2-O2
3	C	501	RUB	O4-C4-C5-O5
3	C	501	RUB	C5-O5-P2-O5P
3	C	501	RUB	C5-O5-P2-O6P
3	D	501	RUB	O2-C2-C3-O3
3	D	501	RUB	C2-C3-C4-C5
3	D	501	RUB	C2-C3-C4-O4
3	D	501	RUB	O3-C3-C4-C5
3	D	501	RUB	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	D	501	RUB	C5-O5-P2-O4P
3	D	501	RUB	C5-O5-P2-O5P
3	D	501	RUB	C5-O5-P2-O6P
3	B	501	RUB	O4-C4-C5-O5
3	D	501	RUB	O4-C4-C5-O5
3	B	501	RUB	C3-C4-C5-O5
3	D	501	RUB	C3-C4-C5-O5
3	A	501	RUB	C1-O1-P1-O1P
3	A	501	RUB	C5-O5-P2-O4P
3	B	501	RUB	C1-O1-P1-O1P
3	C	501	RUB	C5-O5-P2-O4P
3	B	501	RUB	C1-C2-C3-O3
3	A	501	RUB	C5-O5-P2-O5P
3	A	501	RUB	C1-C2-C3-O3
3	B	501	RUB	C4-C5-O5-P2
3	C	501	RUB	C4-C5-O5-P2

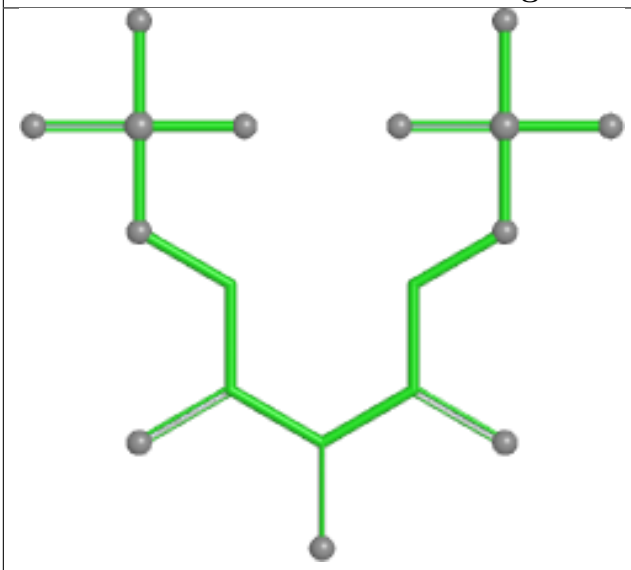
There are no ring outliers.

4 monomers are involved in 13 short contacts:

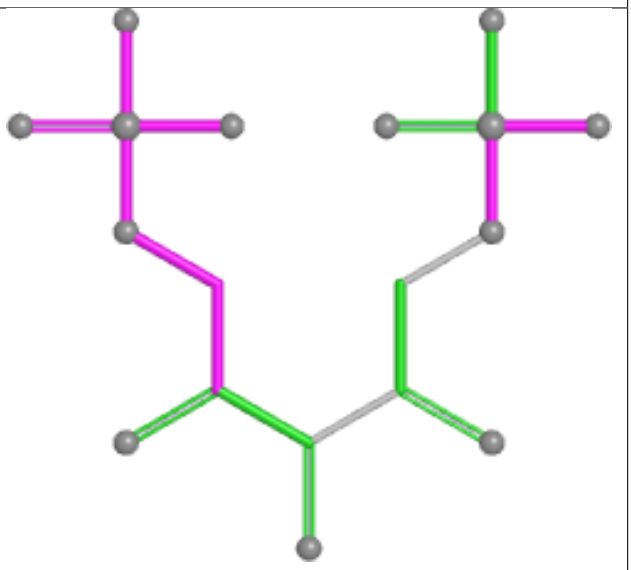
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	RUB	1	0
3	A	501	RUB	4	0
3	C	501	RUB	4	0
3	B	501	RUB	4	0

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

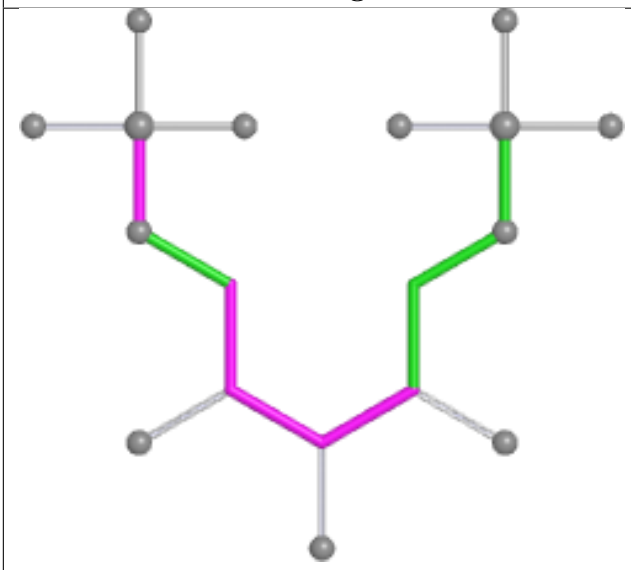
Ligand RUB D 501



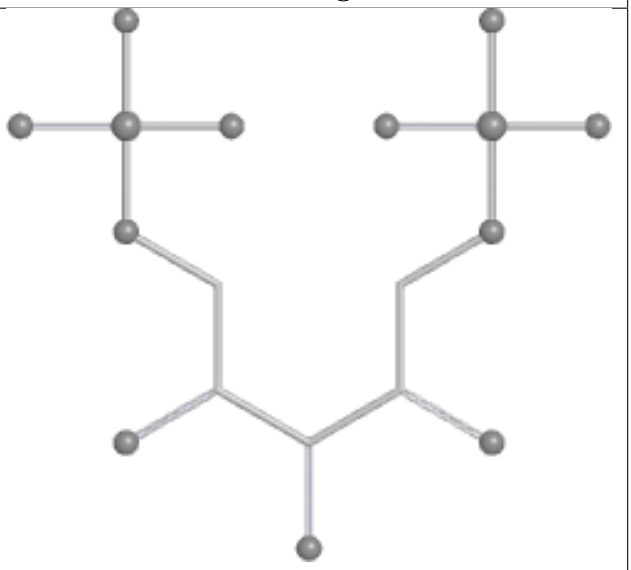
Bond lengths



Bond angles

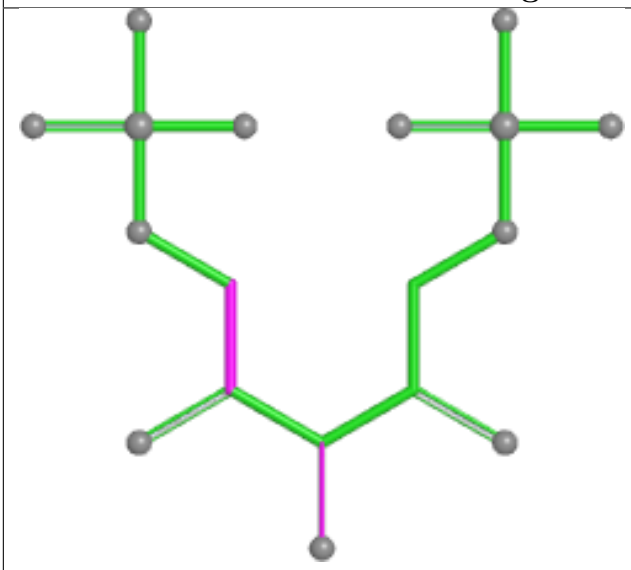


Torsions

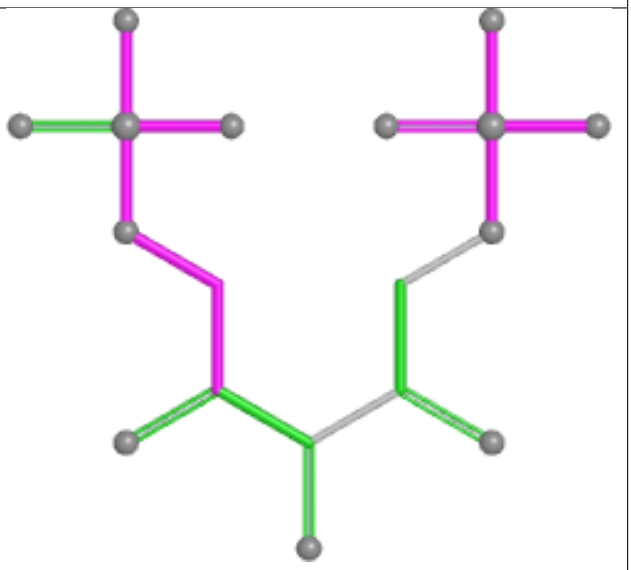


Rings

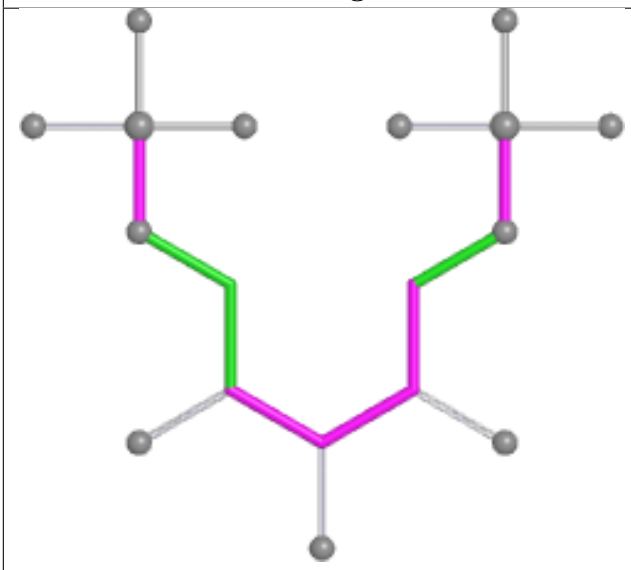
Ligand RUB A 501



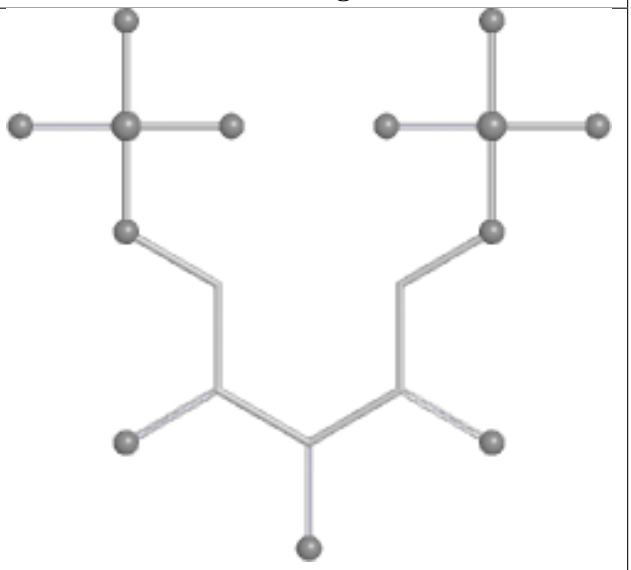
Bond lengths



Bond angles

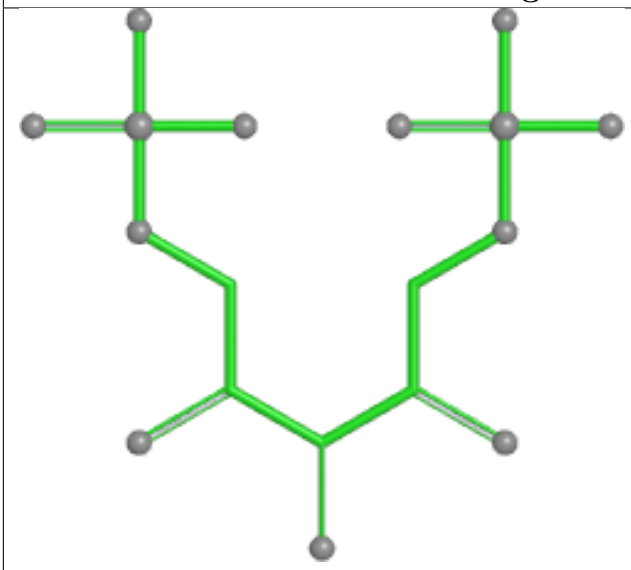


Torsions

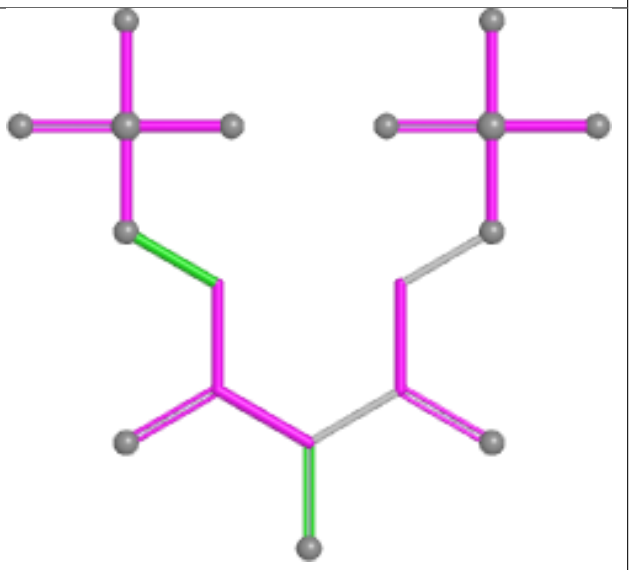


Rings

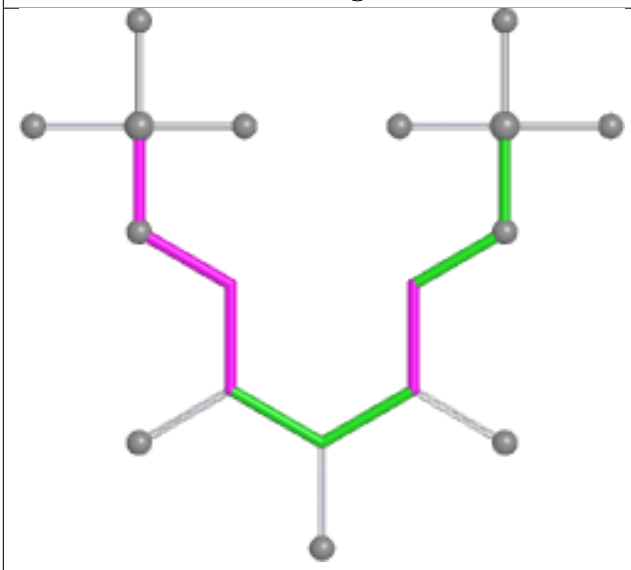
Ligand RUB C 501



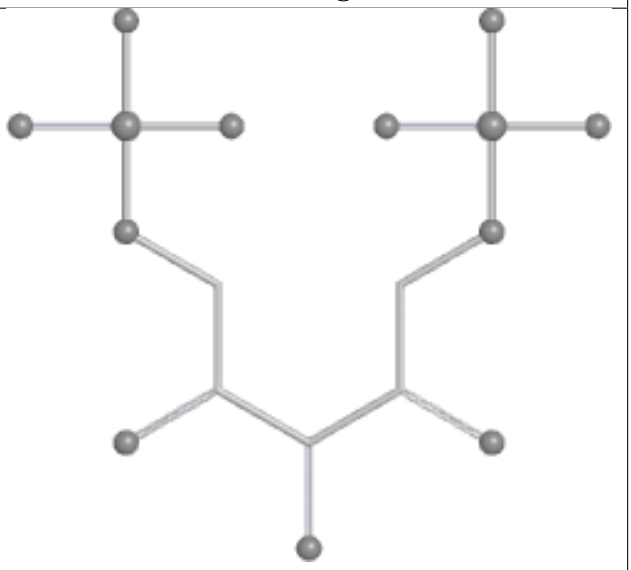
Bond lengths



Bond angles

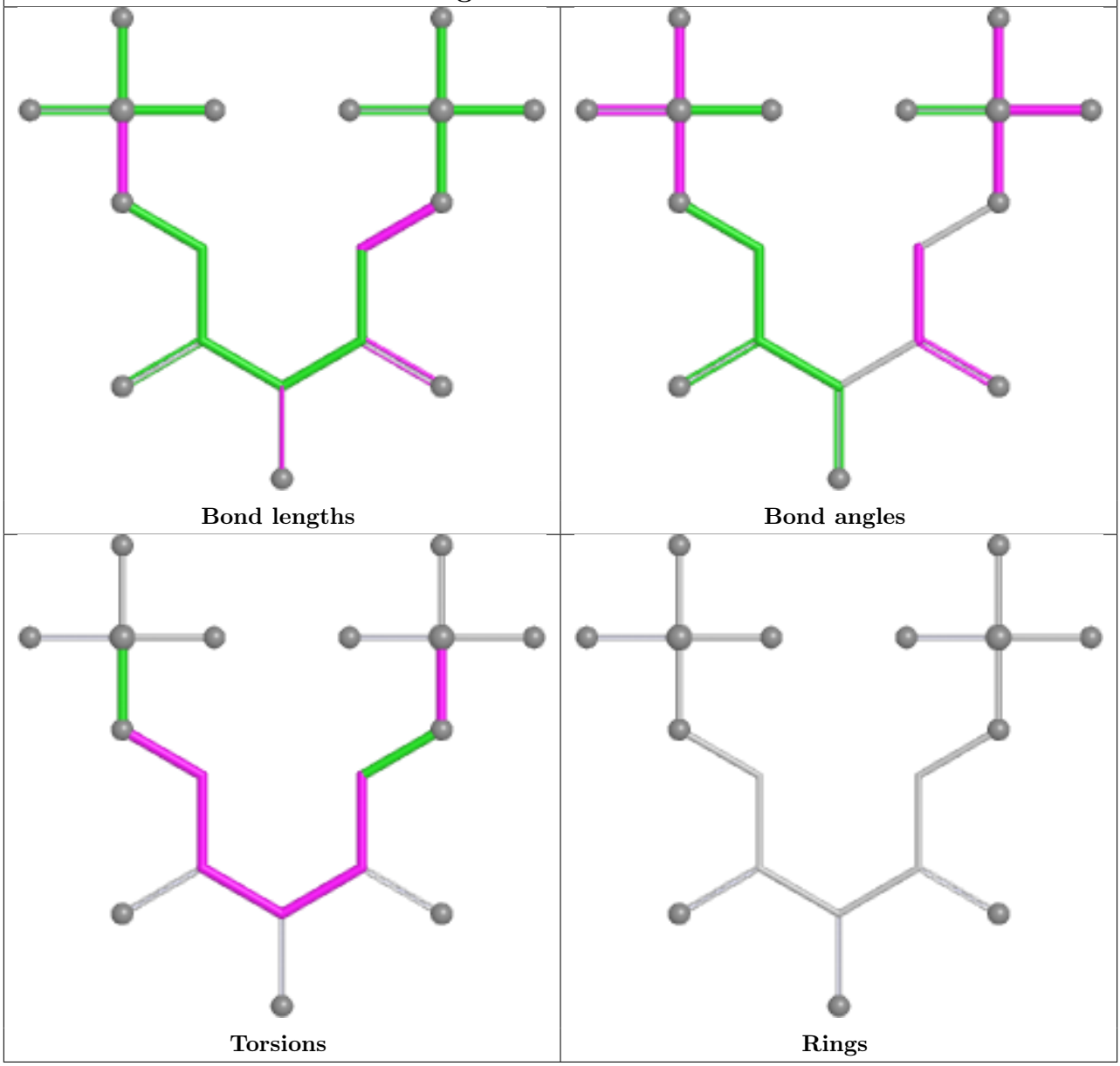


Torsions



Rings

Ligand RUB B 501



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	458/475 (96%)	-0.96	0 100 100	2, 2, 20, 43	0
1	B	458/475 (96%)	-0.97	0 100 100	2, 2, 23, 46	0
1	C	458/475 (96%)	-0.86	0 100 100	2, 9, 28, 34	0
1	D	458/475 (96%)	-0.89	0 100 100	2, 10, 30, 37	0
2	S	123/123 (100%)	-0.80	0 100 100	2, 15, 24, 34	0
2	T	123/123 (100%)	-0.80	0 100 100	2, 14, 27, 52	0
2	U	123/123 (100%)	-0.60	0 100 100	7, 23, 37, 46	0
2	V	123/123 (100%)	-0.62	1 (0%) 86 85	5, 19, 31, 58	0
All	All	2324/2392 (97%)	-0.88	1 (0%) 100 100	2, 8, 29, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	123	TYR	3.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

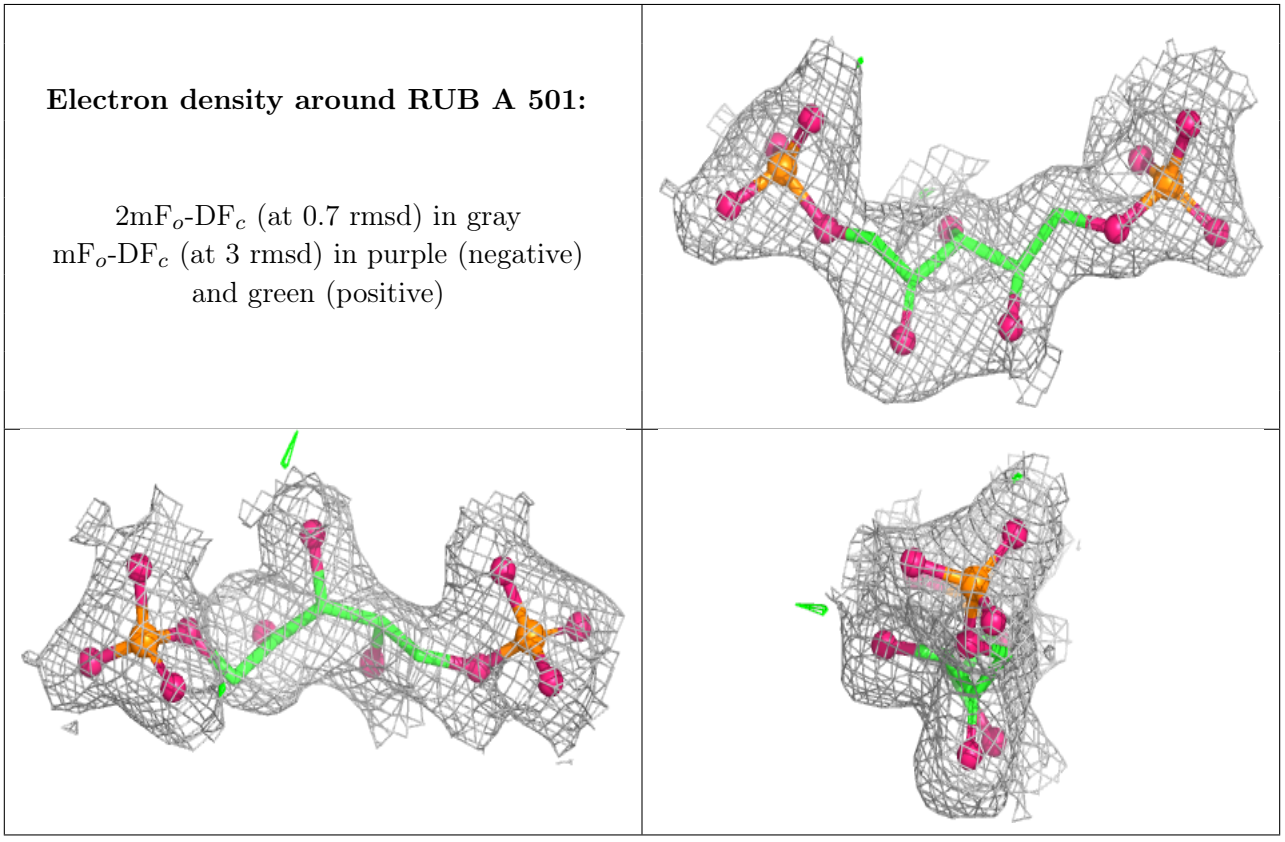
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RUB	A	501	18/18	0.97	0.08	6,10,12,12	0
3	RUB	B	501	18/18	0.98	0.09	2,2,2,2	0
3	RUB	D	501	18/18	0.98	0.07	8,14,18,19	0
3	RUB	C	501	18/18	0.99	0.07	8,11,16,17	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.

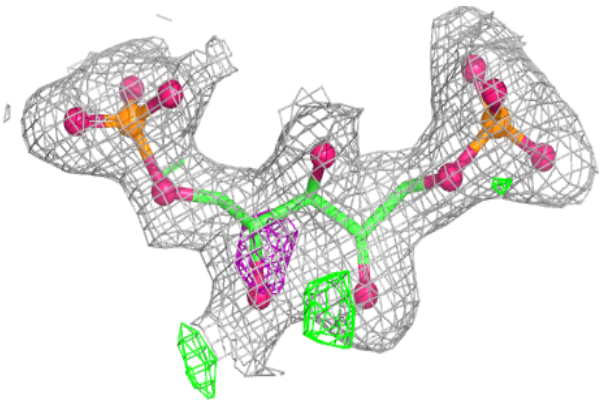
Electron density around RUB A 501:

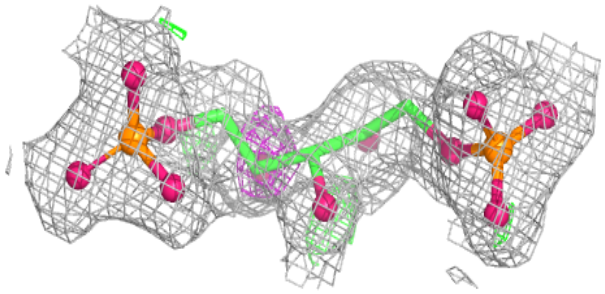
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

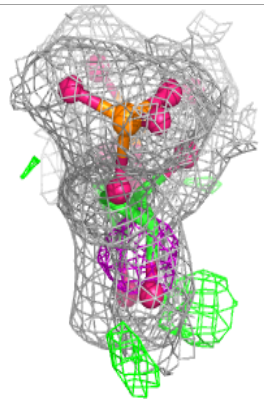


Electron density around RUB B 501:

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

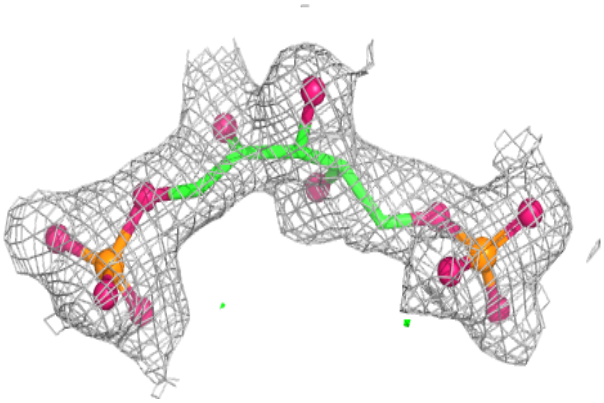


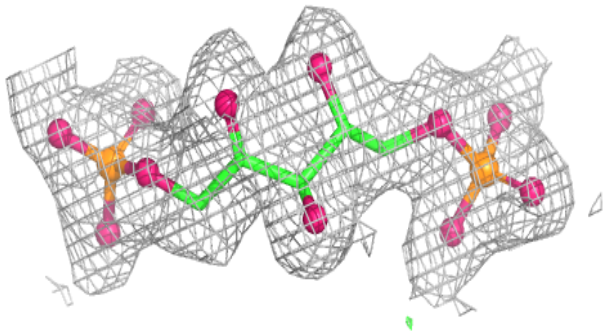


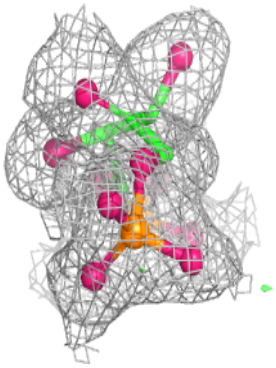


Electron density around RUB D 501:

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

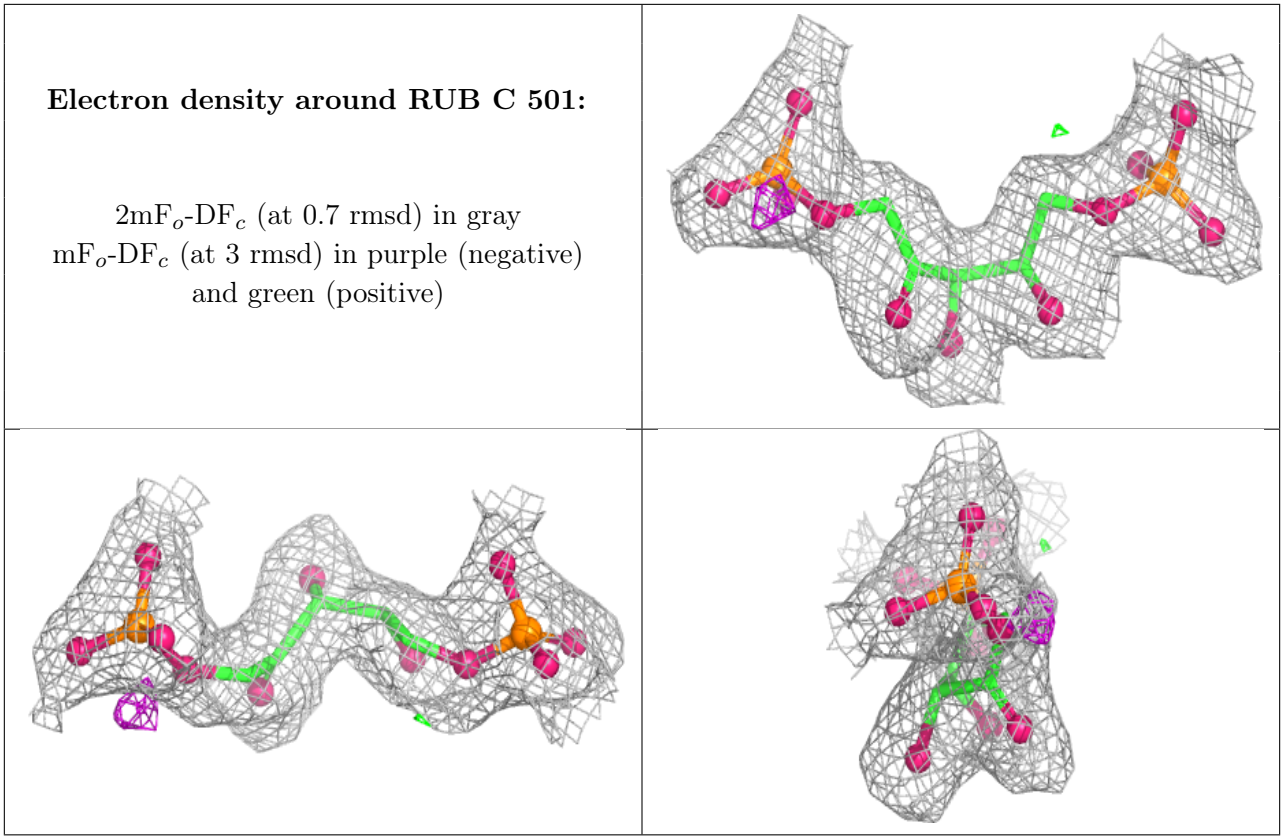






Electron density around RUB C 501:

$2mF_o$-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.