



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:30 AM UTC

PDB ID : 4HHH / pdb_00004hhh
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

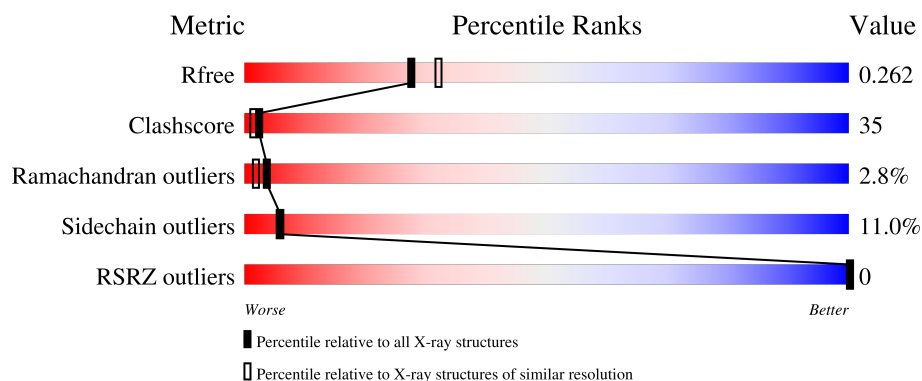
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



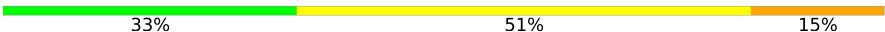
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	
1	C	475	
1	D	475	
2	S	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	T	123	
2	U	123	
2	V	123	

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

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.

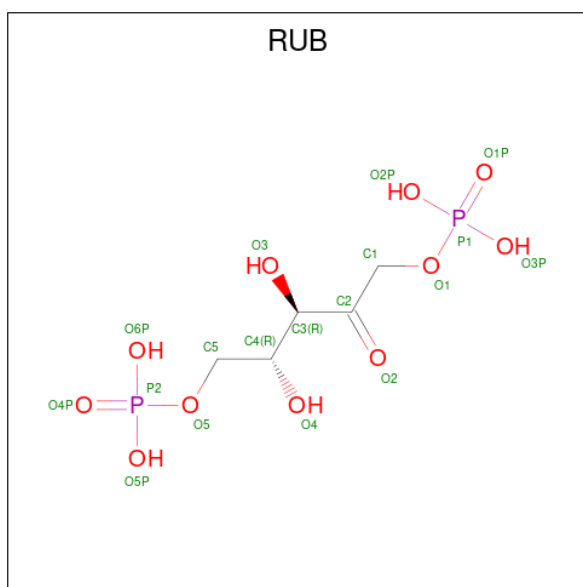
- Molecule 1 is a protein called Ribulose biphosphate carboxylase large chain.

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 biphosphate 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 (CCD ID: RUB) (formula: $C_5H_{12}O_{11}P_2$).



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

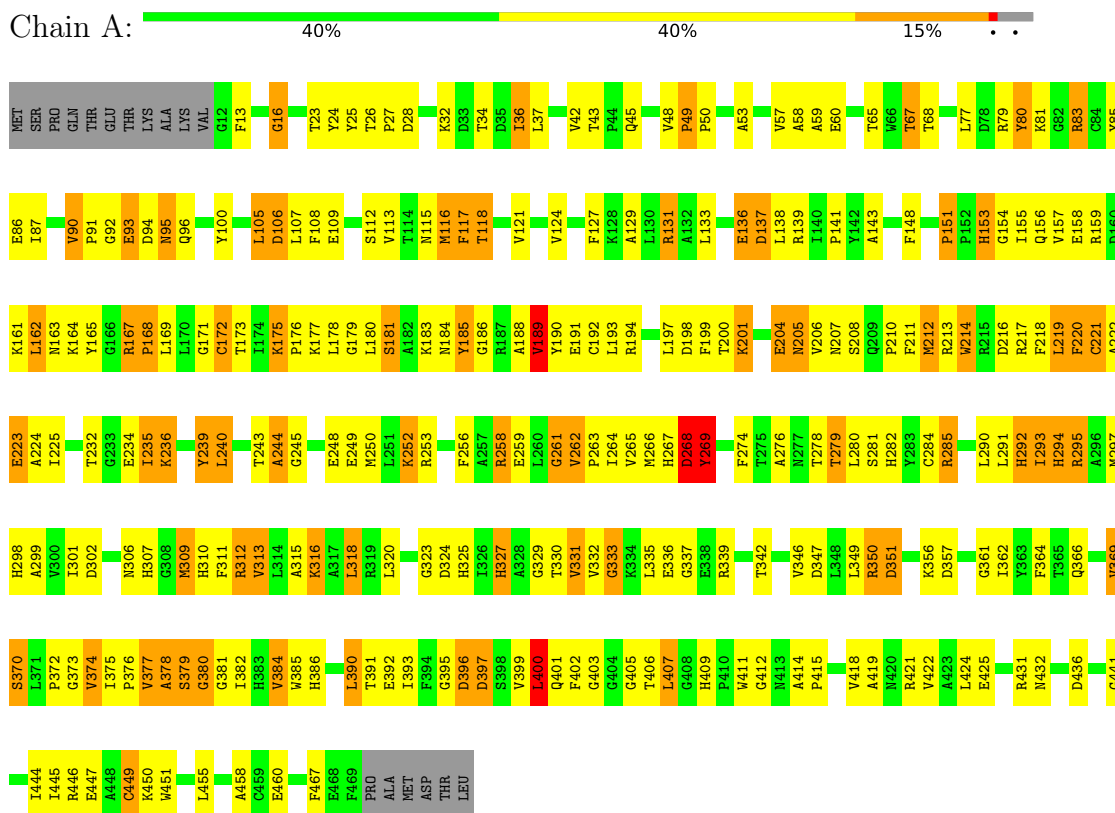
- Molecule 4 is water.

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

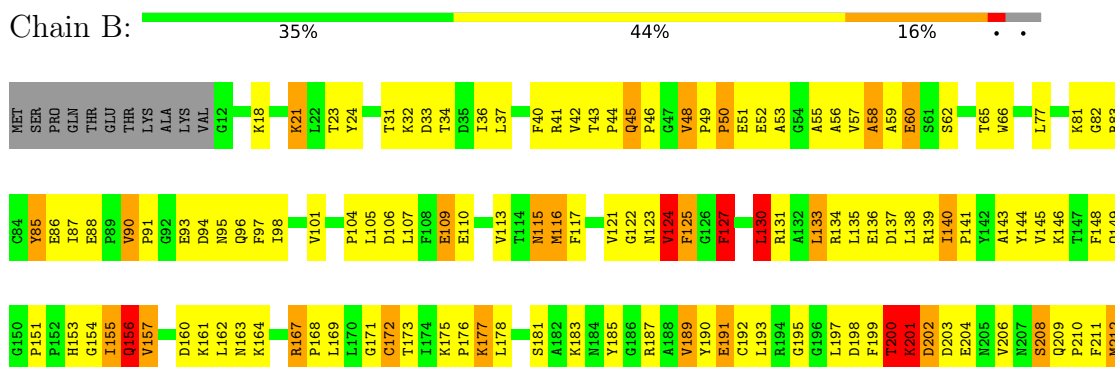
3 Residue-property plots

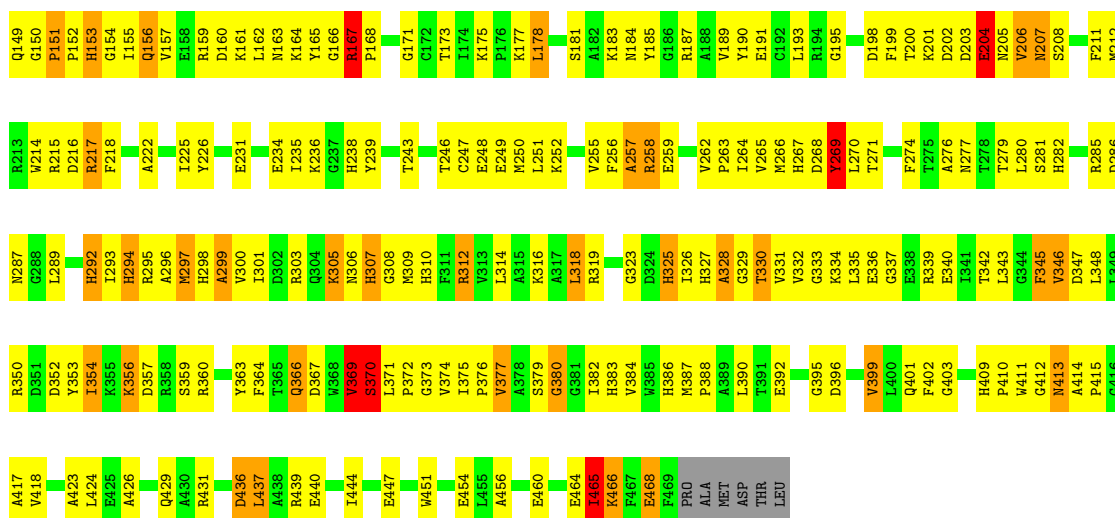
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Ribulose biphosphate carboxylase large chain



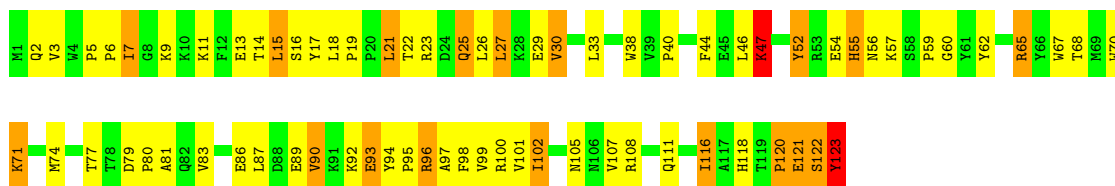
- Molecule 1: Ribulose biphosphate carboxylase large chain





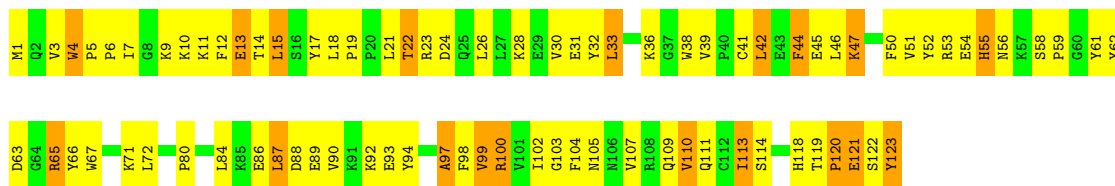
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain S: 41% 42% 15%



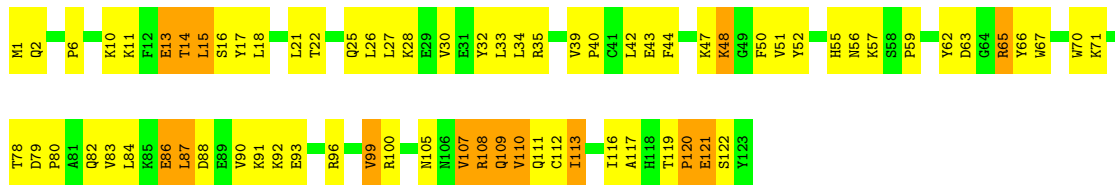
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain T: 33% 51% 15%



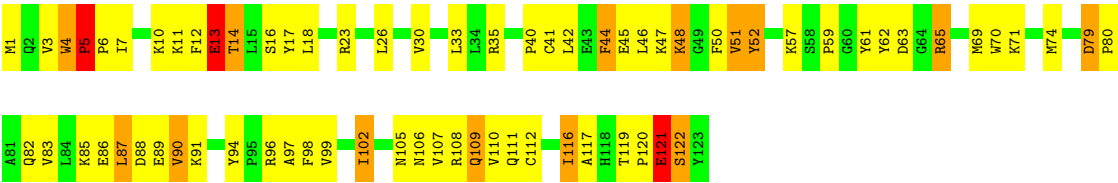
- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain U: 41% 47% 12%



- Molecule 2: Ribulose biphosphate carboxylase small chain

Chain V: 42% 44% 11%



4 Data and refinement statistics

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 – 2.20 109.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (109.95-2.20) 93.1 (109.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.70%)	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)	0.32 , 4.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	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	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.54	32/3765 (0.8%)	1.69	66/5104 (1.3%)
1	B	1.55	32/3783 (0.8%)	1.78	106/5128 (2.1%)
1	C	1.36	20/3790 (0.5%)	1.61	65/5135 (1.3%)
1	D	1.39	22/3758 (0.6%)	1.64	77/5090 (1.5%)
2	S	1.19	3/1089 (0.3%)	1.46	14/1474 (0.9%)
2	T	1.21	2/1099 (0.2%)	1.36	8/1487 (0.5%)
2	U	1.03	0/1087	1.26	6/1472 (0.4%)
2	V	1.04	0/1100	1.24	6/1489 (0.4%)
All	All	1.39	111/19471 (0.6%)	1.61	348/26379 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
2	S	0	1
2	V	0	1
All	All	0	6

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	19	PRO	CA-C	9.53	1.57	1.51
1	A	236	LYS	CA-C	9.01	1.63	1.52
1	A	373	GLY	N-CA	8.33	1.56	1.44
1	D	151	PRO	CA-C	8.08	1.56	1.51
1	B	326	ILE	C-O	-7.91	1.16	1.24
1	A	214	TRP	NE1-CE2	-7.88	1.28	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	LEU	N-CA	7.82	1.55	1.46
1	D	269	TYR	N-CA	7.62	1.55	1.46
1	A	153	HIS	N-CA	7.61	1.56	1.46
1	C	292	HIS	CG-CD2	7.60	1.44	1.35
1	B	167	ARG	N-CA	7.57	1.52	1.45
1	B	393	ILE	N-CA	7.55	1.55	1.46
1	C	327	HIS	CA-C	-7.46	1.43	1.52
1	A	240	LEU	CA-C	7.20	1.61	1.52
1	B	331	VAL	N-CA	7.16	1.55	1.46
1	D	281	SER	N-CA	7.15	1.55	1.46
1	D	33	ASP	CA-C	7.11	1.62	1.52
1	B	214	TRP	N-CA	7.06	1.54	1.46
1	D	292	HIS	CA-C	-7.04	1.44	1.52
1	A	400	LEU	N-CA	6.98	1.54	1.46
1	A	268	ASP	CA-C	6.93	1.62	1.52
1	C	328	ALA	N-CA	-6.92	1.41	1.47
1	C	327	HIS	CE1-NE2	6.85	1.39	1.32
1	A	205	ASN	CA-CB	6.81	1.64	1.53
1	A	105	LEU	CA-C	-6.79	1.43	1.52
1	A	36	ILE	CA-C	6.73	1.60	1.52
1	D	294	HIS	CE1-NE2	6.61	1.39	1.32
2	S	55	HIS	CB-CG	6.61	1.59	1.50
1	A	316	LYS	N-CA	6.58	1.54	1.46
1	B	48	VAL	CA-C	6.49	1.58	1.53
1	D	250	MET	CA-C	-6.48	1.44	1.52
1	A	200	THR	CA-C	6.43	1.61	1.53
1	B	262	VAL	N-CA	-6.37	1.38	1.46
1	D	138	LEU	C-O	-6.29	1.17	1.23
1	A	282	HIS	ND1-CE1	6.28	1.38	1.32
1	B	338	GLU	N-CA	6.25	1.53	1.45
1	A	90	VAL	CA-C	6.24	1.57	1.52
1	B	364	PHE	CA-C	-6.23	1.45	1.52
1	D	276	ALA	N-CA	6.11	1.53	1.46
1	B	187	ARG	CA-CB	-6.09	1.43	1.53
1	D	122	GLY	N-CA	6.08	1.53	1.45
1	A	261	GLY	N-CA	6.08	1.53	1.45
1	B	307	HIS	CG-CD2	5.98	1.42	1.35
1	C	116	MET	C-O	-5.97	1.16	1.24
1	B	48	VAL	N-CA	5.95	1.50	1.46
1	D	292	HIS	ND1-CE1	5.95	1.38	1.32
1	C	294	HIS	CD2-NE2	5.95	1.44	1.37
1	A	210	PRO	C-O	5.92	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	292	HIS	CG-CD2	5.92	1.42	1.35
1	A	327	HIS	CA-C	-5.92	1.45	1.52
1	B	133	LEU	N-CA	5.91	1.53	1.46
1	C	294	HIS	CE1-NE2	5.89	1.38	1.32
1	D	153	HIS	ND1-CE1	5.88	1.38	1.32
1	C	224	ALA	CA-C	5.87	1.60	1.52
1	B	208	SER	N-CA	5.85	1.53	1.46
1	C	292	HIS	ND1-CE1	5.80	1.38	1.32
1	B	143	ALA	CA-CB	-5.77	1.44	1.53
1	A	282	HIS	CG-CD2	5.76	1.42	1.35
1	C	145	VAL	CA-CB	5.76	1.60	1.54
1	A	235	ILE	N-CA	5.67	1.53	1.46
1	B	109	GLU	CA-C	5.67	1.60	1.52
1	B	116	MET	C-O	-5.66	1.17	1.24
1	C	158	GLU	C-O	5.57	1.30	1.24
1	A	181	SER	CA-C	5.55	1.60	1.52
1	D	366	GLN	CA-C	5.55	1.59	1.52
1	A	188	ALA	C-O	5.54	1.31	1.24
1	B	125	PHE	N-CA	5.54	1.53	1.46
1	C	33	ASP	CA-C	-5.54	1.45	1.52
1	C	327	HIS	CG-CD2	5.53	1.42	1.35
1	A	244	ALA	N-CA	5.52	1.53	1.46
1	C	117	PHE	N-CA	5.51	1.53	1.46
1	C	282	HIS	CG-ND1	-5.51	1.32	1.38
1	B	348	LEU	C-O	-5.51	1.17	1.24
1	A	106	ASP	C-O	5.50	1.31	1.24
1	D	383	HIS	CG-CD2	5.49	1.41	1.35
1	B	273	GLY	N-CA	5.49	1.50	1.45
1	B	292	HIS	CA-C	-5.45	1.45	1.52
1	B	156	GLN	CA-C	5.44	1.60	1.52
1	B	172	CYS	N-CA	-5.42	1.40	1.46
1	D	41	ARG	N-CA	-5.41	1.39	1.46
1	D	142	TYR	N-CA	5.40	1.53	1.46
1	B	235	ILE	N-CA	5.38	1.53	1.46
1	A	385	TRP	N-CA	5.36	1.53	1.46
2	T	47	LYS	N-CA	5.36	1.52	1.45
1	C	143	ALA	CA-C	5.34	1.59	1.52
1	D	125	PHE	CA-C	5.33	1.60	1.52
1	B	285	ARG	C-O	5.30	1.30	1.24
1	C	209	GLN	C-O	-5.29	1.19	1.24
1	B	391	THR	CB-CG2	-5.28	1.35	1.52
1	B	371	LEU	C-N	5.27	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	ARG	N-CA	5.26	1.52	1.46
1	D	129	ALA	N-CA	5.24	1.53	1.46
1	A	316	LYS	CA-C	-5.24	1.46	1.52
1	A	280	LEU	C-O	-5.22	1.18	1.24
2	T	47	LYS	CA-C	5.18	1.55	1.52
1	B	305	LYS	N-CA	5.17	1.52	1.46
1	B	189	VAL	CA-C	-5.14	1.45	1.52
1	B	409	HIS	CG-CD2	5.14	1.41	1.35
1	A	214	TRP	CG-CD2	5.14	1.53	1.43
1	A	153	HIS	CE1-NE2	5.13	1.37	1.32
1	A	378	ALA	N-CA	-5.11	1.40	1.45
1	B	310	HIS	CD2-NE2	-5.10	1.32	1.37
1	C	283	TYR	N-CA	5.10	1.52	1.46
2	S	55	HIS	CG-CD2	5.08	1.41	1.35
1	A	284	CYS	N-CA	5.07	1.52	1.46
1	D	271	THR	CA-C	5.07	1.59	1.52
1	A	396	ASP	C-O	5.07	1.30	1.24
1	D	364	PHE	CA-C	-5.06	1.46	1.52
1	C	142	TYR	N-CA	5.02	1.52	1.46
1	B	122	GLY	N-CA	5.01	1.52	1.45
1	D	369	VAL	CA-C	5.00	1.59	1.52

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	VAL	CA-C-N	13.94	134.05	118.85
1	C	262	VAL	C-N-CA	13.94	134.05	118.85
1	A	189	VAL	N-CA-C	-13.36	99.03	111.45
1	D	346	VAL	N-CA-C	-12.70	100.89	111.81
1	C	375	ILE	CA-C-N	-11.24	108.52	119.76
1	C	375	ILE	C-N-CA	-11.24	108.52	119.76
1	B	140[A]	ILE	CA-C-N	-11.13	108.32	119.78
1	B	140[A]	ILE	C-N-CA	-11.13	108.32	119.78
1	B	140[B]	ILE	CA-C-N	-11.13	108.32	119.78
1	B	140[B]	ILE	C-N-CA	-11.13	108.32	119.78
1	A	374	VAL	CA-C-N	-11.01	114.67	122.59
1	A	374	VAL	C-N-CA	-11.01	114.67	122.59
1	D	269	TYR	N-CA-C	10.75	123.07	111.36
1	B	155	ILE	N-CA-C	-10.07	100.55	110.72
1	B	189	VAL	N-CA-C	-9.81	102.32	111.45
1	D	142	TYR	N-CA-C	9.81	124.51	112.54
1	A	259	GLU	N-CA-C	9.77	124.25	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PRO	CA-C-N	-9.47	110.00	119.56
1	B	151	PRO	C-N-CA	-9.47	110.00	119.56
1	B	136	GLU	N-CA-C	9.44	121.33	111.14
1	A	206	VAL	CB-CA-C	-9.39	98.94	111.15
2	T	55	HIS	N-CA-C	9.33	124.46	112.89
1	A	292	HIS	CA-C-N	-9.28	111.06	123.12
1	A	292	HIS	C-N-CA	-9.28	111.06	123.12
1	A	278	THR	N-CA-C	-9.07	102.34	113.50
1	D	359	SER	N-CA-C	-9.01	102.42	113.50
1	B	270	LEU	N-CA-C	-8.87	102.38	113.55
1	D	103	TYR	CA-C-N	-8.76	110.95	119.89
1	D	103	TYR	C-N-CA	-8.76	110.95	119.89
1	B	351	ASP	N-CA-C	8.64	121.93	110.53
1	A	201	LYS	N-CA-C	8.41	121.94	109.24
1	B	293	ILE	N-CA-C	8.36	120.65	108.53
1	C	262	VAL	N-CA-CB	-8.28	99.62	111.21
1	D	149	GLN	N-CA-C	-8.24	100.17	112.04
1	C	149	GLN	N-CA-C	-8.23	101.73	112.68
1	B	58	ALA	N-CA-C	8.18	119.82	111.07
1	D	279	THR	N-CA-C	8.18	119.82	111.07
1	D	299	ALA	N-CA-C	8.14	120.16	111.28
1	D	330	THR	N-CA-C	8.14	123.42	113.17
1	A	293	ILE	N-CA-C	8.10	119.54	107.80
1	C	390	LEU	N-CA-C	8.06	120.79	111.11
1	C	229	GLN	CA-C-N	8.06	131.08	120.28
1	C	229	GLN	C-N-CA	8.06	131.08	120.28
1	A	181	SER	N-CA-C	7.90	121.09	110.35
1	C	242	ALA	N-CA-C	-7.84	102.76	112.88
1	B	235	ILE	N-CA-C	7.81	119.48	108.93
1	B	391	THR	N-CA-C	-7.75	102.91	111.36
1	B	279	THR	N-CA-C	-7.75	102.16	111.69
1	D	281	SER	N-CA-C	7.72	119.70	111.28
2	U	39	VAL	CA-C-N	7.65	127.81	120.31
2	U	39	VAL	C-N-CA	7.65	127.81	120.31
1	A	384[A]	VAL	N-CA-C	7.64	118.38	110.36
1	A	384[B]	VAL	N-CA-C	7.64	118.38	110.36
1	D	250	MET	N-CA-C	-7.60	102.93	111.14
1	C	226	TYR	N-CA-C	7.52	121.56	112.38
2	S	79	ASP	CA-C-N	7.51	128.18	119.47
2	S	79	ASP	C-N-CA	7.51	128.18	119.47
1	A	351	ASP	N-CA-C	7.47	120.39	110.53
1	B	295	ARG	N-CA-C	-7.45	102.73	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	PHE	N-CA-C	7.43	119.46	111.36
1	A	258	ARG	CG-CD-NE	-7.33	95.87	112.00
1	C	352	ASP	N-CA-C	-7.33	104.47	113.41
1	D	64	GLY	N-CA-C	7.30	120.36	112.33
2	S	65	ARG	N-CA-C	-7.29	102.31	112.45
1	D	150	GLY	CA-C-N	-7.28	114.35	119.66
1	D	150	GLY	C-N-CA	-7.28	114.35	119.66
2	S	60	GLY	N-CA-C	-7.26	104.47	114.64
1	A	250	MET	N-CA-C	-7.25	103.38	111.28
2	S	54	GLU	N-CA-C	7.24	122.17	113.12
1	A	192	CYS	N-CA-C	7.17	118.89	111.14
1	A	198	ASP	N-CA-C	-7.14	103.42	111.14
1	B	278	THR	N-CA-C	-7.11	104.07	112.89
1	B	200	THR	CB-CA-C	-7.09	99.42	113.45
1	C	80	TYR	N-CA-C	7.08	122.09	113.17
1	A	262	VAL	CA-C-N	7.07	126.75	119.82
1	A	262	VAL	C-N-CA	7.07	126.75	119.82
1	D	147	THR	N-CA-C	7.06	121.72	113.18
1	A	214	TRP	N-CA-C	7.04	119.60	111.02
1	C	115	ASN	N-CA-C	7.03	118.59	111.07
1	C	286	ASP	N-CA-C	-7.02	103.98	112.54
1	B	426	ALA	CA-C-N	6.99	129.87	120.65
1	B	426	ALA	C-N-CA	6.99	129.87	120.65
2	S	18	LEU	CA-C-N	-6.96	114.58	119.66
2	S	18	LEU	C-N-CA	-6.96	114.58	119.66
1	C	251	LEU	N-CA-C	6.93	119.48	111.02
1	C	116	MET	N-CA-C	-6.93	104.09	112.54
1	D	353	TYR	CB-CA-C	6.92	120.02	110.34
1	C	113	VAL	N-CA-C	-6.91	104.26	111.58
1	B	317	ALA	N-CA-C	-6.91	102.85	112.45
1	A	204	GLU	CA-C-N	6.90	130.22	120.28
1	A	204	GLU	C-N-CA	6.90	130.22	120.28
1	C	198	ASP	N-CA-C	-6.88	103.22	111.69
1	D	265	VAL	N-CA-C	6.83	119.00	109.29
1	A	374	VAL	N-CA-C	-6.83	98.51	108.89
1	C	409	HIS	CA-C-N	6.81	127.09	119.32
1	C	409	HIS	C-N-CA	6.81	127.09	119.32
1	B	305	LYS	N-CA-C	6.76	119.66	111.82
1	C	146	LYS	N-CA-C	6.75	125.17	110.80
2	S	123	TYR	CA-CB-CG	6.75	126.05	113.90
1	B	444	ILE	N-CA-C	-6.74	102.19	111.89
1	B	113	VAL	CB-CA-C	-6.73	103.20	112.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	VAL	CB-CA-C	-6.72	102.56	111.70
1	A	313	VAL	N-CA-C	-6.71	104.22	110.53
1	B	325	HIS	N-CA-C	-6.69	98.86	109.23
1	B	383	HIS	N-CA-C	6.68	116.87	108.45
1	D	382	ILE	N-CA-C	6.66	118.27	109.21
1	B	31	THR	CA-C-N	-6.66	112.73	122.65
1	B	31	THR	C-N-CA	-6.66	112.73	122.65
1	B	181	SER	N-CA-C	-6.66	100.61	110.46
1	B	303	ARG	N-CA-C	6.63	118.50	111.28
1	B	427	CYS	N-CA-C	6.62	118.19	110.97
1	C	37	LEU	N-CA-C	6.62	120.03	109.24
1	C	69	VAL	N-CA-C	-6.54	98.76	108.45
1	B	236	LYS	N-CA-C	6.54	120.05	109.40
1	A	16	GLY	N-CA-C	6.52	118.66	112.08
1	C	271	THR	N-CA-C	-6.52	105.87	113.88
1	A	124	VAL	N-CA-C	6.50	118.03	110.62
1	D	376	PRO	CB-CA-C	-6.49	102.92	111.23
1	B	167	ARG	CA-C-N	6.48	126.46	119.78
1	B	167	ARG	C-N-CA	6.48	126.46	119.78
1	C	217	ARG	N-CA-C	-6.46	103.92	110.97
1	C	332	VAL	N-CA-C	-6.46	105.05	111.77
1	D	156	GLN	N-CA-C	-6.46	104.16	111.14
1	A	302	ASP	N-CA-C	6.46	121.33	113.38
1	B	130	LEU	CA-C-N	6.45	129.22	120.44
1	B	130	LEU	C-N-CA	6.45	129.22	120.44
1	B	151	PRO	N-CA-C	6.45	116.66	110.47
1	B	300	VAL	CA-C-N	6.44	129.95	122.35
1	B	300	VAL	C-N-CA	6.44	129.95	122.35
1	B	273	GLY	CA-C-O	-6.43	117.68	122.37
2	U	18	LEU	CA-C-N	6.42	127.00	120.38
2	U	18	LEU	C-N-CA	6.42	127.00	120.38
1	D	377	VAL	CB-CA-C	6.42	120.13	110.63
1	C	183	LYS	N-CA-C	6.38	117.92	110.97
1	B	292	HIS	CA-C-N	-6.38	114.88	123.10
1	B	292	HIS	C-N-CA	-6.38	114.88	123.10
1	A	318	LEU	N-CA-C	-6.37	103.59	112.45
1	A	92	GLY	N-CA-C	6.31	119.78	111.70
1	B	414	ALA	CA-C-N	6.31	127.73	119.84
1	B	414	ALA	C-N-CA	6.31	127.73	119.84
1	B	139	ARG	CA-C-N	-6.31	118.05	122.59
1	B	139	ARG	C-N-CA	-6.31	118.05	122.59
1	B	191	GLU	CA-C-N	6.28	129.21	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	GLU	C-N-CA	6.28	129.21	120.29
1	B	239	TYR	N-CA-CB	6.28	120.10	109.87
1	A	357	ASP	N-CA-C	6.26	117.65	107.32
2	T	56	ASN	N-CA-C	-6.26	99.93	108.38
1	A	80	TYR	N-CA-C	6.24	121.66	113.30
1	D	282	HIS	N-CA-C	6.24	118.08	111.28
1	A	216	ASP	N-CA-C	-6.23	104.57	111.36
1	C	231	GLU	N-CA-C	6.20	117.84	111.14
1	C	207	ASN	N-CA-C	-6.18	97.63	110.80
2	T	47	LYS	N-CA-C	6.13	118.60	108.48
1	C	280	LEU	N-CA-C	6.13	117.62	111.07
1	D	357	ASP	CA-C-N	6.12	132.38	120.99
1	D	357	ASP	C-N-CA	6.12	132.38	120.99
1	B	109	GLU	N-CA-C	6.10	119.11	109.96
1	D	328	ALA	CA-C-N	6.08	130.26	121.44
1	D	328	ALA	C-N-CA	6.08	130.26	121.44
2	S	5	PRO	N-CA-C	6.06	118.09	110.70
1	D	25	TYR	CA-C-N	-6.05	115.72	123.16
1	D	25	TYR	C-N-CA	-6.05	115.72	123.16
1	D	167	ARG	N-CA-C	6.03	115.25	108.25
1	D	325	HIS	CA-C-N	-6.03	112.73	121.95
1	D	325	HIS	C-N-CA	-6.03	112.73	121.95
1	A	281	SER	N-CA-C	-6.03	105.19	112.54
1	B	340	GLU	CA-C-N	6.00	128.13	120.56
1	B	340	GLU	C-N-CA	6.00	128.13	120.56
1	C	147	THR	N-CA-C	-6.00	105.81	113.02
1	B	332	VAL	N-CA-C	-6.00	105.97	111.67
1	B	214	TRP	N-CA-C	6.00	118.31	111.11
1	A	107	LEU	N-CA-C	5.97	120.04	112.87
1	C	300	VAL	CA-C-N	5.96	129.03	122.77
1	C	300	VAL	C-N-CA	5.96	129.03	122.77
1	D	269	TYR	N-CA-CB	5.96	118.98	110.16
1	C	319	ARG	N-CA-C	-5.95	101.61	111.37
1	A	49	PRO	CA-C-N	5.94	127.26	119.84
1	A	49	PRO	C-N-CA	5.94	127.26	119.84
1	D	82	GLY	N-CA-C	-5.93	104.06	112.37
1	D	268	ASP	CA-C-O	-5.92	113.57	120.62
1	C	316	LYS	N-CA-C	-5.91	104.92	111.36
1	B	371	LEU	CA-C-N	5.91	125.86	119.78
1	B	371	LEU	C-N-CA	5.91	125.86	119.78
1	B	417	ALA	CB-CA-C	-5.88	101.64	110.88
1	C	394	PHE	N-CA-C	5.88	117.68	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	TRP	CA-C-N	5.87	128.39	120.65
1	B	214	TRP	C-N-CA	5.87	128.39	120.65
1	B	273	GLY	N-CA-C	-5.86	106.17	112.08
1	C	267	HIS	CA-C-N	-5.85	115.24	122.84
1	C	267	HIS	C-N-CA	-5.85	115.24	122.84
1	A	390	LEU	N-CA-C	5.84	118.11	111.11
2	T	18	LEU	CA-C-N	-5.83	114.37	120.38
2	T	18	LEU	C-N-CA	-5.83	114.37	120.38
1	D	80	TYR	N-CA-C	5.81	120.65	113.50
1	D	274	PHE	N-CA-C	5.80	117.28	111.07
1	D	294	HIS	N-CA-C	5.79	118.98	110.59
1	D	345	PHE	N-CA-C	5.78	120.07	113.19
1	B	88	GLU	CA-C-N	-5.78	113.83	119.90
1	B	88	GLU	C-N-CA	-5.78	113.83	119.90
1	D	383	HIS	N-CA-C	5.78	118.67	109.65
1	B	177	LYS	O-C-N	5.78	128.24	122.12
1	A	269	TYR	N-CA-C	-5.75	105.37	112.90
1	B	191	GLU	N-CA-C	5.74	118.00	111.11
1	C	145	VAL	N-CA-CB	5.74	116.88	110.51
2	T	97	ALA	N-CA-C	5.71	117.81	108.55
1	A	292	HIS	N-CA-C	5.69	118.00	108.73
1	C	286	ASP	CA-C-N	-5.69	113.73	122.60
1	C	286	ASP	C-N-CA	-5.69	113.73	122.60
1	C	278	THR	N-CA-C	-5.68	104.70	111.69
1	C	248	GLU	N-CA-C	-5.68	105.85	112.89
1	D	343	LEU	N-CA-C	5.67	117.14	111.07
1	B	390	LEU	CA-C-N	5.67	128.34	120.29
1	B	390	LEU	C-N-CA	5.67	128.34	120.29
1	B	45	GLN	CA-C-N	-5.66	112.76	119.84
1	B	45	GLN	C-N-CA	-5.66	112.76	119.84
2	S	7	ILE	CB-CA-C	5.65	119.18	110.82
1	C	376	PRO	CA-C-N	-5.65	115.67	122.90
1	C	376	PRO	C-N-CA	-5.65	115.67	122.90
1	D	465	ILE	N-CA-C	5.64	116.29	108.84
2	U	51	VAL	N-CA-C	5.64	116.55	108.93
1	A	220	PHE	N-CA-C	-5.62	105.14	112.23
1	D	123	ASN	N-CA-C	5.62	119.65	112.12
1	B	130	LEU	CA-CB-CG	5.61	135.93	116.30
1	B	239	TYR	CA-C-N	-5.60	115.56	122.84
1	B	239	TYR	C-N-CA	-5.60	115.56	122.84
1	A	333	GLY	N-CA-C	5.59	120.60	112.60
1	B	213	ARG	CA-C-N	5.59	128.09	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	C-N-CA	5.59	128.09	120.54
1	B	143	ALA	N-CA-C	-5.58	106.61	113.41
1	B	425	GLU	N-CA-C	5.57	122.67	110.80
2	V	5	PRO	N-CA-C	5.55	117.47	110.70
1	C	366	GLN	N-CA-C	5.53	117.42	108.34
1	A	58	ALA	N-CA-C	5.52	117.30	111.28
1	A	377	VAL	N-CA-C	5.52	116.05	107.99
1	B	275	THR	N-CA-C	-5.52	105.17	111.07
1	D	301	ILE	CB-CA-C	-5.51	103.18	112.16
1	B	215	ARG	N-CA-C	5.50	116.96	110.97
1	D	140	ILE	N-CA-C	-5.46	101.66	107.77
1	B	263	PRO	N-CA-C	5.46	121.76	114.18
1	C	157	VAL	N-CA-C	5.45	115.65	110.42
1	D	287	ASN	N-CA-C	5.44	120.59	113.30
1	D	124	VAL	CA-C-N	-5.44	110.42	121.18
1	D	124	VAL	C-N-CA	-5.44	110.42	121.18
1	B	269	TYR	N-CA-C	5.42	119.74	113.18
1	C	215	ARG	N-CA-C	-5.41	105.31	112.34
1	D	350	ARG	N-CA-C	5.41	119.83	111.56
1	B	85	TYR	N-CA-C	5.40	119.86	113.16
1	C	267	HIS	CB-CA-C	-5.40	100.28	110.16
2	S	90	VAL	CB-CA-C	-5.38	104.87	112.14
1	D	247[A]	CYS	N-CA-C	-5.37	105.99	112.54
1	D	247[B]	CYS	N-CA-C	-5.37	105.99	112.54
1	B	390	LEU	N-CA-C	5.36	117.13	111.28
2	V	98	PHE	N-CA-C	-5.34	101.76	110.20
1	D	468	GLU	N-CA-C	5.34	117.34	108.20
1	B	404	GLY	N-CA-C	-5.33	106.32	112.83
1	D	354	ILE	CB-CA-C	5.33	118.74	110.96
1	B	201	LYS	N-CA-C	5.33	116.61	108.52
1	D	413	ASN	N-CA-C	5.32	122.13	110.80
1	D	300	VAL	CB-CA-C	-5.32	104.97	112.14
2	T	44	PHE	N-CA-C	5.32	117.33	108.99
1	A	118	THR	CA-C-N	-5.31	114.59	122.56
1	A	118	THR	C-N-CA	-5.31	114.59	122.56
1	A	244	ALA	N-CA-C	5.31	116.07	108.74
1	C	293	ILE	N-CA-C	5.31	115.72	107.28
1	D	127	PHE	CB-CA-C	-5.31	101.16	109.70
1	A	95	ASN	N-CA-C	-5.30	104.58	111.74
1	C	224	ALA	N-CA-CB	-5.30	102.31	110.16
2	V	4	TRP	CA-C-N	5.30	125.84	120.38
2	V	4	TRP	C-N-CA	5.30	125.84	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	GLU	CA-C-N	5.28	131.21	121.70
1	A	93	GLU	C-N-CA	5.28	131.21	121.70
1	C	181	SER	N-CA-C	5.28	117.67	110.55
1	A	151	PRO	CB-CA-C	-5.27	104.49	110.92
1	D	161	LYS	N-CA-C	-5.26	105.72	111.82
1	B	169	LEU	CA-C-N	-5.26	115.35	122.77
1	B	169	LEU	C-N-CA	-5.26	115.35	122.77
1	B	245	GLY	N-CA-C	-5.26	105.97	113.86
1	B	217	ARG	CB-CG-CD	5.25	123.37	111.30
1	B	86	GLU	N-CA-C	5.25	117.05	108.76
1	A	116	MET	N-CA-C	5.24	118.46	111.75
1	A	131	ARG	CA-C-N	-5.24	113.78	122.11
1	A	131	ARG	C-N-CA	-5.24	113.78	122.11
1	B	413	ASN	N-CA-C	-5.24	105.25	111.69
1	C	92	GLY	N-CA-C	5.24	125.60	113.18
1	A	397	ASP	CB-CA-C	5.24	119.97	112.12
1	C	393	ILE	CA-C-N	5.23	127.28	120.28
1	C	393	ILE	C-N-CA	5.23	127.28	120.28
1	D	279	THR	CA-C-N	5.23	127.71	120.29
1	D	279	THR	C-N-CA	5.23	127.71	120.29
1	A	362	ILE	CB-CA-C	5.21	117.33	111.80
1	B	416	GLY	N-CA-C	-5.21	106.47	112.83
1	B	115	ASN	CA-C-N	5.21	127.52	120.38
1	B	115	ASN	C-N-CA	5.21	127.52	120.38
1	D	293	ILE	N-CA-C	5.21	115.40	108.11
1	A	266	MET	N-CA-CB	-5.21	102.63	111.69
1	C	371	LEU	CA-C-O	-5.21	115.03	120.70
1	D	94	ASP	N-CA-C	-5.20	106.96	113.72
1	C	368	TRP	N-CA-C	-5.19	106.80	112.72
1	D	133	LEU	N-CA-C	5.19	117.86	109.40
1	A	221	CYS	CA-CB-SG	-5.18	102.48	114.40
1	A	347	ASP	N-CA-C	-5.18	106.11	112.90
1	D	370	SER	N-CA-C	5.18	119.44	113.38
1	D	145	VAL	N-CA-CB	5.17	116.24	110.51
1	C	38	ALA	N-CA-C	5.16	117.98	109.72
1	D	86	GLU	N-CA-C	5.16	116.25	108.46
1	B	187	ARG	N-CA-C	-5.16	105.65	111.28
1	B	417	ALA	O-C-N	5.16	127.39	122.07
1	D	147	THR	OG1-CB-CG2	5.16	119.62	109.30
1	D	307	HIS	N-CA-C	5.16	121.79	110.80
1	B	202	ASP	N-CA-CB	5.16	117.85	110.06
1	D	354	ILE	N-CA-C	-5.14	100.35	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	30	VAL	N-CA-C	5.13	115.75	110.36
1	B	307	HIS	N-CA-C	5.13	116.53	107.61
1	B	437	LEU	N-CA-C	5.11	117.59	111.71
1	B	350	ARG	N-CA-C	5.10	119.37	111.56
1	B	90	VAL	CA-C-N	5.10	126.22	119.84
1	B	90	VAL	C-N-CA	5.10	126.22	119.84
2	U	13	GLU	N-CA-C	5.10	116.70	108.08
2	V	44	PHE	N-CA-C	5.10	117.55	109.50
1	C	223	GLU	CA-C-N	5.09	127.51	120.29
1	C	223	GLU	C-N-CA	5.09	127.51	120.29
1	C	265	VAL	CB-CA-C	5.09	118.35	110.82
2	S	68	THR	CB-CA-C	5.08	118.20	109.51
1	D	124	VAL	N-CA-C	5.08	119.91	109.34
1	A	167	ARG	N-CA-C	5.07	114.13	108.25
1	D	399	VAL	N-CA-C	-5.07	101.01	108.11
1	D	95	ASN	N-CA-C	-5.06	105.14	111.92
1	D	243	THR	N-CA-C	-5.05	102.80	110.28
1	D	17	VAL	N-CA-C	5.05	115.62	109.30
1	B	417	ALA	N-CA-C	5.05	116.47	111.07
1	B	326	ILE	CA-C-N	-5.05	113.54	120.71
1	B	326	ILE	C-N-CA	-5.05	113.54	120.71
1	C	253	ARG	CA-CB-CG	-5.04	104.02	114.10
2	V	83	VAL	N-CA-C	-5.04	106.24	111.58
2	T	4	TRP	N-CA-C	-5.03	103.69	109.93
1	B	201	LYS	CB-CA-C	5.03	118.09	109.99
2	S	101	VAL	N-CA-C	5.02	114.98	107.51
1	D	395	GLY	N-CA-C	-5.01	103.70	112.53
1	A	279[A]	THR	CA-C-N	5.01	126.95	120.44
1	A	279[A]	THR	C-N-CA	5.01	126.95	120.44
1	A	279[B]	THR	CA-C-N	5.01	126.95	120.44
1	A	279[B]	THR	C-N-CA	5.01	126.95	120.44
1	B	230	ALA	N-CA-C	-5.01	105.51	110.97
1	C	108	PHE	N-CA-C	5.01	118.37	109.96
1	A	165	TYR	N-CA-C	5.00	116.80	109.24
1	A	178	LEU	N-CA-C	5.00	117.40	109.50
1	D	204	GLU	CA-C-N	5.00	127.91	120.31
1	D	204	GLU	C-N-CA	5.00	127.91	120.31

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

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	273	2
1	B	3653	0	3642	279	1
1	C	3662	0	3632	273	1
1	D	3647	0	3601	251	3
2	S	1049	0	1065	75	1
2	T	1056	0	1076	85	1
2	U	1047	0	1057	74	1
2	V	1057	0	1071	87	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	32	1
4	C	137	0	0	29	1
4	D	147	0	0	31	0
4	S	49	0	0	8	0
4	T	50	0	0	4	0
4	U	30	0	0	3	0
4	V	40	0	0	6	0
All	All	19680	0	18791	1328	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 35.

All (1328) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:214:TRP:CD1	1:B:253:ARG:HH21	1.91	0.88
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
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: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:D:266:MET:HE3	1:D:294:HIS:HD2	1.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:285:ARG:O	1:B:285:ARG:HG3	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:O	1:A:425:GLU:HG3	1.85	0.76
1:C:180:LEU:O	1:C:212:MET:HE2	1.86	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
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:C:229:GLN:NE2	4:C:691:HOH:O	2.21	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:A:136[B]:GLU:O	1:A:137:ASP:HB2	1.86	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
2:T:61:TYR:C	2:T:61:TYR:CD2	2.67	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:309[B]:MET:HE2	1:B:314:LEU:HD21	1.70	0.71
1:C:241:ASN:ND2	1:C:266:MET:HE2	2.05	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
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
1:D:121:VAL:HG11	1:D:309[B]:MET:HE3	1.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:175:LYS:HA	1:A:176:PRO:C	2.21	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:353:TYR:C	1:B:354:ILE:HD12	2.21	0.65
2:S:62:TYR:C	2:S:65:ARG:HD2	2.21	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:A:316:LYS:NZ	1:A:366:GLN:HE21	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:H	1:B:115:ASN:ND2	1.94	0.65
1:C:167:ARG:HH22	1:C:198:ASP:CG	2.04	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: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:B:271:THR:O	1:B:272:GLY:C	2.39	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
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: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:32:LYS:C	1:B:34:THR:H	2.06	0.63
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:B:301:ILE:C	4:B:614:HOH:O	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:160:ASP:OD1	1:D:165:TYR:OH	2.15	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
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: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:C:233:GLY:O	4:C:725:HOH:O	2.15	0.61
1:D:266:MET:CE	1:D:294:HIS:HD2	2.12	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:B:45:GLN:HB3	1:B:46:PRO:CD	2.30	0.61
2:T:32:TYR:OH	4:T:243:HOH:O	2.14	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
2:S:55:HIS:HB3	4:S:242:HOH:O	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:D:121:VAL:HG11	1:D:309[B]:MET:CE	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100:TYR:OH	4:D:685:HOH:O	2.09	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
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:16:GLY:C	1:A:67:THR:HG22	2.28	0.59
1:A:168:PRO:CG	1:A:396:ASP:HA	2.32	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:A:316:LYS:HZ3	1:A:366:GLN:HE21	1.50	0.58
1:D:266:MET:HE3	1:D:294:HIS:CD2	2.31	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:116:MET:HE3	1:B:138:LEU:CD1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:LEU:C	2:T:87:LEU:HD23	2.29	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: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
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
2:V:69:MET:HE3	2:V:71:LYS:O	2.05	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:158:GLU:CD	1:C:325:HIS:HE2	2.14	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
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
2:U:47:LYS:HZ3	2:U:48:LYS:HD2	1.71	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:171:GLY:C	1:C:401:GLN:HG3	2.32	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:B:18[B]:LYS:HB3	1:B:18[B]:LYS:HZ3	1.71	0.55
1:C:368:TRP:O	1:C:369:VAL:C	2.50	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
1:A:37:LEU:HB3	1:A:364:PHE:CE1	2.42	0.55
1:A:252:LYS:NZ	1:D:286:ASP:CG	2.61	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:466:LYS:C	1:D:466:LYS:HD2	2.32	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
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:396:ASP:CG	1:D:431:ARG:HH12	2.15	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:A:117:PHE:CE2	1:A:309[B]:MET:HE1	2.41	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:32:LYS:C	1:B:34:THR:N	2.66	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:183:LYS:O	2:U:66:TYR:OH	2.24	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
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: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
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:D:454:GLU:H	1:D:454:GLU:CD	2.17	0.52
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:C:71:THR:C	1:C:73:GLY:N	2.67	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:102[B]:ILE:HG22	2:T:103:GLY:N	2.23	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:A:330:THR:CG2	1:A:379:SER:C	2.83	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
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
2:U:108:ARG:O	2:U:109:GLN:C	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HB2	1:B:239:TYR:HD2	1.72	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:A:421:ARG:NE	1:A:425:GLU:OE2	2.39	0.51
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
1:B:193:LEU:O	1:B:236:LYS:NZ	2.34	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: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
1:D:97:PHE:C	1:D:97:PHE:CD1	2.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:ALA:O	1:B:418:VAL:HG23	2.11	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
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: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
1:D:295:ARG:O	1:D:296:ALA:C	2.54	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
2:T:14:THR:O	2:T:15:LEU:HB2	2.11	0.50
1:A:222:ALA:C	1:A:224:ALA:N	2.70	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
1:D:269:TYR:OH	1:D:314:LEU:O	2.30	0.50
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:A:127:PHE:C	1:A:129:ALA:H	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:127:PHE:C	1:A:129:ALA:N	2.70	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:B:177:LYS:NZ	1:B:203:ASP:CG	2.71	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:D:257:ALA:O	1:D:258:ARG:C	2.55	0.48
1:C:157:VAL:O	1:C:161:LYS:CG	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:336:GLU:CD	1:A:337:GLY:H	2.20	0.48
1:B:23:THR:CG2	1:B:24:TYR:CE2	2.89	0.48
1:B:294:HIS:NE2	3:B:501:RUB:O4	2.46	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
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:B:309[B]:MET:HE1	1:B:314:LEU:CD2	2.43	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:B:454:GLU:H	1:B:454:GLU:CD	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:S:13:GLU:O	2:S:14:THR:C	2.56	0.47
2:S:122:SER:C	2:S:123:TYR:HD1	2.21	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
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:395:GLY:C	1:A:397:ASP:H	2.21	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
1:D:412:GLY:C	1:D:415:PRO:HD2	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:MET:HE3	1:B:138:LEU:HD13	1.97	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
1:A:85:TYR:CE2	1:A:100:TYR:C	2.93	0.47
1:A:109:GLU:N	1:A:115:ASN:OD1	2.32	0.47
1:A:291:LEU:H	1:A:324:ASP:CG	2.19	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
1:D:211:PHE:CD1	1:D:211:PHE:C	2.93	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
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:HZ1	1:D:294:HIS:CE1	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:340:GLU:CD	4:D:712:HOH:O	2.53	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:241:ASN:HD21	1:C:266:MET:HE2	1.79	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:222:ALA:C	1:A:224:ALA:H	2.24	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
1:D:436:ASP:OD2	1:D:439:ARG:HB2	2.16	0.46
2:T:22:THR:C	2:T:26:LEU:HD12	2.40	0.46
2:U:47:LYS:HZ3	2:U:48:LYS:CD	2.29	0.46
2:U:120:PRO:HB2	2:U:122:SER:HA	1.97	0.46
1:C:71:THR:C	1:C:73:GLY:H	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:244:ALA:C	4:A:607:HOH:O	2.58	0.46
1:B:443:ALA:C	1:B:445:ILE:N	2.68	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: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: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
2:U:107:VAL:C	2:U:109:GLN:H	2.23	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:435:ARG:HH22	1:B:447:GLU:CD	2.22	0.45
1:D:166:GLY:HA2	2:V:112:CYS:O	2.16	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: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
1:C:20:TYR:C	1:C:22:LEU:H	2.24	0.45
1:C:214:TRP:C	1:C:216:ASP:N	2.74	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:26:THR:C	1:A:28:ASP:H	2.25	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:O	1:A:379:SER:HB2	2.17	0.44
1:B:58:ALA:O	1:B:62:SER:OG	2.31	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: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:23:ARG:HH22	2:T:88:ASP:CG	2.25	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:D:103:TYR:O	1:D:104:PRO:C	2.59	0.44
1:D:203:ASP:C	1:D:205:ASN:N	2.72	0.44
1:D:204:GLU:HA	1:D:266:MET:HE1	2.00	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: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:D:178:LEU:HB3	1:D:211:PHE:CZ	2.53	0.44
1:D:256:PHE:O	1:D:257:ALA:C	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:T:11:LYS:HG3	2:T:17:TYR:CE2	2.53	0.43
1:A:185:TYR:CD2	1:A:212:MET:HE1	2.52	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:A:117:PHE:CE2	1:A:309[A]:MET:HE1	2.53	0.43
1:A:418:VAL:O	1:A:419:ALA:C	2.60	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG1	1:A:274:PHE:CD1	2.90	0.43
1:B:309[B]:MET:HE2	1:B:309[B]:MET:HB2	1.48	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
2:V:47:LYS:HE3	2:V:48:LYS:HZ1	1.84	0.43
1:A:23:THR:O	1:A:81:LYS:NZ	2.35	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:T:121:GLU:HG3	2:T:122:SER:N	2.32	0.43
2:V:61:TYR:CD2	2:V:61:TYR:C	2.96	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: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:117:PHE:O	1:A:118:THR:C	2.61	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:B:372:PRO:C	4:B:772:HOH:O	2.62	0.43
1:C:45:GLN:HG2	1:C:129:ALA:C	2.43	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:424:LEU:O	1:B:428:VAL:HG23	2.19	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:176:PRO:O	1:A:177:LYS:C	2.63	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:B:18[B]:LYS:HZ2	1:B:18[B]:LYS:HB2	1.84	0.42
1:B:37:LEU:HD22	1:B:85:TYR:HE2	1.84	0.42
1:B:144:TYR:O	1:B:145:VAL:C	2.63	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
2:S:105:ASN:OD1	2:S:108:ARG:HB2	2.20	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:A:395:GLY:C	1:A:397:ASP:N	2.74	0.42
1:B:18[B]:LYS:NZ	1:B:18[B]:LYS:HB2	2.34	0.42
1:B:185:TYR:CD1	1:B:212:MET:HE1	2.55	0.42
1:B:185:TYR:O	1:B:189:VAL:HG23	2.19	0.42
1:B:204:GLU:HA	1:B:266:MET:HE1	2.01	0.42
1:B:330:THR:HG23	1:B:379:SER:H	1.77	0.42
1:C:150:GLY:C	1:C:322:GLY:HA2	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:156:GLN:HG2	1:B:157:VAL:N	2.30	0.41
1:C:24:TYR:CG	1:C:59:ALA:HB2	2.55	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: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
2:T:89:GLU:HG3	2:T:92:LYS:NZ	2.35	0.41
2:V:96:ARG:C	2:V:120:PRO:HB3	2.45	0.41
1:A:49:PRO:HA	1:A:50:PRO:HD2	1.86	0.41
1:A:267:HIS:CD2	1:A:269:TYR:HA	2.55	0.41
1:C:387:MET:HE1	1:C:402:PHE:CE2	2.56	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
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: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: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:A:436:ASP:OD2	1:A:436:ASP:C	2.63	0.41
1:B:37:LEU:HD22	1:B:85:TYR:CE2	2.56	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:214:TRP:CG	1:C:215:ARG:N	2.87	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:D:258:ARG:C	1:D:258:ARG:CD	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ALA:CB	4:A:627:HOH:O	2.68	0.41
1:A:222:ALA:O	1:A:223:GLU:C	2.63	0.41
1:A:295:ARG:HG3	3:A:501:RUB:O6P	2.21	0.41
1:B:23:THR:O	1:B:81:LYS:NZ	2.41	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:112:SER:O	1:A:113:VAL:C	2.64	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:129:ALA:C	1:D:130:LEU:HD23	2.46	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: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: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:104:PRO:O	1:B:105:LEU:C	2.64	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:35[A]:ARG:HG3	2:V:35[A]:ARG:NH1	2.30	0.41
1:A:412:GLY:C	1:A:415:PRO:HD2	2.46	0.40
1:B:144:TYR:C	1:B:146:LYS:N	2.76	0.40
1:C:330:THR:OG1	1:C:333:GLY:HA3	2.21	0.40
1:D:45:GLN:HG2	1:D:129:ALA:C	2.46	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
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: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:177:LYS:NZ	1:D:203:ASP:OD2	2.29	0.40
1:D:326:ILE:HG22	1:D:374:VAL:CG1	2.51	0.40
2:S:14:THR:O	2:S:15:LEU:HB2	2.20	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
2:V:82:GLN:C	2:V:85:LYS:HB3	2.46	0.40
1:A:26:THR:C	1:A:28:ASP:N	2.79	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LYS:CG	1:C:335:LEU:HD12	2.50	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%)	4	3
1	B	469/475 (99%)	404 (86%)	48 (10%)	17 (4%)	2	1
1	C	468/475 (98%)	411 (88%)	47 (10%)	10 (2%)	5	3
1	D	465/475 (98%)	408 (88%)	47 (10%)	10 (2%)	5	3
2	S	123/123 (100%)	105 (85%)	12 (10%)	6 (5%)	1	0
2	T	124/123 (101%)	109 (88%)	12 (10%)	3 (2%)	4	3
2	U	123/123 (100%)	97 (79%)	20 (16%)	6 (5%)	1	0
2	V	124/123 (101%)	111 (90%)	9 (7%)	4 (3%)	3	1
All	All	2363/2392 (99%)	2050 (87%)	246 (10%)	67 (3%)	4	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/385 (99%)	345 (91%)	36 (9%)	8	9
1	B	383/385 (100%)	342 (89%)	41 (11%)	6	6
1	C	382/385 (99%)	345 (90%)	37 (10%)	8	8
1	D	379/385 (98%)	336 (89%)	43 (11%)	5	5
2	S	115/113 (102%)	98 (85%)	17 (15%)	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	116/113 (103%)	98 (84%)	18 (16%)	2	2
2	U	115/113 (102%)	99 (86%)	16 (14%)	3	3
2	V	116/113 (103%)	99 (85%)	17 (15%)	3	2
All	All	1987/1992 (100%)	1762 (89%)	225 (11%)	6	5

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	83	ARG
1	A	117	PHE
1	A	136[A]	GLU
1	A	136[B]	GLU
1	A	162	LEU
1	A	168	PRO
1	A	172	CYS
1	A	175	LYS
1	A	185	TYR
1	A	189	VAL
1	A	212	MET
1	A	219[A]	LEU
1	A	219[B]	LEU
1	A	252	LYS
1	A	265[A]	VAL
1	A	265[B]	VAL
1	A	268	ASP
1	A	269	TYR
1	A	285	ARG
1	A	294	HIS
1	A	295	ARG
1	A	309[A]	MET
1	A	309[B]	MET
1	A	312	ARG
1	A	332	VAL
1	A	350	ARG
1	A	356	LYS
1	A	370[A]	SER
1	A	370[B]	SER
1	A	382	ILE
1	A	392	GLU
1	A	400	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	407	LEU
1	A	449	CYS
1	A	460	GLU
1	B	21	LYS
1	B	36	ILE
1	B	48	VAL
1	B	51	GLU
1	B	60	GLU
1	B	77	LEU
1	B	107	LEU
1	B	124[A]	VAL
1	B	124[B]	VAL
1	B	127	PHE
1	B	130	LEU
1	B	157	VAL
1	B	183	LYS
1	B	200	THR
1	B	201	LYS
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	268	ASP
1	B	285	ARG
1	B	305	LYS
1	B	314	LEU
1	B	336	GLU
1	B	338	GLU
1	B	339	ARG
1	B	341	ILE
1	B	345	PHE
1	B	354	ILE
1	B	371	LEU
1	B	384	VAL
1	B	392	GLU
1	B	401	GLN
1	B	407	LEU
1	B	429	GLN
1	B	435	ARG
1	B	440	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	445	ILE
1	B	451	TRP
1	C	18	LYS
1	C	21	LYS
1	C	34	THR
1	C	36	ILE
1	C	69	VAL
1	C	77	LEU
1	C	117	PHE
1	C	121	VAL
1	C	156	GLN
1	C	159[A]	ARG
1	C	159[B]	ARG
1	C	161	LYS
1	C	172	CYS
1	C	177	LYS
1	C	183	LYS
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	279	THR
1	C	293	ILE
1	C	336	GLU
1	C	341	ILE
1	C	365[A]	THR
1	C	365[B]	THR
1	C	369	VAL
1	C	384	VAL
1	C	401	GLN
1	C	435	ARG
1	C	439	ARG
1	C	440	GLU
1	C	444	ILE
1	C	465	ILE
1	D	21	LYS
1	D	34	THR
1	D	44	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	125	PHE
1	D	130	LEU
1	D	131	ARG
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	206	VAL
1	D	207	ASN
1	D	212	MET
1	D	217	ARG
1	D	259	GLU
1	D	262	VAL
1	D	269	TYR
1	D	305	LYS
1	D	312	ARG
1	D	318	LEU
1	D	332	VAL
1	D	334	LYS
1	D	346	VAL
1	D	356	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	465	ILE
1	D	466	LYS
2	S	21	LEU
2	S	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	25	GLN
2	S	26	LEU
2	S	27	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	99	VAL
2	S	102	ILE
2	S	107	VAL
2	S	116	ILE
2	S	122	SER
2	S	123	TYR
2	T	1	MET
2	T	7	ILE
2	T	22	THR
2	T	33	LEU
2	T	36	LYS
2	T	42	LEU
2	T	53	ARG
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	107	VAL
2	T	110	VAL
2	T	113	ILE
2	T	121	GLU
2	T	123	TYR
2	U	2	GLN
2	U	14[A]	THR
2	U	14[B]	THR
2	U	28	LYS
2	U	34	LEU
2	U	48	LYS
2	U	65	ARG
2	U	78	THR
2	U	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	U	86	GLU
2	U	87	LEU
2	U	93	GLU
2	U	99	VAL
2	U	110	VAL
2	U	113	ILE
2	U	121	GLU
2	V	7	ILE
2	V	13	GLU
2	V	14	THR
2	V	33	LEU
2	V	42	LEU
2	V	48	LYS
2	V	51	VAL
2	V	52	TYR
2	V	65	ARG
2	V	79[A]	ASP
2	V	79[B]	ASP
2	V	87	LEU
2	V	90	VAL
2	V	102	ILE
2	V	109	GLN
2	V	110	VAL
2	V	116	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	207	ASN
1	A	267	HIS
1	A	282	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	A	442	ASN
1	B	30	GLN
1	B	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	307	HIS
1	B	366	GLN
1	C	45	GLN
1	C	96	GLN
1	C	115	ASN
1	C	123	ASN
1	C	149	GLN
1	C	153	HIS
1	C	156	GLN
1	C	267	HIS
1	C	277	ASN
1	C	292	HIS
1	C	307	HIS
1	C	401	GLN
1	D	96	GLN
1	D	115	ASN
1	D	156	GLN
1	D	184	ASN
1	D	205	ASN
1	D	207	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	82	GLN
2	T	109	GLN
2	U	2	GLN
2	U	25	GLN
2	U	55	HIS
2	U	106	ASN
2	U	111	GLN
2	U	118	HIS
2	V	55	HIS
2	V	105	ASN
2	V	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	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%)
3	RUB	A	501	-	17,17,17	1.22	2 (11%)	17,25,25	2.05	7 (41%)

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

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(°)	Ideal(°)
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
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
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

Continued on next page...

Continued from previous page...

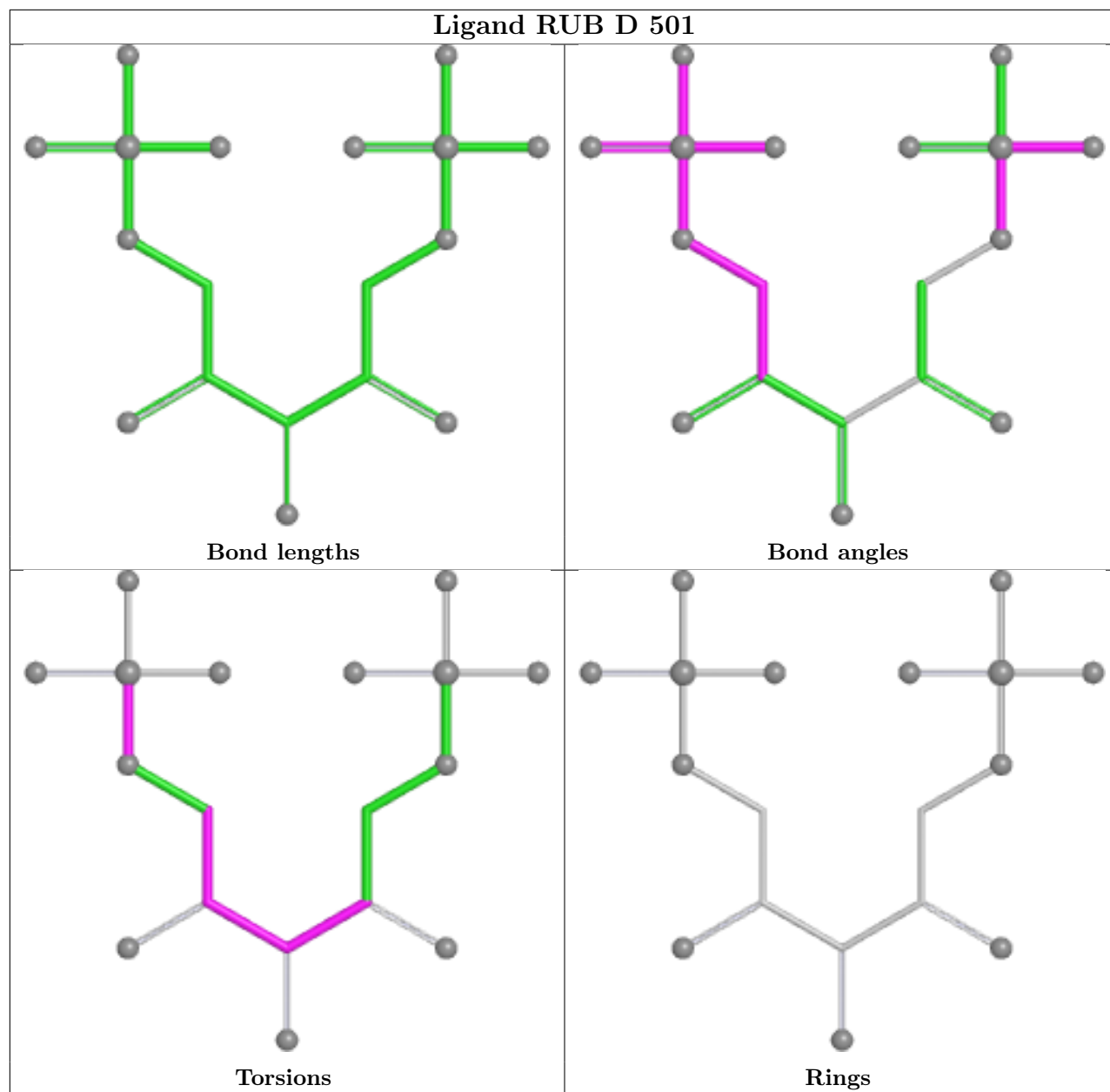
Mol	Chain	Res	Type	Atoms
3	A	501	RUB	C5-O5-P2-O5P
3	A	501	RUB	C1-C2-C3-O3
3	B	501	RUB	C4-C5-O5-P2
3	C	501	RUB	C4-C5-O5-P2

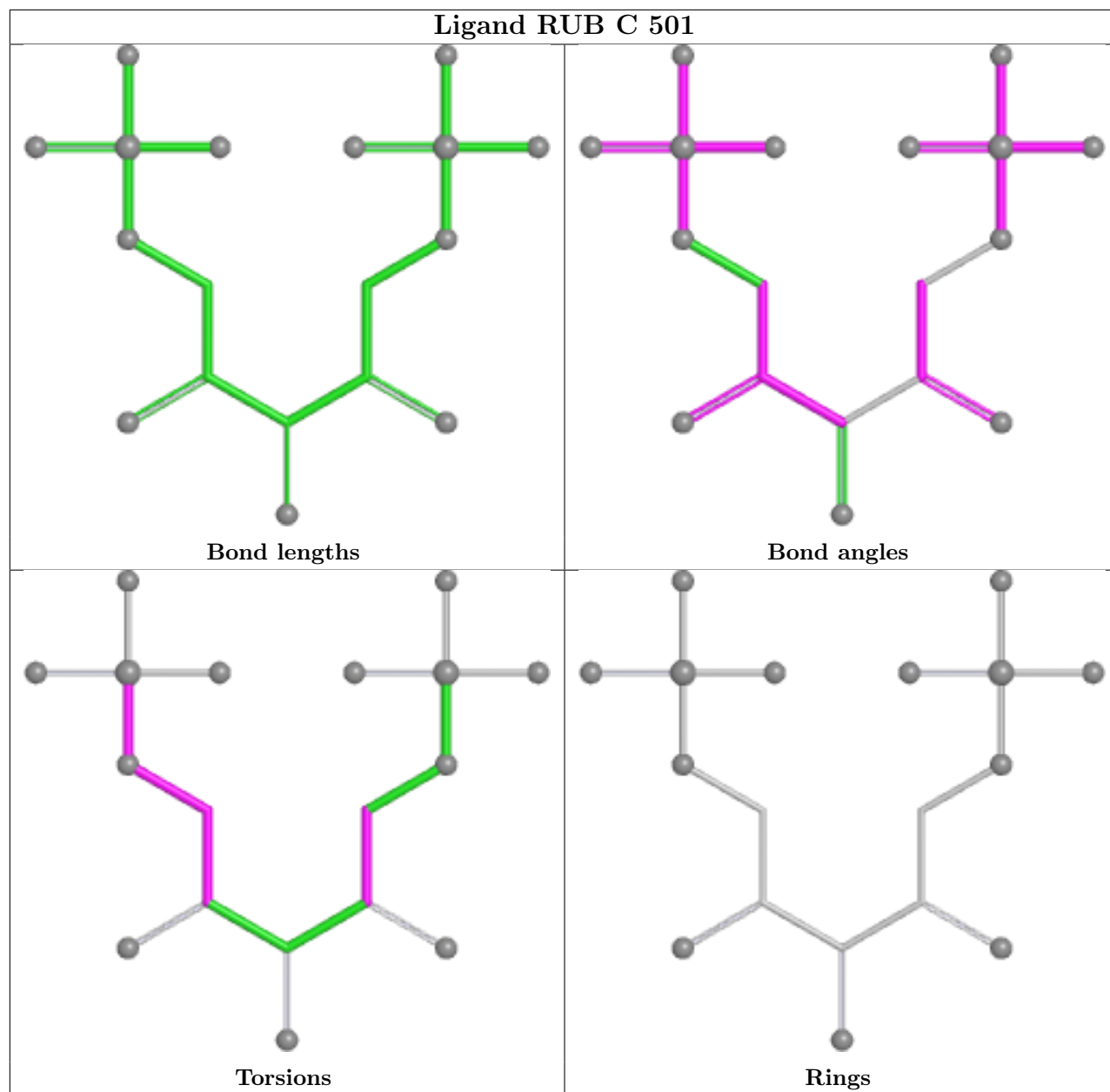
There are no ring outliers.

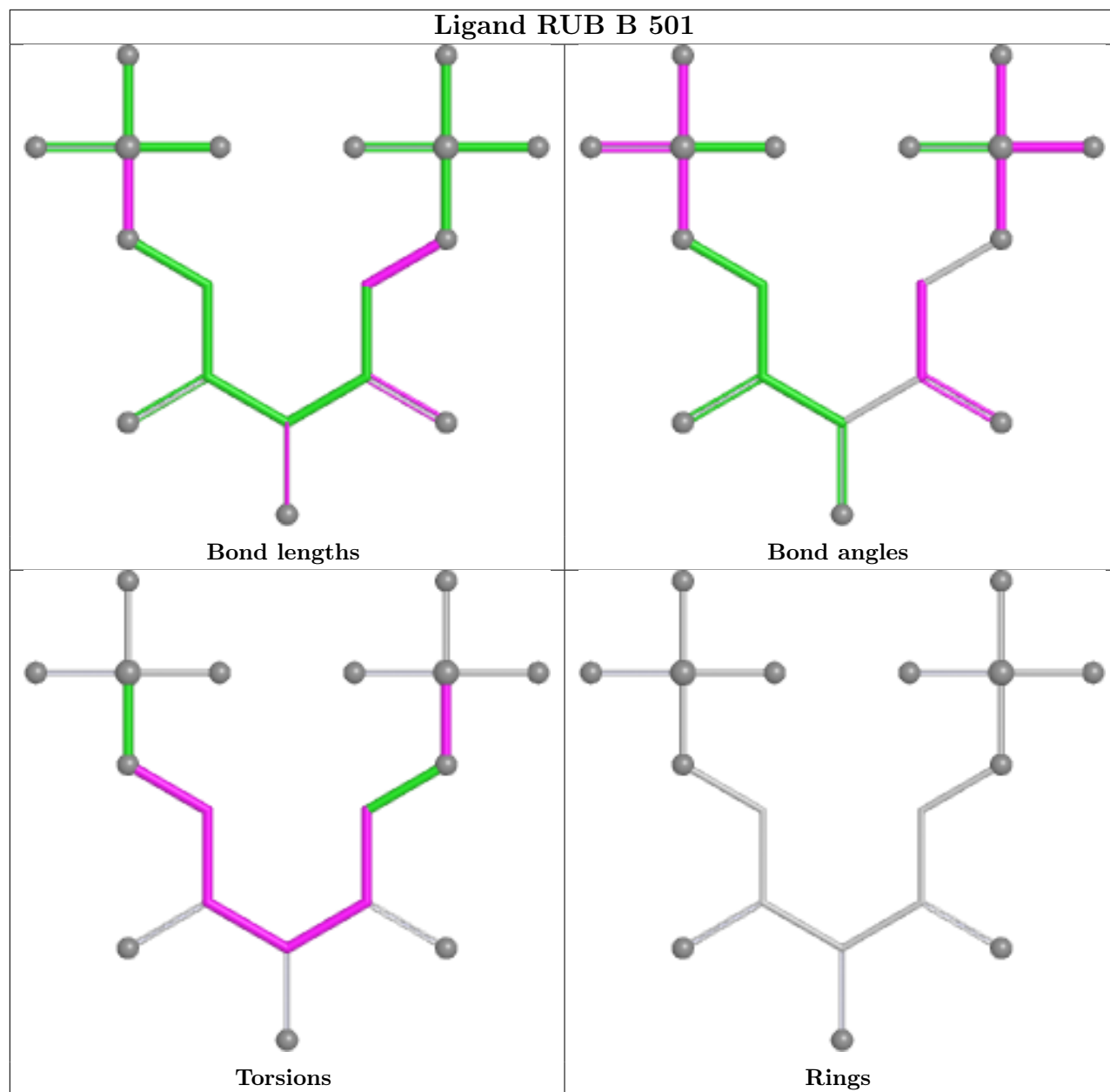
4 monomers are involved in 13 short contacts:

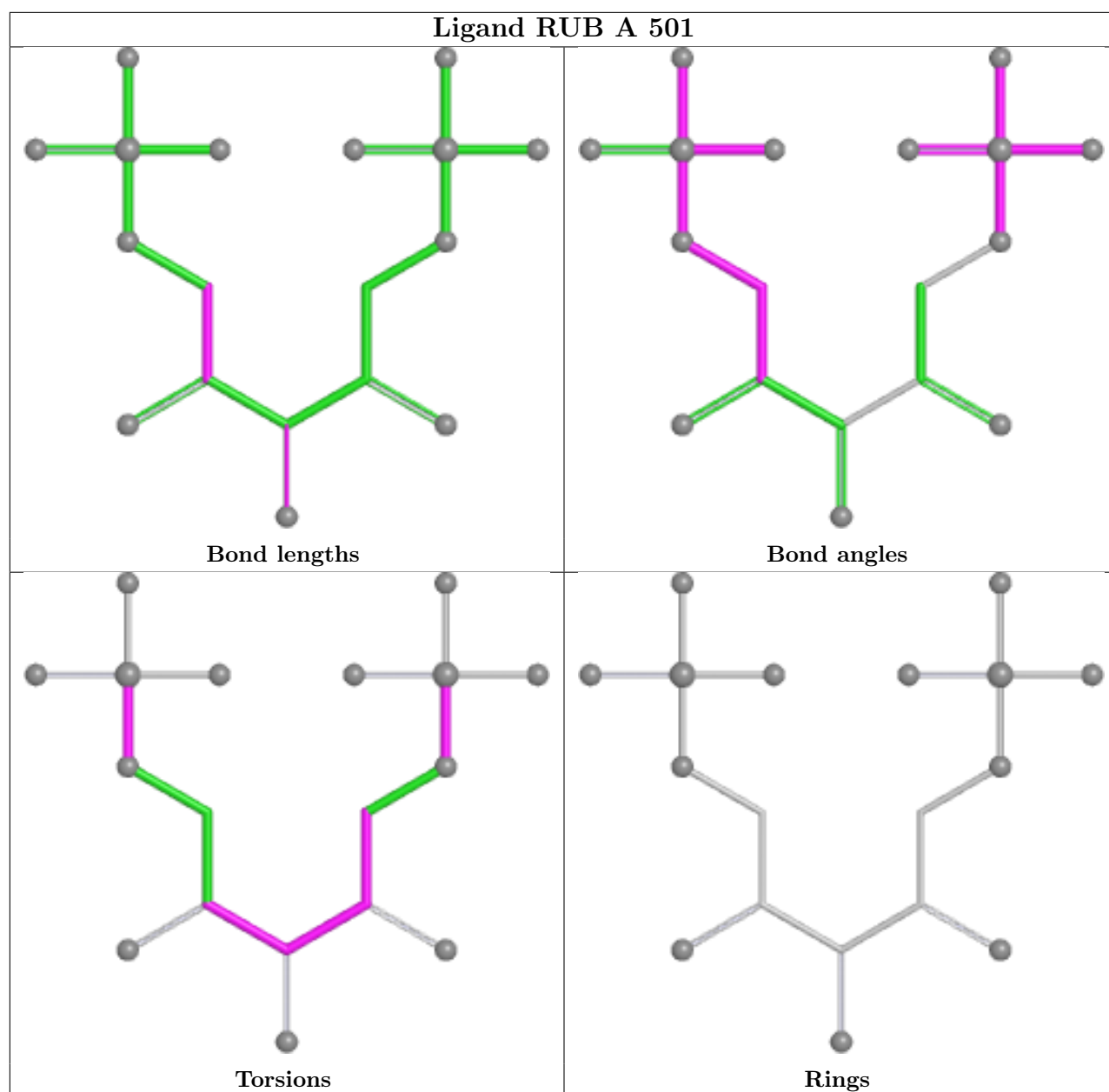
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	RUB	1	0
3	C	501	RUB	4	0
3	B	501	RUB	4	0
3	A	501	RUB	4	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/475 (96%)	-1.56	0 100 100	1, 2, 20, 43	11 (2%)
1	B	458/475 (96%)	-1.57	0 100 100	1, 2, 23, 46	13 (2%)
1	C	458/475 (96%)	-1.51	0 100 100	1, 8, 28, 34	12 (2%)
1	D	458/475 (96%)	-1.54	0 100 100	1, 10, 30, 37	9 (1%)
2	S	123/123 (100%)	-1.51	0 100 100	2, 15, 24, 34	2 (1%)
2	T	123/123 (100%)	-1.50	0 100 100	1, 14, 27, 52	3 (2%)
2	U	123/123 (100%)	-1.40	0 100 100	7, 23, 37, 46	2 (1%)
2	V	123/123 (100%)	-1.43	0 100 100	5, 19, 31, 58	3 (2%)
All	All	2324/2392 (97%)	-1.53	0 100 100	1, 8, 29, 58	55 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

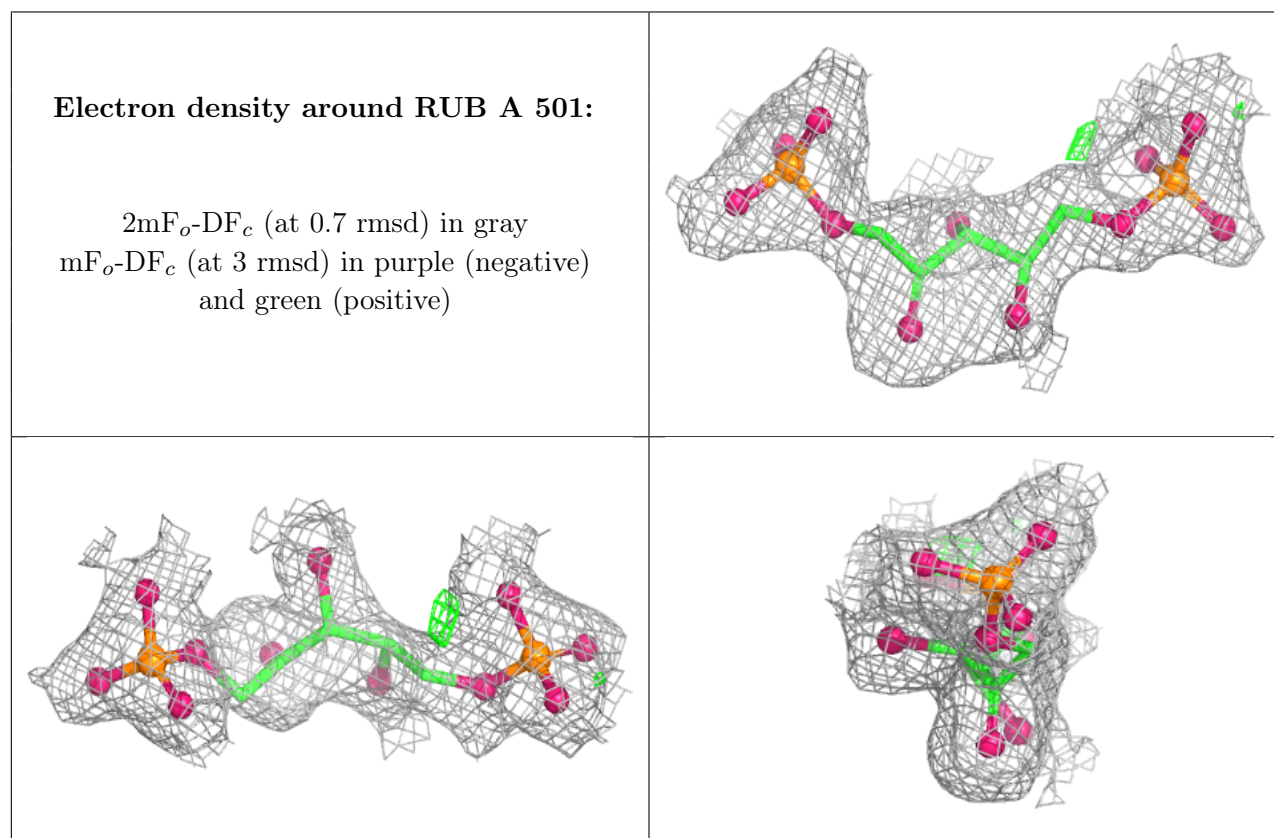
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

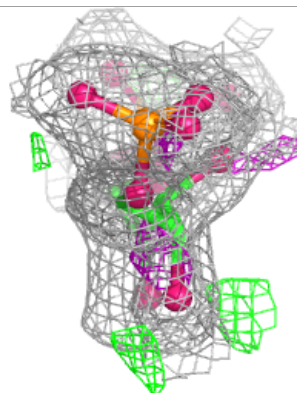
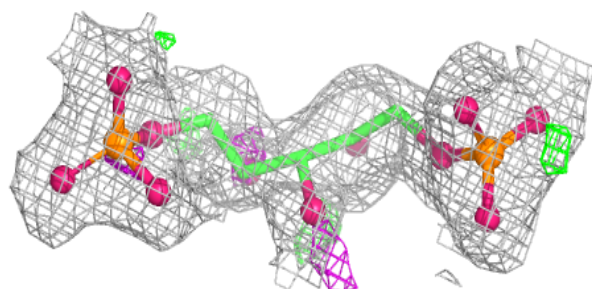
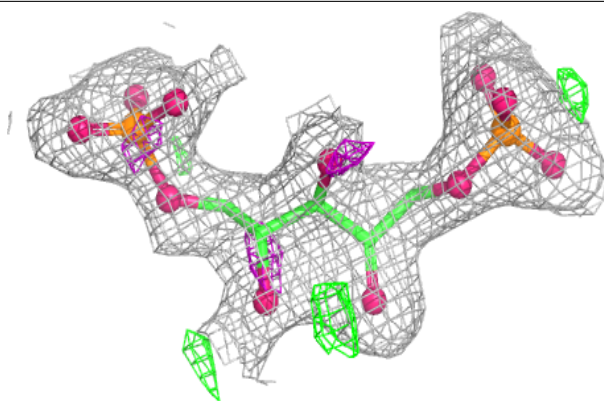
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RUB	A	501	18/18	0.99	0.03	6,10,12,12	0
3	RUB	B	501	18/18	0.99	0.04	2,2,2,2	0
3	RUB	C	501	18/18	1.00	0.02	8,11,16,17	0
3	RUB	D	501	18/18	1.00	0.02	8,14,18,19	0

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.

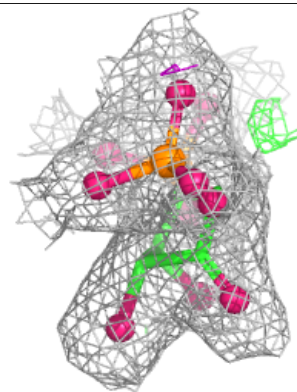
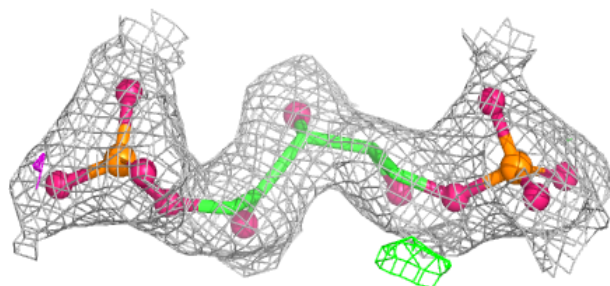
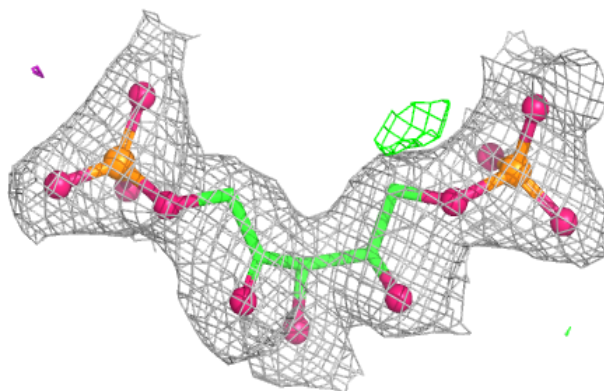


Electron density around RUB B 501:

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

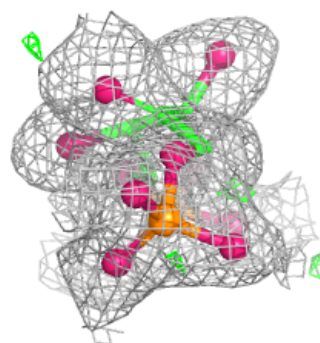
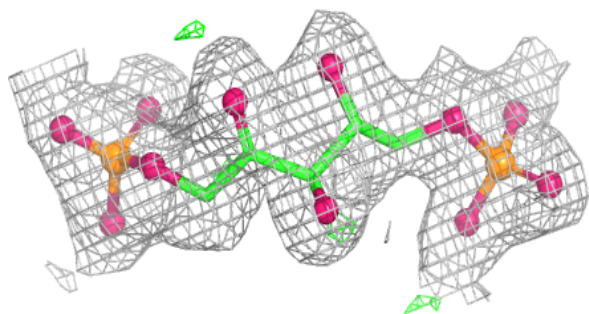
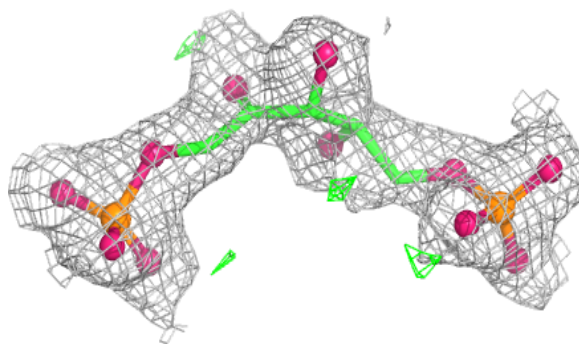
**Electron density around RUB C 501:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.