



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 1T36 / pdb_00001t36
Title : Crystal structure of E. coli carbamoyl phosphate synthetase small subunit mutant C248D complexed with uridine 5'-monophosphate
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2004-04-24
Resolution : 2.10 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

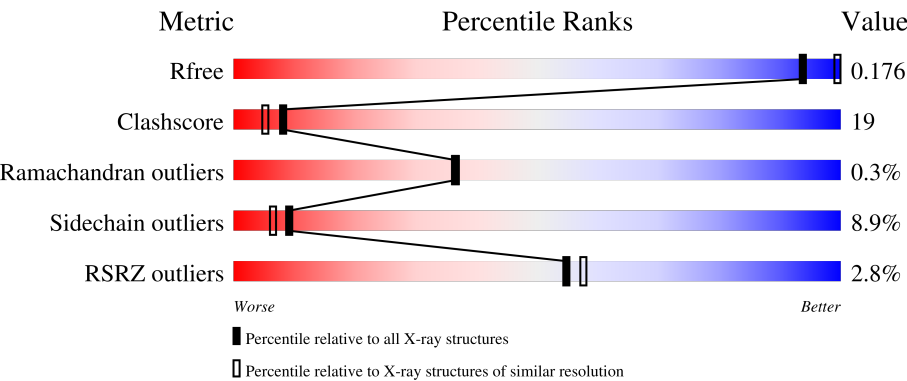
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	1073	2% 66% 28% ..
1	C	1073	2% 63% 29% 6% .
1	E	1073	% 67% 26% 5% .
1	G	1073	2% 54% 37% 7% .
2	B	382	2% 54% 36% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	382	
2	F	382	
2	H	382	

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
5	PO4	E	1078	-	X	-	-
5	PO4	G	1078	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48757 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 Carbamoyl-phosphate synthase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	9	0
			8212	5155	1436	1575	46			
1	C	1058	Total	C	N	O	S	0	8	0
			8197	5146	1426	1579	46			
1	E	1058	Total	C	N	O	S	0	5	0
			8182	5137	1425	1575	45			
1	G	1058	Total	C	N	O	S	0	8	0
			8206	5152	1432	1577	45			

- Molecule 2 is a protein called Carbamoyl-phosphate synthase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	D	379	Total	C	N	O	S	0	1	0
			2904	1830	511	554	9			
2	F	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			
2	H	379	Total	C	N	O	S	0	0	0
			2897	1826	508	554	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	ASP	CYS	engineered mutation	UNP P00907
D	248	ASP	CYS	engineered mutation	UNP P00907
F	248	ASP	CYS	engineered mutation	UNP P00907
H	248	ASP	CYS	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0
3	G	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

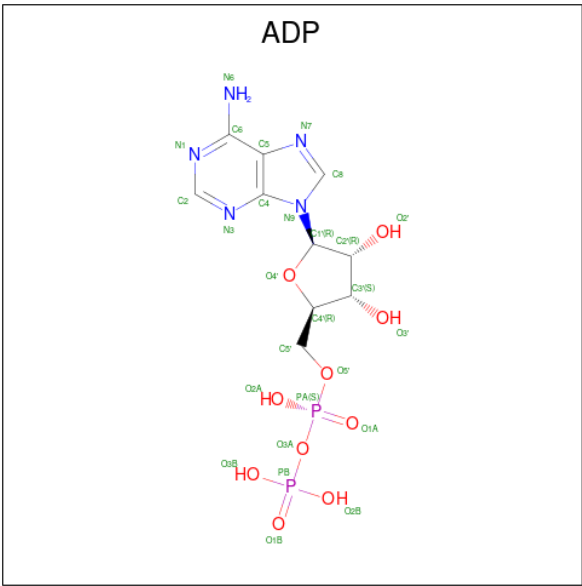


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

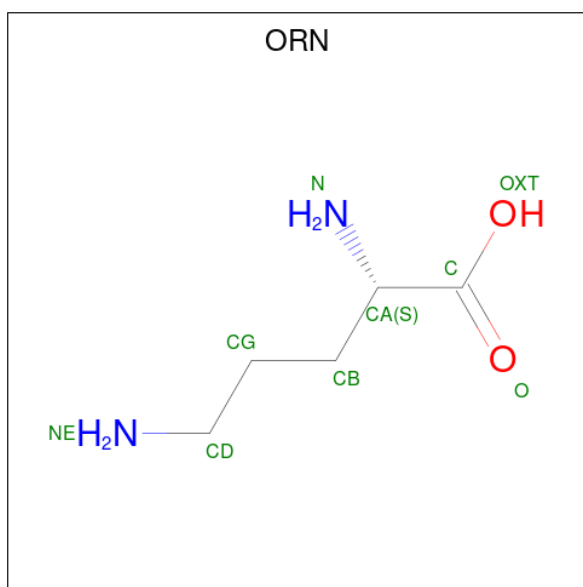
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	Cl	0	0
			5	5		
6	C	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	6	Total	Cl	0	0
			6	6		
6	F	1	Total	Cl	0	0
			1	1		
6	G	6	Total	Cl	0	0
			6	6		
6	H	2	Total	Cl	0	0
			2	2		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



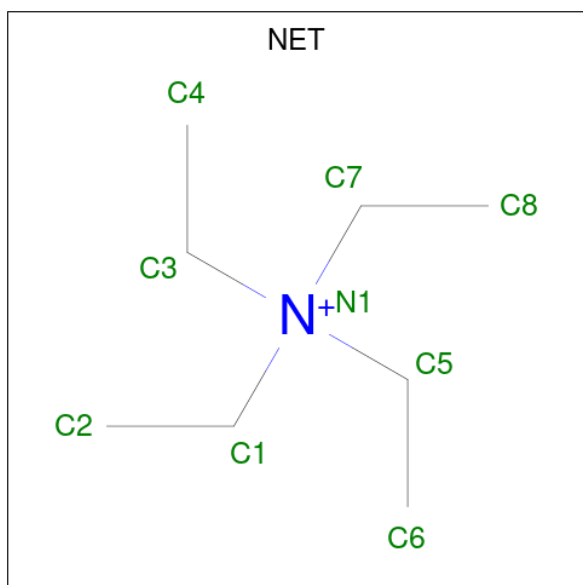
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



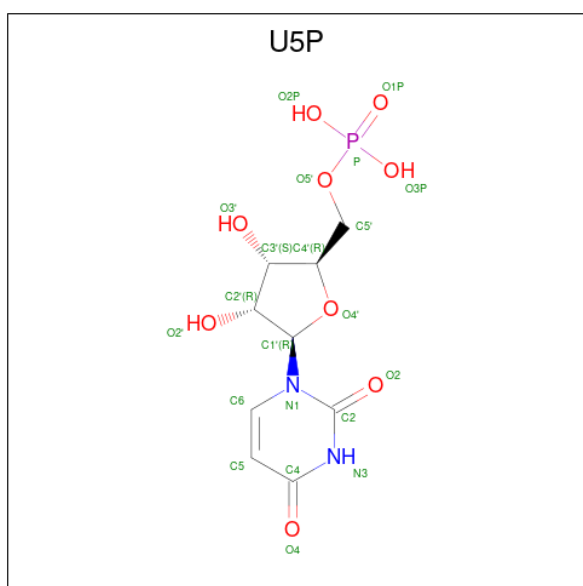
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

- Molecule 10 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O P 21 9 2 9 1	0	0
10	C	1	Total C N O P 21 9 2 9 1	0	0
10	E	1	Total C N O P 21 9 2 9 1	0	0
10	G	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	851	Total O 851 851	0	0
11	B	161	Total O 161 161	0	0

Continued on next page...

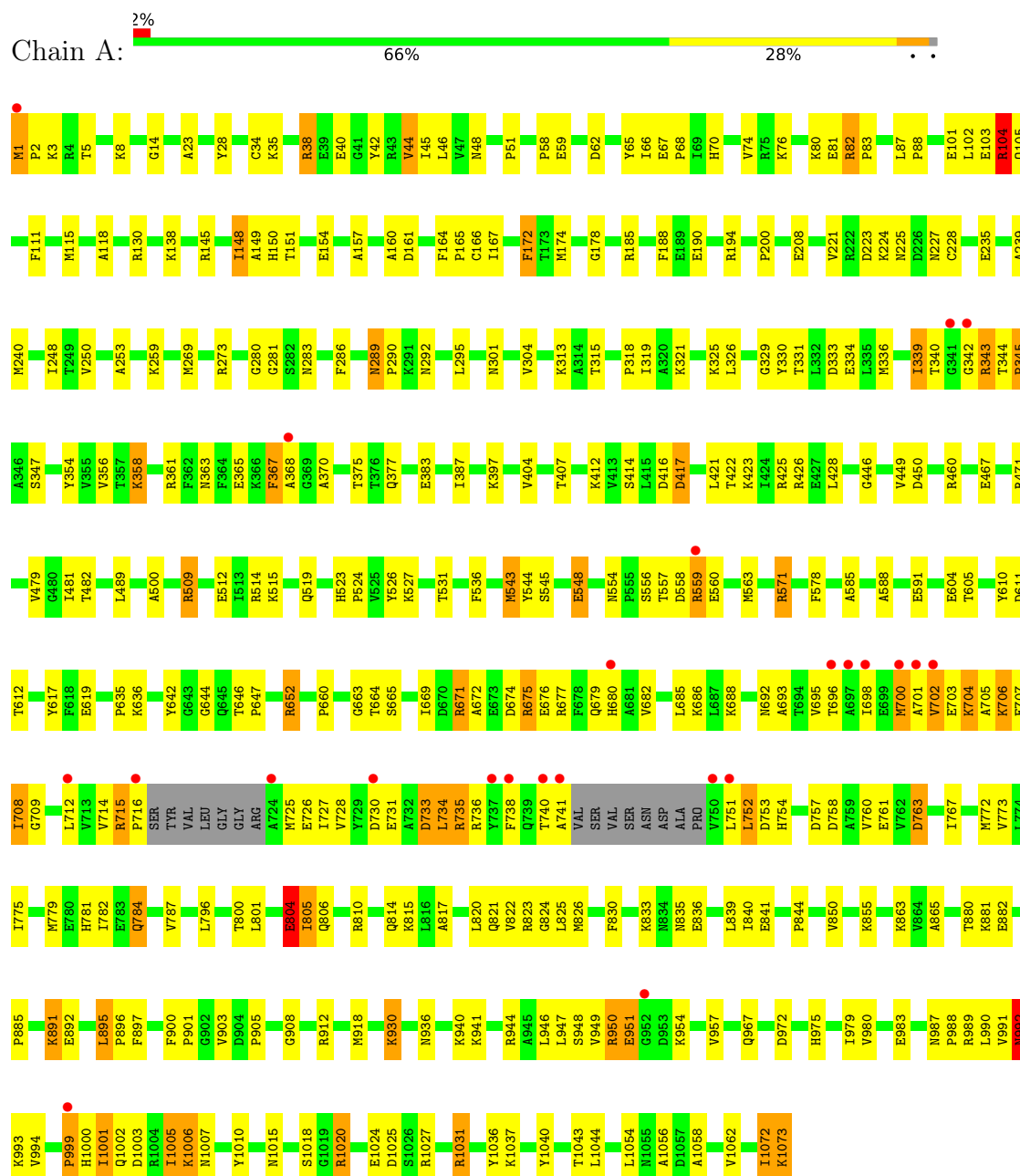
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	819	Total 819	O 819	0	0
11	D	221	Total 221	O 221	0	0
11	E	832	Total 832	O 832	0	0
11	F	200	Total 200	O 200	0	0
11	G	705	Total 705	O 705	0	0
11	H	118	Total 118	O 118	0	0

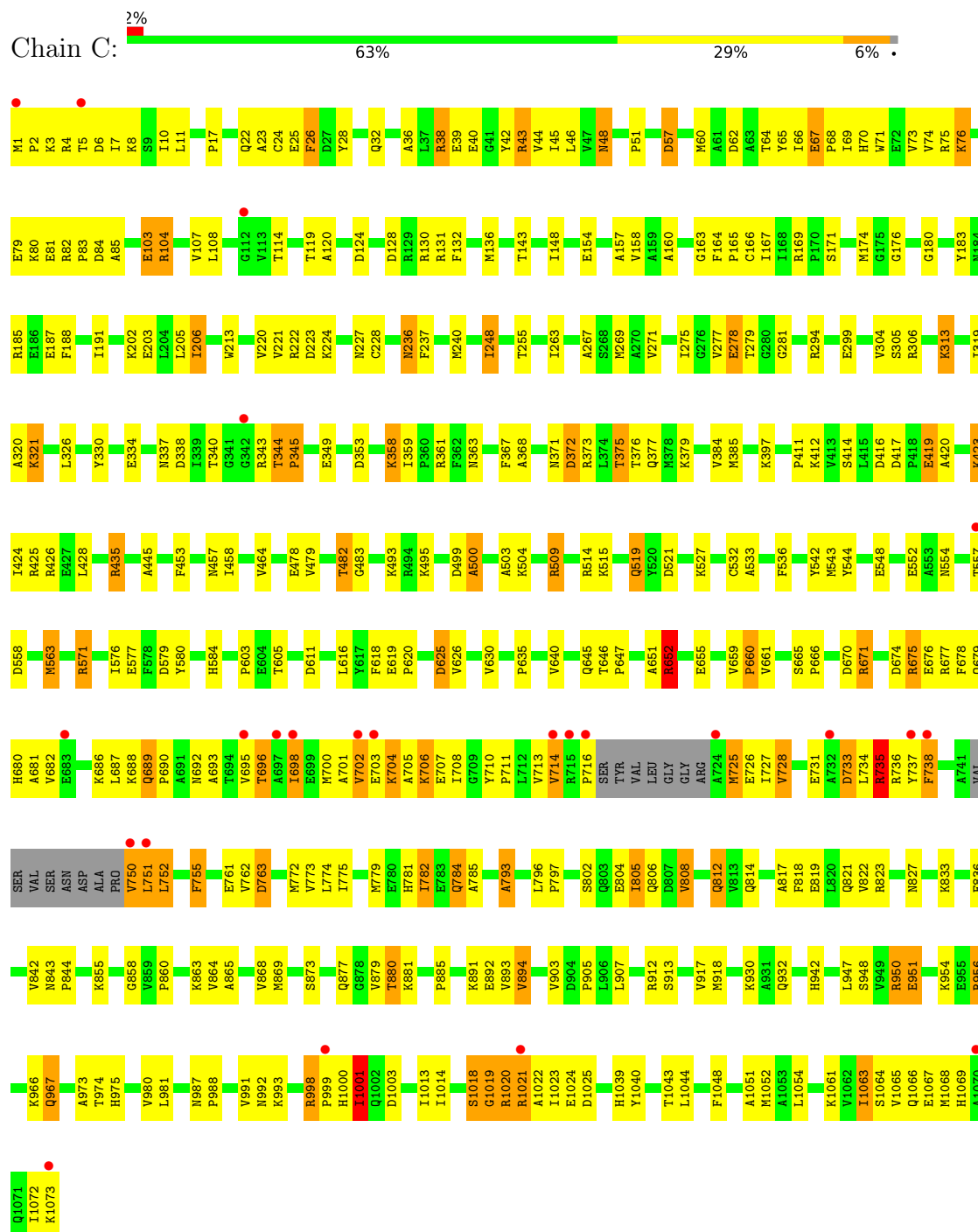
3 Residue-property plots

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.

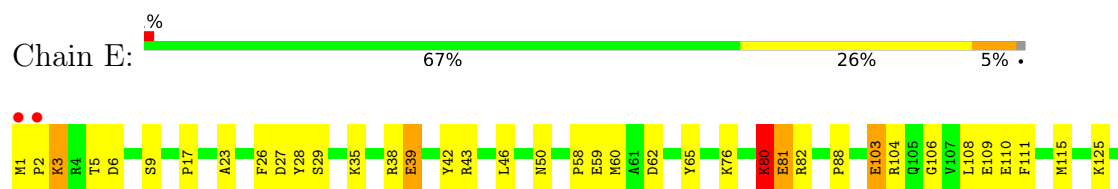
- Molecule 1: Carbamoyl-phosphate synthase large chain

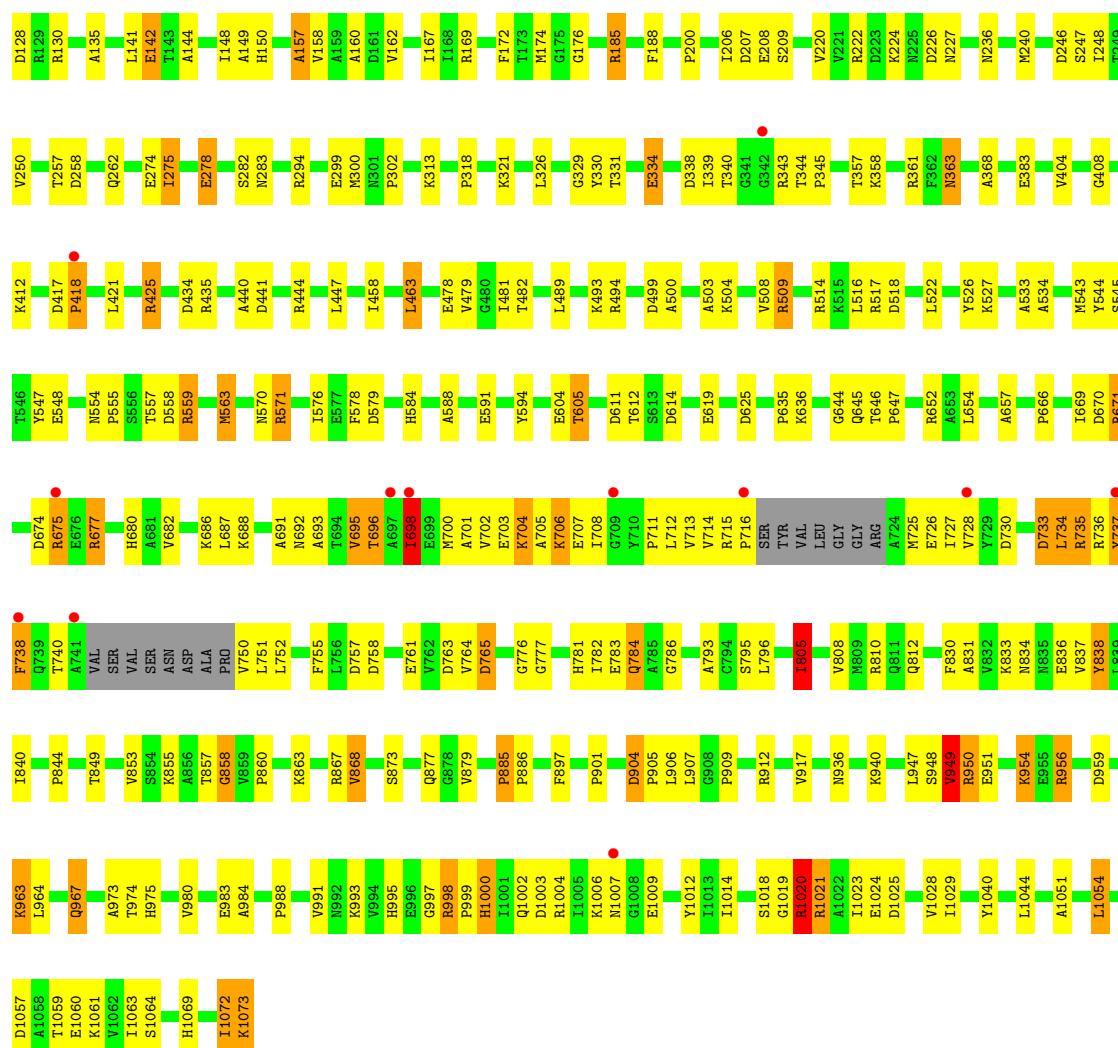


- Molecule 1: Carbamoyl-phosphate synthase large chain

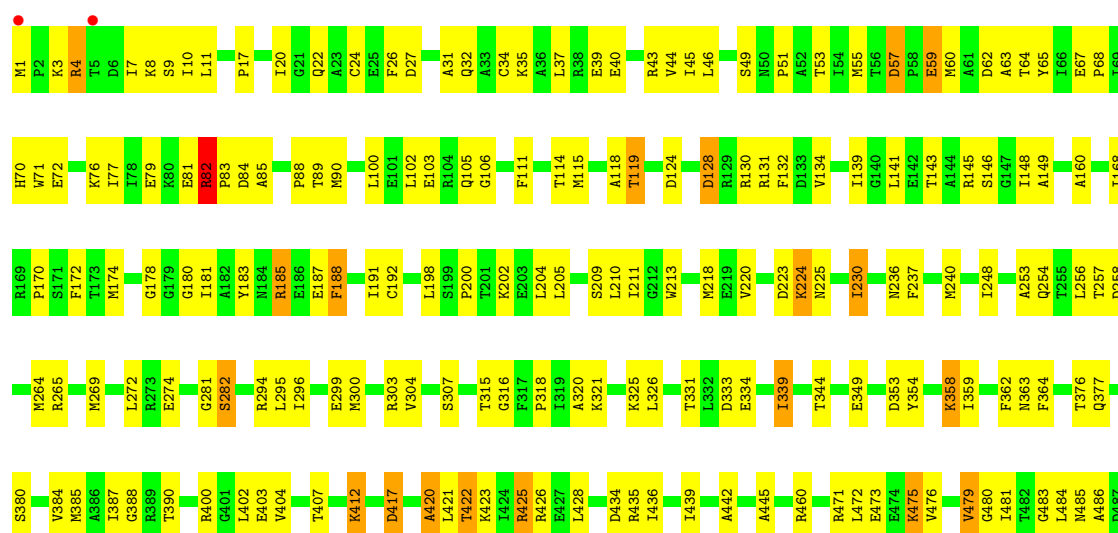


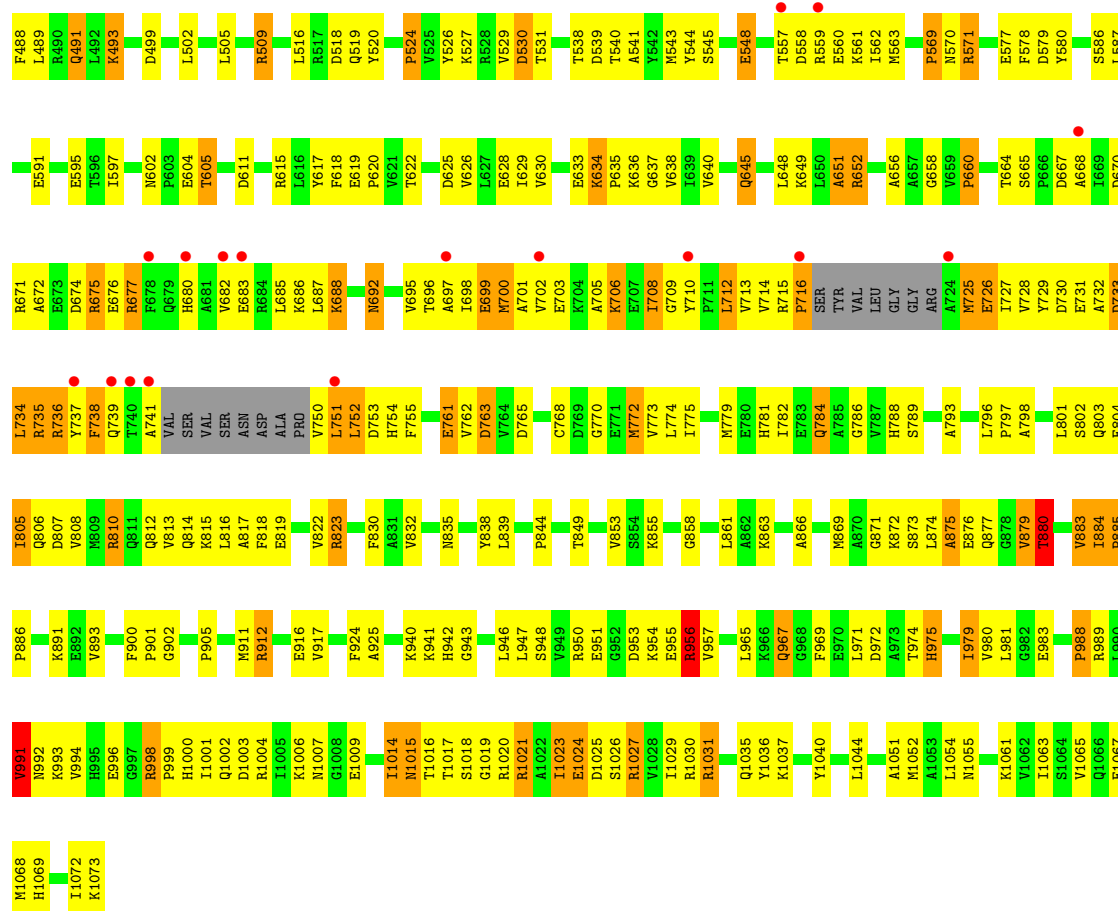
- Molecule 1: Carbamoyl-phosphate synthase large chain



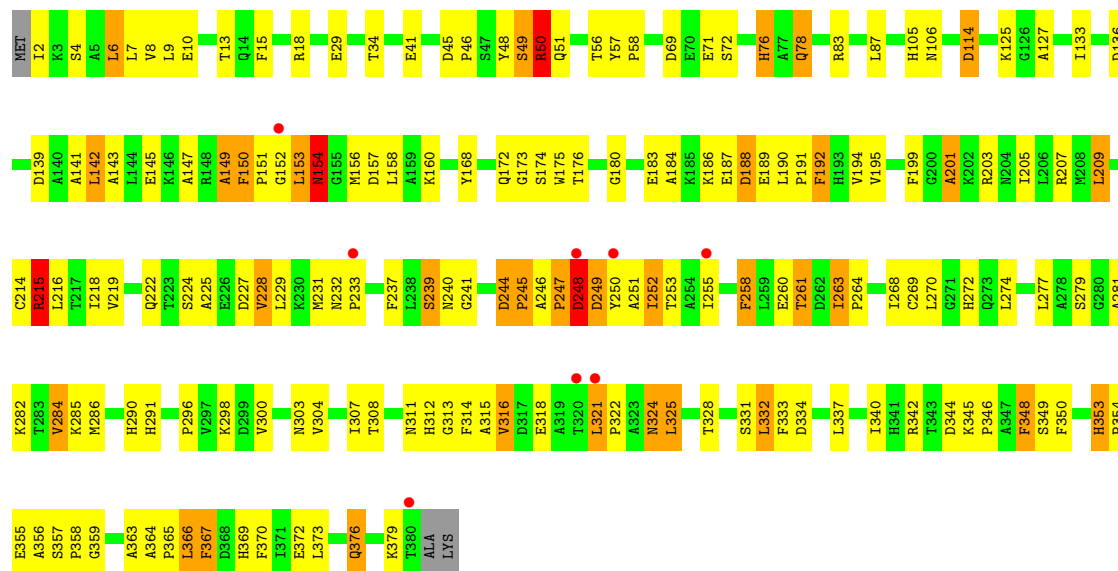


• Molecule 1: Carbamoyl-phosphate synthase large chain

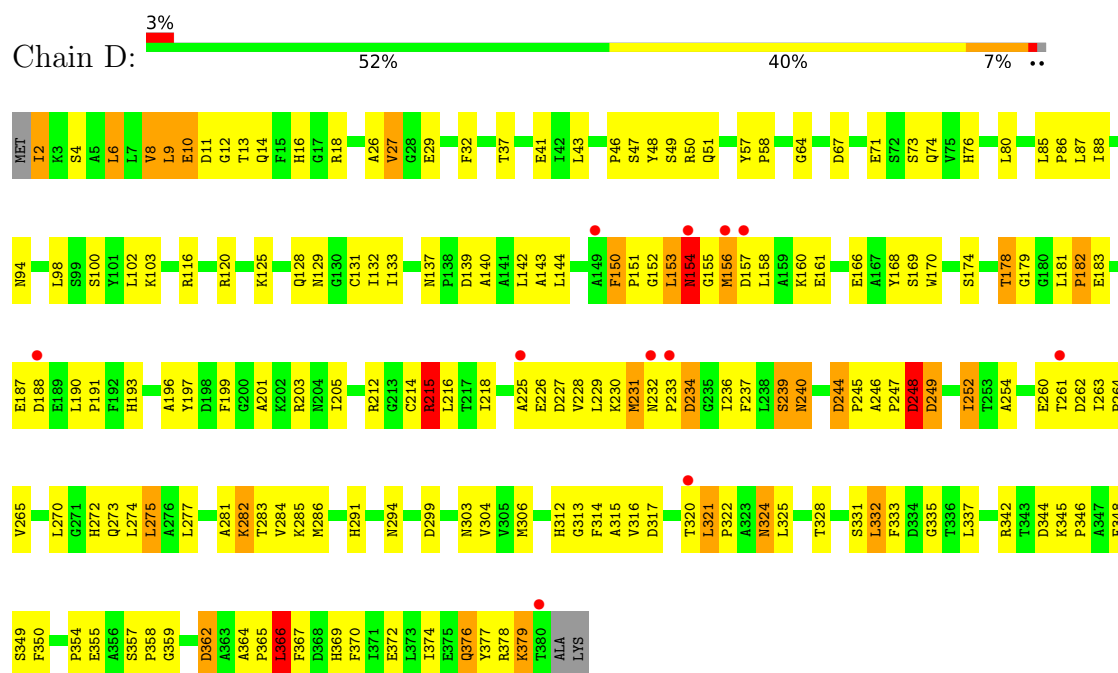




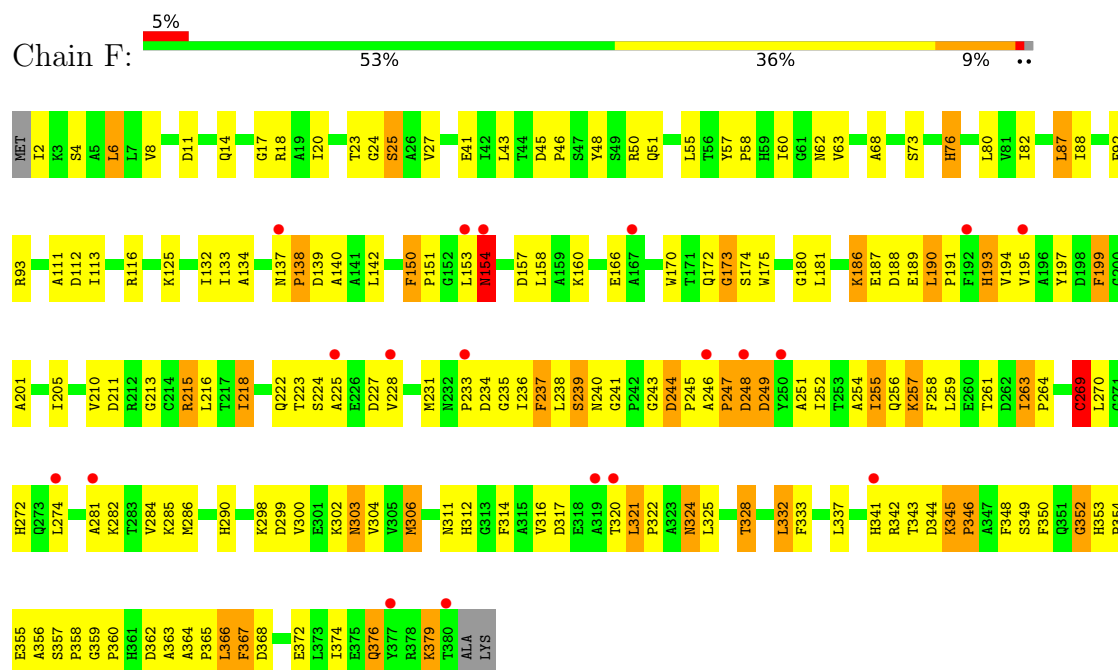
- Molecule 2: Carbamoyl-phosphate synthase small chain



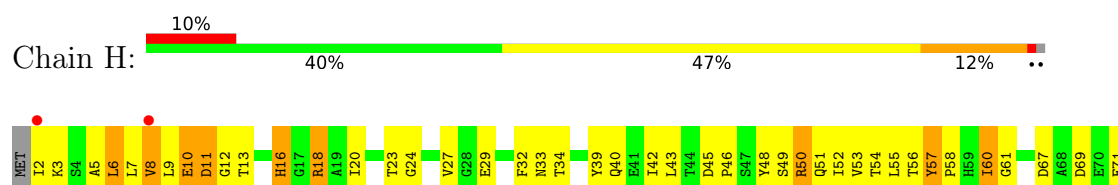
- Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain



• Molecule 2: Carbamoyl-phosphate synthase small chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.50Å 164.90Å 333.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.10) 88.6 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.176 , 0.209 0.175 , 0.176	Depositor DCC
R_{free} test set	42730 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48757	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: MN, NET, CL, PO4, K, ORN, ADP, U5P

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	1.16	1/8374 (0.0%)	1.66	78/11315 (0.7%)
1	C	1.16	5/8355 (0.1%)	1.68	91/11293 (0.8%)
1	E	1.17	4/8328 (0.0%)	1.70	101/11257 (0.9%)
1	G	1.16	1/8368 (0.0%)	1.70	110/11308 (1.0%)
2	B	1.10	0/2959	1.79	50/4019 (1.2%)
2	D	1.14	0/2970	1.78	56/4033 (1.4%)
2	F	1.11	1/2959 (0.0%)	1.76	50/4019 (1.2%)
2	H	1.06	1/2959 (0.0%)	1.73	42/4019 (1.0%)
All	All	1.15	13/45272 (0.0%)	1.71	578/61263 (0.9%)

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
2	B	1	0
2	D	1	0
2	F	1	0
All	All	3	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	ASP	N-CA	-7.31	1.37	1.46
1	C	169	ARG	CA-C	-7.16	1.47	1.52
1	E	808	VAL	CA-CB	-6.91	1.46	1.54
1	E	879	VAL	CA-C	-5.91	1.47	1.52
1	C	371	ASN	C-N	-5.73	1.26	1.33
1	C	319	ILE	CA-CB	-5.63	1.48	1.54
1	C	879	VAL	CA-C	-5.52	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	634	LYS	C-O	-5.43	1.21	1.23
1	E	808	VAL	CA-C	-5.08	1.46	1.52
1	E	614	ASP	CG-OD2	5.04	1.34	1.25
2	H	370	PHE	N-CA	-5.04	1.40	1.46
2	F	372	GLU	CD-OE2	5.02	1.34	1.25
1	A	1010	TYR	CA-C	-5.02	1.46	1.52

All (578) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	557	THR	CA-C-N	11.60	136.41	120.63
1	C	557	THR	C-N-CA	11.60	136.41	120.63
2	B	247	PRO	CA-C-N	11.04	134.79	120.44
2	B	247	PRO	C-N-CA	11.04	134.79	120.44
1	C	885	PRO	O-C-N	10.98	126.36	121.31
2	H	247	PRO	CA-C-N	10.45	134.65	120.44
2	H	247	PRO	C-N-CA	10.45	134.65	120.44
2	D	247	PRO	CA-C-N	10.43	135.28	120.79
2	D	247	PRO	C-N-CA	10.43	135.28	120.79
2	B	105	HIS	CA-CB-CG	-10.31	103.49	113.80
2	B	249	ASP	N-CA-C	9.97	123.49	110.43
2	D	249	ASP	N-CA-C	9.95	123.17	110.24
2	F	154	ASN	CA-CB-CG	-9.90	102.70	112.60
1	G	557	THR	CA-C-N	9.78	134.38	120.79
1	G	557	THR	C-N-CA	9.78	134.38	120.79
1	E	558	ASP	N-CA-CB	-9.56	96.12	109.98
1	E	23	ALA	N-CA-C	9.55	122.76	109.29
1	A	714	VAL	N-CA-C	9.20	116.05	106.21
1	A	554	ASN	CB-CA-C	-9.00	104.81	111.20
1	A	605	THR	N-CA-C	8.93	123.74	110.52
2	D	248	ASP	N-CA-CB	-8.89	96.31	109.82
1	G	793	ALA	N-CA-C	-8.85	98.61	110.55
1	E	1000	HIS	CA-CB-CG	-8.79	105.01	113.80
1	A	652	ARG	CD-NE-CZ	8.78	136.69	124.40
2	H	154	ASN	CB-CA-C	8.78	120.60	109.80
1	E	1054	LEU	N-CA-CB	-8.75	95.08	110.39
1	G	883	VAL	N-CA-CB	8.69	120.20	110.72
1	A	23	ALA	N-CA-C	8.66	121.50	109.29
1	E	557	THR	CA-C-N	8.52	132.22	120.63
1	E	557	THR	C-N-CA	8.52	132.22	120.63
1	G	605	THR	N-CA-C	8.42	122.98	110.52
1	G	738	PHE	CA-CB-CG	-8.36	105.44	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	248	ASP	CA-CB-CG	8.27	120.87	112.60
1	C	353	ASP	CA-CB-CG	8.26	120.86	112.60
1	C	885	PRO	N-CA-CB	8.13	107.74	103.19
2	B	76	HIS	CA-CB-CG	-8.03	105.77	113.80
2	B	106	ASN	CA-CB-CG	-8.00	104.61	112.60
1	G	27	ASP	N-CA-C	-7.97	101.68	111.40
1	A	524	PRO	CB-CA-C	-7.97	99.61	110.60
2	F	249	ASP	N-CA-C	7.94	121.01	110.53
2	H	249	ASP	N-CA-C	7.83	120.68	110.43
1	C	993	LYS	N-CA-C	-7.82	100.21	110.53
1	E	363	ASN	CA-CB-CG	7.79	120.39	112.60
1	C	558	ASP	N-CA-C	7.76	119.64	111.03
1	E	478	GLU	CB-CG-CD	-7.75	99.42	112.60
1	G	339	ILE	N-CA-C	7.73	123.03	111.89
1	C	782	ILE	N-CA-C	-7.67	103.38	110.82
1	G	1015	ASN	CA-CB-CG	7.63	120.23	112.60
2	F	11	ASP	CA-CB-CG	7.58	120.18	112.60
1	E	619	GLU	O-C-N	7.57	126.55	121.71
1	E	993	LYS	N-CA-C	-7.53	100.59	110.53
1	C	344	THR	CA-C-N	7.51	127.47	120.03
1	C	344	THR	C-N-CA	7.51	127.47	120.03
2	B	150	PHE	CA-C-N	7.50	127.37	119.05
2	B	150	PHE	C-N-CA	7.50	127.37	119.05
1	G	57	ASP	CA-C-N	7.48	127.02	119.24
1	G	57	ASP	C-N-CA	7.48	127.02	119.24
2	B	249	ASP	CA-C-N	7.47	130.61	120.38
2	B	249	ASP	C-N-CA	7.47	130.61	120.38
1	G	475[A]	LYS	N-CA-C	-7.46	102.84	110.97
1	G	475[B]	LYS	N-CA-C	-7.46	102.84	110.97
1	G	475[C]	LYS	N-CA-C	-7.46	102.84	110.97
2	H	188	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	283	ASN	CA-CB-CG	7.36	119.96	112.60
1	A	319	ILE	N-CA-C	7.36	118.09	110.36
1	A	557	THR	CA-C-N	7.36	135.59	121.54
1	A	557	THR	C-N-CA	7.36	135.59	121.54
1	E	246	ASP	CA-CB-CG	7.34	119.94	112.60
1	C	543	MET	N-CA-C	7.32	121.00	109.81
2	F	150	PHE	CA-C-N	7.26	127.27	119.28
2	F	150	PHE	C-N-CA	7.26	127.27	119.28
1	E	782	ILE	N-CA-C	-7.24	104.16	110.74
1	E	88	PRO	CB-CA-C	-7.23	101.97	109.92
1	E	514	ARG	NE-CZ-NH2	-7.18	112.74	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	353	HIS	CA-CB-CG	-7.18	106.62	113.80
2	H	346	PRO	N-CA-CB	7.17	107.66	102.28
1	C	345	PRO	CB-CA-C	-7.15	101.58	110.95
2	B	367	PHE	CA-CB-CG	-7.15	106.65	113.80
2	H	321	LEU	N-CA-C	7.13	119.84	109.71
1	C	558	ASP	N-CA-CB	-7.13	99.65	109.98
2	B	174	SER	N-CA-C	7.11	120.54	110.23
2	H	249	ASP	CA-C-N	7.09	131.46	120.82
2	H	249	ASP	C-N-CA	7.09	131.46	120.82
1	A	367	PHE	CA-CB-CG	-7.01	106.79	113.80
1	G	578	PHE	CA-CB-CG	-7.00	106.80	113.80
1	C	367	PHE	CA-CB-CG	-6.99	106.81	113.80
2	F	328	THR	N-CA-CB	6.99	119.89	110.59
1	G	62	ASP	CA-CB-CG	-6.98	105.62	112.60
1	E	885	PRO	CA-C-O	6.96	125.91	120.90
1	A	417	ASP	CA-C-O	6.95	124.47	119.32
2	H	16	HIS	CA-CB-CG	-6.95	106.85	113.80
1	C	605	THR	N-CA-C	6.95	121.19	110.42
1	C	714	VAL	N-CA-C	6.95	117.50	106.32
1	G	716	PRO	N-CA-CB	6.94	110.64	103.00
2	B	45	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	453	PHE	CA-CB-CG	-6.94	106.86	113.80
2	B	353	HIS	CA-CB-CG	-6.93	106.87	113.80
2	H	157	ASP	CA-CB-CG	6.92	119.53	112.60
1	E	463	LEU	N-CA-C	6.88	118.43	111.07
2	D	190	LEU	CA-C-N	6.87	126.47	119.19
2	D	190	LEU	C-N-CA	6.87	126.47	119.19
1	E	150	HIS	CA-CB-CG	-6.87	106.93	113.80
1	C	319	ILE	N-CA-C	6.86	117.56	110.36
1	E	81	GLU	CA-C-N	-6.86	115.42	122.83
1	E	81	GLU	C-N-CA	-6.86	115.42	122.83
1	G	660	PRO	N-CA-CB	6.85	107.21	102.35
1	C	371	ASN	O-C-N	-6.83	114.36	122.96
2	B	244	ASP	CA-CB-CG	6.80	119.40	112.60
2	B	201	ALA	N-CA-C	6.78	120.12	109.96
1	A	345	PRO	CB-CA-C	-6.77	100.31	110.20
1	C	154	GLU	CB-CG-CD	6.77	124.11	112.60
2	B	147	ALA	CA-C-N	6.76	129.34	120.28
2	B	147	ALA	C-N-CA	6.76	129.34	120.28
2	F	346	PRO	N-CA-CB	6.75	106.98	102.25
2	F	193	HIS	CA-C-N	-6.73	113.77	123.06
2	F	193	HIS	C-N-CA	-6.73	113.77	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	SER	N-CA-C	6.72	116.92	108.45
1	C	515	LYS	CA-C-O	6.72	127.87	120.82
1	A	536	PHE	CA-CB-CG	-6.71	107.08	113.80
2	D	321	LEU	N-CA-C	6.71	118.57	109.24
2	D	154	ASN	N-CA-C	6.70	125.07	110.80
2	B	316	VAL	N-CA-CB	-6.69	103.63	111.39
1	E	207	ASP	CA-CB-CG	6.68	119.28	112.60
1	G	417	ASP	CA-CB-CG	6.66	119.26	112.60
1	C	67	GLU	O-C-N	6.66	125.97	121.71
2	D	154	ASN	CA-CB-CG	-6.63	105.97	112.60
2	F	374	ILE	CB-CA-C	-6.63	103.22	111.70
1	E	557	THR	CA-C-O	6.62	126.34	119.05
2	H	132	ILE	CB-CA-C	-6.62	101.64	110.98
2	D	366	LEU	N-CA-C	-6.62	104.10	111.71
1	E	786	GLY	N-CA-C	-6.61	106.61	114.48
2	D	150	PHE	CA-C-N	6.61	126.19	119.19
2	D	150	PHE	C-N-CA	6.61	126.19	119.19
2	F	249	ASP	CA-C-N	6.59	129.44	120.54
2	F	249	ASP	C-N-CA	6.59	129.44	120.54
2	D	181	LEU	CA-C-N	6.58	126.56	119.78
2	D	181	LEU	C-N-CA	6.58	126.56	119.78
1	C	716	PRO	N-CA-CB	6.57	110.23	103.00
1	E	625	ASP	CA-CB-CG	-6.56	106.04	112.60
1	C	514	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	C	536	PHE	CA-CB-CG	-6.53	107.27	113.80
1	G	699	GLU	CA-C-N	6.53	129.27	120.65
1	G	699	GLU	C-N-CA	6.53	129.27	120.65
1	E	959	ASP	CA-C-N	-6.53	111.02	120.29
1	E	959	ASP	C-N-CA	-6.53	111.02	120.29
2	H	152	GLY	CA-C-N	6.52	129.86	120.79
2	H	152	GLY	C-N-CA	6.52	129.86	120.79
1	C	188	PHE	CA-CB-CG	-6.52	107.28	113.80
1	E	38	ARG	CA-C-N	6.51	129.30	120.38
1	E	38	ARG	C-N-CA	6.51	129.30	120.38
1	C	660	PRO	N-CA-CB	6.50	106.97	102.35
1	G	885	PRO	N-CA-CB	6.50	109.38	103.08
2	H	370	PHE	CA-CB-CG	-6.49	107.31	113.80
1	C	435	ARG	N-CA-C	6.48	119.17	111.33
1	G	188	PHE	CA-CB-CG	-6.47	107.33	113.80
1	E	338	ASP	N-CA-C	6.46	118.90	111.02
1	E	1007	ASN	CA-CB-CG	-6.46	106.14	112.60
1	G	390	THR	CA-C-N	6.42	129.21	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	390	THR	C-N-CA	6.42	129.21	120.54
1	E	62	ASP	CA-CB-CG	-6.40	106.20	112.60
1	E	716	PRO	N-CA-CB	6.40	110.04	103.00
1	A	716	PRO	N-CA-CB	6.38	110.02	103.00
1	G	602	ASN	CB-CA-C	6.38	116.48	110.17
2	H	215	ARG	N-CA-CB	-6.37	100.04	110.42
1	A	188	PHE	CA-CB-CG	-6.36	107.44	113.80
1	C	23	ALA	N-CA-C	6.36	120.61	109.80
2	F	244	ASP	CA-CB-CG	6.33	118.93	112.60
1	G	44	VAL	N-CA-C	6.32	117.02	108.17
2	D	248	ASP	CA-CB-CG	6.31	118.91	112.60
2	F	173	GLY	CA-C-N	6.31	130.28	120.75
2	F	173	GLY	C-N-CA	6.31	130.28	120.75
2	H	78	GLN	N-CA-C	6.30	117.94	111.14
1	C	478	GLU	N-CA-C	6.30	118.22	111.36
1	G	953	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	368	ALA	N-CA-C	6.29	118.94	111.33
1	A	304	VAL	N-CA-C	-6.28	103.20	110.05
1	C	1003	ASP	CA-CB-CG	6.28	118.88	112.60
1	E	50	ASN	CA-C-O	6.28	123.37	119.29
1	E	793	ALA	N-CA-C	-6.28	102.08	110.55
1	G	83	PRO	CB-CA-C	-6.27	103.20	111.23
1	A	289	ASN	O-C-N	6.26	126.63	121.31
1	C	1000	HIS	CA-CB-CG	-6.25	107.55	113.80
1	E	612	THR	N-CA-C	6.25	119.07	111.82
2	B	240	ASN	N-CA-C	-6.22	102.50	110.53
1	C	1019	GLY	N-CA-C	-6.22	104.95	112.48
2	B	348	PHE	CA-CB-CG	-6.21	107.59	113.80
1	E	858	GLY	CA-C-N	-6.20	117.33	123.04
1	E	858	GLY	C-N-CA	-6.20	117.33	123.04
2	D	348	PHE	CA-CB-CG	-6.20	107.60	113.80
1	G	570	ASN	CA-CB-CG	6.19	118.79	112.60
1	G	875	ALA	N-CA-C	-6.19	103.47	111.02
1	E	80	LYS	N-CA-C	6.16	118.07	111.36
1	A	248	ILE	N-CA-C	-6.15	100.77	108.89
1	C	808	VAL	CB-CA-C	-6.15	103.83	112.14
1	G	558	ASP	N-CA-CB	-6.14	100.48	109.82
1	G	316	GLY	N-CA-C	-6.13	106.68	115.64
2	B	154	ASN	N-CA-CB	6.11	120.81	110.49
1	G	39	GLU	CB-CA-C	-6.10	99.35	110.63
1	E	275	ILE	CA-C-N	-6.09	114.23	122.63
1	E	275	ILE	C-N-CA	-6.09	114.23	122.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	559	ARG	N-CA-C	6.09	119.47	110.46
1	G	640	VAL	N-CA-CB	-6.08	104.25	112.16
1	E	339	ILE	N-CA-C	6.08	120.91	113.00
1	G	765	ASP	CA-C-N	-6.08	112.44	122.11
1	G	765	ASP	C-N-CA	-6.08	112.44	122.11
1	E	248	ILE	N-CA-C	-6.08	100.87	108.89
1	E	605	THR	N-CA-C	6.07	119.07	110.14
1	A	825	LEU	N-CA-C	6.06	119.05	110.50
1	E	765	ASP	CA-CB-CG	6.05	118.66	112.60
2	D	359	GLY	CA-C-N	6.03	125.99	119.78
2	D	359	GLY	C-N-CA	6.03	125.99	119.78
1	C	557	THR	O-C-N	6.02	128.80	122.23
1	A	804	GLU	N-CA-CB	6.02	119.08	110.16
1	G	557	THR	CA-C-O	6.01	125.76	119.14
2	B	147	ALA	O-C-N	6.01	128.26	122.07
2	D	6	LEU	N-CA-CB	-6.01	100.25	111.13
2	D	182	PRO	CB-CA-C	-6.00	103.55	111.23
2	H	244	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	738	PHE	CA-CB-CG	-6.00	107.80	113.80
1	E	885	PRO	N-CA-CB	6.00	106.55	103.19
2	D	369	HIS	CA-C-O	5.99	126.86	119.97
2	F	360	PRO	N-CA-CB	5.95	108.53	103.35
1	A	82	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	G	991	VAL	CA-CB-CG1	5.95	120.51	110.40
2	B	250	TYR	N-CA-C	5.95	118.53	111.33
1	G	529	VAL	CB-CA-C	5.95	118.28	110.91
2	D	132	ILE	CA-C-N	-5.94	114.73	122.99
2	D	132	ILE	C-N-CA	-5.94	114.73	122.99
2	D	248	ASP	CA-C-N	5.93	129.54	120.82
2	D	248	ASP	C-N-CA	5.93	129.54	120.82
1	A	885	PRO	N-CA-CB	5.93	108.83	103.08
1	C	263	ILE	CB-CA-C	-5.93	104.14	112.14
1	E	707	GLU	CA-C-N	5.93	128.03	120.56
1	E	707	GLU	C-N-CA	5.93	128.03	120.56
2	F	138	PRO	N-CA-CB	5.93	108.58	103.36
1	A	944	ARG	NE-CZ-NH1	5.92	127.42	121.50
2	B	4	SER	N-CA-C	5.92	118.35	110.53
1	C	39	GLU	CB-CA-C	-5.92	100.96	110.79
1	G	1007	ASN	CA-CB-CG	-5.92	106.68	112.60
2	H	89	ALA	N-CA-C	-5.92	100.64	110.17
1	E	868	VAL	CB-CA-C	-5.92	104.31	111.88
1	G	1023	ILE	CB-CA-C	-5.91	104.41	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	MET	N-CA-C	5.91	118.67	109.52
2	B	114	ASP	CA-CB-CG	5.91	118.50	112.60
2	H	57	TYR	CA-C-O	5.90	124.73	119.59
2	H	53	VAL	N-CA-C	5.90	117.08	108.58
1	G	998	ARG	CB-CA-C	5.86	118.53	109.15
1	G	209	SER	N-CA-C	5.86	118.75	109.96
1	C	26	PHE	CA-CB-CG	-5.86	107.94	113.80
1	G	132	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	999	PRO	N-CA-CB	5.85	109.04	102.60
1	C	1039	HIS	CA-CB-CG	-5.85	107.95	113.80
1	C	74	VAL	N-CA-C	-5.85	104.65	110.62
2	D	244	ASP	CB-CA-C	5.85	117.88	109.92
1	E	499	ASP	CA-CB-CG	5.85	118.45	112.60
2	B	136	ASP	N-CA-C	5.84	117.32	111.07
1	C	554	ASN	CB-CA-C	-5.84	107.06	111.20
1	C	998	ARG	N-CA-C	5.83	119.36	110.50
2	F	249	ASP	N-CA-CB	5.83	118.69	110.36
1	A	682	VAL	N-CA-C	-5.80	104.27	110.36
2	D	299	ASP	N-CA-C	-5.80	99.67	108.67
2	D	260	GLU	N-CA-C	-5.80	105.30	112.90
2	H	255	ILE	N-CA-CB	-5.79	104.08	110.51
1	G	420	ALA	N-CA-C	5.79	118.37	111.71
1	E	1012	TYR	N-CA-C	5.78	118.63	108.75
1	A	111	PHE	CA-CB-CG	-5.76	108.03	113.80
2	F	343	THR	N-CA-C	-5.76	104.91	111.14
1	C	660	PRO	CB-CA-C	-5.76	105.26	113.09
1	C	987	ASN	CA-CB-CG	5.76	118.36	112.60
2	H	198	ASP	CA-CB-CG	5.76	118.36	112.60
1	E	1072	ILE	N-CA-C	5.74	117.04	108.54
2	F	62	ASN	CA-CB-CG	5.74	118.34	112.60
2	H	246	ALA	CA-C-N	5.74	127.02	119.84
2	H	246	ALA	C-N-CA	5.74	127.02	119.84
1	C	338	ASP	CA-CB-CG	5.74	118.34	112.60
2	D	249	ASP	CA-C-N	5.74	129.43	120.82
2	D	249	ASP	C-N-CA	5.74	129.43	120.82
1	G	31	ALA	CA-C-N	5.74	127.90	120.44
1	G	31	ALA	C-N-CA	5.74	127.90	120.44
1	G	883	VAL	CB-CA-C	-5.74	103.79	110.91
2	H	307	ILE	N-CA-C	-5.74	100.32	108.58
2	B	50	ARG	CB-CA-C	-5.74	100.22	111.06
1	G	1072	ILE	CB-CA-C	5.73	117.79	111.08
2	D	169	SER	N-CA-C	5.73	118.57	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1001	ILE	N-CA-C	5.72	116.37	110.36
1	A	44	VAL	N-CA-C	5.72	116.54	108.36
1	C	894	VAL	N-CA-CB	5.70	119.84	111.52
1	C	844	PRO	N-CA-CB	5.70	106.24	102.25
1	C	104	ARG	CB-CA-C	-5.70	101.33	110.79
2	D	317	ASP	N-CA-CB	5.70	118.51	109.51
1	C	48	ASN	N-CA-CB	5.70	119.42	110.71
2	H	216	LEU	CA-C-O	5.70	126.75	120.71
1	E	578	PHE	CA-CB-CG	-5.69	108.11	113.80
1	C	817	ALA	CA-C-O	5.69	127.33	121.07
1	G	425	ARG	CA-C-N	5.69	127.84	120.44
1	G	425	ARG	C-N-CA	5.69	127.84	120.44
1	G	991	VAL	CA-CB-CG2	5.69	120.07	110.40
1	A	993	LYS	N-CA-C	-5.69	102.06	110.48
2	D	321	LEU	CA-C-O	5.68	123.53	119.32
1	G	942	HIS	CA-CB-CG	-5.68	108.12	113.80
2	D	178	THR	CB-CA-C	-5.67	102.16	110.95
2	F	248	ASP	CA-CB-CG	-5.67	106.93	112.60
1	E	657	ALA	CA-C-N	-5.67	111.80	122.05
1	E	657	ALA	C-N-CA	-5.67	111.80	122.05
1	A	417	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	557	THR	O-C-N	5.66	129.33	122.48
1	E	554	ASN	CB-CA-C	-5.66	107.18	111.20
2	B	215	ARG	N-CA-C	-5.65	99.20	108.41
2	D	67	ASP	N-CA-C	5.65	117.44	111.28
1	E	209	SER	N-CA-C	5.65	117.89	109.59
1	G	3	LYS	N-CA-C	5.64	118.20	110.24
1	G	88	PRO	CB-CA-C	-5.64	103.71	109.92
2	F	180	GLY	N-CA-C	-5.64	102.60	112.53
1	E	39[A]	GLU	N-CA-C	-5.63	104.51	111.33
1	E	39[B]	GLU	N-CA-C	-5.63	104.51	111.33
1	A	760	VAL	CB-CA-C	-5.63	103.93	110.91
2	B	304	VAL	CA-C-N	-5.63	115.84	123.10
2	B	304	VAL	C-N-CA	-5.63	115.84	123.10
1	C	942	HIS	CA-CB-CG	-5.63	108.17	113.80
1	C	521	ASP	N-CA-C	-5.63	103.64	111.52
2	B	154	ASN	CB-CA-C	5.62	121.61	110.42
1	E	713	VAL	CB-CA-C	-5.62	103.38	111.19
1	C	558	ASP	CB-CA-C	-5.62	102.25	110.95
2	B	173	GLY	CA-C-N	5.61	128.67	120.71
2	B	173	GLY	C-N-CA	5.61	128.67	120.71
2	D	18	ARG	CA-C-O	5.60	126.75	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	THR	CA-C-O	-5.60	114.92	120.80
1	C	625	ASP	CA-CB-CG	-5.60	107.00	112.60
1	G	558	ASP	N-CA-C	5.59	117.84	111.02
1	C	304	VAL	N-CA-C	-5.59	103.96	110.05
2	F	199	PHE	N-CA-C	-5.58	104.70	113.02
1	G	524	PRO	CB-CA-C	-5.58	102.79	111.22
1	A	87	LEU	CA-C-O	5.58	124.05	119.36
1	G	128	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	782	ILE	N-CA-C	-5.58	105.29	110.53
1	G	295	LEU	N-CA-C	5.57	118.32	109.24
1	A	172	PHE	CA-CB-CG	-5.57	108.23	113.80
1	C	255	THR	N-CA-C	5.57	119.07	112.72
1	G	732	ALA	CA-C-N	5.57	128.01	120.38
1	G	732	ALA	C-N-CA	5.57	128.01	120.38
1	A	830	PHE	CB-CA-C	-5.57	99.78	110.24
1	C	79	GLU	CB-CA-C	-5.56	101.91	110.81
2	B	209	LEU	N-CA-C	-5.56	104.85	111.69
1	A	407	THR	N-CA-C	-5.56	105.10	112.94
2	D	239	SER	N-CA-C	5.55	117.49	110.33
1	A	102	LEU	N-CA-C	-5.54	105.14	111.07
2	D	191	PRO	CA-C-N	-5.54	114.11	122.81
2	D	191	PRO	C-N-CA	-5.54	114.11	122.81
1	G	682	VAL	O-C-N	5.54	127.53	121.83
1	G	682	VAL	N-CA-C	-5.54	105.13	110.72
1	A	339	ILE	N-CA-C	5.54	119.79	112.04
1	G	823	ARG	CA-C-N	5.53	128.33	122.63
1	G	823	ARG	C-N-CA	5.53	128.33	122.63
1	G	835	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	824	GLY	N-CA-C	-5.53	105.46	111.21
2	D	137	ASN	CB-CA-C	-5.53	102.03	111.15
1	A	660	PRO	N-CA-CB	5.52	106.67	102.36
2	D	214	CYS	N-CA-C	5.52	118.62	109.46
1	A	104	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	G	491	GLN	N-CA-C	-5.51	105.17	111.07
2	H	356	ALA	CB-CA-C	-5.51	110.20	116.54
2	H	248	ASP	CA-CB-CG	5.51	118.11	112.60
2	B	366	LEU	N-CA-C	-5.51	105.28	111.28
2	F	150	PHE	CA-CB-CG	-5.51	108.29	113.80
1	G	181	ILE	CB-CA-C	-5.50	102.95	110.77
1	A	178	GLY	CA-C-N	-5.50	116.97	122.69
1	A	178	GLY	C-N-CA	-5.50	116.97	122.69
2	D	240	ASN	N-CA-C	-5.50	103.43	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	860	PRO	N-CA-CB	5.50	106.25	102.35
2	H	226	GLU	CB-CG-CD	5.50	121.94	112.60
1	E	1059	THR	CB-CA-C	-5.49	101.28	110.56
1	G	34	CYS	CA-C-N	5.49	127.90	120.38
1	G	34	CYS	C-N-CA	5.49	127.90	120.38
1	A	850	VAL	CA-C-O	5.48	122.88	118.71
1	E	27	ASP	N-CA-C	-5.48	104.95	111.69
2	F	154	ASN	N-CA-CB	5.48	119.75	110.49
1	G	557	THR	N-CA-C	-5.48	106.76	113.50
2	H	232	ASN	CA-C-N	5.47	125.78	119.92
2	H	232	ASN	C-N-CA	5.47	125.78	119.92
2	F	248	ASP	N-CA-CB	-5.47	102.49	110.53
2	F	321	LEU	N-CA-C	5.47	119.34	109.44
1	G	651	ALA	N-CA-C	5.47	117.69	111.02
1	C	652	ARG	CD-NE-CZ	5.45	132.03	124.40
2	D	372	GLU	CB-CA-C	-5.45	102.26	110.92
2	F	237	PHE	CA-CB-CG	-5.45	108.35	113.80
2	F	269	CYS	N-CA-CB	5.45	119.70	110.49
1	G	880	THR	N-CA-CB	-5.45	103.75	111.00
1	C	57	ASP	CA-C-N	5.44	125.52	119.32
1	C	57	ASP	C-N-CA	5.44	125.52	119.32
1	A	674	ASP	CA-C-N	5.44	127.88	120.54
1	A	674	ASP	C-N-CA	5.44	127.88	120.54
1	G	956	ARG	N-CA-C	5.43	118.12	111.82
2	F	17	GLY	CA-C-N	-5.43	114.15	122.62
2	F	17	GLY	C-N-CA	-5.43	114.15	122.62
1	C	500	ALA	N-CA-C	5.43	117.20	111.28
1	C	755	PHE	CA-CB-CG	-5.41	108.39	113.80
1	G	761	GLU	CA-C-N	-5.41	115.42	122.94
1	G	761	GLU	C-N-CA	-5.41	115.42	122.94
2	H	308	THR	N-CA-C	5.41	117.90	109.52
2	B	127	ALA	N-CA-CB	5.40	117.99	109.83
1	A	652	ARG	N-CA-CB	5.40	117.79	109.91
2	B	325	LEU	CB-CA-C	-5.40	101.20	110.16
1	E	278	GLU	CB-CA-C	-5.39	100.32	109.38
2	D	215	ARG	CB-CA-C	5.39	118.64	109.75
1	A	1005	ILE	CA-C-O	5.39	126.56	120.95
1	G	569	PRO	CB-CA-C	-5.39	104.33	111.23
1	A	715	ARG	N-CA-CB	5.39	117.29	110.23
2	D	8	VAL	N-CA-CB	5.39	120.27	111.44
1	A	944	ARG	NH1-CZ-NH2	-5.38	112.30	119.30
1	E	737	TYR	N-CA-C	-5.38	105.10	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	17	GLY	O-C-N	-5.38	119.05	123.14
1	A	680	HIS	N-CA-C	5.38	117.14	111.28
1	E	584	HIS	CA-CB-CG	-5.38	108.42	113.80
2	D	154	ASN	N-CA-CB	5.37	119.56	110.49
1	G	543	MET	N-CA-C	5.37	118.02	109.81
1	A	652	ARG	NE-CZ-NH1	5.37	126.87	121.50
2	D	128	GLN	CB-CA-C	-5.37	98.91	110.45
1	G	994	VAL	N-CA-C	5.36	116.73	110.62
1	E	408	GLY	N-CA-C	-5.36	103.13	110.20
1	E	283	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	523	HIS	CA-CB-CG	-5.35	108.45	113.80
1	E	984	ALA	CA-C-N	-5.35	113.91	122.10
1	E	984	ALA	C-N-CA	-5.35	113.91	122.10
1	A	987	ASN	CA-CB-CG	5.35	117.95	112.60
1	G	980	VAL	N-CA-C	5.34	115.55	110.42
2	H	92	PHE	CA-CB-CG	-5.34	108.46	113.80
1	G	422	THR	CB-CA-C	5.34	119.34	110.90
1	E	714	VAL	N-CA-C	5.34	114.99	106.88
1	A	908	GLY	CA-C-N	5.33	125.42	119.87
1	A	908	GLY	C-N-CA	5.33	125.42	119.87
2	B	260	GLU	N-CA-C	-5.33	106.62	113.23
1	E	805	ILE	CB-CA-C	5.33	119.34	112.14
1	C	445	ALA	CA-C-N	-5.33	114.22	122.69
1	C	445	ALA	C-N-CA	-5.33	114.22	122.69
1	E	998	ARG	CB-CA-C	5.32	116.83	108.63
2	F	241	GLY	CA-C-N	5.32	125.30	120.03
2	F	241	GLY	C-N-CA	5.32	125.30	120.03
1	G	363	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	992	ASN	CA-CB-CG	-5.32	107.28	112.60
1	C	725	MET	CA-C-N	-5.31	113.90	122.82
1	C	725	MET	C-N-CA	-5.31	113.90	122.82
1	E	334	GLU	CB-CA-C	-5.31	98.78	109.55
1	G	518	ASP	CA-CB-CG	-5.30	107.30	112.60
1	A	801	LEU	N-CA-C	5.30	117.91	109.96
2	D	247	PRO	O-C-N	5.30	129.06	122.22
1	E	188	PHE	CA-CB-CG	-5.30	108.50	113.80
2	F	367	PHE	CA-CB-CG	5.29	119.09	113.80
1	E	357	THR	CA-C-N	-5.29	115.53	122.99
1	E	357	THR	C-N-CA	-5.29	115.53	122.99
2	B	308	THR	CA-C-N	5.29	129.44	122.30
2	B	308	THR	C-N-CA	5.29	129.44	122.30
2	D	9	LEU	CA-C-N	5.29	127.67	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	LEU	C-N-CA	5.29	127.67	120.54
1	E	558	ASP	N-CA-C	5.28	116.89	111.03
1	E	418	PRO	O-C-N	5.28	129.03	122.22
2	B	150	PHE	CB-CA-C	5.28	118.34	109.69
1	E	909	PRO	N-CA-CB	5.28	108.37	103.41
2	H	67	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	160	ALA	CA-C-O	5.27	126.06	120.10
1	G	660	PRO	CB-CA-C	-5.27	105.92	113.09
1	G	404	VAL	CB-CA-C	-5.27	105.14	112.36
1	E	142	GLU	N-CA-C	5.26	118.80	109.96
1	C	793	ALA	N-CA-C	-5.26	102.70	110.48
2	H	216	LEU	N-CA-C	5.26	118.06	109.59
2	F	215	ARG	CA-C-N	-5.25	114.57	122.81
2	F	215	ARG	C-N-CA	-5.25	114.57	122.81
1	A	557	THR	N-CA-C	-5.25	107.25	113.97
1	E	157	ALA	O-C-N	5.25	127.47	122.07
1	A	301	ASN	CB-CA-C	5.25	115.99	110.17
2	B	228	VAL	N-CA-C	5.25	115.39	110.30
1	E	963	LYS	CA-C-O	5.25	126.33	120.82
1	E	904	ASP	CA-C-O	5.24	124.32	119.24
1	E	988	PRO	CB-CA-C	-5.24	103.31	111.22
1	G	89	THR	N-CA-CB	-5.23	102.92	110.56
1	G	316	GLY	CA-C-O	5.23	124.61	118.96
1	A	708	ILE	N-CA-C	5.22	115.95	110.62
1	A	787	VAL	N-CA-C	-5.22	100.23	107.80
1	A	248	ILE	N-CA-CB	5.22	116.22	110.53
1	E	810	ARG	NE-CZ-NH1	5.21	126.72	121.50
1	A	280	GLY	CA-C-N	-5.21	117.06	122.69
1	A	280	GLY	C-N-CA	-5.21	117.06	122.69
1	C	1072	ILE	N-CA-C	5.21	116.25	108.54
2	F	359	GLY	CA-C-N	5.21	125.14	119.78
2	F	359	GLY	C-N-CA	5.21	125.14	119.78
1	E	247	SER	CB-CA-C	-5.21	101.21	109.80
1	E	698	ILE	N-CA-C	5.21	115.83	110.36
1	E	404	VAL	N-CA-C	-5.20	107.64	112.43
1	G	253	ALA	N-CA-C	-5.20	103.28	110.35
1	A	559	ARG	N-CA-C	5.20	118.15	110.46
1	C	821	GLN	CB-CA-C	-5.20	104.56	111.63
1	E	654	LEU	CA-C-O	5.19	125.92	120.42
1	G	979	ILE	CA-C-O	5.18	126.83	121.29
1	C	278	GLU	N-CA-CB	-5.17	103.74	110.88
1	C	417	ASP	CA-C-O	5.17	122.65	119.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	692	ASN	CA-CB-CG	-5.17	107.43	112.60
2	H	8	VAL	N-CA-CB	5.17	119.92	111.45
1	C	191	ILE	N-CA-C	5.17	115.38	110.42
1	E	162	VAL	N-CA-C	5.16	118.36	111.44
1	C	735	ARG	CA-C-N	5.16	128.56	120.82
1	C	735	ARG	C-N-CA	5.16	128.56	120.82
2	F	247	PRO	CA-C-O	5.16	125.80	118.99
2	B	149	ALA	CA-C-O	5.16	125.72	119.38
1	C	698	ILE	CB-CA-C	-5.16	105.10	111.70
1	G	407	THR	N-CA-C	-5.15	106.68	113.17
2	B	192	PHE	CA-CB-CG	-5.15	108.65	113.80
2	H	260	GLU	N-CA-C	-5.14	106.85	113.23
2	F	255	ILE	CB-CA-C	-5.14	105.31	112.04
2	F	88	ILE	CB-CA-C	-5.14	101.49	110.38
1	A	578	PHE	CA-CB-CG	-5.14	108.66	113.80
2	B	258	PHE	N-CA-C	-5.14	105.76	112.23
2	D	10	GLU	N-CA-C	-5.14	104.95	111.11
2	F	76	HIS	CA-CB-CG	-5.13	108.67	113.80
2	B	281	ALA	O-C-N	5.13	128.79	122.84
1	C	698	ILE	N-CA-C	5.13	115.57	110.23
1	E	555	PRO	N-CA-CB	5.13	107.81	103.35
2	D	11	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	594	TYR	CA-C-O	-5.13	115.76	121.81
1	A	188	PHE	N-CA-C	5.12	117.26	111.11
2	H	350	PHE	CA-CB-CG	5.12	118.92	113.80
1	E	1020	ARG	CD-NE-CZ	5.12	131.57	124.40
1	G	559	ARG	N-CA-C	5.12	117.64	109.81
1	G	912	ARG	CD-NE-CZ	5.12	131.57	124.40
1	C	618	PHE	CA-CB-CG	-5.12	108.68	113.80
1	E	949	VAL	N-CA-C	5.12	116.67	108.89
2	D	366	LEU	CA-C-O	5.12	125.88	120.10
1	G	530	ASP	O-C-N	5.12	127.35	121.93
1	A	500	ALA	N-CA-C	5.11	116.93	111.36
1	C	248	ILE	N-CA-C	-5.11	101.22	108.58
2	D	183	GLU	N-CA-C	-5.11	103.30	110.50
2	D	328	THR	N-CA-CB	5.11	117.38	110.59
1	G	377	GLN	O-C-N	-5.10	117.50	123.27
1	A	949	VAL	N-CA-C	5.10	116.70	108.85
2	B	245	PRO	N-CA-CB	5.09	108.03	103.19
1	E	834	ASN	CB-CA-C	-5.09	104.36	111.80
1	E	441	ASP	CA-CB-CG	5.09	117.69	112.60
1	G	993	LYS	N-CA-C	-5.09	103.82	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	20	ILE	CA-C-O	5.08	123.43	119.46
1	A	988	PRO	CB-CA-C	-5.08	103.23	110.75
1	G	1024	GLU	N-CA-CB	5.08	117.59	110.12
1	G	364	PHE	N-CA-C	5.07	117.54	111.71
1	E	425	ARG	CD-NE-CZ	-5.07	117.30	124.40
2	B	359	GLY	O-C-N	5.07	126.84	121.77
1	C	43	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	G	539	ASP	CA-C-O	5.07	124.47	118.90
1	A	190	GLU	N-CA-C	5.06	116.49	111.07
1	C	411	PRO	N-CA-CB	5.06	108.04	103.33
1	E	227	ASN	N-CA-C	-5.06	102.79	110.28
2	F	345	LYS	O-C-N	5.06	125.65	121.35
1	G	299	GLU	O-C-N	5.06	128.30	123.04
1	G	230	ILE	CB-CA-C	-5.05	104.17	111.19
1	C	206	ILE	CA-CB-CG1	-5.05	101.81	110.40
2	F	303	ASN	CA-CB-CG	-5.05	107.55	112.60
2	H	245	PRO	N-CA-CB	5.05	107.99	103.19
1	G	1036	TYR	CA-CB-CG	-5.05	104.81	113.90
2	F	352	GLY	O-C-N	-5.05	118.77	122.71
2	H	147	ALA	N-CA-C	5.05	116.59	111.14
1	C	625	ASP	N-CA-C	5.04	116.86	111.36
1	E	543	MET	N-CA-C	5.04	117.81	109.85
1	C	143	THR	CA-C-N	-5.04	111.80	120.97
1	C	143	THR	C-N-CA	-5.04	111.80	120.97
1	A	1007	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	239	ALA	N-CA-C	5.03	116.43	110.19
1	E	563	MET	CB-CA-C	5.03	118.06	109.75
1	A	1025	ASP	N-CA-C	5.03	116.84	111.36
1	G	353	ASP	CA-CB-CG	5.02	117.62	112.60
2	F	359	GLY	O-C-N	5.02	126.79	121.77
1	G	26	PHE	CA-CB-CG	-5.02	108.78	113.80
1	G	988	PRO	CB-CA-C	-5.02	103.32	110.75
1	G	82	ARG	CD-NE-CZ	5.02	131.42	124.40
2	D	234	ASP	N-CA-CB	5.02	118.03	110.30
2	H	154	ASN	N-CA-CB	5.01	116.91	109.19
1	C	674	ASP	CA-C-N	5.01	127.30	120.54
1	C	674	ASP	C-N-CA	5.01	127.30	120.54
1	G	786	GLY	N-CA-C	-5.01	108.52	114.48
1	E	830	PHE	CB-CA-C	-5.01	100.83	110.24
2	F	137	ASN	CA-CB-CG	-5.00	107.60	112.60
1	G	900	PHE	CA-C-N	5.00	125.27	119.47
1	G	900	PHE	C-N-CA	5.00	125.27	119.47

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	154	ASN	CA
2	D	154	ASN	CA
2	F	154	ASN	CA

There are no planarity outliers.

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	8212	0	8255	237	0
1	C	8197	0	8225	266	0
1	E	8182	0	8216	221	0
1	G	8206	0	8247	364	0
2	B	2897	0	2860	157	0
2	D	2904	0	2869	143	0
2	F	2897	0	2860	134	0
2	H	2897	0	2860	222	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	C	10	0	0	1	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	5	0	0	1	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	6	0	0	2	0
6	H	2	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0
7	E	54	0	24	4	0
7	G	54	0	24	1	0
8	A	9	0	11	0	0
8	C	9	0	11	1	0
8	E	9	0	11	2	0
8	G	9	0	11	1	0
9	A	9	0	20	1	0
9	C	9	0	20	1	0
9	E	9	0	20	2	0
9	G	9	0	20	2	0
10	A	21	0	11	1	0
10	C	21	0	11	1	0
10	E	21	0	11	3	0
10	G	21	0	11	2	0
11	A	851	0	0	30	1
11	B	161	0	0	5	0
11	C	819	0	0	22	1
11	D	221	0	0	5	0
11	E	832	0	0	25	0
11	F	200	0	0	2	0
11	G	705	0	0	28	0
11	H	118	0	0	5	0
All	All	48757	0	44656	1734	1

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 19.

All (1734) 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)
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.13	1.10
2:D:227:ASP:HA	2:D:230:LYS:HD2	1.25	1.07
1:G:784:GLN:NE2	1:G:784:GLN:H	1.53	1.05
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.41	1.03
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.38	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.25	1.00
2:H:354:PRO:HG3	2:H:366:LEU:HD22	1.45	0.99
2:H:324:ASN:N	2:H:324:ASN:HD22	1.55	0.98
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.44	0.98
2:B:245:PRO:HD3	2:B:270:LEU:HD11	1.47	0.97
2:H:245:PRO:HD3	2:H:270:LEU:HD11	1.46	0.97
2:H:324:ASN:HD22	2:H:324:ASN:H	0.96	0.95
2:D:324:ASN:H	2:D:324:ASN:HD22	0.99	0.94
2:B:286:MET:HE1	2:B:312:HIS:ND1	1.82	0.94
2:D:228:VAL:HA	2:D:231:MET:HE2	1.50	0.94
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.50	0.94
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.49	0.93
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.50	0.92
1:C:38:ARG:HG3	1:C:38:ARG:HH11	1.33	0.92
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.52	0.92
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.34	0.92
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.33	0.91
2:D:286:MET:HE1	2:D:312:HIS:ND1	1.86	0.91
1:G:784:GLN:HE21	1:G:784:GLN:N	1.67	0.91
2:D:245:PRO:HD3	2:D:270:LEU:HD11	1.51	0.91
2:F:245:PRO:HD3	2:F:270:LEU:HD11	1.51	0.91
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.35	0.91
1:E:1002:GLN:HE22	1:E:1006:LYS:HE3	1.34	0.91
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.87	0.90
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.54	0.90
1:G:1:MET:HB2	1:G:224:LYS:NZ	1.86	0.90
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.87	0.90
2:H:324:ASN:H	2:H:324:ASN:ND2	1.65	0.89
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.08	0.89
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.55	0.88
2:B:228:VAL:HA	2:B:231:MET:HE2	1.55	0.87
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.55	0.87
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.05	0.87
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.39	0.86
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.57	0.86
2:B:50:ARG:HG3	2:B:50:ARG:HH11	1.40	0.86
2:H:245:PRO:CD	2:H:270:LEU:HD11	2.05	0.86
2:D:285:LYS:HG3	2:D:314:PHE:CE1	2.12	0.85
2:D:324:ASN:HD22	2:D:324:ASN:N	1.67	0.85
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.57	0.85
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.57	0.84
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.13	0.84
1:G:708:ILE:HG22	1:G:712:LEU:HD11	1.59	0.83
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.08	0.83
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.59	0.83
1:E:698:ILE:HD12	1:E:698:ILE:H	1.42	0.83
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.07	0.83
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.58	0.83
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.60	0.83
1:G:784:GLN:H	1:G:784:GLN:HE21	0.86	0.83
2:D:324:ASN:H	2:D:324:ASN:ND2	1.77	0.83
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.08	0.83
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.58	0.83
2:H:27:VAL:CG2	2:H:131:CYS:HB2	2.05	0.83
1:A:130[A]:ARG:HB2	1:A:148:ILE:HG13	1.60	0.82
2:D:227:ASP:HA	2:D:230:LYS:CD	2.08	0.82
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.62	0.82
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.62	0.82
1:G:475[B]:LYS:HD2	1:G:488:PHE:CZ	2.14	0.82
2:H:247:PRO:HA	2:H:252:ILE:HD13	1.61	0.82
1:G:563:MET:CE	1:G:635:PRO:HG3	2.10	0.81
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.61	0.81
1:E:967[B]:GLN:HE21	1:E:1054:LEU:HD13	1.43	0.81
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.63	0.80
2:H:272:HIS:HA	2:H:349:SER:HB2	1.63	0.80
1:G:872:LYS:HG2	1:G:877:GLN:HG2	1.64	0.80
2:D:228:VAL:HA	2:D:231:MET:CE	2.11	0.80
1:A:130[B]:ARG:HB2	1:A:148:ILE:HG13	1.64	0.80
1:A:1073:LYS:HD2	1:A:1073:LYS:N	1.95	0.80
1:G:708:ILE:CG2	1:G:712:LEU:HD11	2.12	0.79
1:G:991:VAL:HB	11:G:1721:HOH:O	1.83	0.79
1:G:225:ASN:ND2	1:G:331:THR:HG21	1.97	0.79
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.64	0.78
1:E:509:ARG:CB	1:E:509:ARG:HH11	1.97	0.78
2:F:263:ILE:HG22	2:F:264:PRO:HD2	1.65	0.78
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.19	0.78
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.14	0.77
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.66	0.77
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.99	0.77
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.14	0.77
1:G:726:GLU:HG3	1:G:727:ILE:N	2.00	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:HIS:HD1	1:G:975:HIS:HD1	0.84	0.77
1:A:784:GLN:HE21	1:A:784:GLN:H	1.33	0.77
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.85	0.77
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.15	0.77
2:B:194:VAL:HB	2:B:216:LEU:HD23	1.65	0.77
1:C:652:ARG:HG2	1:C:652:ARG:HH11	1.47	0.76
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.19	0.76
2:D:27:VAL:HG13	2:D:131:CYS:HB2	1.68	0.76
1:G:1020:ARG:O	1:G:1024:GLU:HG3	1.85	0.76
2:F:154:ASN:HD21	2:F:314:PHE:HZ	1.34	0.76
2:B:324:ASN:HD22	2:B:324:ASN:N	1.81	0.76
1:G:1001:ILE:HD12	1:G:1029:ILE:HG12	1.67	0.76
2:F:259:LEU:O	2:F:345:LYS:HE3	1.86	0.76
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.65	0.76
1:C:967[A]:GLN:HG3	1:C:1054:LEU:HD13	1.68	0.76
1:E:157:ALA:HA	11:E:1237:HOH:O	1.84	0.76
2:F:324:ASN:H	2:F:324:ASN:HD22	1.34	0.76
1:A:228:CYS:SG	1:A:269:MET:HG2	2.26	0.76
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.68	0.76
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.85	0.76
1:E:103:GLU:HG3	1:E:104:ARG:N	2.01	0.76
2:H:215:ARG:HH11	2:H:215:ARG:HG2	1.51	0.76
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.85	0.75
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.21	0.75
2:H:71:GLU:O	2:H:203:ARG:HG3	1.87	0.75
2:B:246:ALA:HB1	2:B:248:ASP:CG	2.12	0.75
1:G:57:ASP:HB3	1:G:59:GLU:OE1	1.86	0.75
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.51	0.75
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.22	0.75
1:C:675:ARG:H	1:C:675:ARG:CD	1.99	0.75
2:D:227:ASP:CA	2:D:230:LYS:HD2	2.12	0.75
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.68	0.75
1:A:726:GLU:HG3	1:A:727:ILE:N	2.00	0.74
2:D:50:ARG:HD2	2:D:50:ARG:N	2.01	0.74
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.69	0.74
9:E:1092:NET:H22	9:E:1092:NET:H42	1.66	0.74
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.16	0.74
1:C:1020:ARG:O	1:C:1024:GLU:HG3	1.87	0.74
2:B:324:ASN:HD22	2:B:324:ASN:H	1.36	0.74
2:D:8:VAL:HG22	2:D:14:GLN:HG2	1.70	0.74
2:D:282:LYS:HG3	2:D:320:THR:HG21	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ARG:CD	1:A:675:ARG:H	1.99	0.73
1:A:1001:ILE:HD12	1:A:1002:GLN:N	2.03	0.73
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.89	0.73
1:G:64:THR:O	1:G:1065:VAL:HG23	1.88	0.73
1:A:449:VAL:N	11:A:1435:HOH:O	2.21	0.73
2:D:226:GLU:O	2:D:230:LYS:HG3	1.87	0.73
2:H:16:HIS:O	2:H:113:ILE:HG22	1.88	0.73
1:C:967[B]:GLN:HG2	1:C:1054:LEU:HD13	1.69	0.73
2:D:150:PHE:CE1	2:D:152:GLY:HA2	2.24	0.73
1:G:423:LYS:HB3	11:G:1397:HOH:O	1.89	0.73
2:H:50:ARG:HG3	2:H:50:ARG:HH11	1.52	0.73
1:E:331:THR:OG1	1:E:334:GLU:HG3	1.89	0.72
2:F:154:ASN:ND2	2:F:285:LYS:HE2	2.04	0.72
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.24	0.72
1:E:734:LEU:HD12	1:E:734:LEU:O	1.89	0.72
1:A:344:THR:HB	1:A:345:PRO:HD2	1.71	0.72
1:C:698:ILE:HD12	1:C:698:ILE:H	1.53	0.72
2:B:316:VAL:HG12	2:B:337:LEU:HD23	1.71	0.72
1:C:38:ARG:HG3	1:C:38:ARG:NH1	2.03	0.72
2:B:261:THR:OG1	2:B:263:ILE:HG13	1.89	0.72
1:C:772:MET:SD	1:C:880:THR:HG22	2.30	0.72
2:H:33:ASN:HA	2:H:291:HIS:O	1.90	0.72
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.90	0.72
2:B:50:ARG:HG3	2:B:50:ARG:NH1	2.03	0.72
2:D:263:ILE:HG22	2:D:264:PRO:HD2	1.72	0.72
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.72	0.72
2:F:195:VAL:HG21	2:F:231:MET:HE3	1.72	0.72
2:B:324:ASN:H	2:B:324:ASN:ND2	1.87	0.71
2:H:299:ASP:OD1	2:H:302:LYS:HD2	1.91	0.71
1:G:1004:ARG:HD3	1:G:1009[B]:GLU:OE2	1.91	0.71
1:G:1001:ILE:HD12	1:G:1029:ILE:CG1	2.21	0.71
2:B:286:MET:HE2	2:B:315:ALA:HB2	1.70	0.71
2:D:286:MET:HE1	2:D:312:HIS:CE1	2.26	0.71
1:C:321:LYS:HE3	11:C:1621:HOH:O	1.91	0.70
1:E:967[B]:GLN:NE2	1:E:1054:LEU:HB3	2.06	0.70
2:F:286:MET:HG2	11:F:1893:HOH:O	1.91	0.70
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.56	0.70
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.05	0.70
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.06	0.70
2:B:205:ILE:HG13	2:B:355:GLU:HG3	1.74	0.70
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.07	0.70
1:G:563:MET:HE3	1:G:635:PRO:CG	2.19	0.70
1:C:1:MET:HB2	1:C:224:LYS:NZ	2.05	0.70
1:E:734:LEU:HD11	1:E:738:PHE:CE2	2.27	0.70
1:A:930:LYS:HE3	11:A:1156:HOH:O	1.92	0.69
1:G:668:ALA:O	1:G:671:ARG:HB2	1.92	0.69
1:C:873:SER:O	1:C:877:GLN:HG3	1.93	0.69
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.00	0.69
2:B:190:LEU:HD13	2:B:214:CYS:O	1.91	0.69
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.07	0.69
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.27	0.69
1:G:726:GLU:HG3	1:G:727:ILE:H	1.57	0.69
1:A:725:MET:HE3	11:A:1609:HOH:O	1.91	0.69
2:B:324:ASN:O	2:B:342:ARG:HD2	1.91	0.69
2:F:324:ASN:O	2:F:342:ARG:HD2	1.93	0.69
2:B:279:SER:O	2:B:322:PRO:HG3	1.93	0.69
1:C:1063:ILE:HG12	1:C:1067:GLU:OE2	1.93	0.69
2:H:326:ARG:O	2:H:340:ILE:HG22	1.93	0.69
2:F:254:ALA:O	2:F:257:LYS:HB2	1.92	0.68
1:G:901:PRO:HD2	6:G:1086:CL:CL	2.30	0.68
1:E:644:GLY:O	1:E:647:PRO:HD2	1.92	0.68
1:E:726:GLU:HG3	1:E:727:ILE:H	1.56	0.68
1:A:946:LEU:C	1:A:947:LEU:HD12	2.18	0.68
2:H:50:ARG:HH12	2:H:156:MET:HE1	1.57	0.68
2:H:334:ASP:OD2	2:H:336:THR:HG23	1.94	0.68
1:A:784:GLN:H	1:A:784:GLN:NE2	1.90	0.68
1:G:652[A]:ARG:NH1	1:G:667:ASP:HA	2.09	0.68
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.27	0.68
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.76	0.68
1:C:833:LYS:O	1:C:836:GLU:HB2	1.94	0.68
1:C:228:CYS:SG	1:C:269:MET:HG2	2.34	0.67
1:G:1027:ARG:HE	1:G:1031:ARG:HD3	1.59	0.67
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.22	0.67
1:A:1:MET:HG3	1:A:2:PRO:HD2	1.75	0.67
1:C:43:ARG:NH2	1:C:81:GLU:OE2	2.28	0.67
1:G:967[A]:GLN:HG3	1:G:1054:LEU:HD13	1.76	0.67
1:A:703:GLU:O	1:A:706:LYS:HB2	1.94	0.67
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.08	0.67
2:D:227:ASP:O	2:D:230:LYS:HB2	1.95	0.67
1:A:343:ARG:HD3	11:A:1715:HOH:O	1.92	0.67
2:F:157:ASP:HB3	2:F:160:LYS:HE2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ARG:N	2:B:50:ARG:HD2	1.99	0.67
2:D:50:ARG:HG3	2:D:50:ARG:HH11	1.58	0.67
1:E:1021:ARG:HD3	1:E:1025:ASP:OD2	1.94	0.67
1:C:1:MET:HG3	1:C:2:PRO:HD2	1.77	0.67
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.77	0.67
1:G:974:THR:O	1:G:975:HIS:C	2.38	0.67
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.77	0.67
2:B:225:ALA:O	2:B:228:VAL:HB	1.94	0.67
1:E:905:PRO:HB2	1:E:1040:TYR:OH	1.95	0.67
2:B:263:ILE:HG22	2:B:264:PRO:HD2	1.77	0.67
2:B:322:PRO:HB2	2:B:324:ASN:ND2	2.09	0.67
2:D:282:LYS:HG3	2:D:320:THR:CG2	2.24	0.67
1:E:695:VAL:HA	1:E:700:MET:HE2	1.76	0.67
2:F:251:ALA:O	2:F:252:ILE:C	2.38	0.67
2:H:192:PHE:O	2:H:215:ARG:HB3	1.95	0.67
2:B:222:GLN:HB2	11:B:3567:HOH:O	1.95	0.66
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.77	0.66
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.77	0.66
1:G:687:LEU:HD13	1:G:812:GLN:HG2	1.76	0.66
1:C:726:GLU:HG3	1:C:727:ILE:H	1.59	0.66
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.76	0.66
1:G:863:LYS:O	1:G:866:ALA:HB3	1.94	0.66
2:B:153:LEU:O	2:B:156:MET:HB2	1.95	0.66
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.30	0.66
1:C:419:GLU:HG2	11:C:1718:HOH:O	1.95	0.66
2:D:139:ASP:OD2	2:D:142:LEU:HB2	1.96	0.66
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.76	0.66
2:B:286:MET:HG2	11:B:3570:HOH:O	1.94	0.66
1:C:495:LYS:NZ	11:C:1740:HOH:O	2.27	0.66
1:G:735:ARG:O	1:G:738:PHE:N	2.29	0.66
1:E:757:ASP:O	1:E:833:LYS:NZ	2.28	0.66
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.78	0.66
1:C:482:THR:HB	11:C:1747:HOH:O	1.96	0.66
2:D:50:ARG:HG3	2:D:50:ARG:NH1	2.11	0.66
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.23	0.66
1:G:803:GLN:HG3	1:G:807:ASP:OD1	1.96	0.66
1:E:698:ILE:H	1:E:698:ILE:CD1	2.09	0.66
1:E:907:LEU:HD11	8:E:1091:ORN:HD3	1.76	0.66
2:H:40:GLN:OE1	2:H:69:ASP:HB2	1.95	0.66
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.27	0.65
2:B:228:VAL:HG12	2:B:229:LEU:N	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:ASP:OD2	2:F:245:PRO:HD2	1.97	0.65
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.30	0.65
1:G:873:SER:O	1:G:877:GLN:HG3	1.97	0.65
1:G:475[C]:LYS:HD3	1:G:488:PHE:CZ	2.32	0.65
1:A:509:ARG:NH1	1:A:512[A]:GLU:OE1	2.29	0.65
1:A:735:ARG:O	1:A:738:PHE:N	2.29	0.65
1:A:814:GLN:NE2	11:A:1532:HOH:O	2.30	0.65
1:C:671:ARG:NH2	1:C:819:GLU:O	2.30	0.65
1:C:703:GLU:O	1:C:706:LYS:HB2	1.97	0.65
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.79	0.65
1:A:289:ASN:HB3	1:A:292:ASN:OD1	1.97	0.65
2:B:228:VAL:HA	2:B:231:MET:CE	2.25	0.65
1:G:24:CYS:HB2	1:G:604:GLU:HB2	1.79	0.65
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.96	0.65
2:H:33:ASN:OD1	2:H:292:GLY:HA2	1.97	0.65
1:E:726:GLU:OE1	1:E:1020:ARG:NE	2.30	0.64
1:G:475[A]:LYS:HD3	1:G:488:PHE:CZ	2.32	0.64
2:D:228:VAL:HG22	2:D:231:MET:CE	2.27	0.64
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.32	0.64
1:G:954:LYS:O	1:G:957:VAL:HG12	1.96	0.64
2:H:29:GLU:CD	2:H:153:LEU:HD22	2.22	0.64
2:H:262:ASP:OD1	2:H:345:LYS:NZ	2.31	0.64
1:A:696:THR:HB	1:A:700:MET:SD	2.37	0.64
1:E:703:GLU:O	1:E:706:LYS:HB2	1.97	0.64
2:B:71:GLU:O	2:B:203:ARG:HG3	1.96	0.64
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.79	0.64
1:G:417:ASP:OD1	1:G:423:LYS:NZ	2.29	0.64
2:H:34:THR:HA	2:H:56:THR:OG1	1.97	0.64
2:H:139:ASP:OD2	2:H:142:LEU:HB2	1.97	0.64
1:A:344:THR:HB	1:A:345:PRO:CD	2.27	0.64
2:B:228:VAL:HG11	2:B:258:PHE:CZ	2.33	0.64
1:G:781:HIS:CE1	1:G:789:SER:HB2	2.33	0.64
9:G:1092:NET:H22	9:G:1092:NET:H42	1.79	0.64
1:G:738:PHE:O	1:G:741:ALA:HB3	1.97	0.64
2:H:248:ASP:OD2	2:H:248:ASP:N	2.29	0.64
1:E:1:MET:HB2	1:E:224:LYS:HE3	1.80	0.64
1:G:321:LYS:NZ	1:G:611:ASP:OD1	2.30	0.64
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.13	0.64
2:H:286:MET:HE1	2:H:312:HIS:HE1	1.62	0.64
2:D:158:LEU:O	2:D:161:GLU:HB2	1.98	0.64
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HB2	1:G:224:LYS:CE	2.28	0.64
1:G:950:ARG:NH1	11:G:1675:HOH:O	2.31	0.64
1:A:425[B]:ARG:NH2	11:A:1745:HOH:O	2.31	0.63
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.27	0.63
1:E:321:LYS:NZ	1:E:611:ASP:OD1	2.30	0.63
1:G:339:ILE:HD11	1:G:531:THR:HG23	1.79	0.63
2:H:215:ARG:HG2	2:H:215:ARG:NH1	2.13	0.63
2:D:120:ARG:NH2	11:D:2337:HOH:O	2.29	0.63
2:D:201:ALA:HB2	2:D:239:SER:CB	2.28	0.63
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.61	0.63
1:A:375:THR:HG23	1:A:377:GLN:H	1.63	0.63
1:A:1001:ILE:HD12	1:A:1002:GLN:HB2	1.79	0.63
2:B:344:ASP:O	2:B:345:LYS:HD3	1.99	0.63
2:F:194:VAL:HG13	2:F:235:GLY:O	1.98	0.63
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.79	0.63
1:C:693:ALA:HB1	1:C:704:LYS:HG2	1.81	0.63
1:E:1:MET:N	11:E:1623:HOH:O	2.30	0.63
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.80	0.63
1:A:698:ILE:HD12	1:A:698:ILE:H	1.63	0.63
2:H:46:PRO:HG2	2:H:200:GLY:O	1.99	0.63
1:E:1:MET:HB2	1:E:224:LYS:CE	2.29	0.63
1:E:698:ILE:O	1:E:702:VAL:HG23	1.98	0.63
2:H:74:GLN:HA	11:H:475:HOH:O	1.98	0.63
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.81	0.62
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.98	0.62
2:D:286:MET:HB2	2:D:313:GLY:O	1.98	0.62
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.81	0.62
2:B:353:HIS:ND1	2:B:355:GLU:OE1	2.30	0.62
2:D:153:LEU:O	2:D:156:MET:HB2	1.99	0.62
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.82	0.62
1:E:812:GLN:NE2	11:E:1791:HOH:O	2.27	0.62
2:F:324:ASN:HD22	2:F:324:ASN:N	1.97	0.62
1:C:65:TYR:OH	1:C:80:LYS:HE2	1.99	0.62
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.33	0.62
2:H:46:PRO:HA	2:H:76:HIS:CG	2.35	0.62
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.82	0.62
1:A:1072:ILE:C	1:A:1073:LYS:HD2	2.24	0.62
1:C:698:ILE:O	1:C:702:VAL:HG23	1.99	0.62
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.13	0.62
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.30	0.62
1:G:762:VAL:HG13	1:G:779:MET:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1037:LYS:HE2	11:G:1756:HOH:O	1.98	0.62
2:H:5:ALA:CB	2:H:110:ILE:HG13	2.30	0.62
1:E:997:GLY:O	1:E:1000:HIS:HB3	2.00	0.62
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.08	0.62
1:A:563:MET:CE	1:A:635:PRO:HG3	2.30	0.62
1:G:488:PHE:O	1:G:491:GLN:N	2.33	0.62
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.82	0.62
2:H:286:MET:CE	2:H:315:ALA:HB2	2.29	0.62
2:B:245:PRO:HD3	2:B:270:LEU:CD1	2.27	0.62
2:D:26:ALA:O	2:D:131:CYS:HA	2.00	0.62
2:D:228:VAL:O	2:D:231:MET:HG3	2.00	0.62
1:E:675:ARG:CD	1:E:675:ARG:H	2.12	0.62
1:E:698:ILE:HD12	1:E:698:ILE:N	2.14	0.61
1:E:784:GLN:H	1:E:784:GLN:NE2	1.98	0.61
1:G:76:LYS:HE3	11:G:1740:HOH:O	1.99	0.61
1:G:400:ARG:HD3	11:G:1373:HOH:O	2.00	0.61
2:B:247:PRO:HA	2:B:252:ILE:CD1	2.30	0.61
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.34	0.61
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.35	0.61
2:H:144:LEU:HD12	2:H:144:LEU:O	2.00	0.61
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.63	0.61
1:C:763:ASP:HB3	1:C:779:MET:HE3	1.82	0.61
1:G:59:GLU:OE2	1:G:60:MET:HE2	2.00	0.61
1:G:1063:ILE:HG13	1:G:1067:GLU:OE2	1.99	0.61
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.29	0.61
1:A:738:PHE:O	1:A:741:ALA:HB3	2.01	0.61
1:E:967[B]:GLN:HE21	1:E:1054:LEU:CD1	2.13	0.61
1:G:354:TYR:HB2	1:G:388:GLY:O	2.01	0.61
2:H:236:ILE:HD12	2:H:263:ILE:HG21	1.82	0.61
1:C:44:VAL:N	1:C:62:ASP:OD2	2.29	0.61
1:C:698:ILE:HD12	1:C:698:ILE:N	2.14	0.61
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.36	0.61
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.28	0.61
1:C:998:ARG:CB	1:C:999:PRO:HA	2.30	0.61
1:G:617:TYR:CG	1:G:629:ILE:HD13	2.35	0.61
1:E:1002:GLN:NE2	1:E:1006:LYS:HE3	2.12	0.61
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.19	0.60
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.19	0.60
1:G:804:GLU:O	1:G:808:VAL:HG23	2.00	0.60
1:C:17:PRO:HG3	1:C:917:VAL:HG13	1.83	0.60
1:E:509:ARG:HH11	1:E:509:ARG:HB3	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:946:LEU:CD1	1:G:991:VAL:HG11	2.31	0.60
2:H:342:ARG:HB3	2:H:344:ASP:OD2	2.01	0.60
2:B:34:THR:HA	2:B:56:THR:OG1	2.02	0.60
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.82	0.60
1:C:1020:ARG:O	1:C:1020:ARG:HG3	2.01	0.60
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.82	0.60
1:G:471:ARG:HD2	11:G:1643:HOH:O	2.00	0.60
1:G:1021:ARG:HG3	1:G:1021:ARG:HH11	1.66	0.60
1:C:822:VAL:O	1:C:823:ARG:HD3	2.01	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.48	0.60
1:E:527:LYS:HD2	2:F:116:ARG:HD3	1.84	0.60
2:B:246:ALA:HB1	2:B:248:ASP:OD2	2.01	0.60
2:B:237:PHE:HE1	2:B:268:ILE:HG13	1.66	0.60
2:B:232:ASN:N	2:B:233:PRO:HD3	2.16	0.60
2:B:245:PRO:CG	2:B:274:LEU:HD21	2.32	0.60
1:C:907:LEU:HD11	8:C:1091:ORN:HD3	1.84	0.60
2:F:247:PRO:HA	2:F:252:ILE:HD13	1.82	0.60
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.36	0.60
2:H:367:PHE:O	2:H:370:PHE:HB3	2.01	0.60
1:A:948:SER:OG	10:A:1091:U5P:H5'1	2.01	0.60
1:E:257:THR:HG22	2:F:63:VAL:HG21	1.84	0.60
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.84	0.60
1:A:994:VAL:HG23	1:A:1001:ILE:HD11	1.82	0.59
1:E:344:THR:HB	1:E:345:PRO:HD2	1.83	0.59
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.59
2:H:50:ARG:HD2	2:H:50:ARG:N	2.17	0.59
2:H:232:ASN:N	2:H:233:PRO:HD3	2.17	0.59
1:C:698:ILE:H	1:C:698:ILE:CD1	2.14	0.59
1:E:1021:ARG:HH11	1:E:1021:ARG:CG	2.15	0.59
1:G:620:PRO:HB2	1:G:622:THR:HG23	1.83	0.59
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.30	0.59
1:E:1073:LYS:N	1:E:1073:LYS:HD2	2.17	0.59
2:B:78:GLN:HG2	11:B:3896:HOH:O	2.03	0.59
1:C:519:GLN:NE2	11:C:1768:HOH:O	2.32	0.59
1:C:552:GLU:HB3	11:C:1775:HOH:O	2.01	0.59
2:D:157:ASP:OD2	2:D:160:LYS:HG2	2.03	0.59
2:D:282:LYS:HG3	2:D:320:THR:CB	2.32	0.59
2:F:41:GLU:CB	2:F:358:PRO:HD3	2.33	0.59
1:G:128:ASP:CG	1:G:131:ARG:HG3	2.27	0.59
2:B:269:CYS:O	2:B:272:HIS:HB3	2.02	0.59
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:905:PRO:HB2	1:G:1040:TYR:OH	2.02	0.59
1:A:693:ALA:HB2	1:A:708:ILE:HD11	1.84	0.59
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.49	0.59
1:C:784:GLN:H	1:C:784:GLN:HE21	1.50	0.59
2:D:178:THR:HG22	2:D:179:GLY:N	2.15	0.59
1:C:46:LEU:HD12	1:C:46:LEU:C	2.28	0.59
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.68	0.59
2:H:334:ASP:CG	2:H:336:THR:HG23	2.28	0.59
1:G:734:LEU:HD12	1:G:734:LEU:O	2.02	0.59
2:H:215:ARG:HH11	2:H:215:ARG:CG	2.16	0.59
1:A:115:MET:HG2	1:A:118:ALA:O	2.01	0.59
1:G:597:ILE:HG12	1:G:615:ARG:HB2	1.85	0.59
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.84	0.58
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.39	0.58
1:E:904:ASP:O	1:E:906:LEU:N	2.36	0.58
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.85	0.58
1:C:1:MET:N	1:C:224:LYS:HE3	2.17	0.58
1:C:1021:ARG:HH11	1:C:1021:ARG:HG3	1.67	0.58
2:B:245:PRO:HG2	2:B:274:LEU:CD2	2.34	0.58
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.18	0.58
1:G:698:ILE:O	1:G:702:VAL:HG23	2.03	0.58
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.30	0.58
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.33	0.58
2:F:92:PHE:CE1	2:F:93:ARG:HG2	2.38	0.58
2:F:322:PRO:CD	2:F:325:LEU:HD12	2.33	0.58
1:G:1067:GLU:O	1:G:1068:MET:C	2.46	0.58
2:H:247:PRO:HA	2:H:252:ILE:CD1	2.31	0.58
1:C:998:ARG:HA	1:C:999:PRO:C	2.28	0.58
1:G:676:GLU:O	1:G:680:HIS:ND1	2.36	0.58
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.39	0.58
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.38	0.58
2:H:153:LEU:O	2:H:156:MET:HB2	2.03	0.58
2:H:363:ALA:C	2:H:365:PRO:HD2	2.28	0.58
2:B:272:HIS:ND1	2:B:349:SER:OG	2.32	0.58
1:C:646:THR:HB	1:C:647:PRO:HD3	1.86	0.58
1:G:773:VAL:HG21	1:G:817:ALA:CB	2.33	0.58
2:H:50:ARG:NH1	2:H:156:MET:HE1	2.19	0.58
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.19	0.58
1:E:440:ALA:O	1:E:444:ARG:HG3	2.03	0.58
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.38	0.58
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:H3	1:C:224:LYS:HE3	1.69	0.58
2:D:275:LEU:HD23	2:D:349:SER:OG	2.04	0.58
1:E:734:LEU:HD12	1:E:734:LEU:C	2.28	0.58
2:F:186:LYS:HB2	2:F:189:GLU:OE2	2.04	0.58
1:G:481:ILE:HA	1:G:484:LEU:HD12	1.86	0.58
1:A:941:LYS:NZ	1:A:1056:ALA:O	2.33	0.58
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.85	0.58
1:E:735:ARG:O	1:E:738:PHE:N	2.37	0.58
1:G:784:GLN:NE2	1:G:784:GLN:N	2.36	0.58
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.38	0.57
2:B:46:PRO:HA	2:B:76:HIS:CG	2.39	0.57
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.34	0.57
2:H:201:ALA:HB2	2:H:239:SER:CB	2.34	0.57
1:C:814:GLN:HG3	1:C:818:PHE:HE2	1.69	0.57
1:E:340:THR:O	1:E:343:ARG:HB2	2.04	0.57
1:G:118:ALA:HA	11:G:1763:HOH:O	2.03	0.57
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.04	0.57
1:G:702:VAL:O	1:G:706:LYS:HD2	2.05	0.57
1:G:902:GLY:O	1:G:1027:ARG:NH2	2.38	0.57
1:A:726:GLU:HG3	1:A:727:ILE:H	1.67	0.57
1:C:157:ALA:O	1:C:160:ALA:HB3	2.05	0.57
1:C:678:PHE:CE1	1:C:842:VAL:HG23	2.40	0.57
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.34	0.57
1:G:1021:ARG:HH11	1:G:1021:ARG:CG	2.17	0.57
11:G:1440:HOH:O	2:H:123:ARG:HD2	2.02	0.57
2:H:272:HIS:HA	2:H:349:SER:CB	2.32	0.57
2:H:361:HIS:ND1	11:H:399:HOH:O	2.30	0.57
1:C:419:GLU:HB3	1:C:423[B]:LYS:NZ	2.18	0.57
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.19	0.57
2:H:142:LEU:O	2:H:146:LYS:HG3	2.05	0.57
2:H:369:HIS:O	2:H:372:GLU:HB2	2.05	0.57
1:C:24:CYS:SG	1:C:576:ILE:HD12	2.44	0.57
2:D:225:ALA:HB2	2:D:254:ALA:HB1	1.87	0.57
1:E:1006:LYS:HG3	1:E:1006:LYS:O	2.04	0.57
1:G:702:VAL:HG13	1:G:731:GLU:HG3	1.86	0.57
2:F:286:MET:HE1	2:F:312:HIS:CE1	2.39	0.57
1:G:516:LEU:HD11	1:G:520:TYR:CZ	2.40	0.57
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.87	0.57
1:A:460:ARG:HG3	11:A:1299:HOH:O	2.04	0.57
1:A:936:ASN:HB2	11:A:1109:HOH:O	2.04	0.57
1:E:947:LEU:HD12	1:E:947:LEU:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:695:VAL:CG1	1:G:700:MET:HB3	2.34	0.57
2:B:286:MET:HE1	2:B:312:HIS:CE1	2.39	0.56
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.86	0.56
2:H:286:MET:HE2	2:H:315:ALA:HB2	1.87	0.56
2:B:324:ASN:N	2:B:324:ASN:ND2	2.45	0.56
1:A:1001:ILE:O	1:A:1005:ILE:HG13	2.06	0.56
2:B:150:PHE:CE1	2:B:152:GLY:HA2	2.40	0.56
2:B:237:PHE:CE1	2:B:268:ILE:HG13	2.41	0.56
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.69	0.56
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.86	0.56
1:C:814:GLN:HG3	1:C:818:PHE:CE2	2.39	0.56
2:D:201:ALA:HA	2:D:240:ASN:OD1	2.05	0.56
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.04	0.56
1:G:105:GLN:NE2	1:G:105:GLN:HA	2.20	0.56
1:A:730:ASP:H	1:A:733:ASP:HB2	1.71	0.56
1:E:503:ALA:HB1	1:E:508:VAL:O	2.06	0.56
2:H:342:ARG:NH2	2:H:344:ASP:OD1	2.33	0.56
2:B:286:MET:HE2	2:B:315:ALA:CB	2.36	0.56
1:E:950:ARG:HD3	11:E:1593:HOH:O	2.04	0.56
2:F:290:HIS:HB2	2:F:312:HIS:CD2	2.40	0.56
1:C:423[A]:LYS:HE2	11:C:1420:HOH:O	2.04	0.56
1:C:426:ARG:HD3	1:C:426:ARG:C	2.30	0.56
1:E:142:GLU:OE2	1:E:294:ARG:NH2	2.38	0.56
2:H:133:ILE:HD11	2:H:143:ALA:HA	1.87	0.56
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.87	0.56
1:G:695:VAL:HG11	1:G:701:ALA:N	2.21	0.56
1:A:698:ILE:O	1:A:702:VAL:HG23	2.06	0.56
1:G:698:ILE:HD12	1:G:698:ILE:N	2.20	0.56
2:H:295:HIS:HD2	2:H:296:PRO:O	1.89	0.56
1:E:796:LEU:C	1:E:796:LEU:HD23	2.31	0.56
1:E:1057:ASP:HB3	1:E:1060:GLU:HB2	1.87	0.56
1:G:703:GLU:HA	1:G:706:LYS:HD3	1.88	0.56
1:C:695:VAL:HG21	1:C:701:ALA:CA	2.28	0.55
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.70	0.55
2:D:345:LYS:HB3	2:D:346:PRO:CD	2.35	0.55
1:E:995:HIS:ND1	11:E:1847:HOH:O	2.33	0.55
1:G:223:ASP:OD1	1:G:225:ASN:N	2.39	0.55
1:C:571:ARG:HD3	1:C:571:ARG:N	2.21	0.55
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.88	0.55
1:A:40:GLU:HG3	1:A:325:LYS:HE2	1.88	0.55
2:D:201:ALA:HB2	2:D:239:SER:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:GLU:HA	1:E:706:LYS:HD3	1.89	0.55
1:E:967[B]:GLN:NE2	1:E:1054:LEU:HD13	2.17	0.55
1:G:240:MET:HE3	7:G:1089:ADP:C4	2.40	0.55
1:E:494:ARG:HG2	1:E:547:TYR:HB2	1.89	0.55
1:G:874:LEU:HB3	1:G:879:VAL:O	2.05	0.55
2:H:9:LEU:O	2:H:10:GLU:C	2.49	0.55
2:H:218:ILE:N	2:H:218:ILE:HD13	2.21	0.55
2:H:363:ALA:O	2:H:366:LEU:HD13	2.06	0.55
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.06	0.55
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.36	0.55
1:G:950:ARG:HG2	1:G:1016:THR:OG1	2.07	0.55
2:F:153:LEU:HG	2:F:158:LEU:HD11	1.88	0.55
2:B:168:TYR:O	2:B:218:ILE:N	2.29	0.55
1:C:423[B]:LYS:NZ	11:C:1420:HOH:O	2.38	0.55
1:E:108:LEU:HB2	11:E:1179:HOH:O	2.07	0.55
1:E:1061:LYS:NZ	11:E:1828:HOH:O	2.39	0.55
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.72	0.55
1:G:274:GLU:HB2	11:G:1205:HOH:O	2.06	0.55
1:G:802:SER:O	1:G:806:GLN:HG3	2.07	0.55
1:A:130[A]:ARG:NE	11:A:1197:HOH:O	2.38	0.55
1:A:663:GLY:O	1:A:664:THR:C	2.48	0.55
2:F:224:SER:OG	2:F:227:ASP:HB2	2.07	0.55
1:G:645[A]:GLN:HG3	1:G:649:LYS:HE3	1.89	0.55
1:A:76:LYS:HD3	11:A:1163:HOH:O	2.07	0.55
2:B:263:ILE:CG2	2:B:264:PRO:HD2	2.36	0.55
1:C:509:ARG:HD3	11:C:1763:HOH:O	2.07	0.55
1:A:1001:ILE:HD12	1:A:1002:GLN:H	1.69	0.55
2:B:172:GLN:O	2:B:207:ARG:HA	2.07	0.55
1:E:3:LYS:NZ	11:E:1094:HOH:O	2.39	0.55
1:G:948:SER:OG	10:G:1093:U5P:H5'1	2.07	0.55
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.89	0.54
1:A:446:GLY:O	1:E:447:LEU:HD23	2.07	0.54
1:C:64:THR:O	1:C:1065:VAL:HG23	2.07	0.54
1:G:213:TRP:CZ3	1:G:296:ILE:HD12	2.42	0.54
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.40	0.54
2:F:246:ALA:C	2:F:248:ASP:H	2.13	0.54
2:H:186:LYS:O	2:H:189:GLU:HB2	2.06	0.54
2:H:350:PHE:CG	2:H:366:LEU:HD21	2.42	0.54
1:A:588:ALA:HB2	1:A:863:LYS:HG2	1.90	0.54
1:A:701:ALA:O	1:A:705:ALA:N	2.30	0.54
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:N	1:E:224:LYS:HE3	2.21	0.54
1:G:788:HIS:ND1	1:G:911:MET:HB2	2.23	0.54
1:A:646:THR:HB	1:A:647:PRO:HD3	1.88	0.54
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.72	0.54
1:C:661:VAL:HB	11:C:1801:HOH:O	2.08	0.54
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.89	0.54
1:G:1001:ILE:HD11	11:G:1537:HOH:O	2.07	0.54
1:A:167:ILE:HD12	1:A:167:ILE:N	2.21	0.54
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.21	0.54
2:F:342:ARG:HB3	2:F:345:LYS:H	1.71	0.54
1:G:294:ARG:HD2	6:G:1085:CL:CL	2.45	0.54
1:A:833:LYS:O	1:A:836:GLU:HB2	2.08	0.54
2:D:324:ASN:ND2	2:D:324:ASN:N	2.41	0.54
2:F:228:VAL:O	2:F:231:MET:HG3	2.08	0.54
1:G:493:LYS:NZ	1:G:499:ASP:OD2	2.34	0.54
2:B:201:ALA:HB2	2:B:239:SER:CB	2.38	0.54
2:B:355:GLU:OE2	2:B:355:GLU:N	2.30	0.54
2:B:364:ALA:N	2:B:365:PRO:HD2	2.23	0.54
1:E:670:ASP:HB2	11:E:1785:HOH:O	2.08	0.54
2:F:50:ARG:HD2	2:F:50:ARG:N	2.21	0.54
1:G:991:VAL:HG21	1:G:1001:ILE:HG22	1.89	0.54
2:H:257:LYS:O	2:H:261:THR:HG23	2.06	0.54
2:B:186:LYS:O	2:B:187:GLU:C	2.50	0.54
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.89	0.54
1:C:762:VAL:HG13	1:C:779:MET:O	2.08	0.54
2:D:10:GLU:OE2	2:D:129:ASN:N	2.29	0.54
1:E:185:ARG:NH2	11:E:1238:HOH:O	2.40	0.54
1:G:967[B]:GLN:HG2	1:G:1054:LEU:HD13	1.90	0.54
2:H:132:ILE:HG22	2:H:133:ILE:N	2.23	0.54
1:C:43:ARG:HA	1:C:62:ASP:OD2	2.08	0.54
2:F:50:ARG:HG2	2:F:158:LEU:HD22	1.90	0.54
2:H:69:ASP:HA	11:H:500:HOH:O	2.07	0.54
1:A:145:ARG:HH12	1:A:161:ASP:CG	2.16	0.54
2:D:277:LEU:HD23	2:D:281:ALA:O	2.08	0.54
1:E:125:LYS:NZ	11:E:1188:HOH:O	2.41	0.54
1:E:144:ALA:HB1	1:E:208:GLU:CG	2.38	0.54
1:E:901:PRO:HD2	6:E:1086:CL:CL	2.45	0.54
9:A:1090:NET:H82	9:A:1090:NET:H62	1.91	0.53
2:B:6:LEU:HD12	2:B:7:LEU:N	2.23	0.53
1:C:827:ASN:HB3	1:C:843:ASN:HB2	1.90	0.53
2:D:262:ASP:HB2	11:D:2882:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:HIS:HA	2:D:349:SER:HB2	1.88	0.53
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.73	0.53
1:G:698:ILE:HD12	1:G:698:ILE:H	1.73	0.53
2:H:275:LEU:HD23	2:H:349:SER:CB	2.39	0.53
1:E:1051:ALA:O	1:E:1054:LEU:HB2	2.08	0.53
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.44	0.53
1:G:622:THR:O	1:G:626:VAL:HG23	2.08	0.53
1:A:772[B]:MET:SD	1:A:880:THR:HG22	2.49	0.53
1:E:482:THR:HB	11:E:1442:HOH:O	2.08	0.53
2:F:43:LEU:HD21	2:F:80:LEU:HD13	1.90	0.53
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.39	0.53
1:G:139:ILE:HD11	1:G:141:LEU:HD12	1.90	0.53
1:A:709:GLY:O	1:A:754:HIS:ND1	2.41	0.53
1:C:171:SER:HB2	1:C:203:GLU:HB3	1.90	0.53
1:C:1019:GLY:O	1:C:1023:ILE:HD12	2.08	0.53
1:E:675:ARG:H	1:E:675:ARG:HD3	1.72	0.53
1:E:954:LYS:O	1:E:980:VAL:HG11	2.09	0.53
1:G:710:TYR:HB3	1:G:729:TYR:O	2.07	0.53
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.74	0.53
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.38	0.53
1:A:70:HIS:O	1:A:74:VAL:HG23	2.09	0.53
2:B:322:PRO:HG2	2:B:324:ASN:ND2	2.21	0.53
2:F:41:GLU:HB2	2:F:358:PRO:HD3	1.91	0.53
1:G:423:LYS:HA	1:G:426[B]:ARG:NH2	2.24	0.53
1:G:946:LEU:HD11	1:G:991:VAL:HG11	1.89	0.53
2:H:236:ILE:CD1	2:H:263:ILE:HG21	2.39	0.53
2:H:275:LEU:HD23	2:H:349:SER:OG	2.09	0.53
1:E:2:PRO:O	1:E:3:LYS:C	2.48	0.53
2:F:201:ALA:HB2	2:F:239:SER:CB	2.38	0.53
2:H:8:VAL:HG12	2:H:9:LEU:N	2.24	0.53
2:H:205:ILE:HG13	2:H:355:GLU:HG3	1.90	0.53
1:A:979:ILE:O	1:A:983:GLU:HG3	2.08	0.53
2:B:49:SER:O	2:B:50:ARG:HB2	2.08	0.53
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.07	0.53
1:G:272:LEU:HD21	1:G:282:SER:HB2	1.89	0.53
2:H:279:SER:OG	2:H:342:ARG:NH1	2.30	0.53
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.08	0.53
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.08	0.53
1:A:665:SER:O	1:A:669:ILE:HG13	2.09	0.53
2:B:367:PHE:O	2:B:370:PHE:HB3	2.08	0.53
1:C:1:MET:CG	1:C:2:PRO:HD2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.91	0.53
2:D:188:ASP:OD2	2:D:188:ASP:N	2.31	0.53
1:G:100:LEU:N	1:G:100:LEU:HD12	2.24	0.53
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.18	0.52
2:B:247:PRO:HA	2:B:252:ILE:HD12	1.90	0.52
1:G:751:LEU:O	1:G:752:LEU:HD12	2.08	0.52
1:A:695:VAL:HG12	1:A:696:THR:N	2.22	0.52
2:D:228:VAL:HG22	2:D:231:MET:HE1	1.92	0.52
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.90	0.52
1:G:530:ASP:C	1:G:531:THR:HG23	2.35	0.52
2:H:48:TYR:O	2:H:51:GLN:HB2	2.09	0.52
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.57	0.52
2:F:41:GLU:HB3	2:F:358:PRO:HD3	1.92	0.52
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.90	0.52
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.91	0.52
1:E:278:GLU:HG2	11:E:1310:HOH:O	2.09	0.52
1:E:726:GLU:HG3	1:E:727:ILE:N	2.24	0.52
1:G:1:MET:HB2	1:G:224:LYS:HE3	1.90	0.52
1:G:178:GLY:HA3	1:G:198:LEU:HD23	1.91	0.52
1:A:28:TYR:CZ	1:A:313:LYS:HE3	2.43	0.52
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.40	0.52
1:C:419:GLU:CB	1:C:423[B]:LYS:NZ	2.73	0.52
2:F:193:HIS:O	2:F:234:ASP:HB2	2.10	0.52
1:G:384:VAL:HG22	1:G:385:MET:N	2.24	0.52
2:H:176:THR:O	2:H:180:GLY:N	2.37	0.52
1:A:822:VAL:O	1:A:823:ARG:HD3	2.10	0.52
1:C:420:ALA:HA	1:C:423[B]:LYS:HD2	1.91	0.52
1:C:542:TYR:CD1	1:C:616:LEU:HD23	2.45	0.52
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.24	0.52
1:G:1035:GLN:NE2	11:G:1544:HOH:O	2.43	0.52
1:A:954:LYS:O	1:A:957:VAL:HG12	2.10	0.52
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.44	0.52
1:E:998:ARG:HA	1:E:999:PRO:C	2.33	0.52
1:A:671:ARG:HG3	1:A:677:ARG:NH1	2.24	0.52
1:C:998:ARG:HB3	1:C:999:PRO:HA	1.91	0.52
2:D:245:PRO:HD3	2:D:270:LEU:CD1	2.33	0.52
2:D:282:LYS:HG3	2:D:320:THR:HB	1.92	0.52
2:F:363:ALA:C	2:F:365:PRO:HD2	2.34	0.52
1:G:708:ILE:HG21	1:G:712:LEU:HD11	1.92	0.52
2:H:54:THR:HG23	2:H:81:VAL:HG12	1.90	0.52
2:H:202:LYS:NZ	2:H:356:ALA:O	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:VAL:CG1	2:B:337:LEU:HD23	2.38	0.52
2:D:286:MET:HE2	2:D:314:PHE:C	2.35	0.52
2:F:199:PHE:HB3	2:F:270:LEU:HD23	1.92	0.52
1:A:370:ALA:HB2	1:A:903:VAL:CG2	2.40	0.52
1:A:891:LYS:HG2	1:A:892:GLU:N	2.25	0.52
2:B:50:ARG:HG2	2:B:158:LEU:CD2	2.40	0.52
2:D:46:PRO:HA	2:D:76:HIS:CG	2.45	0.52
1:E:517:ARG:HG2	1:E:522:LEU:HD23	1.91	0.52
1:A:138:LYS:NZ	11:A:1921:HOH:O	2.40	0.51
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.10	0.51
2:D:362:ASP:OD2	2:D:362:ASP:N	2.41	0.51
2:F:247:PRO:HD2	2:F:248:ASP:OD1	2.10	0.51
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.90	0.51
2:B:340:ILE:O	2:B:348:PHE:HB2	2.10	0.51
1:C:174:MET:HB2	5:C:1078:PO4:O1	2.09	0.51
2:D:196:ALA:HA	2:D:237:PHE:O	2.10	0.51
1:E:873:SER:O	1:E:877:GLN:HG3	2.09	0.51
1:G:701:ALA:O	1:G:705:ALA:N	2.33	0.51
2:H:160:LYS:HE3	2:H:161:GLU:OE2	2.09	0.51
1:E:967[B]:GLN:NE2	1:E:1054:LEU:CB	2.74	0.51
1:E:998:ARG:CB	1:E:999:PRO:HA	2.40	0.51
1:G:784:GLN:HB3	11:G:1480:HOH:O	2.11	0.51
2:H:286:MET:HE1	2:H:312:HIS:CE1	2.44	0.51
2:H:317:ASP:HB3	2:H:320:THR:HG23	1.92	0.51
1:A:224:LYS:HE2	1:A:329:GLY:O	2.10	0.51
1:A:450:ASP:N	11:A:1435:HOH:O	2.27	0.51
2:B:83:ARG:HH11	2:B:83:ARG:HG3	1.75	0.51
1:G:225:ASN:ND2	11:G:1296:HOH:O	2.42	0.51
1:G:762:VAL:HG12	1:G:763:ASP:N	2.25	0.51
2:H:50:ARG:HG3	2:H:50:ARG:NH1	2.16	0.51
2:H:317:ASP:OD2	2:H:319:ALA:HB3	2.09	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
1:E:109:GLU:O	1:E:110:GLU:C	2.50	0.51
1:G:435:ARG:O	1:G:436:ILE:C	2.52	0.51
1:A:685:LEU:O	1:A:686:LYS:HB2	2.09	0.51
1:C:7:ILE:HG23	1:C:84:ASP:HB2	1.91	0.51
1:C:373:ARG:O	1:C:379:LYS:NZ	2.40	0.51
1:C:784:GLN:H	1:C:784:GLN:NE2	2.08	0.51
1:E:500:ALA:O	1:E:504:LYS:HG3	2.10	0.51
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.46	0.51
2:H:6:LEU:HD12	2:H:7:LEU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:CYS:HB2	1:A:273:ARG:NH2	2.26	0.51
1:C:167:ILE:HD12	1:C:167:ILE:N	2.25	0.51
1:C:973:ALA:O	1:C:991:VAL:HG12	2.10	0.51
1:E:361:ARG:CZ	1:E:571:ARG:HG2	2.41	0.51
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.90	0.51
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.76	0.51
1:G:773:VAL:HG21	1:G:817:ALA:HB3	1.91	0.51
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.28	0.51
1:C:69:ILE:O	1:C:69:ILE:HG22	2.10	0.51
1:G:695:VAL:CG2	1:G:752:LEU:HD22	2.40	0.51
1:A:730:ASP:OD2	1:A:733:ASP:HB2	2.11	0.51
1:A:948:SER:O	1:A:1015:ASN:HA	2.11	0.51
1:A:991:VAL:HG22	1:A:992:ASN:N	2.26	0.51
2:B:248:ASP:OD2	2:B:248:ASP:N	2.41	0.51
1:C:119:THR:O	1:C:120:ALA:C	2.53	0.51
1:C:385:MET:HB2	1:C:603:PRO:HG3	1.92	0.51
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.93	0.51
1:E:258:ASP:O	1:E:262:GLN:HG2	2.10	0.51
1:E:526:TYR:CE1	1:E:545:SER:HB3	2.46	0.51
9:E:1092:NET:H42	9:E:1092:NET:C2	2.33	0.51
1:A:772[A]:MET:SD	1:A:880:THR:HG22	2.51	0.51
1:A:1027[B]:ARG:HB3	1:A:1027[B]:ARG:CZ	2.40	0.51
2:D:174:SER:O	2:D:182:PRO:HD3	2.11	0.51
1:E:973:ALA:O	1:E:991:VAL:HG12	2.10	0.51
1:G:143:THR:HA	1:G:296:ILE:HG23	1.93	0.51
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.93	0.51
1:G:479:VAL:HG21	1:G:483:GLY:HA3	1.92	0.51
1:G:891:LYS:NZ	11:G:1678:HOH:O	2.43	0.51
1:A:240:MET:HE3	7:A:1087:ADP:C4	2.45	0.50
2:B:72:SER:HB2	11:B:3543:HOH:O	2.10	0.50
2:B:194:VAL:HB	2:B:216:LEU:CD2	2.38	0.50
1:C:782:ILE:HD13	1:C:793:ALA:C	2.36	0.50
2:F:190:LEU:HD23	2:F:213:GLY:HA2	1.93	0.50
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.39	0.50
1:G:119:THR:HG23	11:G:1763:HOH:O	2.11	0.50
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.11	0.50
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.11	0.50
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.26	0.50
2:H:141:ALA:O	2:H:145:GLU:N	2.39	0.50
1:A:951:GLU:HA	1:A:951:GLU:OE1	2.06	0.50
1:C:1:MET:HB2	1:C:224:LYS:HZ1	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ARG:O	2:D:120:ARG:HG3	2.11	0.50
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.92	0.50
1:G:1:MET:O	1:G:334:GLU:OE1	2.29	0.50
2:H:82:ILE:O	2:H:111:ALA:HA	2.12	0.50
1:A:333:ASP:OD1	1:A:333:ASP:N	2.44	0.50
2:B:245:PRO:HG2	2:B:274:LEU:HD21	1.93	0.50
2:D:246:ALA:HB1	2:D:248:ASP:HB2	1.94	0.50
1:G:577:GLU:O	1:G:580:TYR:HB3	2.12	0.50
2:H:49:SER:O	2:H:50:ARG:HB2	2.11	0.50
2:H:316:VAL:HG12	2:H:337:LEU:HD23	1.93	0.50
1:A:715:ARG:NH2	7:A:1088:ADP:O1A	2.44	0.50
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.41	0.50
2:B:318:GLU:HA	2:B:321:LEU:HD13	1.91	0.50
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.93	0.50
2:D:316:VAL:CG1	2:D:337:LEU:HD23	2.41	0.50
1:G:814:GLN:CG	1:G:818:PHE:HE2	2.25	0.50
2:H:10:GLU:HB2	2:H:128:GLN:HG2	1.94	0.50
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.42	0.50
2:H:153:LEU:O	2:H:154:ASN:C	2.54	0.50
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.47	0.50
2:B:6:LEU:HD11	2:B:8:VAL:HG23	1.94	0.50
1:C:948:SER:OG	10:C:1093:U5P:H5'1	2.11	0.50
2:D:12:GLY:HA2	2:D:144:LEU:HD13	1.92	0.50
1:G:40:GLU:OE1	1:G:325:LYS:HE2	2.12	0.50
1:G:412:LYS:HE2	1:G:434:ASP:CG	2.37	0.50
1:G:796:LEU:HD23	1:G:797:PRO:N	2.27	0.50
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.41	0.50
1:A:467:GLU:O	1:A:471:ARG:HG2	2.12	0.50
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.47	0.50
1:C:675:ARG:H	1:C:675:ARG:HD3	1.77	0.50
1:C:802:SER:O	1:C:806:GLN:HG3	2.12	0.50
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.42	0.50
1:G:358:LYS:HG2	1:G:359:ILE:N	2.19	0.50
2:H:324:ASN:O	2:H:342:ARG:HA	2.10	0.50
1:C:372:ASP:N	11:C:1371:HOH:O	2.30	0.50
1:E:425:ARG:HD3	11:E:1422:HOH:O	2.11	0.50
2:F:154:ASN:ND2	2:F:314:PHE:HZ	2.08	0.50
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.36	0.50
1:G:579:ASP:OD1	1:G:605:THR:HB	2.12	0.50
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.46	0.50
1:C:349:GLU:O	2:D:294:ASN:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:THR:HG22	2:F:24:GLY:N	2.25	0.50
2:F:342:ARG:NE	2:F:344:ASP:OD2	2.45	0.50
2:H:32:PHE:HA	2:H:54:THR:O	2.11	0.50
2:H:161:GLU:OE1	2:H:161:GLU:HA	2.12	0.50
2:B:224:SER:O	2:B:225:ALA:C	2.51	0.49
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.47	0.49
2:D:9:LEU:HD12	2:D:13:THR:HB	1.94	0.49
2:F:281:ALA:HB2	2:F:322:PRO:HD3	1.94	0.49
1:G:9:SER:O	1:G:84:ASP:HB2	2.11	0.49
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.11	0.49
1:G:439:ILE:O	1:G:442:ALA:HB3	2.12	0.49
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.36	0.49
1:A:421:LEU:HB3	1:E:421:LEU:HD13	1.94	0.49
1:C:930:LYS:HE3	11:C:1159:HOH:O	2.11	0.49
1:C:1066:GLN:HB2	11:C:1156:HOH:O	2.12	0.49
1:G:569:PRO:O	1:G:571:ARG:HD2	2.13	0.49
1:A:416:ASP:N	1:A:416:ASP:OD2	2.34	0.49
1:G:697:ALA:HB3	1:G:700:MET:HB2	1.95	0.49
2:H:48:TYR:CZ	2:H:311:ASN:ND2	2.80	0.49
1:C:702:VAL:O	1:C:706:LYS:HD3	2.12	0.49
1:E:735:ARG:O	1:E:738:PHE:HB2	2.13	0.49
1:C:951:GLU:O	1:C:954:LYS:HB2	2.13	0.49
1:E:963:LYS:O	1:E:964:LEU:C	2.53	0.49
2:F:154:ASN:HD22	2:F:285:LYS:HE2	1.76	0.49
1:G:735:ARG:O	1:G:738:PHE:HB2	2.12	0.49
1:A:59:GLU:HG3	11:A:1503:HOH:O	2.13	0.49
2:B:157:ASP:OD1	2:B:160:LYS:HD3	2.13	0.49
1:C:1:MET:CB	1:C:2:PRO:HD2	2.43	0.49
1:C:223:ASP:OD2	1:C:227:ASN:HB2	2.12	0.49
1:C:772:MET:HE1	1:C:880:THR:CA	2.42	0.49
2:D:263:ILE:HG22	2:D:264:PRO:CD	2.40	0.49
2:D:370:PHE:O	2:D:374:ILE:HG13	2.12	0.49
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.48	0.49
1:C:337:ASN:HB3	1:C:340:THR:OG1	2.13	0.49
2:D:2:ILE:HD11	11:D:2829:HOH:O	2.12	0.49
1:E:559:ARG:NH1	11:E:1893:HOH:O	2.44	0.49
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.95	0.49
1:E:695:VAL:HG21	1:E:701:ALA:CA	2.37	0.49
1:G:702:VAL:CG1	1:G:731:GLU:HG3	2.43	0.49
1:G:781:HIS:HE1	1:G:789:SER:HB2	1.76	0.49
2:H:246:ALA:C	2:H:248:ASP:H	2.21	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:O	1:A:334:GLU:OE1	2.30	0.49
1:A:365:GLU:OE2	1:A:365:GLU:N	2.39	0.49
1:A:767:ILE:CD1	1:A:865:ALA:HB2	2.42	0.49
1:C:686:LYS:O	1:C:687:LEU:HD23	2.13	0.49
1:C:950:ARG:HD3	11:C:1583:HOH:O	2.12	0.49
1:E:157:ALA:O	1:E:160:ALA:HB3	2.12	0.49
1:G:1017:THR:HG21	1:G:1023:ILE:CA	2.40	0.49
1:A:358:LYS:HE3	11:A:1128:HOH:O	2.11	0.49
2:B:199:PHE:O	2:B:241:GLY:HA3	2.13	0.49
2:B:376:GLN:O	2:B:376:GLN:HG3	2.13	0.49
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.48	0.49
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.42	0.49
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.43	0.49
1:G:772:MET:HE1	1:G:880:THR:HA	1.94	0.49
2:H:274:LEU:O	2:H:275:LEU:C	2.55	0.49
2:H:310:GLN:OE1	2:H:312:HIS:NE2	2.46	0.49
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.77	0.49
1:A:150:HIS:N	1:A:154:GLU:OE2	2.30	0.49
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.28	0.49
1:A:675:ARG:H	1:A:675:ARG:HD3	1.76	0.49
1:A:735:ARG:O	1:A:736:ARG:C	2.54	0.49
1:A:1006:LYS:O	1:A:1006:LYS:HG3	2.12	0.49
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.43	0.49
1:C:420:ALA:HA	1:C:423[A]:LYS:HD2	1.95	0.49
2:D:342:ARG:HE	2:D:344:ASP:CG	2.19	0.49
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HD13	1.94	0.49
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.94	0.49
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.13	0.48
1:E:110:GLU:HG2	1:E:111:PHE:CD1	2.47	0.48
1:E:493:LYS:HE2	1:E:517:ARG:CD	2.43	0.48
1:E:693:ALA:CB	1:E:708:ILE:HD11	2.38	0.48
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.95	0.48
1:G:170:PRO:HA	1:G:204:LEU:HD23	1.94	0.48
1:G:354:TYR:CD2	1:G:387:ILE:HG23	2.48	0.48
1:G:1021:ARG:O	1:G:1025:ASP:OD2	2.31	0.48
2:H:275:LEU:HD23	2:H:349:SER:HB3	1.95	0.48
2:H:286:MET:HE3	2:H:315:ALA:HB2	1.95	0.48
1:A:347:SER:O	2:B:296:PRO:HB3	2.12	0.48
6:A:1083:CL:CL	11:A:1622:HOH:O	2.57	0.48
1:G:315:THR:O	1:G:531:THR:HG22	2.12	0.48
1:G:772:MET:HE1	1:G:880:THR:CA	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:298:LYS:O	2:H:329:HIS:HA	2.14	0.48
1:A:65:TYR:OH	1:A:80[A]:LYS:HE3	2.14	0.48
1:A:515:LYS:HG3	11:A:1774:HOH:O	2.12	0.48
1:C:68:PRO:HG3	1:C:930:LYS:O	2.13	0.48
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.95	0.48
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.48	0.48
1:G:460:ARG:HG3	11:G:1283:HOH:O	2.11	0.48
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.61	0.48
2:H:355:GLU:OE2	2:H:355:GLU:N	2.42	0.48
1:A:101:GLU:O	1:A:105:GLN:HG2	2.13	0.48
2:B:284:VAL:O	2:B:314:PHE:HA	2.14	0.48
1:E:509:ARG:HH11	1:E:509:ARG:HB2	1.75	0.48
1:E:636:LYS:HD3	11:E:1773:HOH:O	2.12	0.48
1:E:853:VAL:O	1:E:857:THR:HG23	2.13	0.48
1:C:751:LEU:O	1:C:752:LEU:HD12	2.13	0.48
1:E:1004:ARG:NH1	1:E:1009:GLU:OE1	2.41	0.48
2:H:43:LEU:HD21	2:H:80:LEU:HD13	1.95	0.48
2:H:227:ASP:HA	2:H:230:LYS:HD2	1.95	0.48
1:A:145:ARG:HB3	1:A:208:GLU:CD	2.39	0.48
1:C:174:MET:HB3	11:C:1191:HOH:O	2.13	0.48
1:C:361:ARG:NH2	1:C:571:ARG:HG2	2.28	0.48
1:C:726:GLU:HG3	1:C:727:ILE:N	2.27	0.48
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.96	0.48
1:E:128:ASP:OD1	1:E:130:ARG:HB3	2.14	0.48
1:E:1021:ARG:HH11	1:E:1021:ARG:HG3	1.79	0.48
2:F:45:ASP:OD2	2:F:46:PRO:HD2	2.13	0.48
1:G:730:ASP:O	1:G:733:ASP:HB2	2.12	0.48
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.48
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.46	0.48
1:C:626:VAL:O	1:C:630:VAL:HG23	2.13	0.48
2:D:342:ARG:NH2	2:D:344:ASP:OD1	2.30	0.48
1:E:35:LYS:O	1:E:39[B]:GLU:HB2	2.13	0.48
2:F:25:SER:HA	2:F:132:ILE:O	2.14	0.48
1:G:488:PHE:O	1:G:489:LEU:C	2.55	0.48
1:A:151:THR:OG1	1:A:154:GLU:HG3	2.13	0.48
1:A:340:THR:O	1:A:343:ARG:HB2	2.14	0.48
1:A:426:ARG:HD3	1:A:426:ARG:C	2.39	0.48
1:C:267:ALA:O	1:C:271:VAL:HG23	2.14	0.48
2:F:158:LEU:HD12	2:F:243:GLY:HA3	1.95	0.48
2:B:50:ARG:HG2	2:B:158:LEU:HD22	1.95	0.48
2:D:153:LEU:O	2:D:155:GLY:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:LEU:HD21	2:F:140:ALA:HA	1.94	0.48
2:F:195:VAL:HG11	2:F:231:MET:HE1	1.94	0.48
2:F:263:ILE:HG22	2:F:264:PRO:CD	2.40	0.48
1:G:183:TYR:HB2	1:G:187:GLU:OE1	2.14	0.48
1:G:796:LEU:HD23	1:G:796:LEU:C	2.38	0.48
2:H:18:ARG:NH1	2:H:20:ILE:HG22	2.29	0.48
2:H:210:VAL:O	2:H:211:ASP:C	2.57	0.48
2:H:295:HIS:NE2	2:H:333:PHE:HB2	2.29	0.48
1:A:703:GLU:HA	1:A:703:GLU:OE2	2.14	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.13	0.48
2:D:154:ASN:ND2	2:D:314:PHE:HZ	2.12	0.48
1:E:704:LYS:O	1:E:705:ALA:C	2.56	0.48
1:E:950:ARG:HH11	1:E:950:ARG:HD2	1.55	0.48
2:F:342:ARG:NH2	2:F:344:ASP:OD1	2.47	0.48
1:G:563:MET:HB2	1:G:638:VAL:HG22	1.96	0.48
1:G:692:ASN:C	1:G:708:ILE:HD11	2.39	0.48
1:G:1027:ARG:NE	1:G:1031:ARG:HD3	2.28	0.48
1:A:509:ARG:HB2	1:A:509:ARG:CZ	2.44	0.47
2:D:234:ASP:CG	2:D:378:ARG:HH11	2.22	0.47
1:E:494:ARG:HG2	1:E:547:TYR:CB	2.44	0.47
1:E:736:ARG:O	1:E:740:THR:HG23	2.13	0.47
2:F:186:LYS:HB3	2:F:188:ASP:OD2	2.13	0.47
2:H:237:PHE:CE2	2:H:239:SER:HA	2.48	0.47
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.14	0.47
1:A:315:THR:O	1:A:531:THR:HG22	2.14	0.47
1:A:703:GLU:OE2	1:A:706:LYS:NZ	2.36	0.47
2:F:68:ALA:HA	2:F:181:LEU:HD11	1.96	0.47
1:G:563:MET:CB	1:G:638:VAL:HG22	2.44	0.47
2:H:296:PRO:HB2	2:H:332:LEU:HB2	1.97	0.47
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.45	0.47
1:C:70:HIS:O	1:C:73:VAL:N	2.45	0.47
1:C:130:ARG:HG3	1:C:148:ILE:HG13	1.96	0.47
1:C:772:MET:CE	1:C:880:THR:HG22	2.44	0.47
2:D:170:TRP:HB3	2:D:216:LEU:HB2	1.96	0.47
2:H:32:PHE:O	2:H:291:HIS:HB2	2.15	0.47
1:A:1:MET:HB2	1:A:224:LYS:HE3	1.95	0.47
1:E:224:LYS:NZ	11:E:1624:HOH:O	2.42	0.47
1:E:897:PHE:HB3	11:E:1557:HOH:O	2.14	0.47
1:G:49:SER:O	1:G:51:PRO:HD3	2.15	0.47
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.44	0.47
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:HA	1:A:165:PRO:C	2.40	0.47
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.96	0.47
1:C:860:PRO:HB2	1:C:863:LYS:HB2	1.97	0.47
2:D:157:ASP:CG	2:D:160:LYS:HG2	2.40	0.47
2:D:272:HIS:HA	2:D:349:SER:CB	2.44	0.47
1:E:696:THR:OG1	1:E:700:MET:HE1	2.14	0.47
1:G:168:ILE:HG23	1:G:204:LEU:HD22	1.96	0.47
1:G:349:GLU:O	2:H:294:ASN:HB2	2.15	0.47
1:G:698:ILE:H	1:G:698:ILE:CD1	2.27	0.47
1:G:943:GLY:O	1:G:969:PHE:HA	2.14	0.47
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.35	0.47
1:A:446:GLY:C	1:E:447:LEU:HD23	2.40	0.47
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.14	0.47
2:B:272:HIS:HA	2:B:349:SER:HB2	1.95	0.47
2:D:197:TYR:HB3	2:D:199:PHE:CZ	2.50	0.47
2:D:286:MET:HG2	11:D:2883:HOH:O	2.13	0.47
2:D:316:VAL:HG12	2:D:337:LEU:CD2	2.44	0.47
1:E:368:ALA:HA	11:E:1708:HOH:O	2.14	0.47
1:G:772:MET:SD	1:G:880:THR:HG22	2.54	0.47
2:H:251:ALA:O	2:H:255:ILE:HG13	2.15	0.47
2:H:370:PHE:CZ	2:H:374:ILE:HD11	2.49	0.47
1:A:796:LEU:HD23	1:A:796:LEU:C	2.40	0.47
1:A:950:ARG:HD3	11:A:1597:HOH:O	2.14	0.47
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.80	0.47
2:B:291:HIS:HD2	2:B:311:ASN:OD1	1.98	0.47
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.15	0.47
1:C:25:GLU:HG3	1:C:306:ARG:HA	1.96	0.47
1:C:228:CYS:SG	1:C:269:MET:HE2	2.55	0.47
1:C:240:MET:HE3	7:C:1089:ADP:C4	2.50	0.47
1:C:640:VAL:HG21	1:C:651:ALA:HB2	1.97	0.47
1:C:676:GLU:O	1:C:680:HIS:ND1	2.48	0.47
1:C:710:TYR:HA	1:C:711:PRO:C	2.39	0.47
2:D:29:GLU:CD	2:D:153:LEU:HD22	2.39	0.47
2:D:245:PRO:CG	2:D:274:LEU:HD21	2.44	0.47
2:F:174:SER:HB2	2:F:211:ASP:OD2	2.13	0.47
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.49	0.47
1:G:675:ARG:CD	1:G:675:ARG:H	2.26	0.47
1:G:814:GLN:O	1:G:815:LYS:C	2.54	0.47
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.95	0.47
2:H:45:ASP:OD2	2:H:46:PRO:HD2	2.14	0.47
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:363:ALA:HB1	2:H:366:LEU:HD13	1.97	0.47
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.50	0.47
1:C:124:ASP:OD1	1:C:131:ARG:HD3	2.15	0.47
2:D:205:ILE:HG21	2:D:237:PHE:CZ	2.49	0.47
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.96	0.47
2:F:298:LYS:HG2	2:F:299:ASP:N	2.30	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.29	0.47
1:G:699:GLU:OE2	1:G:699:GLU:HA	2.15	0.47
1:A:767:ILE:HD13	1:A:865:ALA:HB2	1.97	0.47
1:C:75:ARG:HG3	1:C:107:VAL:CG1	2.45	0.47
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.96	0.47
1:C:702:VAL:CG1	1:C:731:GLU:HG3	2.45	0.47
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.50	0.47
1:C:1018:SER:O	1:C:1022:ALA:HB3	2.14	0.47
1:E:836:GLU:HB2	1:E:838:TYR:CE2	2.50	0.47
2:F:187:GLU:CG	2:F:215:ARG:HD2	2.43	0.47
2:H:111:ALA:O	2:H:112:ASP:HB2	2.15	0.47
2:H:267:GLY:O	2:H:349:SER:HA	2.14	0.47
1:A:692:ASN:HA	1:A:752:LEU:O	2.15	0.47
1:C:223:ASP:CG	1:C:227:ASN:HB2	2.39	0.47
1:C:695:VAL:HG23	1:C:752:LEU:HD22	1.97	0.47
1:E:1051:ALA:HA	1:E:1054:LEU:HD12	1.96	0.47
2:F:55:LEU:HD13	2:F:60:ILE:HD12	1.95	0.47
1:G:185:ARG:O	1:G:188:PHE:HB3	2.14	0.47
1:G:1004:ARG:O	1:G:1009[B]:GLU:HB2	2.14	0.47
1:A:763:ASP:HB3	1:A:779:MET:HE3	1.96	0.46
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.81	0.46
1:C:689:GLN:O	1:C:690:PRO:C	2.58	0.46
1:E:757:ASP:O	1:E:758:ASP:C	2.58	0.46
1:E:1019:GLY:O	1:E:1023:ILE:HG13	2.15	0.46
1:G:656:ALA:C	1:G:658:GLY:H	2.24	0.46
2:H:318:GLU:HG2	2:H:318:GLU:O	2.14	0.46
1:A:947:LEU:HD12	1:A:947:LEU:N	2.30	0.46
2:D:98:LEU:HD12	2:D:98:LEU:O	2.16	0.46
1:E:481:ILE:HG23	1:E:482:THR:N	2.29	0.46
2:F:324:ASN:ND2	2:F:324:ASN:H	2.07	0.46
1:G:90:MET:HA	1:G:304:VAL:HG22	1.96	0.46
1:G:423:LYS:H	1:G:423:LYS:HG3	1.50	0.46
1:A:514:ARG:HD3	11:A:1461:HOH:O	2.14	0.46
1:C:532:CYS:O	1:C:533:ALA:HB3	2.16	0.46
1:C:784:GLN:O	1:C:784:GLN:HG2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:ARG:HD2	11:G:1750:HOH:O	2.15	0.46
2:D:228:VAL:HG13	2:D:231:MET:HE3	1.98	0.46
2:D:252:ILE:HD13	2:D:277:LEU:HB3	1.97	0.46
2:D:376:GLN:HA	2:D:379:LYS:NZ	2.30	0.46
1:G:735:ARG:O	1:G:736:ARG:C	2.58	0.46
2:H:254:ALA:O	2:H:257:LYS:HB2	2.15	0.46
2:H:301:GLU:OE1	2:H:328:THR:HG22	2.15	0.46
1:A:612:THR:HG22	1:A:612:THR:O	2.15	0.46
1:A:992:ASN:HB2	1:A:999:PRO:O	2.14	0.46
2:B:355:GLU:O	2:B:356:ALA:C	2.58	0.46
2:F:379:LYS:NZ	2:F:379:LYS:HB2	2.30	0.46
1:G:486:ALA:HB2	1:G:520:TYR:CG	2.51	0.46
1:G:734:LEU:HD11	1:G:738:PHE:HE2	1.79	0.46
1:A:166:CYS:C	1:A:167:ILE:HD12	2.41	0.46
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.15	0.46
2:B:41:GLU:HG3	2:B:69:ASP:O	2.16	0.46
2:D:263:ILE:CG2	2:D:264:PRO:HD2	2.42	0.46
1:G:124:ASP:OD1	1:G:131:ARG:HD3	2.16	0.46
1:G:484:LEU:HD22	1:G:489:LEU:HD13	1.98	0.46
1:G:665:SER:HB2	11:G:1668:HOH:O	2.16	0.46
1:G:726:GLU:OE1	1:G:1020:ARG:NE	2.36	0.46
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.45	0.46
1:A:805:ILE:HG22	1:A:806:GLN:N	2.29	0.46
1:E:176:GLY:N	7:E:1089:ADP:O2B	2.41	0.46
1:E:318:PRO:HB2	1:E:321:LYS:HB2	1.97	0.46
1:G:685:LEU:O	1:G:686:LYS:HB2	2.15	0.46
1:G:905:PRO:HB2	1:G:1040:TYR:HH	1.81	0.46
2:H:10:GLU:O	2:H:12:GLY:N	2.48	0.46
2:B:46:PRO:HA	2:B:76:HIS:CB	2.46	0.46
1:C:236:ASN:N	1:C:236:ASN:HD22	2.14	0.46
2:D:331:SER:O	2:D:335:GLY:HA2	2.15	0.46
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.51	0.46
1:G:625:ASP:O	1:G:629:ILE:HG13	2.15	0.46
1:A:157:ALA:O	1:A:160:ALA:HB3	2.16	0.46
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.41	0.46
2:B:363:ALA:C	2:B:365:PRO:HD2	2.41	0.46
1:E:434:ASP:O	1:E:435:ARG:C	2.57	0.46
1:E:783:GLU:OE1	8:E:1091:ORN:NE	2.49	0.46
2:F:269:CYS:O	2:F:270:LEU:C	2.59	0.46
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.46
8:G:1091:ORN:N	11:G:1554:HOH:O	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:ASP:HB3	2:H:48:TYR:CD2	2.50	0.46
2:H:169:SER:HA	2:H:216:LEU:O	2.16	0.46
2:H:364:ALA:O	2:H:366:LEU:N	2.48	0.46
1:A:367:PHE:HB3	1:A:903:VAL:HG21	1.98	0.46
1:A:414:SER:OG	1:A:416:ASP:OD2	2.30	0.46
2:D:154:ASN:ND2	2:D:314:PHE:CZ	2.84	0.46
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.46
1:E:169:ARG:HG2	11:E:1874:HOH:O	2.15	0.46
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.97	0.46
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.98	0.46
1:G:806:GLN:HB3	1:G:810:ARG:NH1	2.31	0.46
2:H:27:VAL:O	2:H:78:GLN:HG2	2.16	0.46
2:H:344:ASP:OD2	2:H:345:LYS:N	2.48	0.46
1:A:585:ALA:HB2	1:A:642:TYR:CE2	2.52	0.45
2:B:263:ILE:HG22	2:B:264:PRO:CD	2.45	0.45
1:C:11:LEU:HA	1:C:45:ILE:O	2.17	0.45
1:E:240:MET:HE3	7:E:1089:ADP:C4	2.51	0.45
1:G:597:ILE:HA	1:G:615:ARG:O	2.15	0.45
2:H:154:ASN:C	2:H:154:ASN:HD22	2.24	0.45
2:H:218:ILE:N	2:H:218:ILE:CD1	2.79	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
1:C:891:LYS:HG2	1:C:892:GLU:N	2.30	0.45
1:E:489:LEU:HD22	1:E:516:LEU:HD23	1.98	0.45
1:E:579:ASP:OD1	1:E:605:THR:HB	2.16	0.45
2:F:222:GLN:HB2	11:F:1487:HOH:O	2.16	0.45
1:G:775:ILE:CD1	1:G:813:VAL:HG11	2.46	0.45
2:H:8:VAL:CG1	2:H:9:LEU:N	2.80	0.45
2:H:158:LEU:O	2:H:159:ALA:C	2.58	0.45
2:H:170:TRP:CD1	2:H:172:GLN:H	2.33	0.45
1:A:671:ARG:CG	1:A:677:ARG:NH1	2.80	0.45
2:B:205:ILE:HG13	2:B:355:GLU:CG	2.46	0.45
1:C:726:GLU:CG	1:C:727:ILE:N	2.79	0.45
1:E:59:GLU:CG	1:E:60:MET:HE2	2.42	0.45
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.34	0.45
1:G:339:ILE:O	1:G:538:THR:OG1	2.29	0.45
1:G:688:LYS:HD2	1:G:838:TYR:CE1	2.52	0.45
2:H:11:ASP:OD2	2:H:13:THR:OG1	2.30	0.45
2:H:272:HIS:CA	2:H:349:SER:HB2	2.41	0.45
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.52	0.45
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.12	0.45
1:C:164:PHE:HA	1:C:165:PRO:C	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:O	1:C:281:GLY:HA2	2.16	0.45
1:C:424:ILE:O	1:C:425:ARG:C	2.58	0.45
2:F:272:HIS:HA	2:F:349:SER:OG	2.15	0.45
1:G:22:GLN:HG3	1:G:174:MET:HE1	1.98	0.45
1:G:502:LEU:O	1:G:505:LEU:HB2	2.17	0.45
2:H:246:ALA:O	2:H:248:ASP:N	2.50	0.45
2:H:352:GLY:O	2:H:354:PRO:HD3	2.16	0.45
2:H:364:ALA:N	2:H:365:PRO:HD2	2.31	0.45
1:A:286:PHE:CD1	1:A:295:LEU:HD11	2.51	0.45
1:A:695:VAL:CG1	1:A:696:THR:N	2.80	0.45
1:C:796:LEU:HD23	1:C:796:LEU:C	2.42	0.45
1:G:70:HIS:O	1:G:71:TRP:C	2.59	0.45
1:G:102:LEU:HD23	1:G:102:LEU:HA	1.82	0.45
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.80	0.45
1:G:941:LYS:HE3	11:G:1704:HOH:O	2.15	0.45
2:H:284:VAL:O	2:H:315:ALA:N	2.45	0.45
1:A:644:GLY:O	1:A:647:PRO:HD2	2.17	0.45
1:A:947:LEU:N	1:A:947:LEU:CD1	2.80	0.45
1:C:103:GLU:HG3	1:C:104:ARG:N	2.31	0.45
1:C:103:GLU:HB2	1:C:108:LEU:HD12	1.99	0.45
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.98	0.45
1:C:577:GLU:O	1:C:580:TYR:HB3	2.17	0.45
1:C:802:SER:OG	1:C:805:ILE:HB	2.16	0.45
1:C:865:ALA:O	1:C:869:MET:HG3	2.16	0.45
1:C:1001:ILE:HD11	11:C:1576:HOH:O	2.16	0.45
2:D:316:VAL:HB	2:D:337:LEU:HD23	1.97	0.45
1:G:257:THR:O	1:G:258:ASP:C	2.56	0.45
2:H:350:PHE:CD1	2:H:366:LEU:HD21	2.51	0.45
1:A:321:LYS:NZ	1:A:611:ASP:OD1	2.45	0.45
1:C:695:VAL:CG1	1:C:696:THR:N	2.80	0.45
1:C:1064:SER:O	1:C:1068:MET:HG3	2.17	0.45
1:E:141:LEU:HD23	1:E:141:LEU:HA	1.69	0.45
1:E:1021:ARG:O	1:E:1025:ASP:OD2	2.34	0.45
2:F:272:HIS:HA	2:F:349:SER:CB	2.47	0.45
1:G:734:LEU:HD12	1:G:734:LEU:C	2.41	0.45
1:G:813:VAL:HA	1:G:816:LEU:HD12	1.98	0.45
2:H:121:LEU:HD11	2:H:125:LYS:HD3	1.99	0.45
2:H:176:THR:O	2:H:177:LEU:C	2.57	0.45
1:A:481:ILE:HG22	11:A:1762:HOH:O	2.16	0.45
1:C:213:TRP:HH2	1:C:294:ARG:HD2	1.82	0.45
1:C:344:THR:HB	1:C:345:PRO:CD	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:PHE:O	1:C:679:GLN:C	2.59	0.45
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.17	0.45
2:F:82:ILE:O	2:F:111:ALA:HA	2.17	0.45
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.47	0.45
2:F:365:PRO:O	2:F:366:LEU:C	2.59	0.45
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.50	0.45
1:G:812:GLN:O	1:G:813:VAL:C	2.60	0.45
2:H:23:THR:HG22	2:H:24:GLY:N	2.31	0.45
1:A:35:LYS:HA	11:A:1142:HOH:O	2.17	0.45
2:B:6:LEU:HD12	2:B:7:LEU:H	1.81	0.45
2:B:369:HIS:O	2:B:373:LEU:HG	2.16	0.45
1:E:726:GLU:CG	1:E:727:ILE:N	2.80	0.45
2:F:111:ALA:O	2:F:112:ASP:HB2	2.17	0.45
1:G:333:ASP:OD1	1:G:333:ASP:N	2.49	0.45
1:G:703:GLU:O	1:G:706:LYS:HB2	2.17	0.45
1:G:998:ARG:HA	1:G:999:PRO:C	2.40	0.45
2:H:153:LEU:N	2:H:153:LEU:CD1	2.79	0.45
1:A:167:ILE:N	1:A:167:ILE:CD1	2.80	0.45
1:A:882:GLU:HB3	11:A:1828:HOH:O	2.17	0.45
1:C:166:CYS:C	1:C:167:ILE:HD12	2.42	0.45
1:C:735:ARG:O	1:C:738:PHE:HB2	2.17	0.45
2:D:50:ARG:NH1	2:D:156:MET:CE	2.80	0.45
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.80	0.45
1:G:65:TYR:CE2	1:G:77:ILE:HG23	2.52	0.45
1:G:265:ARG:O	1:G:269:MET:HG3	2.16	0.45
2:H:232:ASN:N	2:H:233:PRO:CD	2.80	0.45
1:A:148:ILE:CG2	1:A:149:ALA:N	2.80	0.44
2:B:83:ARG:HG3	2:B:83:ARG:NH1	2.32	0.44
1:C:419:GLU:CB	1:C:423[B]:LYS:HZ3	2.29	0.44
2:D:232:ASN:N	2:D:233:PRO:HD3	2.33	0.44
2:F:225:ALA:HB2	2:F:254:ALA:HB1	1.99	0.44
1:G:561:LYS:HG2	1:G:595:GLU:OE2	2.17	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.80	0.44
1:A:82:ARG:N	1:A:83:PRO:CD	2.81	0.44
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.52	0.44
2:B:199:PHE:HB3	2:B:270:LEU:HD23	1.99	0.44
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.44
1:E:730:ASP:OD2	1:E:733:ASP:HB2	2.17	0.44
1:E:1028:VAL:CG1	1:E:1029:ILE:N	2.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:ASP:OD1	2:F:302:LYS:HD2	2.17	0.44
1:G:866:ALA:O	1:G:869:MET:HB2	2.17	0.44
1:G:1021:ARG:CG	1:G:1021:ARG:NH1	2.80	0.44
2:H:18:ARG:NH1	11:H:502:HOH:O	2.50	0.44
2:H:281:ALA:HB2	2:H:322:PRO:HD3	2.00	0.44
1:A:34:CYS:SG	1:A:46:LEU:HD22	2.58	0.44
2:B:272:HIS:HA	2:B:349:SER:CB	2.48	0.44
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.59	0.44
1:G:436:ILE:HG22	11:G:1304:HOH:O	2.16	0.44
1:G:730:ASP:H	1:G:733:ASP:HB2	1.83	0.44
2:H:50:ARG:NH1	2:H:156:MET:CE	2.80	0.44
2:H:286:MET:CE	2:H:312:HIS:CE1	3.00	0.44
2:B:149:ALA:O	2:B:151:PRO:HD3	2.17	0.44
2:B:176:THR:O	2:B:180:GLY:N	2.39	0.44
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.53	0.44
1:C:659:VAL:HG13	1:C:660:PRO:HD2	2.00	0.44
1:C:736:ARG:CZ	1:C:736:ARG:HB3	2.47	0.44
1:E:563:MET:CE	1:E:635:PRO:HG3	2.45	0.44
1:E:692:ASN:HA	1:E:752:LEU:O	2.17	0.44
1:E:734:LEU:O	1:E:737:TYR:HB3	2.16	0.44
1:G:473:GLU:HG2	1:G:505:LEU:HD11	1.98	0.44
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.82	0.44
1:G:1051:ALA:O	1:G:1052:MET:C	2.57	0.44
1:A:702:VAL:O	1:A:706:LYS:HD3	2.17	0.44
1:C:464:VAL:HG21	2:D:88:ILE:HG12	2.00	0.44
1:C:620:PRO:O	1:C:625:ASP:HB2	2.18	0.44
2:D:205:ILE:HG21	2:D:237:PHE:CE2	2.52	0.44
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.83	0.44
1:E:344:THR:HB	1:E:345:PRO:CD	2.46	0.44
1:E:588:ALA:HB2	1:E:863:LYS:HG2	1.99	0.44
1:E:755:PHE:CE1	7:E:1090:ADP:C2	3.05	0.44
2:F:172:GLN:HG2	2:F:173:GLY:N	2.29	0.44
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.82	0.44
1:G:796:LEU:HD23	1:G:797:PRO:CA	2.48	0.44
2:H:324:ASN:N	2:H:324:ASN:ND2	2.30	0.44
2:D:6:LEU:HD21	2:D:140:ALA:HB2	1.99	0.44
1:E:148:ILE:CG2	1:E:149:ALA:N	2.80	0.44
1:E:222:ARG:NE	1:E:226:ASP:OD2	2.49	0.44
1:E:784:GLN:H	1:E:784:GLN:HE21	1.66	0.44
2:F:23:THR:CG2	2:F:24:GLY:N	2.81	0.44
2:F:150:PHE:HA	2:F:151:PRO:HD2	1.88	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:GLY:O	2:F:354:PRO:HD3	2.17	0.44
2:F:365:PRO:O	2:F:368:ASP:N	2.49	0.44
1:G:45:ILE:HA	1:G:63:ALA:O	2.18	0.44
2:H:120:ARG:HD2	11:H:413:HOH:O	2.18	0.44
2:H:153:LEU:CD1	2:H:153:LEU:H	2.30	0.44
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.18	0.44
1:A:560:GLU:OE1	1:A:636:LYS:HD2	2.18	0.44
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.88	0.44
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.53	0.44
1:C:1:MET:O	1:C:334:GLU:OE1	2.36	0.44
2:D:332:LEU:HA	2:D:332:LEU:HD12	1.68	0.44
1:E:755:PHE:CD1	7:E:1090:ADP:C2	3.06	0.44
1:G:1052:MET:O	1:G:1055:ASN:HB2	2.18	0.44
1:A:250:VAL:HA	1:A:356:VAL:O	2.18	0.44
1:A:900:PHE:N	1:A:901:PRO:HD3	2.33	0.44
1:A:994:VAL:CG2	1:A:1001:ILE:HD11	2.48	0.44
2:B:29:GLU:HB2	2:B:153:LEU:HD22	1.99	0.44
2:H:104:ARG:HG2	2:H:105:HIS:HD2	1.82	0.44
1:C:60[A]:MET:HE2	11:C:1495:HOH:O	2.17	0.44
1:C:221:VAL:O	1:C:228:CYS:HA	2.17	0.44
1:C:361:ARG:CZ	1:C:571:ARG:HG2	2.48	0.44
2:D:10:GLU:C	2:D:12:GLY:H	2.26	0.44
2:D:379:LYS:HB3	2:D:379:LYS:HE2	1.75	0.44
1:G:35:LYS:HD2	11:G:1144:HOH:O	2.17	0.44
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.83	0.44
1:G:713:VAL:HG23	1:G:755:PHE:HB2	2.00	0.44
1:G:873:SER:OG	1:G:876:GLU:HB2	2.18	0.44
1:G:1027:ARG:HE	1:G:1031:ARG:CD	2.29	0.44
2:H:350:PHE:CG	2:H:366:LEU:CD2	3.01	0.44
1:A:1001:ILE:HD12	1:A:1002:GLN:CB	2.47	0.43
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.18	0.43
1:C:82:ARG:N	1:C:83:PRO:CD	2.80	0.43
1:C:894:VAL:O	1:C:913:SER:HB2	2.17	0.43
1:E:691:ALA:CB	1:E:708:ILE:HG23	2.47	0.43
1:E:967[B]:GLN:NE2	1:E:1054:LEU:CD1	2.78	0.43
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.98	0.43
2:F:245:PRO:CG	2:F:274:LEU:HD21	2.48	0.43
1:G:664:THR:HG22	1:G:668:ALA:HB3	2.00	0.43
2:H:27:VAL:HG21	2:H:146:LYS:HB3	2.00	0.43
2:B:58:PRO:HA	2:B:83:ARG:HB3	2.00	0.43
1:C:24:CYS:CB	1:C:576:ILE:HD12	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:VAL:HG12	1:C:696:THR:N	2.33	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.99	0.43
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.18	0.43
2:D:376:GLN:HA	2:D:379:LYS:HZ3	1.83	0.43
1:E:674:ASP:O	1:E:675:ARG:C	2.60	0.43
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.83	0.43
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.30	0.43
1:G:560:GLU:OE1	1:G:636:LYS:HE3	2.17	0.43
1:G:738:PHE:HA	1:G:741:ALA:HB3	2.00	0.43
9:G:1092:NET:H22	9:G:1092:NET:C4	2.43	0.43
1:A:45:ILE:HD13	1:A:81:GLU:HB3	2.01	0.43
1:A:235:GLU:HB2	1:A:253:ALA:HA	2.01	0.43
1:A:571:ARG:NH2	11:A:1415:HOH:O	2.27	0.43
2:B:307:ILE:N	2:B:307:ILE:HD13	2.33	0.43
1:C:701:ALA:O	1:C:705:ALA:N	2.40	0.43
1:C:702:VAL:HG11	1:C:735:ARG:HH21	1.79	0.43
2:D:43:LEU:HD21	2:D:80:LEU:HD13	2.00	0.43
1:E:533:ALA:O	1:E:534:ALA:HB3	2.18	0.43
1:E:936:ASN:ND2	11:E:1156:HOH:O	2.52	0.43
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.34	0.43
2:H:195:VAL:HG11	2:H:228:VAL:HG13	1.99	0.43
2:H:270:LEU:HA	2:H:270:LEU:HD12	1.57	0.43
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.53	0.43
1:C:704:LYS:O	1:C:707:GLU:HB2	2.19	0.43
1:C:735:ARG:O	1:C:738:PHE:N	2.50	0.43
9:C:1092:NET:H83	9:C:1092:NET:H11	1.80	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.34	0.43
1:G:178:GLY:CA	1:G:198:LEU:HD23	2.48	0.43
1:G:709:GLY:O	1:G:754:HIS:ND1	2.50	0.43
2:H:132:ILE:CG2	2:H:133:ILE:N	2.81	0.43
2:H:193:HIS:O	2:H:234:ASP:HB2	2.18	0.43
1:C:397:LYS:NZ	1:C:619:GLU:OE1	2.50	0.43
1:C:424:ILE:HD13	1:C:424:ILE:HG21	1.83	0.43
1:C:693:ALA:HB3	1:C:752:LEU:HB2	2.01	0.43
2:D:50:ARG:NH1	2:D:156:MET:HE1	2.34	0.43
2:D:74:GLN:HB2	11:D:2853:HOH:O	2.18	0.43
2:D:199:PHE:CE2	2:D:274:LEU:HD12	2.53	0.43
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.54	0.43
1:E:81:GLU:O	1:E:82:ARG:C	2.57	0.43
1:E:831:ALA:HB2	1:E:840:ILE:HD11	2.01	0.43
1:E:949:VAL:O	1:E:954:LYS:NZ	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:190:LEU:HA	2:F:191:PRO:HD2	1.80	0.43
2:F:342:ARG:HE	2:F:344:ASP:CG	2.27	0.43
2:H:16:HIS:CD2	2:H:16:HIS:N	2.86	0.43
2:H:199:PHE:CE2	2:H:274:LEU:CD1	3.02	0.43
2:H:219:VAL:O	2:H:220:PRO:C	2.62	0.43
2:H:354:PRO:HB3	2:H:363:ALA:O	2.17	0.43
1:A:740:THR:H	1:A:740:THR:HG23	1.51	0.43
1:A:784:GLN:HE22	1:A:1043:THR:HB	1.83	0.43
2:D:350:PHE:HB2	2:D:366:LEU:CD2	2.48	0.43
1:E:998:ARG:HG2	1:E:999:PRO:HA	2.01	0.43
2:F:342:ARG:HD2	2:F:342:ARG:HA	1.79	0.43
2:F:364:ALA:N	2:F:365:PRO:HD2	2.32	0.43
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.18	0.43
2:B:285:LYS:HG3	2:B:314:PHE:CZ	2.52	0.43
1:C:163:GLY:O	1:C:166:CYS:HB3	2.18	0.43
2:D:50:ARG:HH12	2:D:156:MET:CE	2.32	0.43
1:E:17:PRO:HG3	1:E:917:VAL:HG13	2.00	0.43
1:G:106:GLY:HA2	11:G:1176:HOH:O	2.18	0.43
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.19	0.43
1:G:814:GLN:HG3	1:G:818:PHE:CE2	2.53	0.43
1:G:822:VAL:C	1:G:823:ARG:HG2	2.44	0.43
1:A:194:ARG:NH2	11:A:1266:HOH:O	2.30	0.43
1:A:891:LYS:NZ	11:A:1825:HOH:O	2.51	0.43
2:B:350:PHE:CD1	2:B:366:LEU:HD21	2.53	0.43
1:C:28:TYR:CE1	1:C:313:LYS:HE3	2.53	0.43
1:C:678:PHE:O	1:C:681:ALA:N	2.52	0.43
2:D:6:LEU:HD13	2:D:16:HIS:ND1	2.34	0.43
2:D:41:GLU:HB2	2:D:358:PRO:HD3	2.01	0.43
2:D:168:TYR:O	2:D:218:ILE:N	2.43	0.43
2:D:272:HIS:HB2	2:D:349:SER:HB2	2.01	0.43
1:E:761:GLU:HG2	1:E:781:HIS:CE1	2.54	0.43
1:E:974:THR:O	1:E:975:HIS:C	2.62	0.43
2:F:46:PRO:HA	2:F:76:HIS:CG	2.53	0.43
1:G:218:MET:HE3	1:G:264:MET:SD	2.59	0.43
1:G:772:MET:HE1	1:G:880:THR:CB	2.49	0.43
2:H:300:VAL:HG22	2:H:328:THR:O	2.19	0.43
2:B:187:GLU:C	2:B:189:GLU:H	2.26	0.43
1:C:375:THR:HG23	1:C:377:GLN:H	1.84	0.43
1:C:772:MET:HE1	1:C:880:THR:HA	1.99	0.43
2:D:201:ALA:CB	2:D:239:SER:HB2	2.48	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:LEU:O	1:G:211:ILE:C	2.61	0.43
1:G:472:LEU:O	1:G:476:VAL:HG23	2.18	0.43
2:H:201:ALA:HB2	2:H:239:SER:HB2	2.01	0.43
2:H:332:LEU:HA	2:H:332:LEU:HD12	1.59	0.43
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.43
2:B:201:ALA:HB2	2:B:239:SER:HB2	1.99	0.43
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.54	0.43
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.43
1:C:891:LYS:HE3	1:C:893:VAL:HG12	2.01	0.43
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.49	0.43
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.48	0.43
2:H:54:THR:HG23	2:H:81:VAL:CG1	2.48	0.43
1:A:702:VAL:HG11	1:A:735:ARG:NH2	2.34	0.42
2:B:342:ARG:NE	2:B:344:ASP:OD2	2.51	0.42
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.74	0.42
1:E:646:THR:HB	1:E:647:PRO:HD3	2.00	0.42
1:E:836:GLU:HG3	11:E:1817:HOH:O	2.18	0.42
1:E:948:SER:OG	10:E:1093:U5P:H5'1	2.18	0.42
2:F:87:LEU:HD12	2:F:87:LEU:HA	1.69	0.42
1:G:82:ARG:NH1	11:G:1744:HOH:O	2.52	0.42
1:G:692:ASN:HB3	1:G:753:ASP:OD2	2.19	0.42
1:G:738:PHE:C	1:G:741:ALA:HB3	2.43	0.42
1:G:762:VAL:CG1	1:G:763:ASP:N	2.81	0.42
2:H:210:VAL:HA	2:H:214:CYS:O	2.19	0.42
1:A:425[A]:ARG:NH1	11:A:1430:HOH:O	2.32	0.42
2:B:268:ILE:HD13	2:B:354:PRO:HD2	2.00	0.42
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	2.00	0.42
1:E:458:ILE:O	1:E:463:LEU:HD11	2.19	0.42
1:E:1021:ARG:CG	1:E:1021:ARG:NH1	2.80	0.42
2:F:379:LYS:NZ	2:F:379:LYS:CB	2.82	0.42
1:G:652[A]:ARG:HH12	1:G:667:ASP:HA	1.81	0.42
1:G:885:PRO:HA	1:G:886:PRO:HD3	1.66	0.42
2:H:5:ALA:HB1	2:H:110:ILE:HG13	2.01	0.42
2:H:132:ILE:C	2:H:133:ILE:HG13	2.43	0.42
2:H:163:THR:OG1	2:H:198:ASP:O	2.37	0.42
2:H:219:VAL:HG23	2:H:220:PRO:O	2.19	0.42
1:A:67:GLU:OE1	1:A:1062:VAL:HA	2.19	0.42
1:A:840:ILE:O	1:A:841:GLU:HB3	2.19	0.42
2:B:255:ILE:HD13	2:B:274:LEU:HB3	2.01	0.42
1:C:579:ASP:O	1:C:580:TYR:C	2.62	0.42
1:C:681:ALA:O	1:C:682:VAL:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:ILE:HD13	1:C:775:ILE:HA	1.84	0.42
1:E:26:PHE:HA	1:E:29[B]:SER:OG	2.19	0.42
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.19	0.42
1:G:671:ARG:NH2	1:G:819:GLU:O	2.52	0.42
2:H:168:TYR:CD1	2:H:168:TYR:N	2.87	0.42
2:B:369:HIS:O	2:B:372:GLU:HB2	2.20	0.42
1:C:864:VAL:O	1:C:868:VAL:HG23	2.19	0.42
1:E:867:ARG:O	1:E:868:VAL:C	2.59	0.42
2:F:23:THR:HG23	2:F:134:ALA:O	2.19	0.42
1:G:51:PRO:C	1:G:53:THR:H	2.28	0.42
2:H:29:GLU:HA	2:H:129:ASN:HA	1.99	0.42
2:H:256:GLN:HG3	2:H:278:ALA:HB1	2.01	0.42
1:C:435:ARG:HB2	11:C:1376:HOH:O	2.20	0.42
2:F:218:ILE:HD13	2:F:218:ILE:N	2.34	0.42
1:G:105:GLN:NE2	1:G:105:GLN:CA	2.82	0.42
1:G:191:ILE:O	1:G:192:CYS:C	2.63	0.42
1:G:421:LEU:HD21	1:G:445:ALA:HB1	2.00	0.42
1:G:479:VAL:HG23	1:G:480:GLY:O	2.19	0.42
1:G:734:LEU:O	1:G:737:TYR:HB3	2.18	0.42
1:G:772:MET:CE	1:G:880:THR:HA	2.49	0.42
2:H:45:ASP:O	2:H:76:HIS:HB2	2.18	0.42
2:H:275:LEU:CD2	2:H:349:SER:HB3	2.48	0.42
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.62	0.42
1:C:932:GLN:HG3	11:C:1554:HOH:O	2.19	0.42
2:D:325:LEU:HA	2:D:325:LEU:HD23	1.52	0.42
1:E:1:MET:O	1:E:329:GLY:O	2.38	0.42
1:E:6:ASP:OD2	1:E:6:ASP:N	2.42	0.42
2:F:188:ASP:OD2	2:F:188:ASP:N	2.52	0.42
1:G:630:VAL:HG13	1:G:635:PRO:CD	2.50	0.42
1:G:924:PHE:O	1:G:925:ALA:C	2.58	0.42
2:B:172:GLN:HA	11:B:3559:HOH:O	2.18	0.42
1:C:737:TYR:O	1:C:738:PHE:C	2.62	0.42
2:D:71:GLU:O	2:D:203:ARG:HG3	2.20	0.42
2:D:286:MET:HE2	2:D:315:ALA:HB2	2.02	0.42
2:F:6:LEU:HD23	2:F:138:PRO:HB2	2.02	0.42
2:F:205:ILE:HG12	2:F:355:GLU:HG3	2.02	0.42
1:G:130:ARG:O	1:G:134:VAL:HG23	2.19	0.42
1:A:339:ILE:HD13	1:A:339:ILE:HG21	1.79	0.42
1:C:980:VAL:HG13	11:C:1568:HOH:O	2.20	0.42
2:D:228:VAL:O	2:D:229:LEU:C	2.63	0.42
2:D:236:ILE:HB	2:D:265:VAL:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:764:VAL:HA	1:E:777:GLY:O	2.20	0.42
1:G:40:GLU:CD	1:G:325:LYS:HE2	2.45	0.42
1:G:318:PRO:HB2	1:G:321:LYS:HB2	2.01	0.42
1:G:762:VAL:CG2	1:G:801:LEU:HD11	2.49	0.42
1:G:874:LEU:O	1:G:875:ALA:C	2.63	0.42
2:H:208:MET:SD	2:H:355:GLU:HA	2.59	0.42
1:A:954:LYS:HB3	1:A:980:VAL:HG21	2.01	0.42
1:C:183:TYR:N	1:C:187:GLU:OE1	2.33	0.42
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.41	0.42
1:C:827:ASN:N	1:C:843:ASN:O	2.51	0.42
1:C:954:LYS:HG2	1:C:980:VAL:HG21	2.01	0.42
2:D:85:LEU:HD12	2:D:86:PRO:HD2	2.02	0.42
1:E:863:LYS:NZ	11:E:1496:HOH:O	2.51	0.42
2:F:195:VAL:HG11	2:F:231:MET:CE	2.50	0.42
2:F:274:LEU:HD23	2:F:274:LEU:HA	1.61	0.42
1:G:530:ASP:O	1:G:531:THR:OG1	2.29	0.42
1:G:948:SER:O	1:G:1015:ASN:HA	2.19	0.42
2:H:158:LEU:O	2:H:161:GLU:HB2	2.19	0.42
2:H:318:GLU:HA	2:H:337:LEU:HD22	2.01	0.42
1:A:44:VAL:O	1:A:62:ASP:HB2	2.20	0.42
1:A:185:ARG:HH11	1:A:185:ARG:HD3	1.73	0.42
1:A:370:ALA:HB2	1:A:903:VAL:HG23	2.00	0.42
1:A:897:PHE:HB3	11:A:1561:HOH:O	2.20	0.42
1:C:132:PHE:O	1:C:136:MET:HG2	2.20	0.42
1:C:974:THR:O	1:C:975:HIS:C	2.63	0.42
1:E:65:TYR:OH	1:E:80:LYS:HE3	2.20	0.42
2:F:303:ASN:C	2:F:304:VAL:HG13	2.45	0.42
1:G:37:LEU:HD23	1:G:37:LEU:HA	1.81	0.42
1:G:256:LEU:HD23	1:G:256:LEU:HA	1.91	0.42
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.23	0.42
1:G:698:ILE:N	1:G:698:ILE:CD1	2.83	0.42
1:G:893:VAL:HA	1:G:916:GLU:HA	2.02	0.42
2:H:193:HIS:HD2	2:H:194:VAL:N	2.18	0.42
2:H:272:HIS:HE1	2:H:340:ILE:HG12	1.83	0.42
1:A:14:GLY:HA2	11:A:1098:HOH:O	2.20	0.41
1:A:804:GLU:HB3	11:A:1837:HOH:O	2.19	0.41
1:A:817:ALA:HB2	1:A:826:MET:SD	2.60	0.41
2:B:29:GLU:CB	2:B:153:LEU:HD22	2.50	0.41
2:D:102:LEU:O	2:D:103:LYS:C	2.63	0.41
1:E:1:MET:H1	1:E:224:LYS:HE3	1.83	0.41
1:E:76:LYS:HA	1:E:76:LYS:HD2	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:677:ARG:O	1:E:680:HIS:HB2	2.20	0.41
2:F:239:SER:OG	2:F:240:ASN:O	2.38	0.41
1:G:425:ARG:NH1	11:G:1403:HOH:O	2.50	0.41
2:H:49:SER:C	2:H:51:GLN:H	2.28	0.41
2:H:289:GLY:O	2:H:290:HIS:HD2	2.03	0.41
2:H:307:ILE:O	2:H:362:ASP:HB2	2.20	0.41
1:A:318:PRO:HG3	1:A:610:TYR:OH	2.20	0.41
1:A:757:ASP:O	1:A:758:ASP:C	2.63	0.41
1:A:990:LEU:HD21	1:G:975:HIS:CE1	2.55	0.41
2:B:190:LEU:HD12	2:B:215:ARG:HB2	2.02	0.41
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.57	0.41
1:C:222:ARG:HD3	1:C:277:VAL:O	2.20	0.41
1:C:679:GLN:HG3	1:C:689:GLN:HE22	1.84	0.41
1:C:779:MET:HE3	1:C:779:MET:HB2	1.88	0.41
1:C:956:ARG:HD3	1:C:1044:LEU:HD23	2.02	0.41
1:E:652:ARG:HD3	1:E:666:PRO:HB2	2.01	0.41
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.50	0.41
1:G:686:LYS:O	1:G:687:LEU:HD23	2.21	0.41
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.34	0.41
2:H:272:HIS:ND1	2:H:349:SER:OG	2.51	0.41
2:H:299:ASP:HB3	2:H:304:VAL:HG22	2.01	0.41
2:H:354:PRO:HA	2:H:363:ALA:HB3	2.03	0.41
1:A:221:VAL:HA	1:A:281:GLY:HA2	2.01	0.41
1:A:225:ASN:CG	1:A:331:THR:HG21	2.45	0.41
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.48	0.41
2:B:228:VAL:CG1	2:B:258:PHE:CE1	3.00	0.41
1:C:6:ASP:OD2	1:C:6:ASP:N	2.43	0.41
1:C:57:ASP:OD1	1:C:584:HIS:NE2	2.46	0.41
1:C:384:VAL:HG22	1:C:385:MET:N	2.35	0.41
1:E:106:GLY:HA2	11:E:1178:HOH:O	2.20	0.41
1:G:1001:ILE:CD1	1:G:1029:ILE:HD11	2.51	0.41
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.55	0.41
2:D:8:VAL:HG12	2:D:9:LEU:O	2.20	0.41
2:D:324:ASN:O	2:D:342:ARG:HA	2.20	0.41
1:E:734:LEU:CD1	1:E:738:PHE:CE2	3.00	0.41
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.56	0.41
1:G:402:LEU:O	1:G:403:GLU:HB2	2.20	0.41
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.49	0.41
1:G:992:ASN:HA	1:G:996:GLU:OE1	2.19	0.41
2:H:272:HIS:HD2	2:H:351:GLN:NE2	2.19	0.41
1:A:543:MET:CE	1:A:617:TYR:CZ	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LEU:HA	1:A:896:PRO:HD3	1.90	0.41
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.45	0.41
2:B:141:ALA:O	2:B:145:GLU:HB2	2.20	0.41
2:B:286:MET:HE3	2:B:313:GLY:C	2.46	0.41
1:C:48:ASN:O	1:C:66:ILE:HA	2.20	0.41
1:C:176:GLY:HA3	1:C:376:THR:O	2.20	0.41
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.20	0.41
1:C:457:ASN:ND2	11:C:1288:HOH:O	2.53	0.41
1:C:493:LYS:NZ	1:C:499:ASP:OD2	2.51	0.41
2:D:48:TYR:HA	2:D:51:GLN:NE2	2.35	0.41
1:E:1:MET:CB	1:E:224:LYS:NZ	2.80	0.41
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.55	0.41
1:E:671:ARG:CG	1:E:677:ARG:NH1	2.84	0.41
1:E:715:ARG:HG2	1:E:725:MET:HE2	2.03	0.41
2:F:237:PHE:CE2	2:F:239:SER:HA	2.56	0.41
2:F:270:LEU:HD12	2:F:270:LEU:HA	1.79	0.41
2:F:317:ASP:CG	2:F:320:THR:HG23	2.45	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.83	0.41
1:G:633:GLU:O	1:G:634:LYS:C	2.63	0.41
1:G:637:GLY:HA2	1:G:660:PRO:O	2.20	0.41
1:G:772:MET:HE1	1:G:880:THR:HG22	2.01	0.41
1:G:948:SER:HG	10:G:1093:U5P:H5'1	1.84	0.41
1:G:992:ASN:ND2	1:G:996:GLU:HB3	2.35	0.41
1:A:367:PHE:O	1:A:370:ALA:HB3	2.20	0.41
2:B:357:SER:HA	2:B:358:PRO:HA	1.76	0.41
1:C:278:GLU:C	1:C:279:THR:HG23	2.45	0.41
1:C:761:GLU:OE2	1:C:785:ALA:HA	2.20	0.41
2:D:245:PRO:HG2	2:D:274:LEU:CD2	2.50	0.41
1:E:954:LYS:NZ	10:E:1093:U5P:O3P	2.30	0.41
1:G:804:GLU:HB3	11:G:1688:HOH:O	2.21	0.41
1:G:853:VAL:HG12	1:G:861:LEU:HD11	2.03	0.41
1:G:1065:VAL:O	1:G:1068:MET:HB2	2.21	0.41
2:H:23:THR:HG23	2:H:134:ALA:O	2.21	0.41
2:H:158:LEU:HD23	2:H:158:LEU:HA	1.70	0.41
1:A:1001:ILE:CD1	1:A:1002:GLN:N	2.80	0.41
2:B:251:ALA:O	2:B:252:ILE:C	2.64	0.41
2:B:300:VAL:HG22	2:B:328:THR:O	2.20	0.41
1:C:75:ARG:HG3	1:C:107:VAL:HG11	2.02	0.41
1:C:903:VAL:HG22	11:C:1369:HOH:O	2.20	0.41
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.36	0.41
2:F:324:ASN:O	2:F:342:ARG:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:CB	1:G:224:LYS:HZ2	2.18	0.41
1:G:11:LEU:HA	1:G:45:ILE:O	2.21	0.41
1:G:362:PHE:CE1	1:G:380:SER:HB3	2.55	0.41
1:G:618:PHE:C	1:G:619:GLU:HG2	2.46	0.41
1:G:701:ALA:O	1:G:702:VAL:C	2.64	0.41
1:G:805:ILE:HD13	1:G:832:VAL:HG11	2.02	0.41
1:G:883:VAL:HG12	1:G:884:ILE:N	2.33	0.41
1:G:1000:HIS:O	1:G:1001:ILE:C	2.64	0.41
2:H:20:ILE:O	2:H:99:SER:OG	2.35	0.41
1:A:130[B]:ARG:HD2	11:A:1197:HOH:O	2.19	0.41
1:A:259:LYS:HD3	2:B:175:TRP:CD2	2.55	0.41
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.56	0.41
2:B:255:ILE:CD1	2:B:274:LEU:HB3	2.50	0.41
2:B:332:LEU:HA	2:B:332:LEU:HD12	1.76	0.41
1:C:655:GLU:CD	1:C:666:PRO:HG2	2.46	0.41
1:C:761:GLU:CG	1:C:781:HIS:CE1	3.03	0.41
2:D:303:ASN:C	2:D:304:VAL:HG13	2.46	0.41
2:F:286:MET:CE	2:F:312:HIS:ND1	2.82	0.41
1:G:115:MET:HG2	1:G:118:ALA:O	2.21	0.41
1:G:667:ASP:O	1:G:668:ALA:C	2.64	0.41
2:H:23:THR:CG2	2:H:24:GLY:N	2.84	0.41
2:H:247:PRO:CA	2:H:252:ILE:CD1	2.99	0.41
2:H:350:PHE:CD2	2:H:354:PRO:HD3	2.56	0.41
2:H:374:ILE:O	2:H:378:ARG:HG3	2.20	0.41
1:A:773:VAL:CG2	1:A:814:GLN:HG3	2.51	0.41
2:B:133:ILE:HD13	2:B:133:ILE:HG21	1.73	0.41
2:B:187:GLU:O	2:B:189:GLU:N	2.53	0.41
2:B:246:ALA:C	2:B:248:ASP:H	2.29	0.41
2:B:246:ALA:C	2:B:248:ASP:N	2.79	0.41
2:B:350:PHE:HB2	2:B:366:LEU:HD23	2.01	0.41
1:C:205:LEU:C	1:C:206:ILE:HG13	2.45	0.41
1:C:503:ALA:O	1:C:504:LYS:C	2.63	0.41
1:C:750:VAL:HG12	1:C:752:LEU:CD1	2.51	0.41
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.21	0.41
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.01	0.41
1:E:1063:ILE:CG1	1:E:1064:SER:N	2.84	0.41
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.56	0.41
1:G:187:GLU:O	1:G:191:ILE:HG13	2.20	0.41
1:G:812:GLN:O	1:G:816:LEU:HD12	2.21	0.41
1:G:830:PHE:CE1	1:G:839:LEU:CD1	3.04	0.41
1:G:875:ALA:HB2	11:G:1504:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:883:VAL:CG1	1:G:884:ILE:N	2.80	0.41
2:H:245:PRO:HG3	2:H:274:LEU:HG	2.02	0.41
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.51	0.41
1:A:677:ARG:HD2	11:A:1807:HOH:O	2.21	0.41
1:A:820:LEU:O	1:A:821:GLN:HB2	2.20	0.41
1:C:1051:ALA:HA	1:C:1054:LEU:HD12	2.03	0.41
2:D:228:VAL:HG12	2:D:229:LEU:N	2.34	0.41
2:D:376:GLN:O	2:D:377:TYR:C	2.62	0.41
1:E:570:ASN:HB2	11:E:1629:HOH:O	2.21	0.41
1:E:576:ILE:HD13	1:E:576:ILE:HG21	1.88	0.41
10:E:1093:U5P:H6	10:E:1093:U5P:H2'	1.95	0.41
2:F:356:ALA:O	2:F:357:SER:HB3	2.21	0.41
1:G:148:ILE:HG22	1:G:149:ALA:N	2.36	0.41
1:G:524:PRO:CG	1:G:628:GLU:HG3	2.50	0.41
1:G:814:GLN:CG	1:G:818:PHE:CE2	3.03	0.41
1:G:947:LEU:HD12	1:G:947:LEU:N	2.36	0.41
2:B:9:LEU:O	2:B:10:GLU:C	2.64	0.40
1:C:500:ALA:O	1:C:504:LYS:HG3	2.21	0.40
1:C:796:LEU:HA	1:C:797:PRO:HA	1.94	0.40
2:D:32:PHE:O	2:D:291:HIS:HB2	2.21	0.40
2:D:150:PHE:HA	2:D:151:PRO:HD3	1.76	0.40
1:G:339:ILE:HG22	1:G:540:THR:OG1	2.21	0.40
1:G:561:LYS:HE2	1:G:595:GLU:OE2	2.21	0.40
1:G:715:ARG:HG2	1:G:725:MET:HE2	2.03	0.40
1:G:1001:ILE:HG21	1:G:1001:ILE:HD13	1.69	0.40
2:H:228:VAL:C	2:H:230:LYS:N	2.80	0.40
1:A:48:ASN:O	1:A:66:ILE:HA	2.21	0.40
1:A:999:PRO:HD2	1:G:983:GLU:OE1	2.20	0.40
1:C:85:ALA:HA	1:C:114:THR:O	2.21	0.40
1:C:1021:ARG:O	1:C:1025:ASP:OD2	2.39	0.40
2:D:246:ALA:CB	2:D:248:ASP:HB2	2.51	0.40
2:D:270:LEU:O	2:D:273:GLN:HB2	2.20	0.40
2:D:365:PRO:O	2:D:366:LEU:C	2.63	0.40
1:E:9:SER:HA	1:E:43:ARG:O	2.20	0.40
1:E:135:ALA:HB1	1:E:274:GLU:CG	2.51	0.40
1:G:67:GLU:HB3	1:G:68:PRO:HD2	2.02	0.40
1:G:479:VAL:HG23	1:G:483:GLY:CA	2.48	0.40
1:G:586:SER:O	1:G:587:LEU:C	2.61	0.40
1:G:775:ILE:HD11	1:G:813:VAL:HG11	2.02	0.40
1:G:991:VAL:HG22	1:G:1001:ILE:HG23	2.03	0.40
2:H:199:PHE:CE2	2:H:274:LEU:HD12	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:ASP:CG	2:H:378:ARG:HH11	2.27	0.40
1:A:51:PRO:HG3	1:A:918:MET:HB2	2.02	0.40
1:A:354:TYR:CD2	1:A:387:ILE:HG23	2.56	0.40
1:A:397:LYS:NZ	1:A:619:GLU:OE1	2.50	0.40
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.87	0.40
1:A:726:GLU:CG	1:A:727:ILE:N	2.79	0.40
2:B:187:GLU:C	2:B:189:GLU:N	2.80	0.40
2:B:277:LEU:C	2:B:279:SER:H	2.27	0.40
1:C:22:GLN:HG3	1:C:26:PHE:CE2	2.57	0.40
1:C:36:ALA:O	1:C:40:GLU:HG2	2.21	0.40
1:C:237:PHE:HB3	1:C:248:ILE:O	2.20	0.40
2:F:367:PHE:O	2:F:368:ASP:C	2.62	0.40
1:G:972:ASP:HA	1:G:989:ARG:O	2.21	0.40
1:A:58:PRO:HD2	1:A:59:GLU:OE2	2.22	0.40
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.39	0.40
1:A:930:LYS:NZ	1:A:1058:ALA:O	2.51	0.40
1:A:992:ASN:O	1:A:1000:HIS:HA	2.22	0.40
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.97	0.40
2:B:186:LYS:HB3	2:B:188:ASP:OD2	2.22	0.40
1:C:4:ARG:NE	1:C:7:ILE:HD12	2.37	0.40
1:C:76:LYS:HA	1:C:76:LYS:HD2	1.96	0.40
2:D:98:LEU:HD12	2:D:98:LEU:C	2.45	0.40
2:D:193:HIS:CD2	2:D:193:HIS:C	2.99	0.40
1:E:110:GLU:CD	1:E:111:PHE:CE1	3.00	0.40
1:E:765:ASP:O	1:E:776:GLY:N	2.49	0.40
2:F:316:VAL:HB	2:F:337:LEU:HD23	2.03	0.40
1:G:540:THR:HG22	1:G:541:ALA:N	2.36	0.40
1:G:695:VAL:HG23	1:G:752:LEU:HD22	2.03	0.40
2:H:225:ALA:O	2:H:229:LEU:HD12	2.22	0.40
2:H:277:LEU:HD23	2:H:277:LEU:HA	1.95	0.40
1:A:702:VAL:CG1	1:A:731:GLU:CG	2.99	0.40
2:B:142:LEU:O	2:B:143:ALA:C	2.65	0.40
2:B:183:GLU:O	2:B:184:ALA:C	2.65	0.40
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.66	0.40
1:C:70:HIS:O	1:C:71:TRP:C	2.64	0.40
1:C:124:ASP:O	1:C:128:ASP:HB3	2.22	0.40
1:C:677:ARG:O	1:C:680:HIS:HB2	2.22	0.40
1:E:361:ARG:NH2	1:E:571:ARG:HG2	2.37	0.40
1:E:695:VAL:CG1	1:E:696:THR:N	2.84	0.40
1:G:85:ALA:HA	1:G:114:THR:O	2.22	0.40
1:G:220:VAL:O	1:G:281:GLY:HA2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:HH12	2:H:156:MET:CE	2.30	0.40

All (1) 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)
11:A:1848:HOH:O	11:C:1912:HOH:O[4_555]	2.14	0.06

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	1061/1073 (99%)	1015 (96%)	44 (4%)	2 (0%)	43	44
1	C	1060/1073 (99%)	1005 (95%)	54 (5%)	1 (0%)	48	50
1	E	1057/1073 (98%)	1013 (96%)	42 (4%)	2 (0%)	43	44
1	G	1061/1073 (99%)	996 (94%)	59 (6%)	6 (1%)	21	18
2	B	377/382 (99%)	348 (92%)	26 (7%)	3 (1%)	16	12
2	D	378/382 (99%)	354 (94%)	23 (6%)	1 (0%)	36	36
2	F	377/382 (99%)	355 (94%)	21 (6%)	1 (0%)	36	36
2	H	377/382 (99%)	346 (92%)	27 (7%)	4 (1%)	11	8
All	All	5748/5820 (99%)	5432 (94%)	296 (5%)	20 (0%)	36	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154	ASN
2	D	154	ASN
1	E	738	PHE
1	G	485	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	975	HIS
2	H	11	ASP
1	A	558	ASP
2	F	311	ASN
2	H	247	PRO
1	G	798	ALA
2	B	188	ASP
1	C	368	ALA
1	E	954	LYS
1	G	739	GLN
1	G	736	ARG
2	H	10	GLU
2	H	365	PRO
1	A	88	PRO
2	B	191	PRO
1	G	871	GLY

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	874/878 (100%)	806 (92%)	68 (8%)	11	9
1	C	873/878 (99%)	802 (92%)	71 (8%)	11	8
1	E	870/878 (99%)	806 (93%)	64 (7%)	13	10
1	G	874/878 (100%)	790 (90%)	84 (10%)	8	5
2	B	308/310 (99%)	276 (90%)	32 (10%)	7	4
2	D	309/310 (100%)	276 (89%)	33 (11%)	6	4
2	F	308/310 (99%)	272 (88%)	36 (12%)	5	3
2	H	308/310 (99%)	269 (87%)	39 (13%)	4	2
All	All	4724/4752 (99%)	4297 (91%)	427 (9%)	9	6

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	8	LYS
1	A	38	ARG
1	A	103	GLU
1	A	104	ARG
1	A	148	ILE
1	A	174	MET
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	412	LYS
1	A	422	THR
1	A	428	LEU
1	A	479	VAL
1	A	482	THR
1	A	509	ARG
1	A	519	GLN
1	A	548	GLU
1	A	556	SER
1	A	559	ARG
1	A	571	ARG
1	A	591	GLU
1	A	652	ARG
1	A	671	ARG
1	A	675	ARG
1	A	676	GLU
1	A	679	GLN
1	A	688	LYS
1	A	700	MET
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	751	LEU
1	A	752	LEU
1	A	763	ASP
1	A	784	GLN
1	A	800	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	804	GLU
1	A	805	ILE
1	A	815	LYS
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	881	LYS
1	A	891	LYS
1	A	895	LEU
1	A	912	ARG
1	A	930	LYS
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	967[A]	GLN
1	A	967[B]	GLN
1	A	992	ASN
1	A	1001	ILE
1	A	1006	LYS
1	A	1018	SER
1	A	1020	ARG
1	A	1031	ARG
1	A	1044	LEU
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	18	ARG
2	B	49	SER
2	B	50	ARG
2	B	78	GLN
2	B	87	LEU
2	B	125	LYS
2	B	142	LEU
2	B	153	LEU
2	B	154	ASN
2	B	192	PHE
2	B	195	VAL
2	B	215	ARG
2	B	219	VAL
2	B	227	ASP
2	B	239	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	248	ASP
2	B	249	ASP
2	B	252	ILE
2	B	253	THR
2	B	261	THR
2	B	263	ILE
2	B	282	LYS
2	B	284	VAL
2	B	321	LEU
2	B	324	ASN
2	B	331	SER
2	B	332	LEU
2	B	333	PHE
2	B	376	GLN
2	B	379	LYS
1	C	5	THR
1	C	8	LYS
1	C	10	ILE
1	C	38	ARG
1	C	76	LYS
1	C	103	GLU
1	C	185	ARG
1	C	202	LYS
1	C	236	ASN
1	C	275	ILE
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	419	GLU
1	C	423[A]	LYS
1	C	423[B]	LYS
1	C	428	LEU
1	C	482	THR
1	C	509	ARG
1	C	519	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	548	GLU
1	C	563	MET
1	C	571	ARG
1	C	645	GLN
1	C	652	ARG
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	688	LYS
1	C	689	GLN
1	C	696	THR
1	C	702	VAL
1	C	704	LYS
1	C	706	LYS
1	C	714	VAL
1	C	725	MET
1	C	728	VAL
1	C	733	ASP
1	C	735	ARG
1	C	750	VAL
1	C	751	LEU
1	C	752	LEU
1	C	763	ASP
1	C	774	LEU
1	C	784	GLN
1	C	805	ILE
1	C	812	GLN
1	C	855	LYS
1	C	880	THR
1	C	881	LYS
1	C	912	ARG
1	C	950	ARG
1	C	951	GLU
1	C	956	ARG
1	C	966	LYS
1	C	967[A]	GLN
1	C	967[B]	GLN
1	C	1001	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1061	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1063	ILE
1	C	1073	LYS
2	D	2	ILE
2	D	4	SER
2	D	27	VAL
2	D	37	THR
2	D	47	SER
2	D	49	SER
2	D	73	SER
2	D	87	LEU
2	D	100	SER
2	D	125	LYS
2	D	153	LEU
2	D	154	ASN
2	D	156	MET
2	D	166	GLU
2	D	215	ARG
2	D	231	MET
2	D	248	ASP
2	D	249	ASP
2	D	252	ILE
2	D	261	THR
2	D	275	LEU
2	D	282	LYS
2	D	284	VAL
2	D	306	MET
2	D	321	LEU
2	D	324	ASN
2	D	332	LEU
2	D	333	PHE
2	D	357	SER
2	D	362	ASP
2	D	366	LEU
2	D	376	GLN
2	D	379	LYS
1	E	3	LYS
1	E	5	THR
1	E	46	LEU
1	E	80	LYS
1	E	103	GLU
1	E	115	MET
1	E	167	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	174	MET
1	E	185	ARG
1	E	220	VAL
1	E	236	ASN
1	E	250	VAL
1	E	275	ILE
1	E	299	GLU
1	E	300	MET
1	E	326	LEU
1	E	358	LYS
1	E	363	ASN
1	E	412	LYS
1	E	479	VAL
1	E	509	ARG
1	E	518	ASP
1	E	548	GLU
1	E	571	ARG
1	E	591	GLU
1	E	645[A]	GLN
1	E	645[B]	GLN
1	E	671	ARG
1	E	675	ARG
1	E	677	ARG
1	E	686	LYS
1	E	688	LYS
1	E	695	VAL
1	E	696	THR
1	E	698	ILE
1	E	704	LYS
1	E	706	LYS
1	E	712	LEU
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	763	ASP
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	838	TYR
1	E	849	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	855	LYS
1	E	912	ARG
1	E	940	LYS
1	E	949	VAL
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	983	GLU
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1072	ILE
1	E	1073	LYS
2	F	2	ILE
2	F	4	SER
2	F	6	LEU
2	F	18	ARG
2	F	25	SER
2	F	27	VAL
2	F	73	SER
2	F	87	LEU
2	F	113	ILE
2	F	125	LYS
2	F	154	ASN
2	F	166	GLU
2	F	175	TRP
2	F	186	LYS
2	F	190	LEU
2	F	210	VAL
2	F	218	ILE
2	F	236	ILE
2	F	238	LEU
2	F	239	SER
2	F	249	ASP
2	F	256	GLN
2	F	257	LYS
2	F	261	THR
2	F	263	ILE
2	F	269	CYS
2	F	282	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	284	VAL
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	333	PHE
2	F	366	LEU
2	F	376	GLN
2	F	379	LYS
1	G	4	ARG
1	G	8	LYS
1	G	20	ILE
1	G	46	LEU
1	G	55	MET
1	G	59	GLU
1	G	82	ARG
1	G	103	GLU
1	G	119	THR
1	G	145	ARG
1	G	185	ARG
1	G	202	LYS
1	G	224	LYS
1	G	230	ILE
1	G	236	ASN
1	G	282	SER
1	G	300	MET
1	G	303	ARG
1	G	307	SER
1	G	326	LEU
1	G	344	THR
1	G	358	LYS
1	G	412	LYS
1	G	422	THR
1	G	428	LEU
1	G	479	VAL
1	G	493	LYS
1	G	509	ARG
1	G	519	GLN
1	G	548	GLU
1	G	562	ILE
1	G	571	ARG
1	G	591	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	645[A]	GLN
1	G	645[B]	GLN
1	G	648	LEU
1	G	652[A]	ARG
1	G	652[B]	ARG
1	G	675	ARG
1	G	677	ARG
1	G	683	GLU
1	G	688	LYS
1	G	692	ASN
1	G	696	THR
1	G	700	MET
1	G	706	LYS
1	G	708	ILE
1	G	712	LEU
1	G	714	VAL
1	G	725	MET
1	G	726	GLU
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	763	ASP
1	G	772	MET
1	G	774	LEU
1	G	782	ILE
1	G	784	GLN
1	G	805	ILE
1	G	810	ARG
1	G	849	THR
1	G	855	LYS
1	G	879	VAL
1	G	880	THR
1	G	884	ILE
1	G	912	ARG
1	G	940	LYS
1	G	951	GLU
1	G	955	GLU
1	G	956	ARG
1	G	967[A]	GLN
1	G	967[B]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	991	VAL
1	G	1006	LYS
1	G	1014	ILE
1	G	1018	SER
1	G	1021	ARG
1	G	1027	ARG
1	G	1031	ARG
1	G	1061	LYS
1	G	1073	LYS
2	H	2	ILE
2	H	3	LYS
2	H	6	LEU
2	H	18	ARG
2	H	42	ILE
2	H	50	ARG
2	H	52	ILE
2	H	60	ILE
2	H	104	ARG
2	H	108	VAL
2	H	110	ILE
2	H	120	ARG
2	H	125	LYS
2	H	128	GLN
2	H	131	CYS
2	H	154	ASN
2	H	166	GLU
2	H	174	SER
2	H	215	ARG
2	H	217	THR
2	H	218	ILE
2	H	219	VAL
2	H	239	SER
2	H	248	ASP
2	H	249	ASP
2	H	257	LYS
2	H	261	THR
2	H	263	ILE
2	H	279	SER
2	H	282	LYS
2	H	284	VAL
2	H	285	LYS
2	H	306	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	324	ASN
2	H	332	LEU
2	H	333	PHE
2	H	340	ILE
2	H	376	GLN
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	337	ASN
1	A	391	GLN
1	A	679	GLN
1	A	689	GLN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	827	ASN
1	A	834	ASN
1	A	835	ASN
1	A	843	ASN
1	A	898	ASN
1	A	936	ASN
1	A	992	ASN
1	A	995	HIS
1	A	1000	HIS
1	A	1015	ASN
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	154	ASN
2	B	232	ASN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	391	GLN
1	C	457	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	689	GLN
1	C	692	ASN
1	C	784	GLN
1	C	806	GLN
1	C	827	ASN
1	C	835	ASN
1	C	843	ASN
1	C	936	ASN
1	C	942	HIS
1	C	992	ASN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	291	HIS
2	D	324	ASN
1	E	105	GLN
1	E	225	ASN
1	E	266	ASN
1	E	391	GLN
1	E	491	GLN
1	E	679	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	806	GLN
1	E	814	GLN
1	E	898	ASN
1	E	936	ASN
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1002	GLN
1	E	1035	GLN
1	E	1055	ASN
2	F	51	GLN
2	F	78	GLN
2	F	154	ASN
2	F	273	GLN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	337	ASN
1	G	523	HIS
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN
1	G	803	GLN
1	G	843	ASN
1	G	898	ASN
1	G	936	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	78	GLN
2	H	154	ASN
2	H	291	HIS
2	H	311	ASN
2	H	324	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 61 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NET	E	1092	-	8,8,8	0.41	0	10,10,10	0.78	0
8	ORN	C	1091	-	7,8,8	1.20	1 (14%)	6,9,9	1.15	1 (16%)
10	U5P	E	1093	-	22,22,22	0.99	1 (4%)	32,33,33	1.64	6 (18%)
5	PO4	E	1078	3	4,4,4	2.59	3 (75%)	6,6,6	1.39	1 (16%)
7	ADP	E	1090	3	28,29,29	1.28	3 (10%)	43,45,45	0.93	2 (4%)
7	ADP	A	1088	3	28,29,29	1.27	1 (3%)	43,45,45	0.87	1 (2%)
8	ORN	G	1091	-	7,8,8	0.87	0	6,9,9	0.90	0
10	U5P	A	1091	-	22,22,22	0.87	1 (4%)	32,33,33	0.84	0
9	NET	C	1092	-	8,8,8	0.52	0	10,10,10	0.79	0
9	NET	G	1092	-	8,8,8	0.75	0	10,10,10	0.49	0
10	U5P	G	1093	-	22,22,22	0.96	1 (4%)	32,33,33	1.48	3 (9%)
7	ADP	C	1090	3	28,29,29	1.07	1 (3%)	43,45,45	1.01	3 (6%)
7	ADP	E	1089	3	28,29,29	1.33	3 (10%)	43,45,45	0.97	2 (4%)
7	ADP	G	1090	3	28,29,29	1.16	2 (7%)	43,45,45	0.92	3 (6%)
5	PO4	G	1078	3	4,4,4	2.39	3 (75%)	6,6,6	1.24	1 (16%)
10	U5P	C	1093	-	22,22,22	0.85	1 (4%)	32,33,33	0.93	1 (3%)
7	ADP	G	1089	3	28,29,29	1.22	3 (10%)	43,45,45	1.10	4 (9%)
8	ORN	E	1091	-	7,8,8	1.11	1 (14%)	6,9,9	0.97	0
5	PO4	C	1078	3	4,4,4	2.37	3 (75%)	6,6,6	1.09	0
7	ADP	C	1089	3	28,29,29	1.88	5 (17%)	43,45,45	1.05	2 (4%)
7	ADP	A	1087	3	28,29,29	1.39	3 (10%)	43,45,45	0.82	0
5	PO4	C	1088	-	4,4,4	2.60	3 (75%)	6,6,6	1.01	0
5	PO4	A	1078	3	4,4,4	2.00	1 (25%)	6,6,6	1.43	1 (16%)
8	ORN	A	1089	-	7,8,8	0.91	0	6,9,9	1.70	1 (16%)
9	NET	A	1090	-	8,8,8	0.75	0	10,10,10	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NET	E	1092	-	-	0/12/12/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ORN	C	1091	-	-	6/8/8/8	-
10	U5P	E	1093	-	-	6/10/26/26	0/2/2/2
7	ADP	E	1090	3	-	4/16/32/32	0/3/3/3
7	ADP	A	1088	3	-	4/16/32/32	0/3/3/3
8	ORN	G	1091	-	-	6/8/8/8	-
10	U5P	A	1091	-	-	6/10/26/26	0/2/2/2
9	NET	C	1092	-	-	0/12/12/12	-
9	NET	G	1092	-	-	0/12/12/12	-
10	U5P	G	1093	-	-	6/10/26/26	0/2/2/2
7	ADP	C	1090	3	-	4/16/32/32	0/3/3/3
7	ADP	E	1089	3	-	2/16/32/32	0/3/3/3
7	ADP	G	1090	3	-	0/16/32/32	0/3/3/3
10	U5P	C	1093	-	-	5/10/26/26	0/2/2/2
7	ADP	G	1089	3	-	2/16/32/32	0/3/3/3
8	ORN	E	1091	-	-	6/8/8/8	-
7	ADP	A	1087	3	-	1/16/32/32	0/3/3/3
7	ADP	C	1089	3	-	2/16/32/32	0/3/3/3
8	ORN	A	1089	-	-	6/8/8/8	-
9	NET	A	1090	-	-	3/12/12/12	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1089	ADP	PA-O3A	-6.95	1.52	1.59
7	A	1087	ADP	PA-O3A	-4.43	1.54	1.59
7	A	1088	ADP	PA-O3A	-4.21	1.55	1.59
5	C	1088	PO4	P-O2	-3.58	1.44	1.54
7	E	1089	ADP	PA-O3A	-3.48	1.55	1.59
5	E	1078	PO4	P-O3	-3.39	1.44	1.54
7	E	1090	ADP	O2'-C2'	3.12	1.50	1.43
5	G	1078	PO4	P-O2	-3.09	1.45	1.54
5	C	1078	PO4	P-O2	-3.08	1.45	1.54
5	E	1078	PO4	P-O2	-3.04	1.45	1.54
10	E	1093	U5P	P-O3P	3.00	1.65	1.54
10	C	1093	U5P	P-O3P	3.00	1.65	1.54
7	C	1089	ADP	O2'-C2'	2.99	1.50	1.43
7	E	1090	ADP	O3'-C3'	2.96	1.50	1.43
7	G	1089	ADP	O2'-C2'	2.93	1.50	1.43
10	A	1091	U5P	P-O3P	2.90	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1093	U5P	P-O3P	2.80	1.65	1.54
5	C	1078	PO4	P-O3	-2.75	1.46	1.54
7	G	1090	ADP	O3'-C3'	2.74	1.49	1.43
7	A	1087	ADP	C2-N1	2.69	1.38	1.33
5	C	1088	PO4	P-O3	-2.67	1.46	1.54
7	E	1089	ADP	O3'-C3'	2.66	1.49	1.43
7	C	1089	ADP	C2-N1	2.62	1.38	1.33
7	A	1087	ADP	O3'-C3'	2.62	1.49	1.43
7	C	1089	ADP	C8-N7	2.57	1.36	1.31
7	E	1090	ADP	C2-N1	2.57	1.38	1.33
5	G	1078	PO4	P-O3	-2.53	1.47	1.54
5	C	1088	PO4	P-O4	-2.50	1.47	1.54
5	A	1078	PO4	P-O1	-2.46	1.45	1.50
7	C	1090	ADP	O3'-C3'	2.44	1.49	1.43
8	C	1091	ORN	O-C	2.27	1.28	1.22
7	G	1089	ADP	C2-N1	2.24	1.37	1.33
7	G	1090	ADP	O2'-C2'	2.21	1.48	1.43
5	G	1078	PO4	P-O4	-2.20	1.48	1.54
8	E	1091	ORN	O-C	2.15	1.28	1.22
7	E	1089	ADP	O2'-C2'	2.14	1.48	1.43
5	C	1078	PO4	P-O4	-2.14	1.48	1.54
7	G	1089	ADP	O4'-C1'	-2.14	1.37	1.42
5	E	1078	PO4	P-O4	-2.13	1.48	1.54
7	C	1089	ADP	C4-N9	2.10	1.42	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	1093	U5P	O3P-P-O5'	-5.05	93.51	106.67
10	G	1093	U5P	O3P-P-O5'	-4.42	95.14	106.67
10	G	1093	U5P	O2P-P-O5'	3.35	115.41	106.67
7	E	1090	ADP	O2A-PA-O3A	3.24	116.03	107.27
7	G	1089	ADP	N6-C6-N1	3.13	125.34	118.38
8	A	1089	ORN	CB-CA-C	-3.10	102.24	110.45
7	E	1089	ADP	O2A-PA-O3A	2.95	115.24	107.27
7	C	1089	ADP	O2'-C2'-C3'	2.71	120.51	111.82
10	E	1093	U5P	O5'-P-O1P	2.69	113.71	106.44
7	C	1090	ADP	O3'-C3'-C2'	2.68	120.40	111.82
5	A	1078	PO4	O2-P-O1	-2.67	101.49	110.95
10	E	1093	U5P	O2P-P-O5'	2.52	113.24	106.67
7	C	1090	ADP	O2A-PA-O3A	2.50	114.03	107.27
7	G	1090	ADP	C2'-C3'-C4'	-2.43	97.91	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1090	ADP	O4'-C4'-C5'	-2.42	101.57	109.33
10	G	1093	U5P	O4'-C1'-N1	2.32	113.61	108.36
7	G	1089	ADP	O3'-C3'-C2'	2.29	119.14	111.82
7	G	1090	ADP	O2'-C2'-C3'	2.26	119.05	111.82
7	E	1090	ADP	O3'-C3'-C2'	2.21	118.89	111.82
10	E	1093	U5P	O2'-C2'-C1'	2.20	117.69	110.10
7	G	1089	ADP	O4'-C1'-N9	-2.14	103.98	108.09
5	E	1078	PO4	O2-P-O1	-2.12	103.44	110.95
5	G	1078	PO4	O4-P-O3	2.12	114.50	107.91
7	E	1089	ADP	O3'-C3'-C2'	2.10	118.54	111.82
8	C	1091	ORN	CB-CA-C	-2.07	104.95	110.45
10	E	1093	U5P	C3'-C2'-C1'	2.07	105.38	101.46
10	E	1093	U5P	C6-N1-C2	-2.05	118.50	121.00
7	A	1088	ADP	O2'-C2'-C3'	2.04	118.37	111.82
10	C	1093	U5P	O2P-P-O5'	2.02	111.92	106.67
7	G	1089	ADP	O4'-C4'-C3'	-2.01	101.17	105.15
7	C	1089	ADP	N9-C8-N7	-2.00	111.09	113.94
7	C	1090	ADP	O2B-PB-O3A	2.00	111.35	104.64

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1090	ADP	PA-O3A-PB-O3B
7	E	1090	ADP	PA-O3A-PB-O3B
8	A	1089	ORN	N-CA-CB-CG
8	A	1089	ORN	C-CA-CB-CG
8	C	1091	ORN	N-CA-CB-CG
8	C	1091	ORN	C-CA-CB-CG
8	E	1091	ORN	N-CA-CB-CG
8	E	1091	ORN	C-CA-CB-CG
8	G	1091	ORN	N-CA-CB-CG
8	G	1091	ORN	C-CA-CB-CG
10	E	1093	U5P	O4'-C4'-C5'-O5'
10	G	1093	U5P	O4'-C4'-C5'-O5'
10	E	1093	U5P	C3'-C4'-C5'-O5'
8	G	1091	ORN	CA-CB-CG-CD
8	C	1091	ORN	OXT-C-CA-N
10	C	1093	U5P	C2'-C1'-N1-C6
10	E	1093	U5P	C2'-C1'-N1-C6
10	G	1093	U5P	C2'-C1'-N1-C6
8	E	1091	ORN	OXT-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	G	1091	ORN	OXT-C-CA-N
10	G	1093	U5P	C3'-C4'-C5'-O5'
8	E	1091	ORN	CA-CB-CG-CD
8	C	1091	ORN	CA-CB-CG-CD
8	C	1091	ORN	O-C-CA-N
8	E	1091	ORN	O-C-CA-N
8	G	1091	ORN	O-C-CA-N
10	A	1091	U5P	C2'-C1'-N1-C6
7	A	1088	ADP	PA-O3A-PB-O1B
7	A	1088	ADP	PA-O3A-PB-O3B
7	C	1089	ADP	PA-O3A-PB-O2B
8	A	1089	ORN	NE-CD-CG-CB
8	G	1091	ORN	NE-CD-CG-CB
10	G	1093	U5P	C2'-C1'-N1-C2
10	E	1093	U5P	O4'-C1'-N1-C6
10	G	1093	U5P	O4'-C1'-N1-C2
10	E	1093	U5P	C2'-C1'-N1-C2
10	A	1091	U5P	O4'-C1'-N1-C6
10	C	1093	U5P	O4'-C1'-N1-C6
10	A	1091	U5P	O4'-C4'-C5'-O5'
7	C	1089	ADP	C5'-O5'-PA-O1A
7	E	1089	ADP	C5'-O5'-PA-O1A
10	E	1093	U5P	O4'-C1'-N1-C2
7	E	1090	ADP	PA-O3A-PB-O1B
10	C	1093	U5P	C2'-C1'-N1-C2
8	A	1089	ORN	OXT-C-CA-N
9	A	1090	NET	C8-C7-N1-C1
10	C	1093	U5P	O4'-C1'-N1-C2
10	G	1093	U5P	O4'-C1'-N1-C6
9	A	1090	NET	C8-C7-N1-C5
7	A	1088	ADP	PB-O3A-PA-O2A
8	A	1089	ORN	CA-CB-CG-CD
8	C	1091	ORN	NE-CD-CG-CB
8	A	1089	ORN	O-C-CA-N
7	E	1090	ADP	PB-O3A-PA-O2A
10	A	1091	U5P	O4'-C1'-N1-C2
10	A	1091	U5P	C3'-C4'-C5'-O5'
10	C	1093	U5P	C5'-O5'-P-O2P
7	C	1090	ADP	PA-O3A-PB-O1B
7	A	1087	ADP	PB-O3A-PA-O2A
7	A	1088	ADP	PB-O3A-PA-O1A
7	C	1090	ADP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	1091	U5P	C2'-C1'-N1-C2
8	E	1091	ORN	O-C-CA-CB
9	A	1090	NET	C8-C7-N1-C3
7	C	1090	ADP	PB-O3A-PA-O1A
7	E	1089	ADP	PB-O3A-PA-O2A
7	E	1090	ADP	PB-O3A-PA-O1A
7	G	1089	ADP	PB-O3A-PA-O1A
7	G	1089	ADP	PB-O3A-PA-O2A

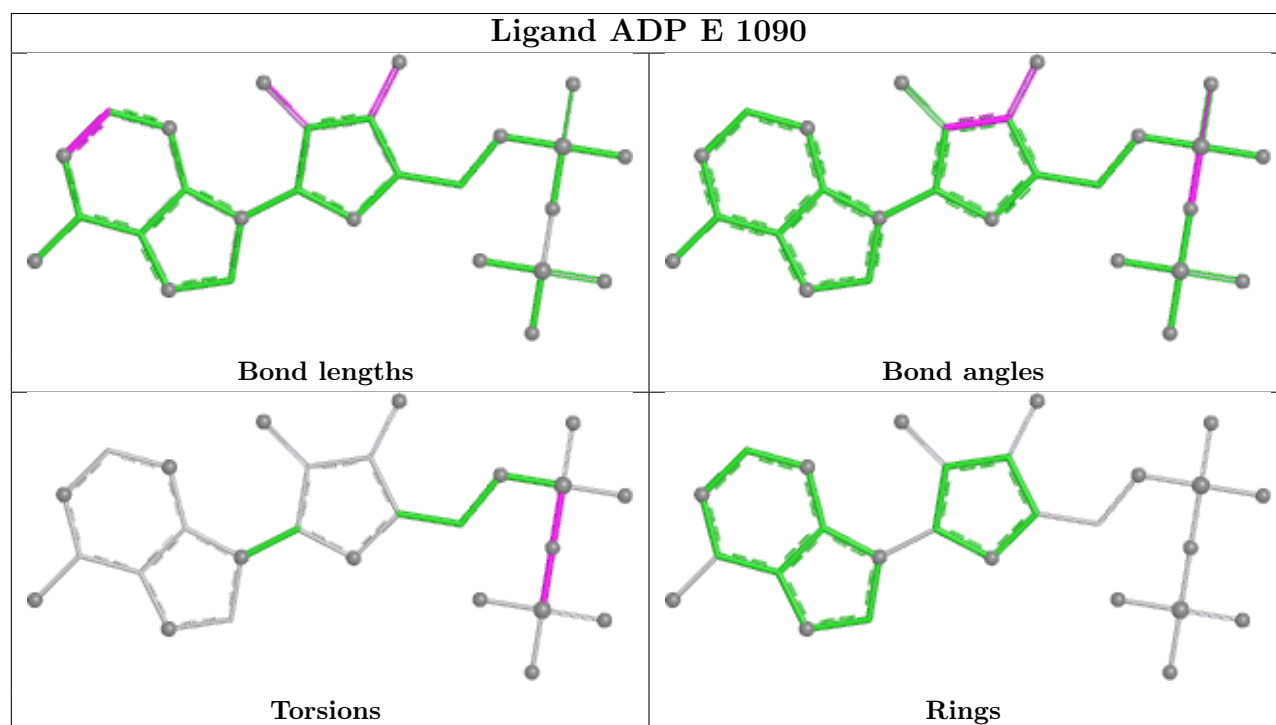
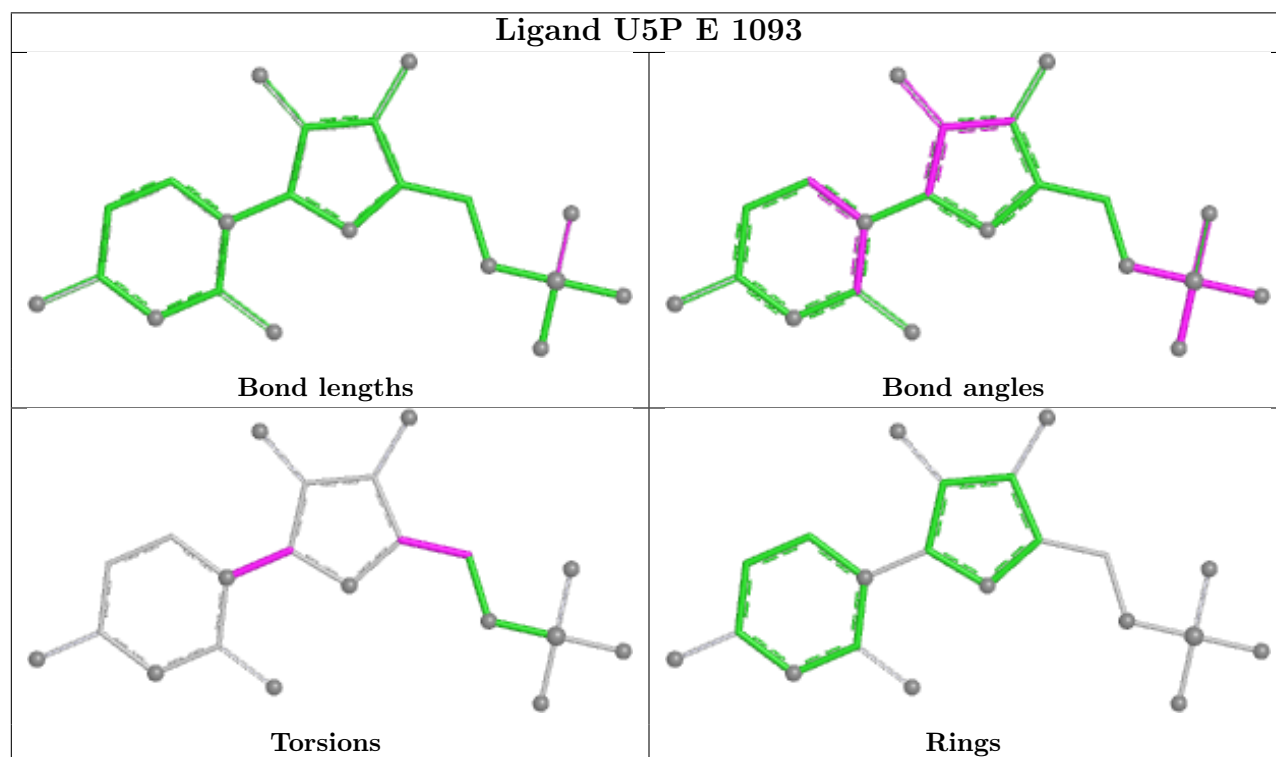
There are no ring outliers.

18 monomers are involved in 26 short contacts:

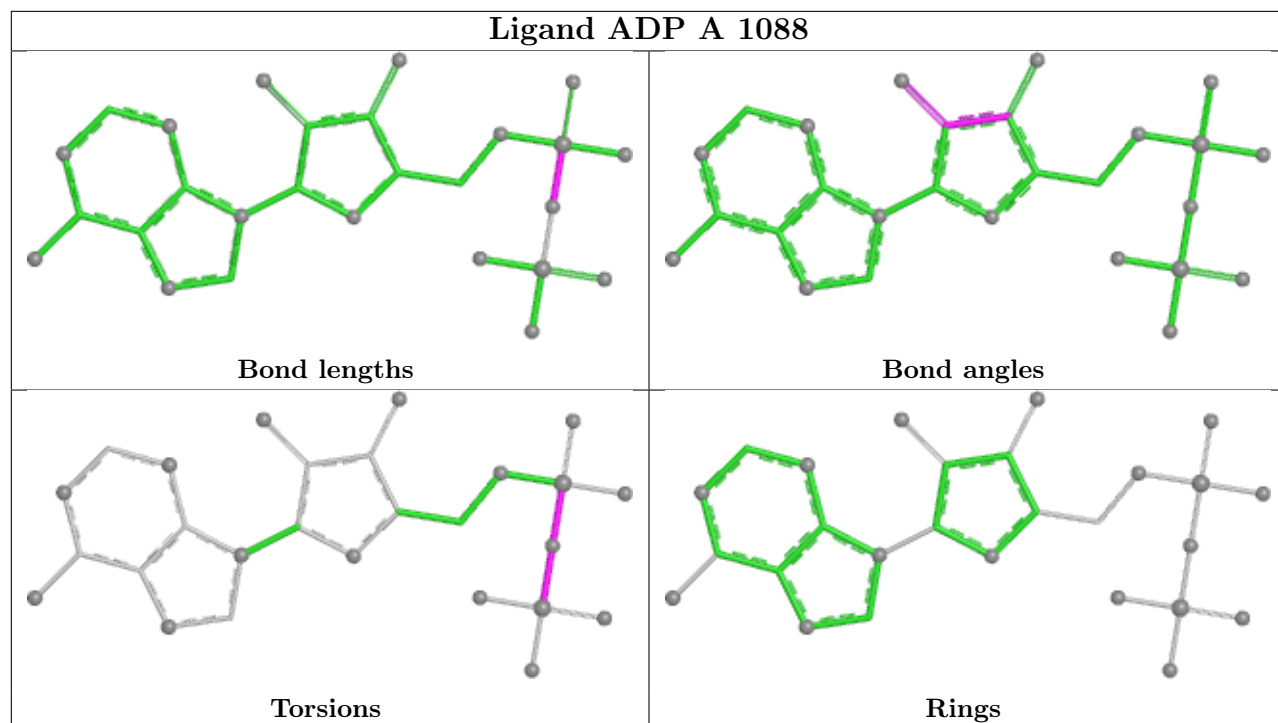
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	1092	NET	2	0
8	C	1091	ORN	1	0
10	E	1093	U5P	3	0
7	E	1090	ADP	2	0
7	A	1088	ADP	1	0
8	G	1091	ORN	1	0
10	A	1091	U5P	1	0
9	C	1092	NET	1	0
9	G	1092	NET	2	0
10	G	1093	U5P	2	0
7	E	1089	ADP	2	0
10	C	1093	U5P	1	0
7	G	1089	ADP	1	0
8	E	1091	ORN	2	0
5	C	1078	PO4	1	0
7	C	1089	ADP	1	0
7	A	1087	ADP	1	0
9	A	1090	NET	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

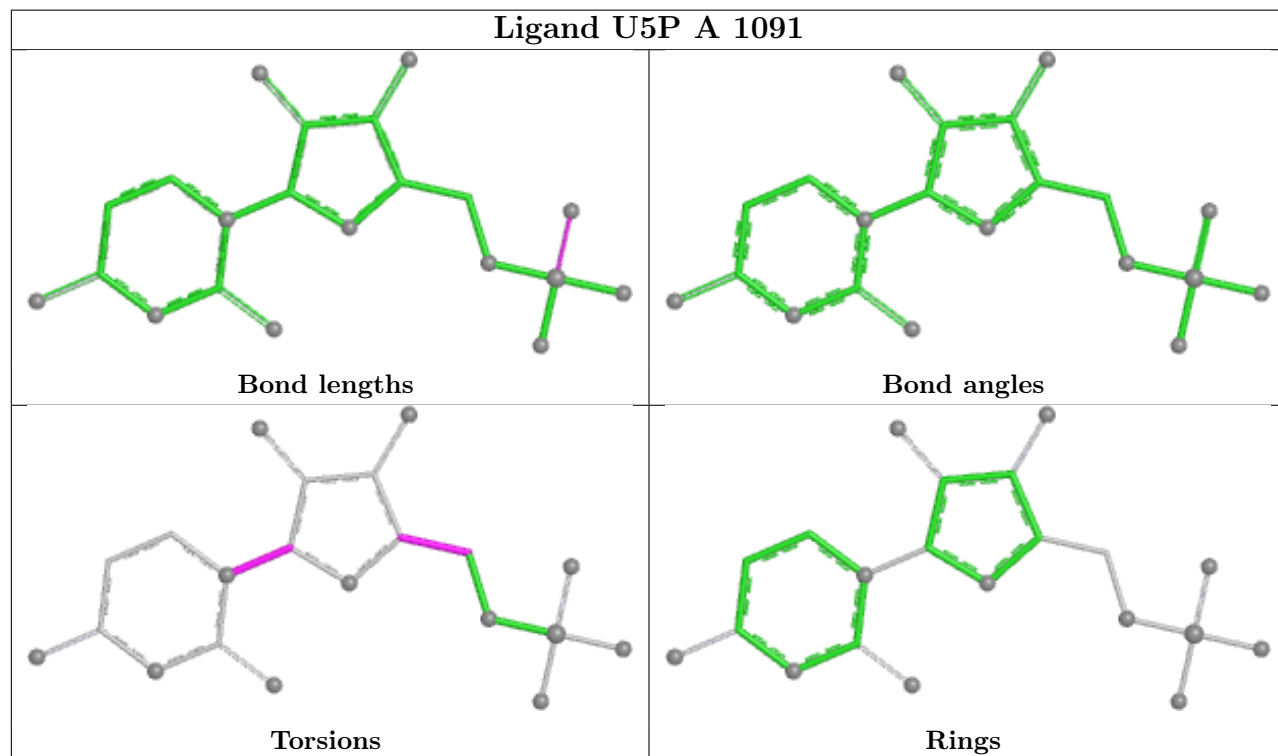
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



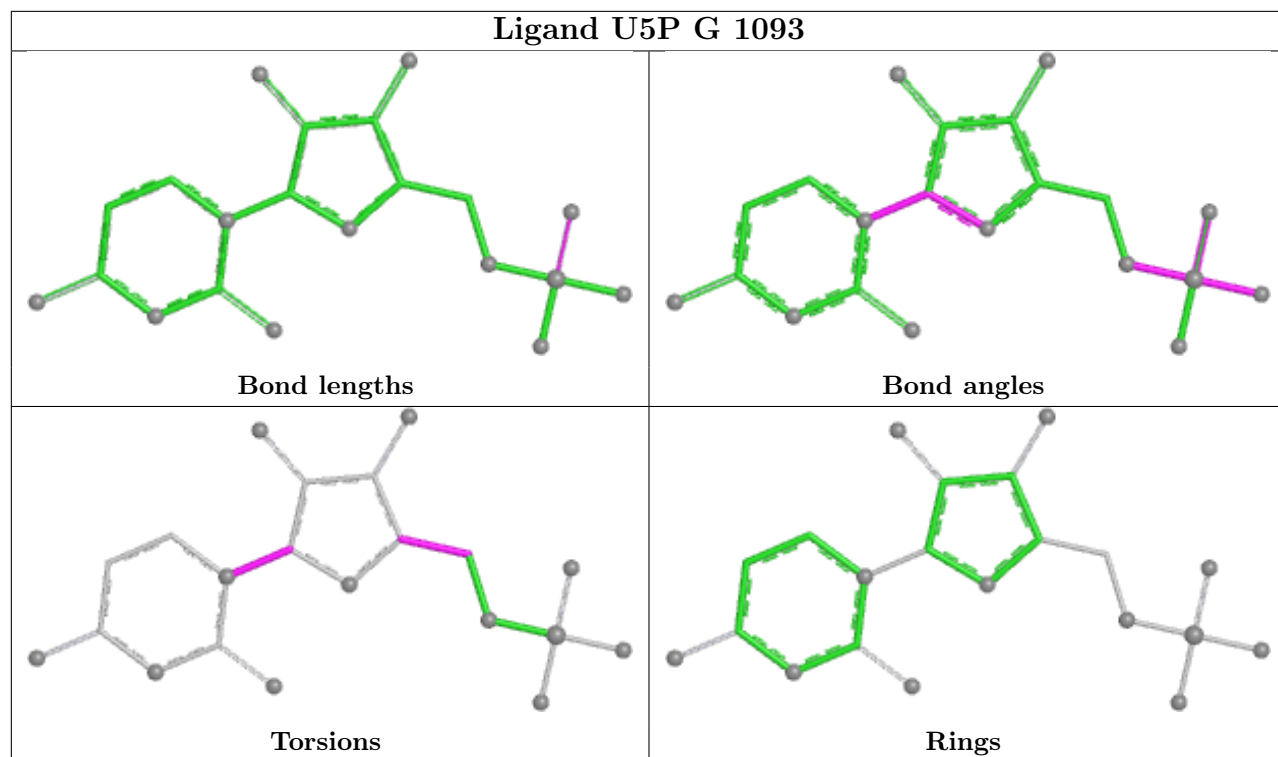
Ligand ADP A 1088



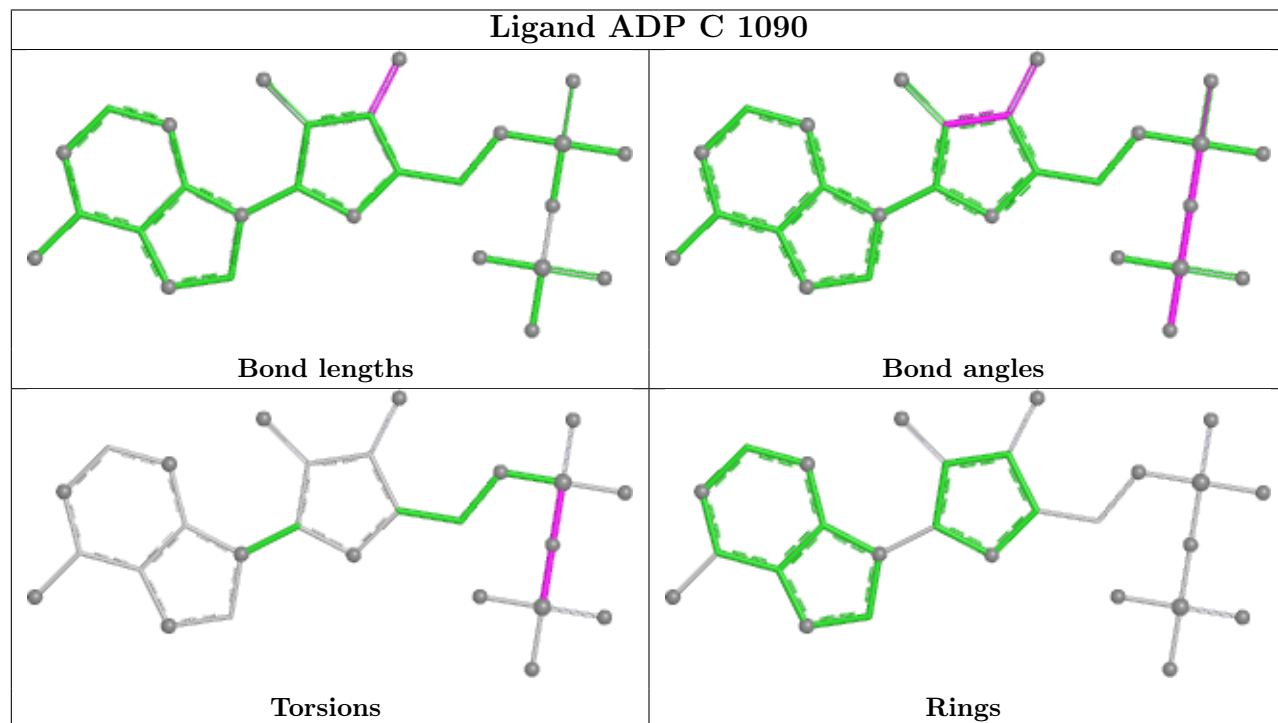
Ligand U5P A 1091



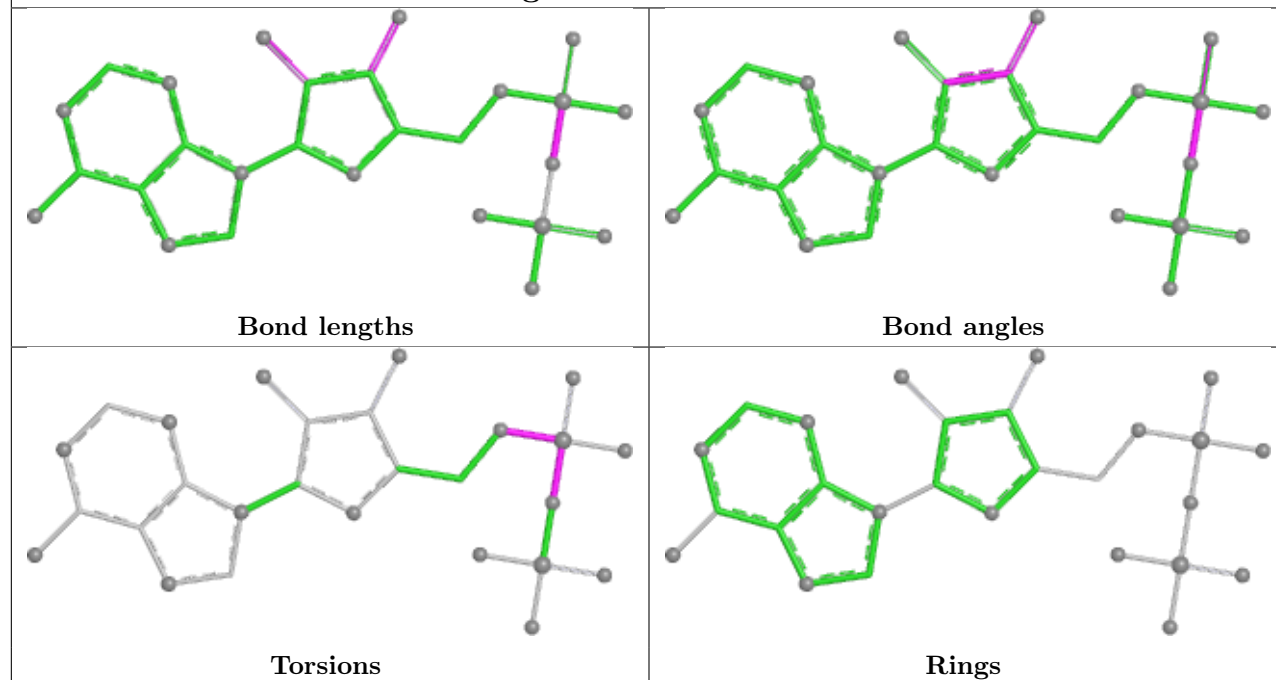
Ligand U5P G 1093



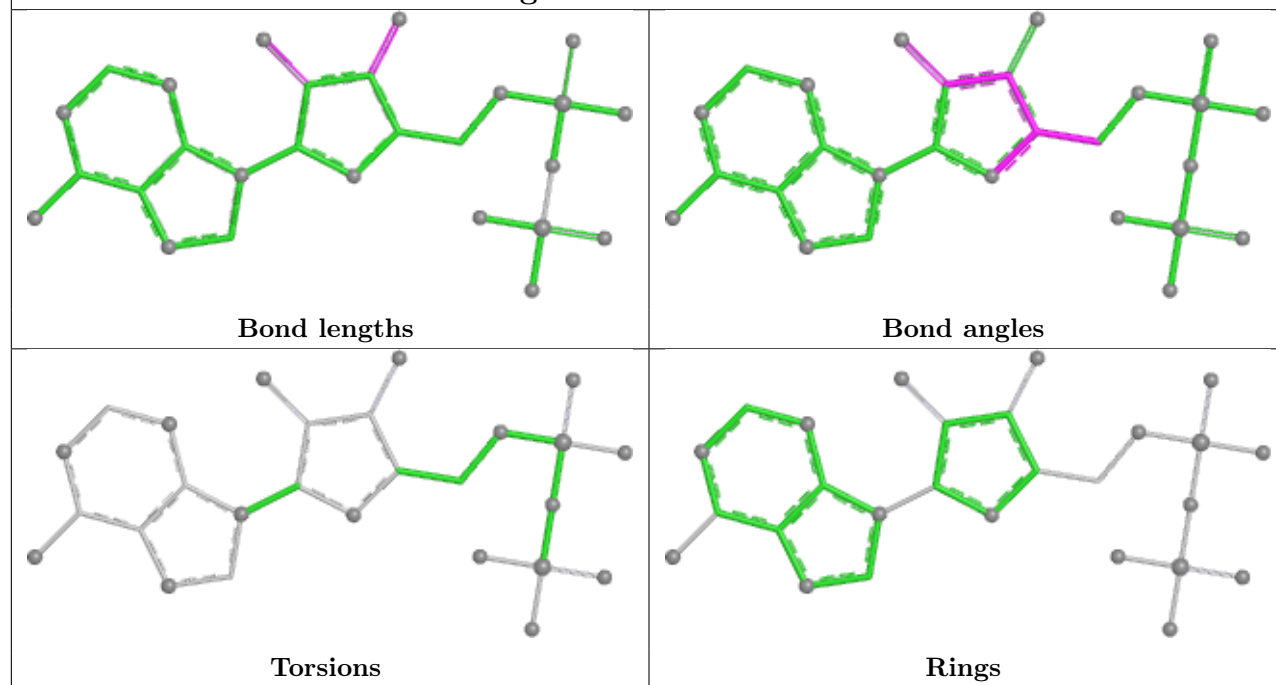
Ligand ADP C 1090

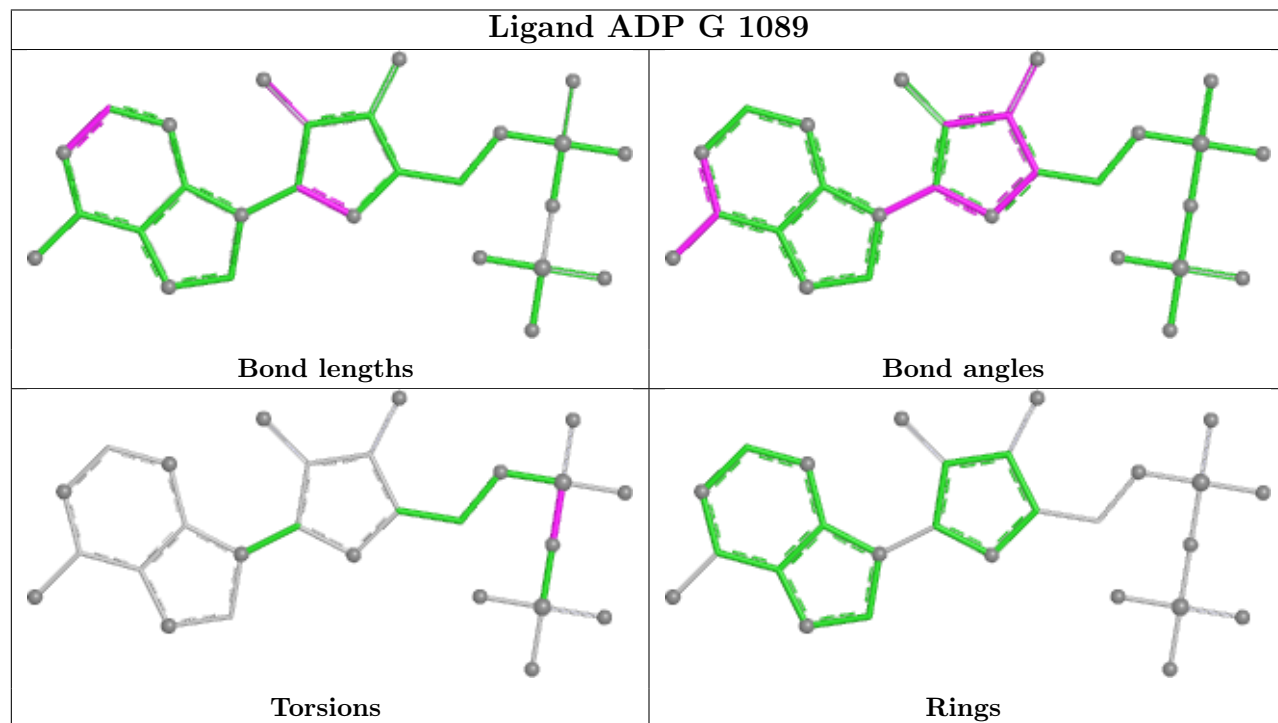
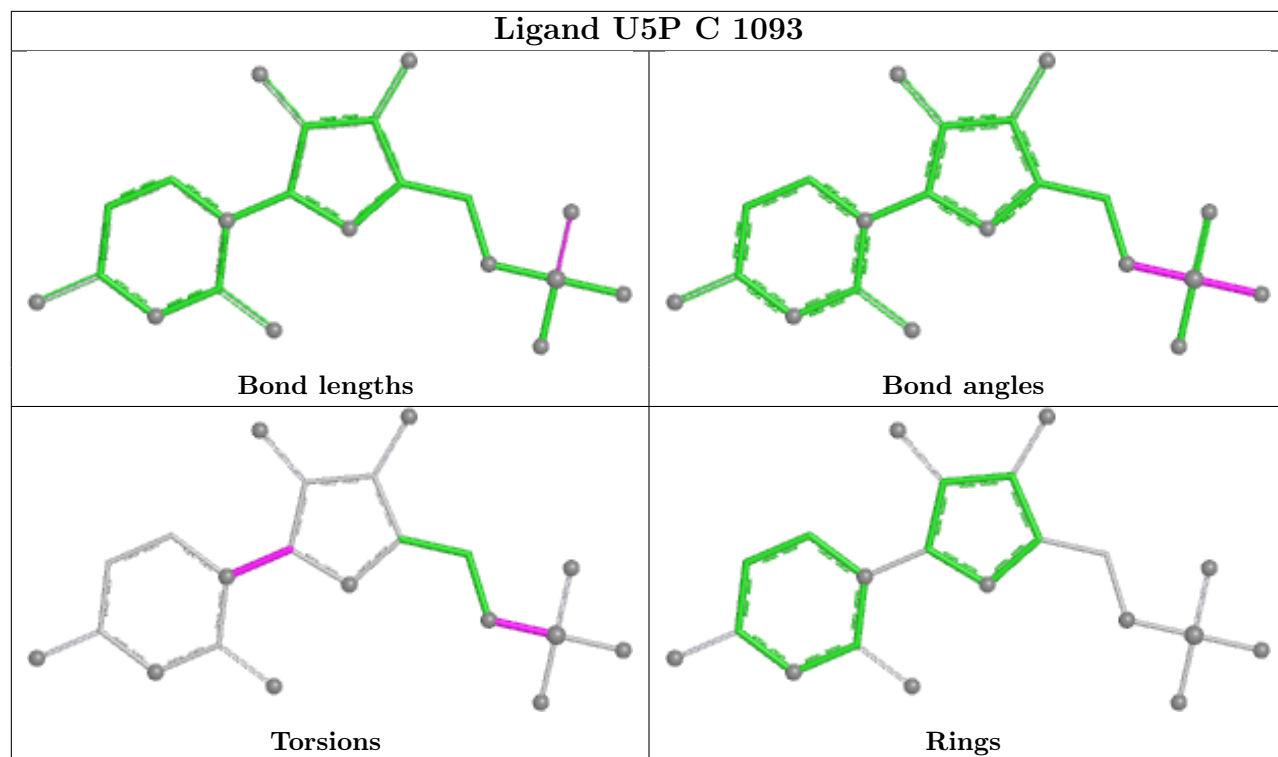


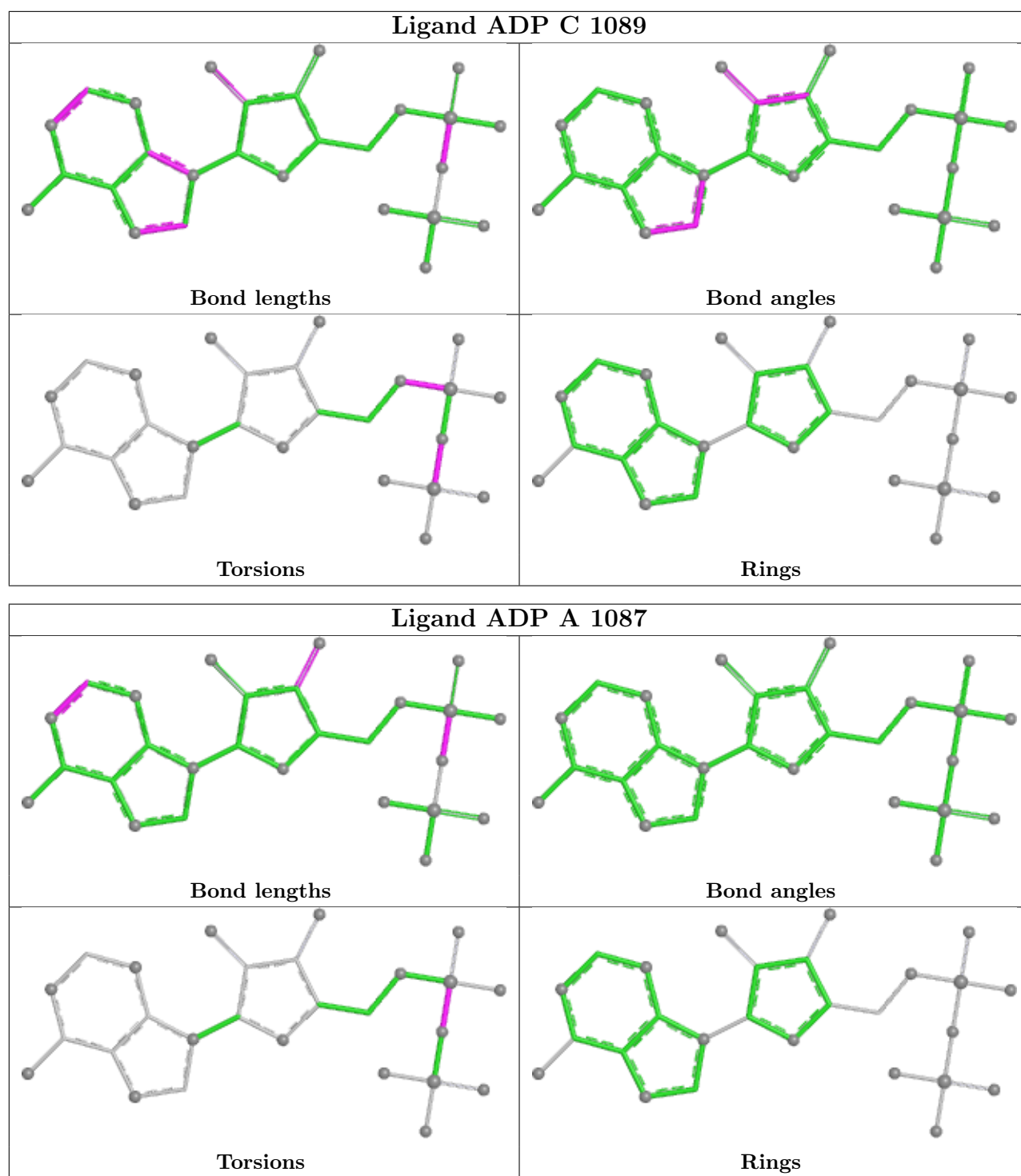
Ligand ADP E 1089



Ligand ADP G 1090







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1058/1073 (98%)	-0.50	24 (2%) 61 64	17, 33, 73, 100	9 (0%)
1	C	1058/1073 (98%)	-0.40	24 (2%) 61 64	18, 35, 81, 100	8 (0%)
1	E	1058/1073 (98%)	-0.58	14 (1%) 75 77	17, 31, 75, 100	5 (0%)
1	G	1058/1073 (98%)	-0.16	19 (1%) 67 70	20, 41, 84, 100	8 (0%)
2	B	379/382 (99%)	0.11	8 (2%) 63 66	21, 48, 87, 100	0
2	D	379/382 (99%)	-0.03	11 (2%) 53 56	21, 40, 78, 100	1 (0%)
2	F	379/382 (99%)	0.17	19 (5%) 34 36	20, 47, 92, 100	0
2	H	379/382 (99%)	0.72	40 (10%) 11 12	33, 63, 97, 100	0
All	All	5748/5820 (98%)	-0.24	159 (2%) 55 57	17, 38, 84, 100	31 (0%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	PRO	5.6
1	A	751	LEU	4.5
1	E	1	MET	4.5
1	C	697	ALA	4.2
2	H	134	ALA	4.2
2	H	246	ALA	4.1
1	G	737	TYR	4.0
1	E	675	ARG	3.9
1	A	716	PRO	3.9
1	A	341	GLY	3.9
1	G	697	ALA	3.8
1	A	724	ALA	3.7
1	E	741	ALA	3.7
2	F	233	PRO	3.6
2	F	192	PHE	3.6
2	F	246	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	738	PHE	3.5
2	H	156	MET	3.4
2	H	141	ALA	3.4
1	E	738	PHE	3.4
2	H	159	ALA	3.3
1	C	695	VAL	3.3
2	H	150	PHE	3.3
2	H	232	ASN	3.3
1	E	709	GLY	3.2
1	C	750	VAL	3.1
1	C	732	ALA	3.1
1	G	724	ALA	3.1
1	A	740	THR	3.1
2	B	250	TYR	3.1
1	C	1	MET	3.1
1	A	952	GLY	3.0
1	A	999	PRO	3.0
2	H	377	TYR	3.0
1	C	716	PRO	3.0
1	G	751	LEU	3.0
2	F	250	TYR	3.0
2	H	288	PHE	3.0
1	C	724	ALA	2.9
2	H	251	ALA	2.9
1	E	342	GLY	2.9
1	G	1	MET	2.9
2	F	274	LEU	2.9
2	H	339	GLY	2.9
1	A	750	VAL	2.9
1	A	1	MET	2.9
2	H	314	PHE	2.9
2	H	321	LEU	2.8
1	C	714	VAL	2.8
1	G	5	THR	2.8
1	G	557	THR	2.8
1	G	559	ARG	2.8
2	F	377	TYR	2.8
2	B	380	THR	2.8
2	D	380	THR	2.8
1	A	702	VAL	2.8
2	H	2	ILE	2.8
1	G	680	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	700	MET	2.8
2	H	188	ASP	2.8
1	A	680	HIS	2.7
1	A	342	GLY	2.7
1	A	741	ALA	2.7
2	F	228	VAL	2.7
1	A	701	ALA	2.7
1	C	5	THR	2.7
1	A	698	ILE	2.6
2	D	225	ALA	2.6
1	A	737	TYR	2.6
2	H	228	VAL	2.6
1	E	716	PRO	2.6
2	H	165	ALA	2.6
1	C	737	TYR	2.5
2	F	319	ALA	2.5
1	E	737	TYR	2.5
1	G	710	TYR	2.5
1	C	683	GLU	2.5
2	H	278	ALA	2.5
1	A	696	THR	2.4
1	A	368	ALA	2.4
2	H	276	ALA	2.4
1	C	738	PHE	2.4
1	C	557	THR	2.4
1	A	559	ARG	2.4
2	H	225	ALA	2.4
2	F	341	HIS	2.4
2	F	137	ASN	2.4
2	H	8	VAL	2.4
2	D	156	MET	2.4
2	H	343	THR	2.4
1	G	716	PRO	2.4
1	C	698	ILE	2.4
1	G	682	VAL	2.4
1	C	999	PRO	2.4
2	F	248	ASP	2.3
2	D	320	THR	2.3
2	H	250	TYR	2.3
1	C	112	GLY	2.3
2	H	248	ASP	2.3
2	H	73	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	715	ARG	2.3
1	G	678	PHE	2.3
2	H	266	PHE	2.3
1	G	702	VAL	2.3
2	H	380	THR	2.3
1	A	697	ALA	2.3
2	H	224	SER	2.2
1	C	702	VAL	2.2
1	E	728	VAL	2.2
1	C	1021	ARG	2.2
2	D	157	ASP	2.2
2	H	157	ASP	2.2
2	D	149	ALA	2.2
2	H	152	GLY	2.2
2	F	153	LEU	2.2
2	B	320	THR	2.2
2	D	261	THR	2.2
2	B	152	GLY	2.2
2	H	135	GLY	2.2
1	C	703	GLU	2.2
1	E	697	ALA	2.2
2	F	225	ALA	2.2
1	G	740	THR	2.2
2	F	195	VAL	2.2
2	H	201	ALA	2.2
2	H	151	PRO	2.1
1	G	741	ALA	2.1
2	F	281	ALA	2.1
2	H	149	ALA	2.1
2	F	154	ASN	2.1
1	E	698	ILE	2.1
1	G	668	ALA	2.1
1	A	712	LEU	2.1
2	B	248	ASP	2.1
1	E	418	PRO	2.1
2	B	321	LEU	2.1
2	H	274	LEU	2.1
2	D	154	ASN	2.1
2	D	232	ASN	2.1
1	G	739	GLN	2.1
2	F	320	THR	2.1
2	F	380	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	138	PRO	2.1
2	F	167	ALA	2.1
1	E	1007	ASN	2.0
2	H	227	ASP	2.0
2	H	233	PRO	2.0
1	C	342	GLY	2.0
2	B	255	ILE	2.0
1	G	683	GLU	2.0
1	C	1070	ALA	2.0
2	H	143	ALA	2.0
1	C	751	LEU	2.0
2	H	373	LEU	2.0
1	A	730	ASP	2.0
2	D	188	ASP	2.0
1	C	1073	LYS	2.0
2	B	233	PRO	2.0
2	D	233	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PO4	C	1088	5/5	0.77	0.12	80,80,80,80	0
6	CL	G	1084	1/1	0.84	0.20	72,72,72,72	0
6	CL	E	1084	1/1	0.87	0.15	74,74,74,74	0
6	CL	A	1083	1/1	0.92	0.10	66,66,66,66	0
6	CL	H	385	1/1	0.93	0.12	82,82,82,82	0
6	CL	G	1087	1/1	0.94	0.10	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	C	1083	1/1	0.94	0.12	77,77,77,77	0
8	ORN	G	1091	9/9	0.94	0.08	28,33,36,63	0
6	CL	G	1088	1/1	0.95	0.14	67,67,67,67	0
4	K	H	383	1/1	0.95	0.09	64,64,64,64	0
8	ORN	A	1089	9/9	0.95	0.08	24,29,36,37	0
6	CL	E	1087	1/1	0.95	0.08	54,54,54,54	0
10	U5P	G	1093	21/21	0.95	0.10	31,57,80,85	0
8	ORN	C	1091	9/9	0.96	0.07	20,29,35,39	0
8	ORN	E	1091	9/9	0.96	0.06	16,25,37,40	0
6	CL	C	1086	1/1	0.96	0.09	67,67,67,67	0
10	U5P	A	1091	21/21	0.96	0.09	28,58,80,81	0
10	U5P	C	1093	21/21	0.96	0.10	33,51,83,89	0
10	U5P	E	1093	21/21	0.96	0.09	37,54,80,89	0
6	CL	H	384	1/1	0.96	0.10	67,67,67,67	0
6	CL	C	1084	1/1	0.97	0.06	43,43,43,43	0
9	NET	A	1090	9/9	0.97	0.06	18,23,28,38	0
7	ADP	G	1090	27/27	0.97	0.07	29,47,80,89	0
4	K	E	1083	1/1	0.97	0.08	58,58,58,58	0
4	K	G	1083	1/1	0.97	0.06	52,52,52,52	0
4	K	E	1081	1/1	0.97	0.06	42,42,42,42	0
7	ADP	E	1090	27/27	0.98	0.05	23,35,48,56	0
6	CL	E	1085	1/1	0.98	0.05	49,49,49,49	0
4	K	C	1082	1/1	0.98	0.05	44,44,44,44	0
4	K	G	1081	1/1	0.98	0.06	46,46,46,46	0
6	CL	G	1086	1/1	0.98	0.08	54,54,54,54	0
4	K	B	383	1/1	0.98	0.04	45,45,45,45	0
6	CL	C	1087	1/1	0.98	0.11	63,63,63,63	0
9	NET	C	1092	9/9	0.98	0.05	16,21,23,29	0
9	NET	E	1092	9/9	0.98	0.06	15,23,27,28	0
9	NET	G	1092	9/9	0.98	0.06	18,28,29,37	0
6	CL	D	384	1/1	0.98	0.04	34,34,34,34	0
6	CL	A	1086	1/1	0.98	0.06	56,56,56,56	0
7	ADP	A	1088	27/27	0.98	0.05	20,33,47,60	0
7	ADP	C	1090	27/27	0.98	0.06	26,42,61,77	0
5	PO4	G	1078	5/5	0.99	0.04	17,24,31,35	0
4	K	E	1077	1/1	0.99	0.03	30,30,30,30	0
6	CL	A	1084	1/1	0.99	0.04	40,40,40,40	0
6	CL	A	1085	1/1	0.99	0.06	39,39,39,39	0
4	K	A	1077	1/1	0.99	0.02	27,27,27,27	0
7	ADP	A	1087	27/27	0.99	0.04	16,22,31,38	0
6	CL	C	1081	1/1	0.99	0.03	29,29,29,29	0
7	ADP	C	1089	27/27	0.99	0.05	16,23,31,44	0

Continued on next page...

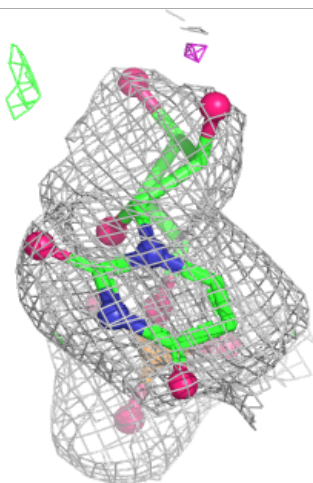
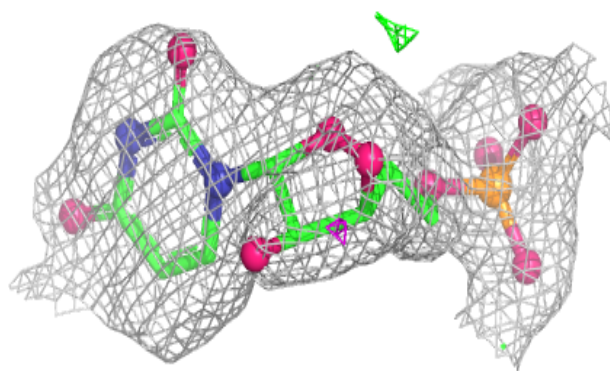
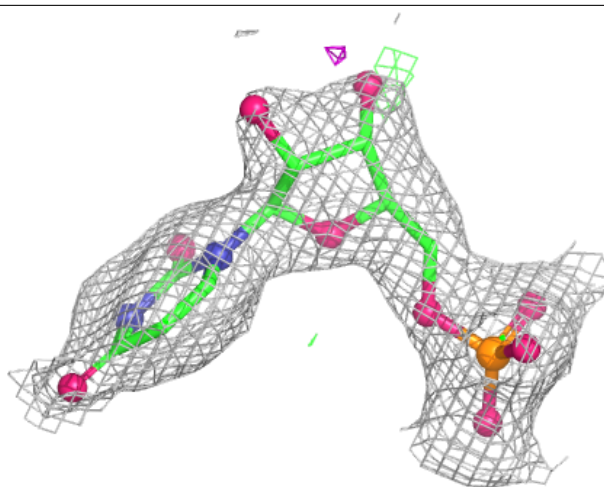
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	A	1082	1/1	0.99	0.02	41,41,41,41	0
7	ADP	E	1089	27/27	0.99	0.04	15,26,34,36	0
4	K	F	383	1/1	0.99	0.02	36,36,36,36	0
7	ADP	G	1089	27/27	0.99	0.04	17,27,35,41	0
6	CL	C	1085	1/1	0.99	0.05	39,39,39,39	0
4	K	G	1077	1/1	0.99	0.03	38,38,38,38	0
3	MN	G	1079	1/1	0.99	0.03	47,47,47,47	0
4	K	C	1077	1/1	0.99	0.03	27,27,27,27	0
4	K	C	1080	1/1	0.99	0.03	36,36,36,36	0
5	PO4	A	1078	5/5	0.99	0.03	17,21,24,29	0
6	CL	E	1086	1/1	0.99	0.04	41,41,41,41	0
5	PO4	C	1078	5/5	0.99	0.04	16,22,24,25	0
6	CL	E	1088	1/1	0.99	0.05	44,44,44,44	0
6	CL	F	384	1/1	0.99	0.04	32,32,32,32	0
6	CL	G	1082	1/1	0.99	0.04	29,29,29,29	0
4	K	A	1076	1/1	0.99	0.01	21,21,21,21	0
6	CL	G	1085	1/1	0.99	0.04	46,46,46,46	0
4	K	E	1080	1/1	1.00	0.02	27,27,27,27	0
3	MN	G	1074	1/1	1.00	0.03	31,31,31,31	0
3	MN	G	1075	1/1	1.00	0.03	28,28,28,28	0
3	MN	A	1074	1/1	1.00	0.03	25,25,25,25	0
4	K	G	1076	1/1	1.00	0.01	28,28,28,28	0
3	MN	A	1075	1/1	1.00	0.03	23,23,23,23	0
4	K	G	1080	1/1	1.00	0.03	38,38,38,38	0
6	CL	E	1082	1/1	1.00	0.04	24,24,24,24	0
3	MN	A	1079	1/1	1.00	0.03	37,37,37,37	0
4	K	A	1080	1/1	1.00	0.03	29,29,29,29	0
3	MN	C	1074	1/1	1.00	0.04	27,27,27,27	0
3	MN	C	1075	1/1	1.00	0.03	25,25,25,25	0
4	K	C	1076	1/1	1.00	0.02	22,22,22,22	0
3	MN	C	1079	1/1	1.00	0.03	46,46,46,46	0
5	PO4	E	1078	5/5	1.00	0.03	19,22,26,27	0
3	MN	E	1074	1/1	1.00	0.03	27,27,27,27	0
6	CL	A	1081	1/1	1.00	0.02	28,28,28,28	0
3	MN	E	1075	1/1	1.00	0.03	27,27,27,27	0
4	K	D	383	1/1	1.00	0.02	34,34,34,34	0
4	K	E	1076	1/1	1.00	0.02	25,25,25,25	0
3	MN	E	1079	1/1	1.00	0.03	41,41,41,41	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.

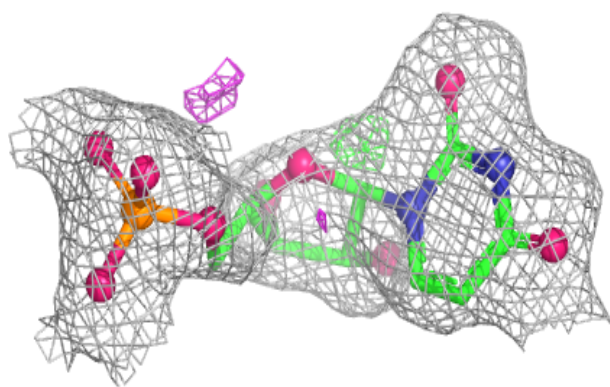
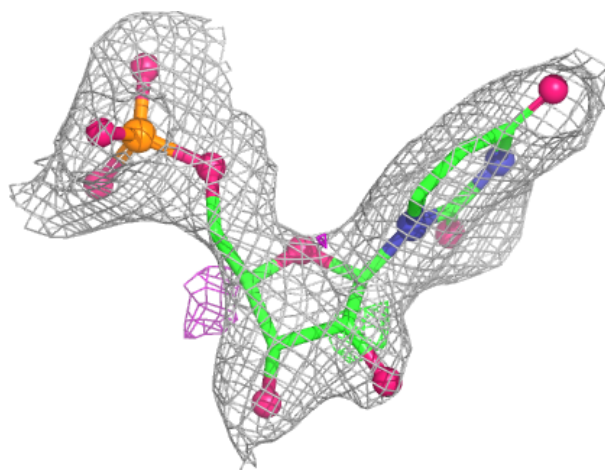
Electron density around U5P G 1093:

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



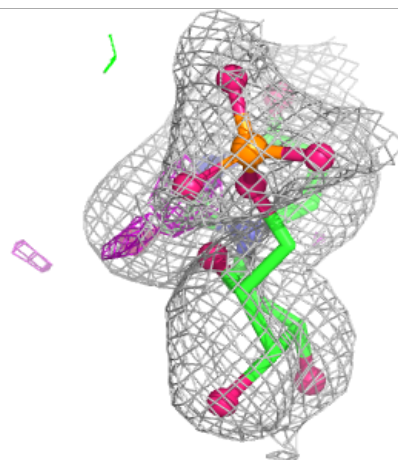
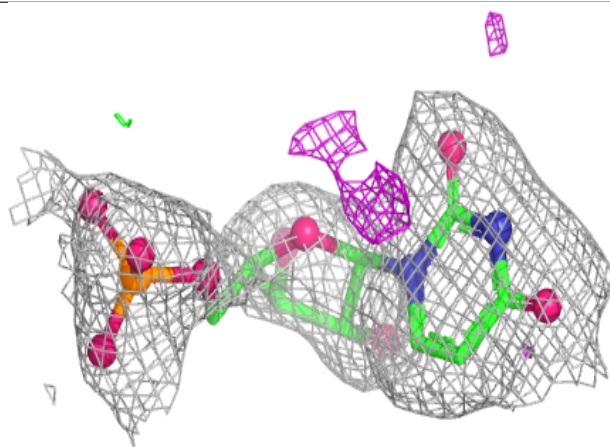
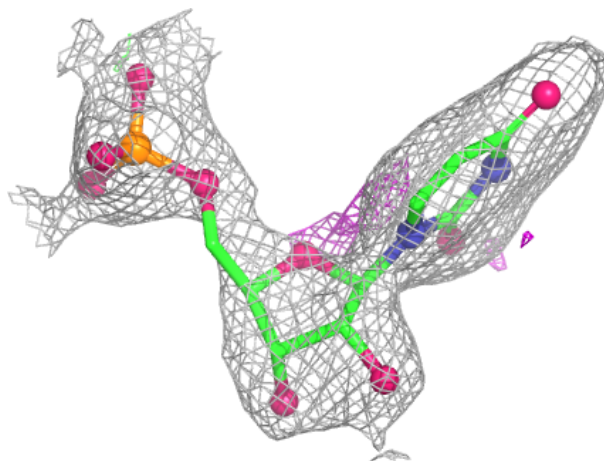
Electron density around U5P A 1091:

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



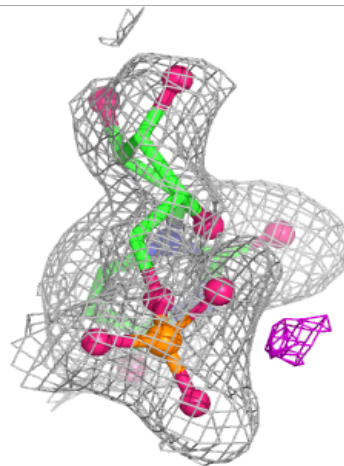
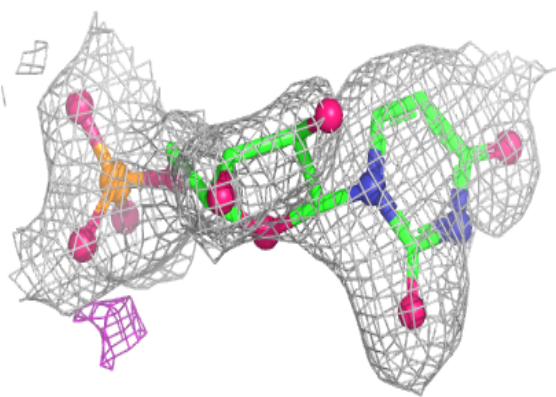
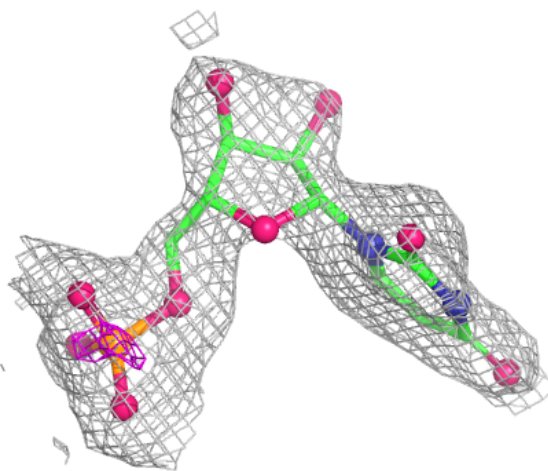
Electron density around U5P C 1093:

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



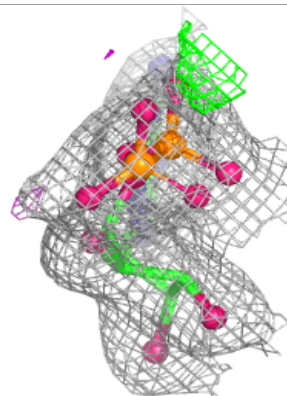
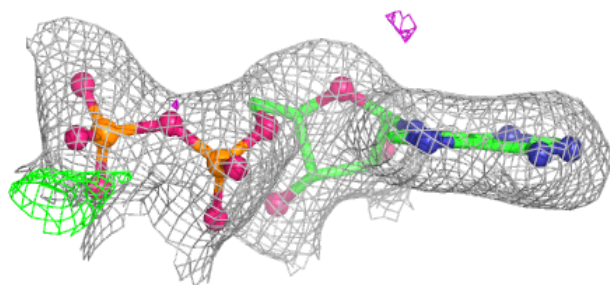
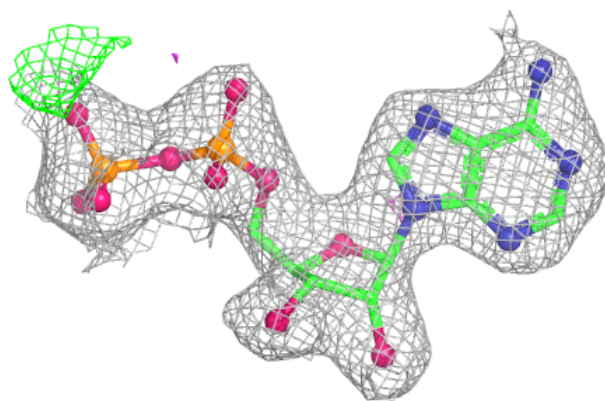
Electron density around U5P E 1093:

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

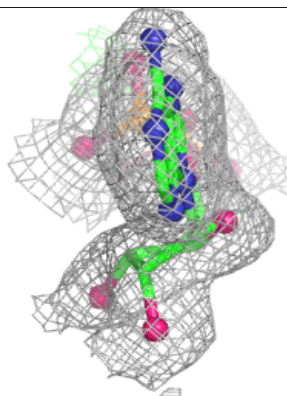
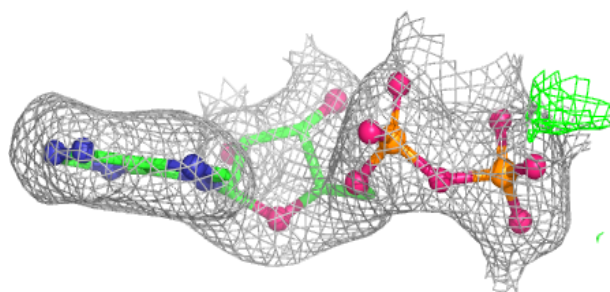
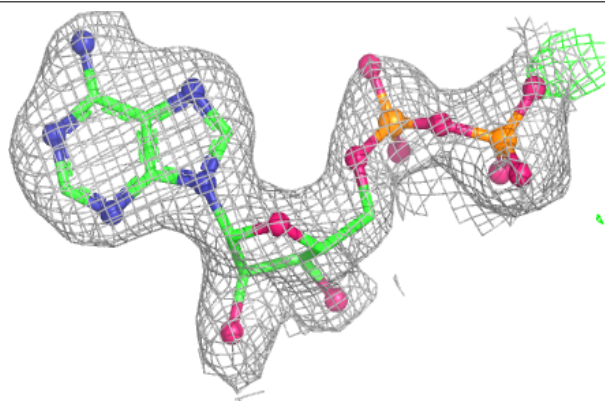


Electron density around ADP G 1090:

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

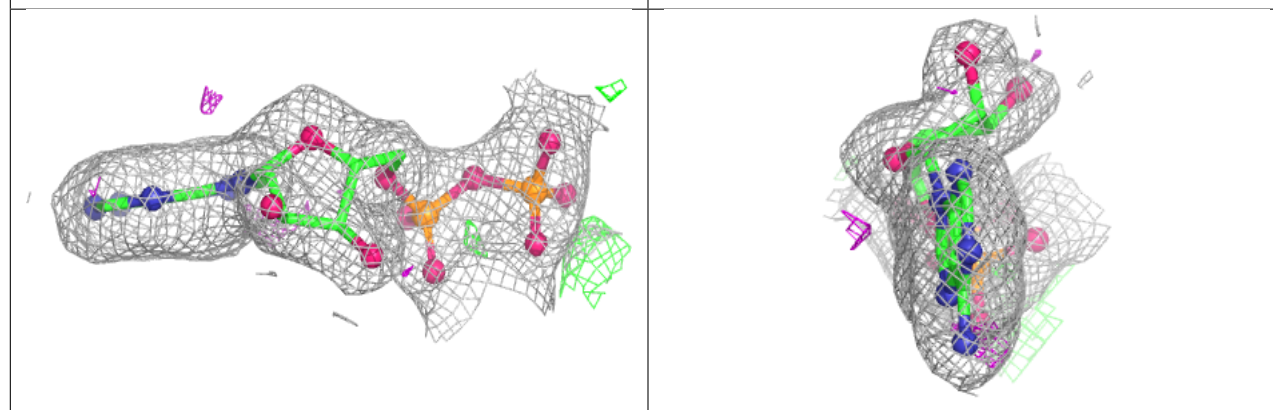
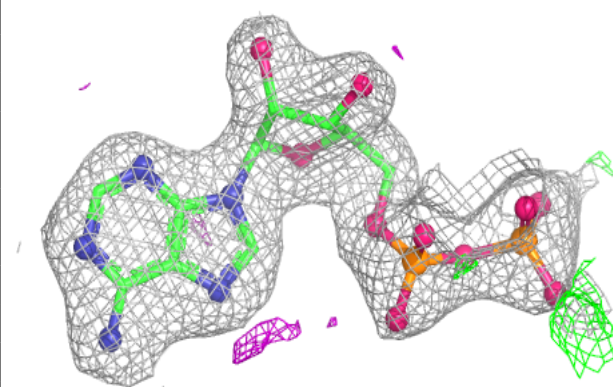
**Electron density around ADP E 1090:**

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

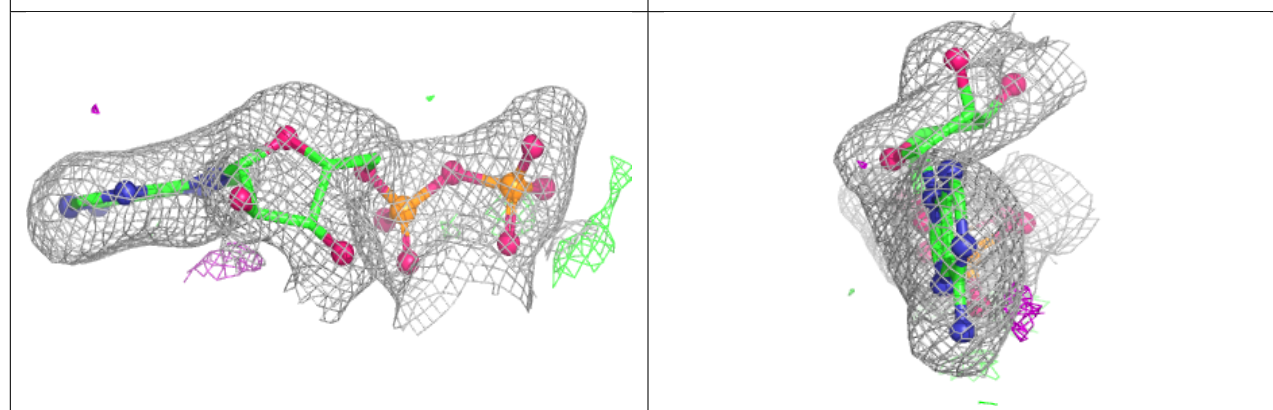
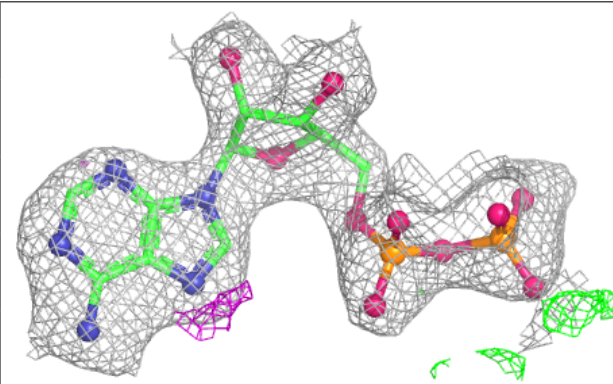


Electron density around ADP A 1088:

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

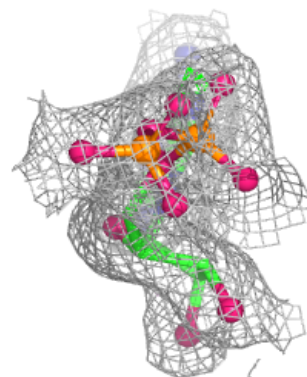
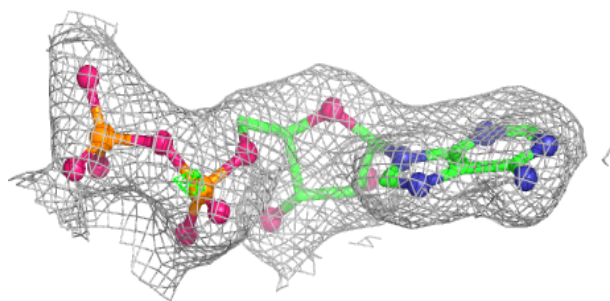
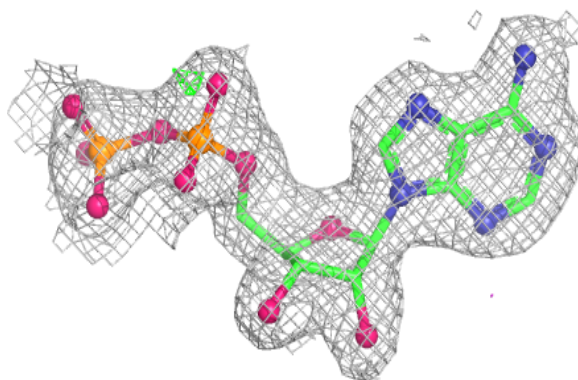
**Electron density around ADP C 1090:**

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

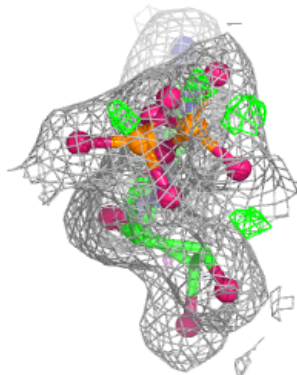
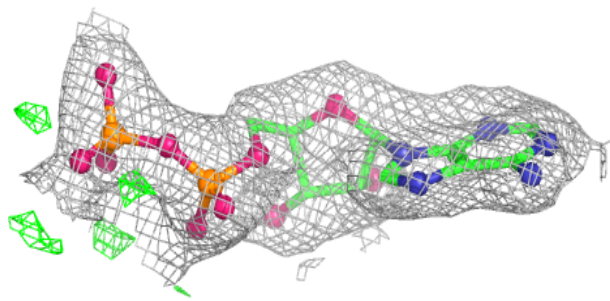
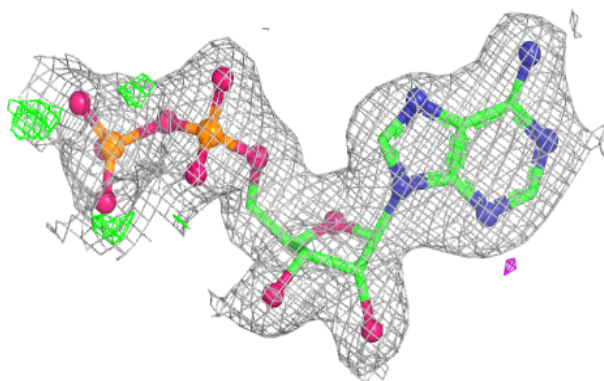


Electron density around ADP A 1087:

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

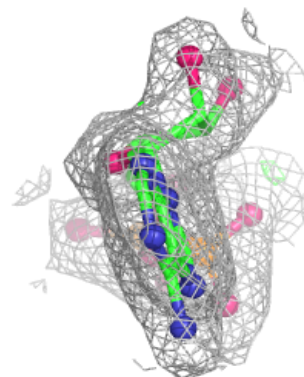
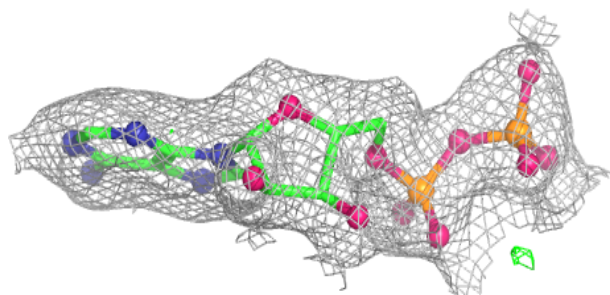
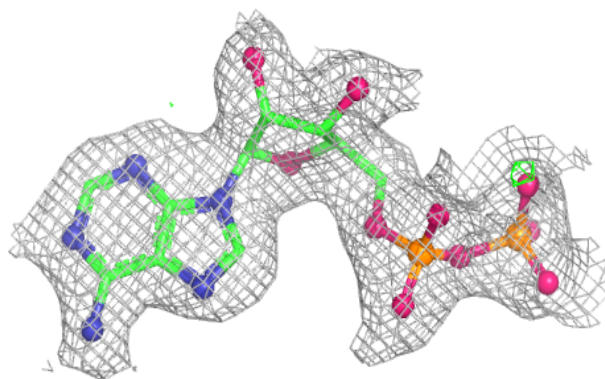
**Electron density around ADP C 1089:**

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

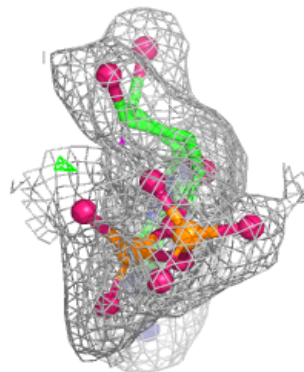
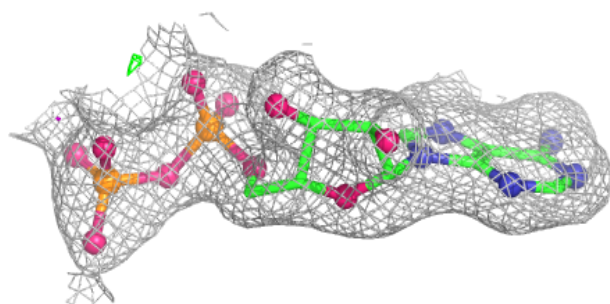
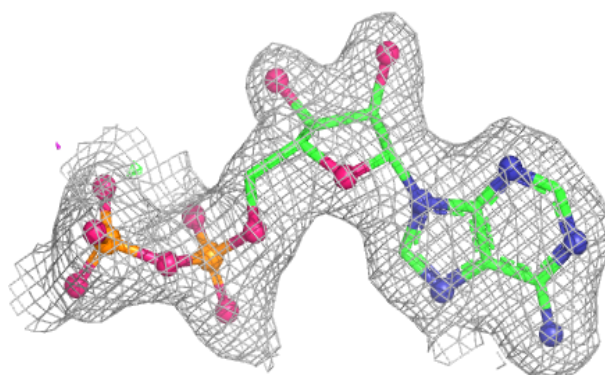


Electron density around ADP E 1089:

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

**Electron density around ADP G 1089:**

$2mF_o-DF_c$ (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.