



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:04 am GMT

PDB ID : 1M6V
Title : Crystal Structure of the G359F (small subunit) Point Mutant of Carbamoyl Phosphate Synthetase
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2002-07-17
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

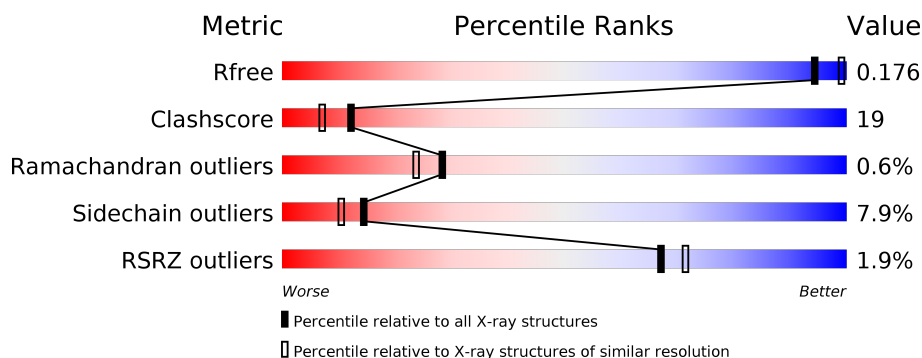
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>61%</div> <div>30%</div> <div>7%</div> <div>•</div> </div>
1	C	1073	<div> <div>2%</div> <div>62%</div> <div>30%</div> <div>7%</div> <div>••</div> </div>
1	E	1073	<div> <div>2%</div> <div>61%</div> <div>29%</div> <div>8%</div> <div>••</div> </div>
1	G	1073	<div> <div>2%</div> <div>52%</div> <div>37%</div> <div>8%</div> <div>••</div> </div>
2	B	382	<div> <div>2%</div> <div>37%</div> <div>46%</div> <div>14%</div> <div>••</div> </div>
2	D	382	<div> <div>59%</div> <div>32%</div> <div>8%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
8	ORN	A	4011	-	-	-	X
8	ORN	C	4031	-	-	-	X
8	ORN	E	4054	-	-	-	X
8	ORN	G	4076	-	-	-	X
9	NET	G	4077	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48206 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 synthetase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1059	Total	C	N	O	S	0	6	0
			8190	5140	1425	1579	46			
1	C	1059	Total	C	N	O	S	0	5	0
			8196	5144	1431	1576	45			
1	E	1059	Total	C	N	O	S	0	6	0
			8189	5141	1426	1576	46			
1	G	1059	Total	C	N	O	S	0	6	0
			8197	5144	1428	1580	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	SEE REMARK 999	UNP P00968
C	46	ASN	LEU	SEE REMARK 999	UNP P00968
E	46	ASN	LEU	SEE REMARK 999	UNP P00968
G	46	ASN	LEU	SEE REMARK 999	UNP P00968

- Molecule 2 is a protein called carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			
2	D	375	Total	C	N	O	S	0	2	0
			2877	1814	507	546	10			
2	F	375	Total	C	N	O	S	0	3	0
			2880	1818	505	546	11			
2	H	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	SEE REMARK 999	UNP P00907
B	359	PHE	GLY	ENGINEERED	UNP P00907
D	183	GLN	GLU	SEE REMARK 999	UNP P00907
D	359	PHE	GLY	ENGINEERED	UNP P00907
F	183	GLN	GLU	SEE REMARK 999	UNP P00907
F	359	PHE	GLY	ENGINEERED	UNP P00907
H	183	GLN	GLU	SEE REMARK 999	UNP P00907
H	359	PHE	GLY	ENGINEERED	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
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

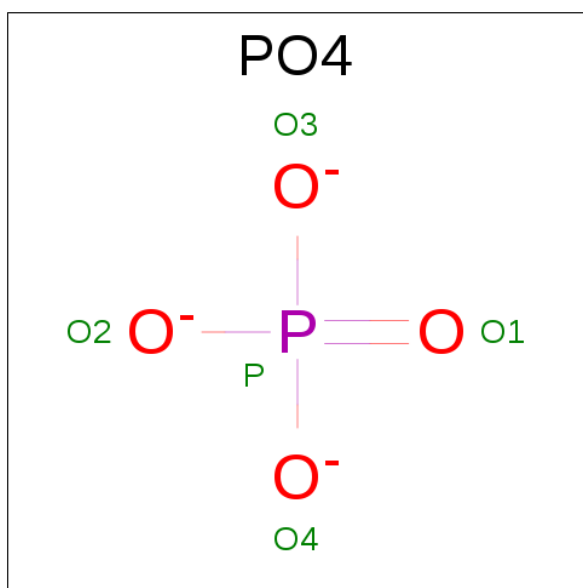
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	A	5	Total K 5 5	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

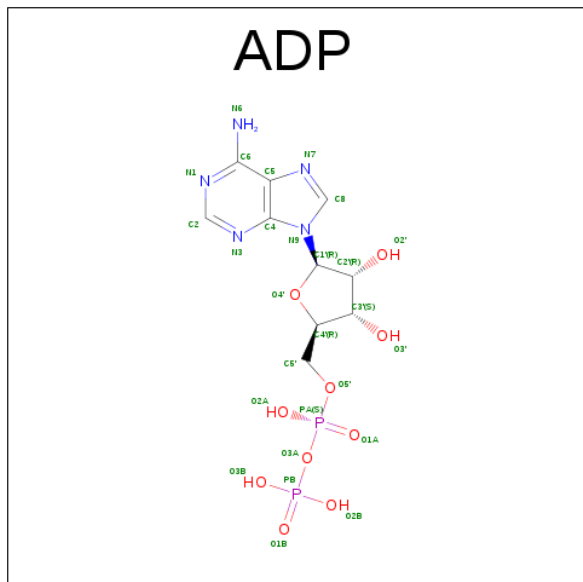
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	6	Total Cl 6 6	0	0
5	D	1	Total Cl 1 1	0	0
5	E	6	Total Cl 6 6	0	0
5	H	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	7	Total Cl 7 7	0	0
5	A	5	Total Cl 5 5	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



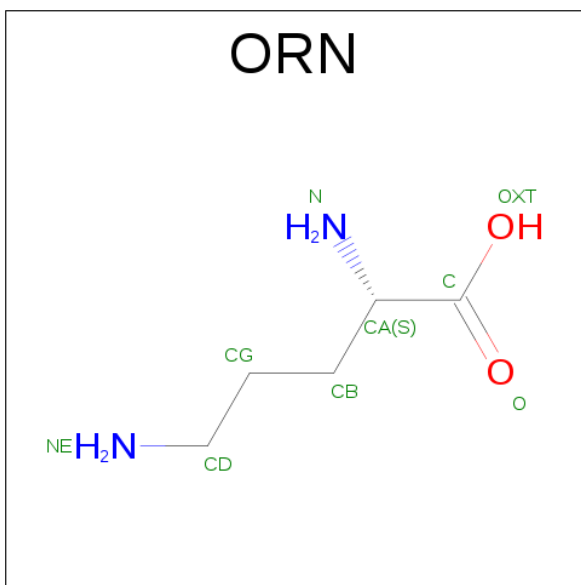
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



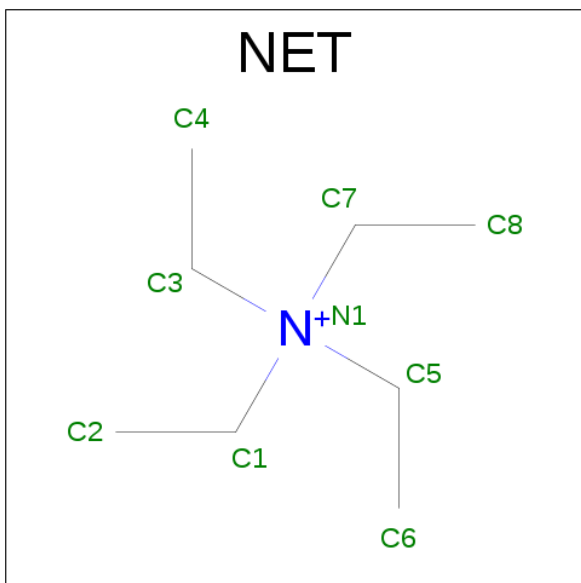
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	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 (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



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 (three-letter code: NET) (formula: $C_8H_{20}N$).



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

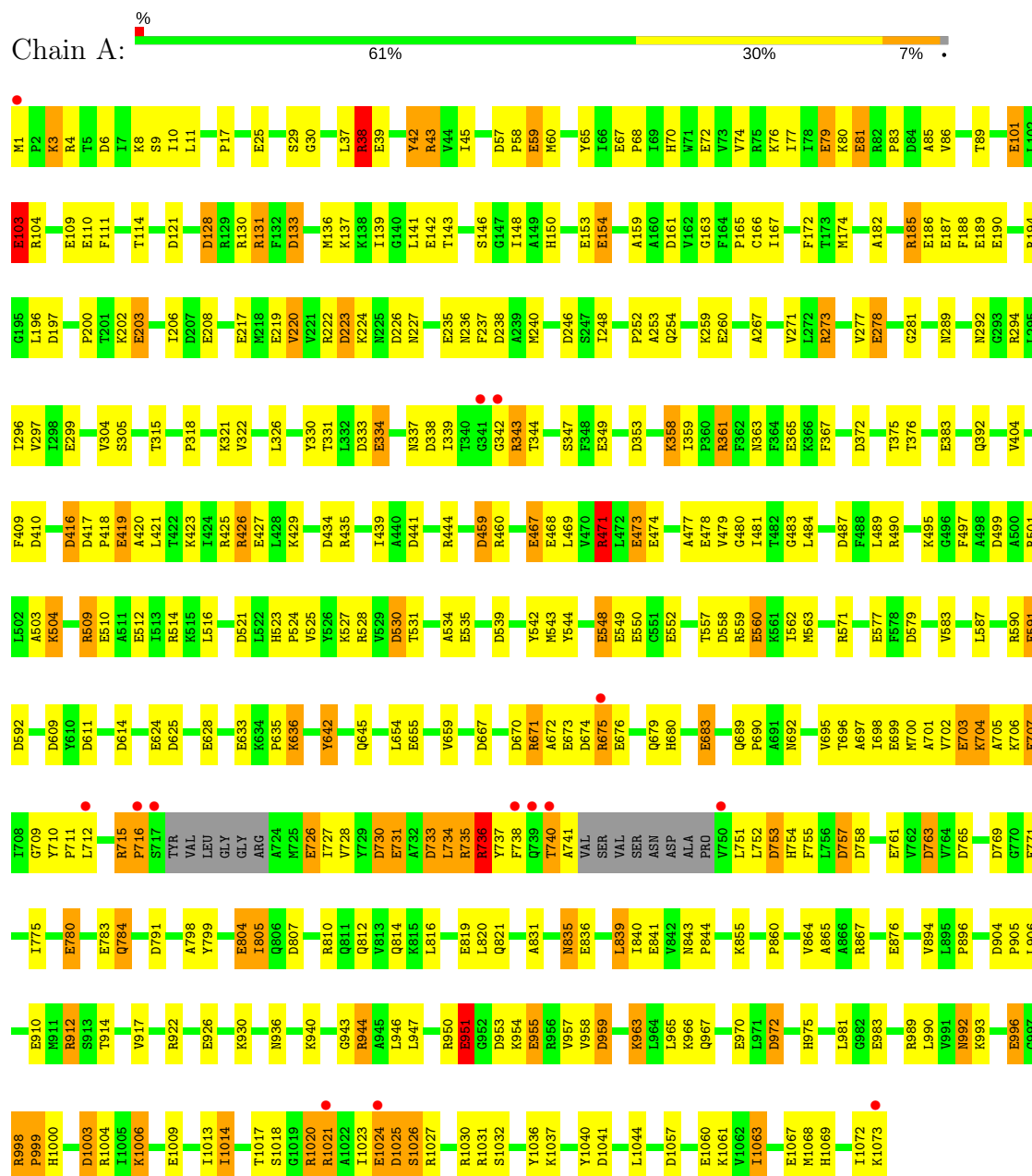
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	793	Total O 793 793	0	0
10	B	130	Total O 130 130	0	0
10	C	681	Total O 681 681	0	0
10	D	177	Total O 177 177	0	0
10	E	813	Total O 813 813	0	0
10	F	205	Total O 205 205	0	0
10	G	645	Total O 645 645	0	0
10	H	117	Total O 117 117	0	0

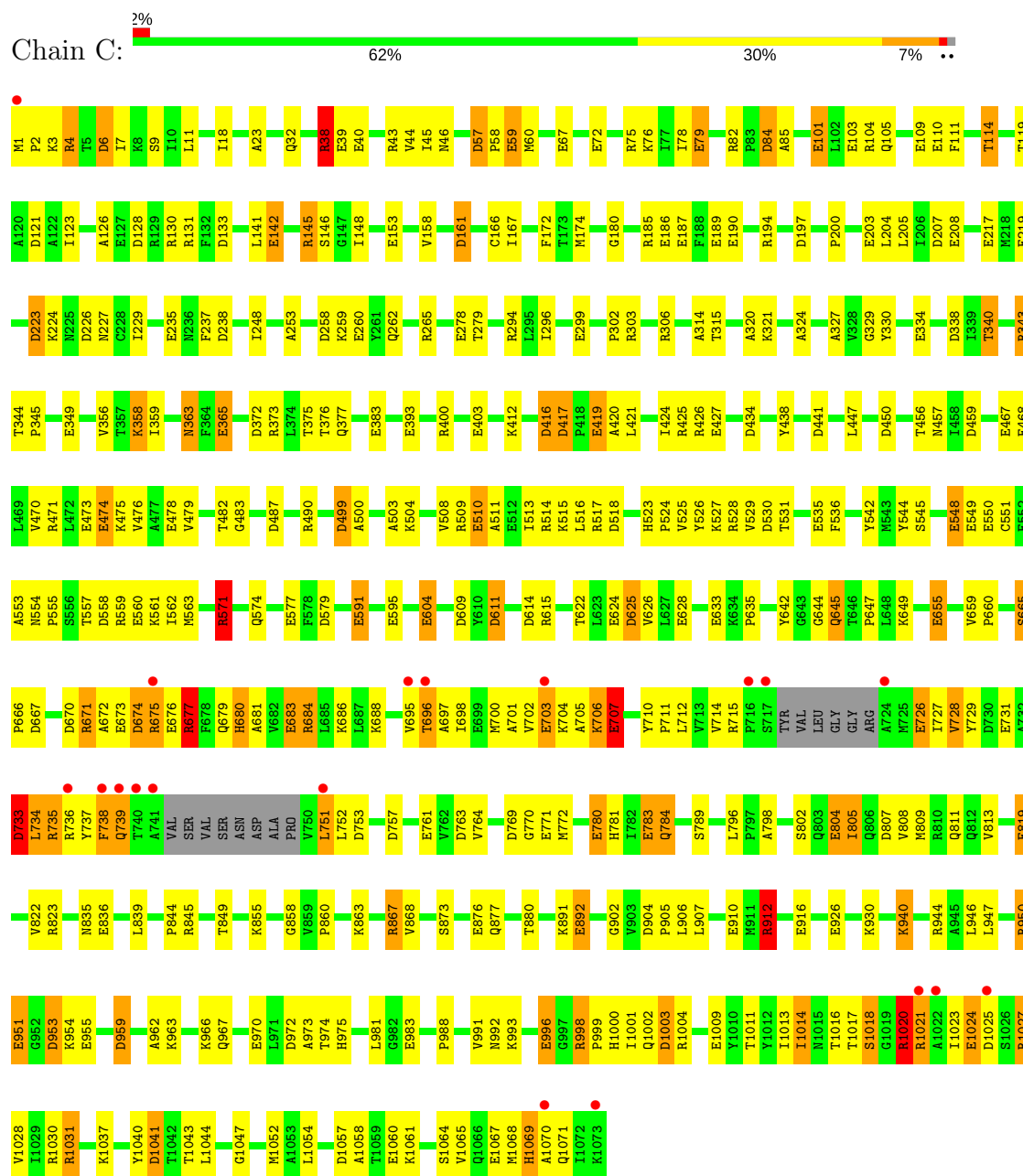
3 Residue-property plots

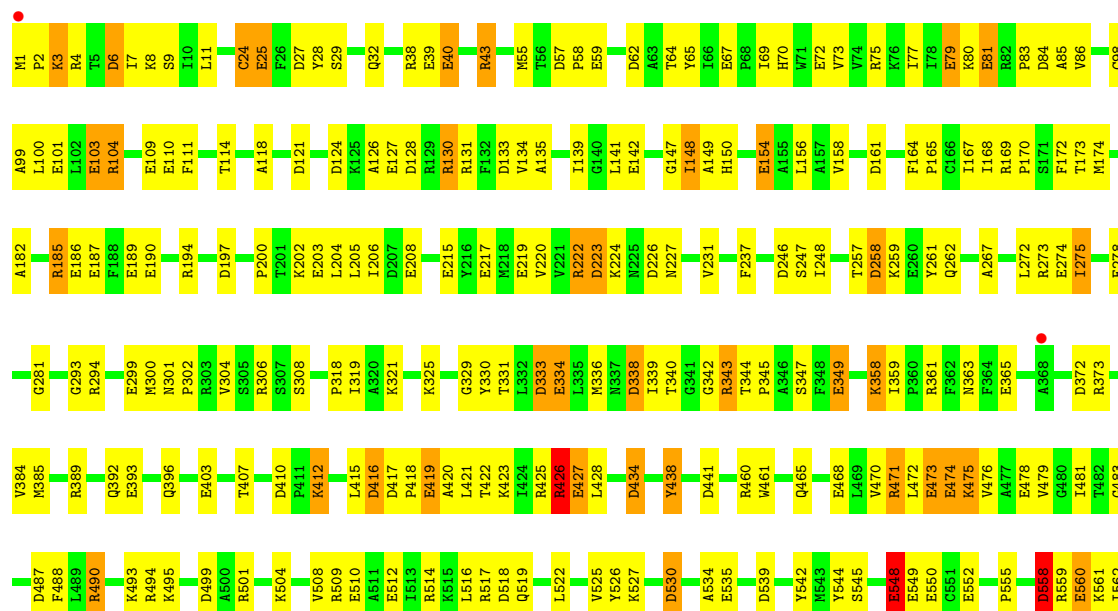
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

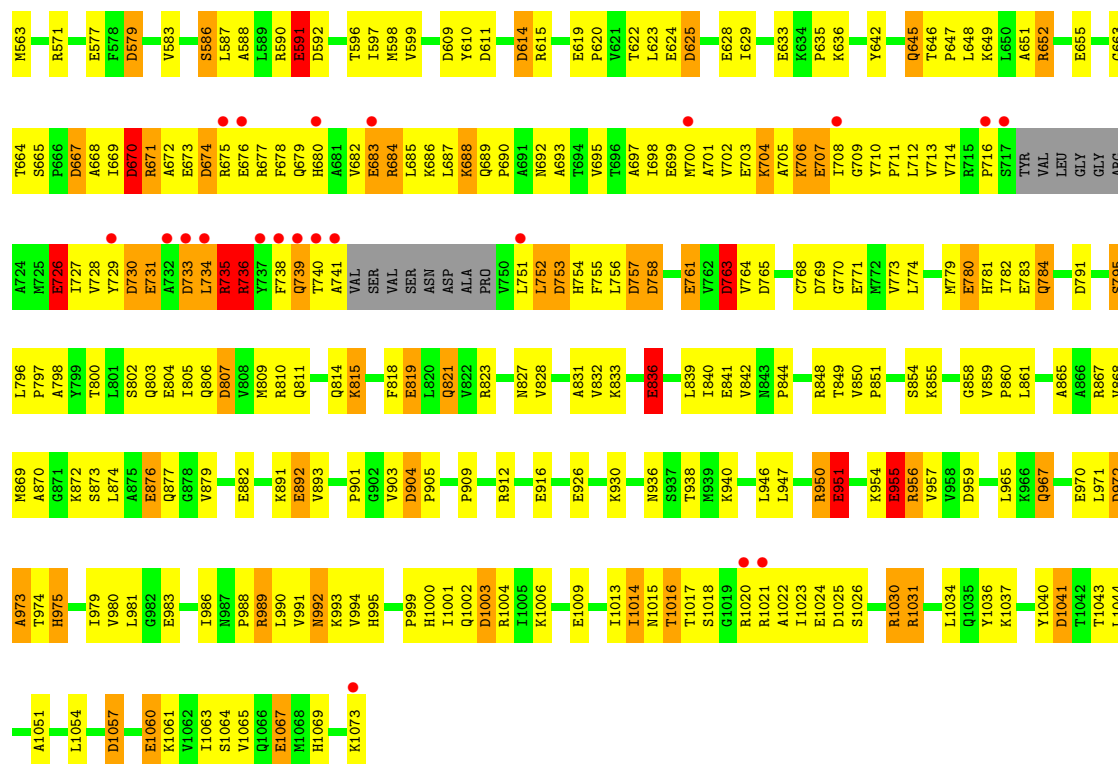
- Molecule 1: carbamoyl phosphate synthetase large chain



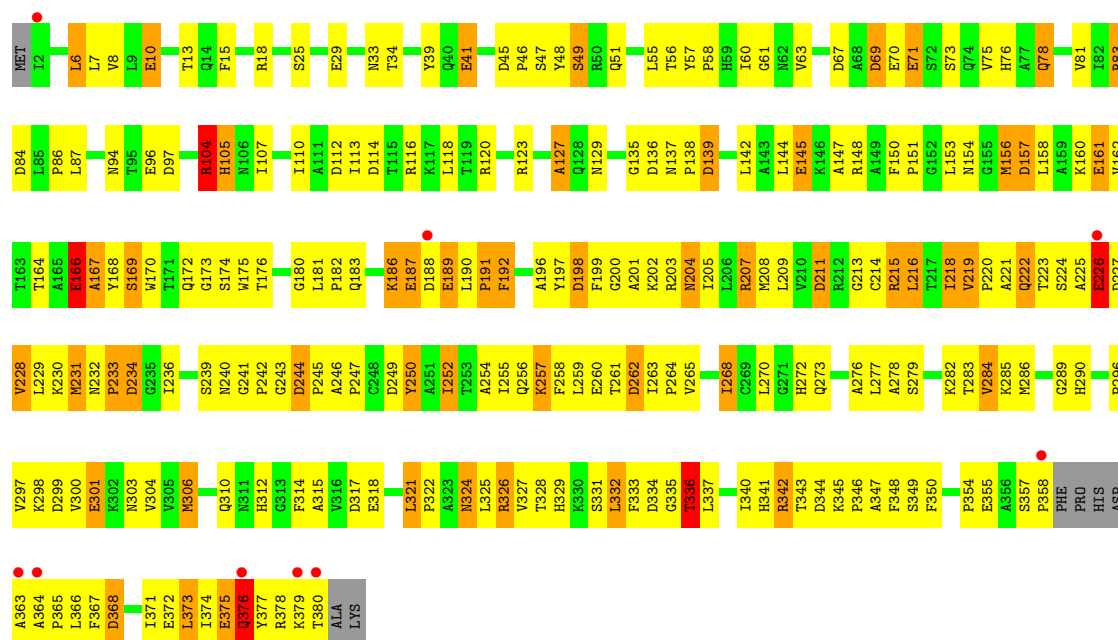
• Molecule 1: carbamoyl phosphate synthetase large chain





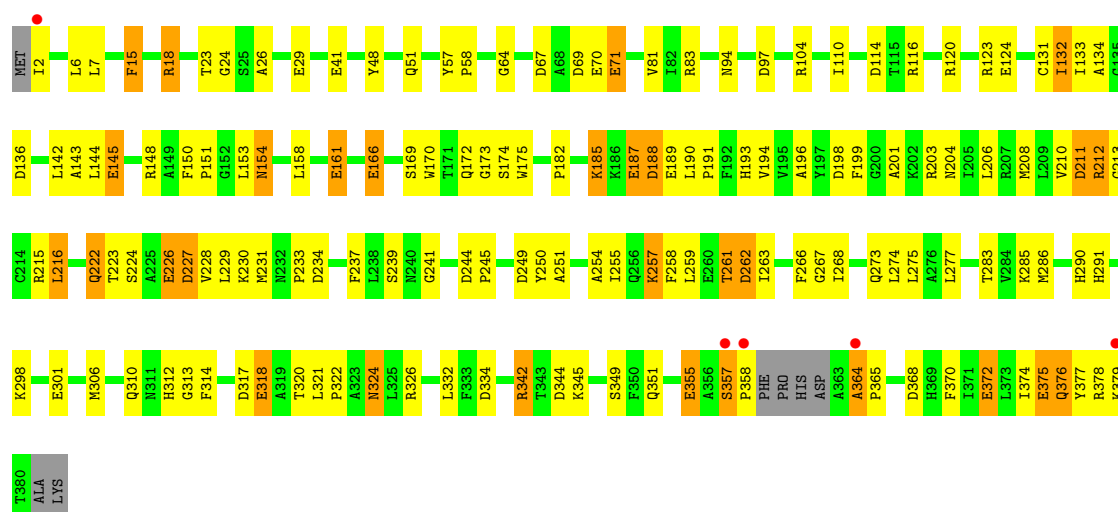


• Molecule 2: carbamoyl-phosphate synthetase small chain



• Molecule 2: carbamoyl-phosphate synthetase small chain



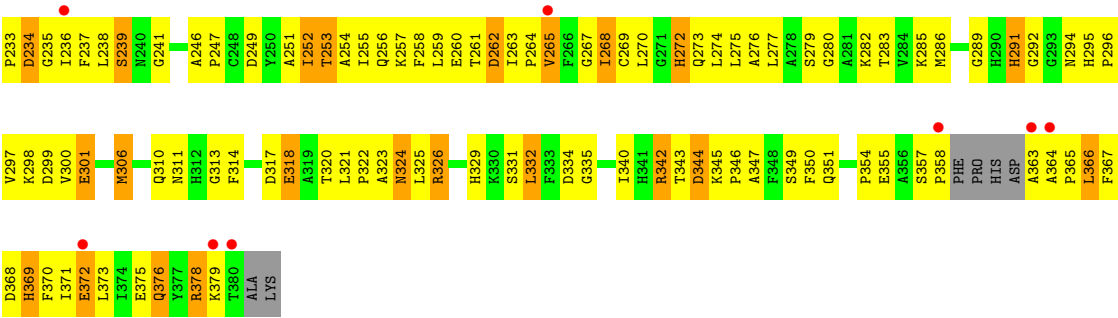


• Molecule 2: carbamoyl-phosphate synthetase small chain



• Molecule 2: carbamoyl-phosphate synthetase 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	151.50Å 164.20Å 331.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 19.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.10) 92.0 (19.93-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , 0.245 0.176 , 0.176	Depositor DCC
R_{free} test set	44042 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 104.7	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	48206	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: ADP, CL, K, MN, ORN, NET, PO4

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	1.07	77/8340 (0.9%)	1.42	118/11273 (1.0%)
1	C	1.05	74/8350 (0.9%)	1.44	124/11288 (1.1%)
1	E	1.06	67/8339 (0.8%)	1.45	136/11272 (1.2%)
1	G	1.04	72/8351 (0.9%)	1.46	139/11291 (1.2%)
2	B	0.94	18/2934 (0.6%)	1.40	39/3981 (1.0%)
2	D	0.96	16/2944 (0.5%)	1.44	41/3996 (1.0%)
2	F	0.94	16/2951 (0.5%)	1.40	42/4003 (1.0%)
2	H	0.93	18/2934 (0.6%)	1.40	42/3981 (1.1%)
All	All	1.03	358/45143 (0.8%)	1.43	681/61085 (1.1%)

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	H	1	0

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	GLU	CD-OE2	9.30	1.35	1.25
1	C	1009	GLU	CD-OE2	8.99	1.35	1.25
1	E	804	GLU	CD-OE2	8.31	1.34	1.25
1	C	955	GLU	CD-OE2	8.07	1.34	1.25
1	A	876	GLU	CD-OE2	8.00	1.34	1.25
1	A	955	GLU	CD-OE2	7.99	1.34	1.25
1	E	478	GLU	CD-OE2	7.92	1.34	1.25
2	H	166	GLU	CD-OE2	7.84	1.34	1.25
2	F	145	GLU	CD-OE2	7.83	1.34	1.25
1	E	955	GLU	CD-OE2	7.79	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	166	GLU	CD-OE2	7.76	1.34	1.25
1	G	1009	GLU	CD-OE2	7.75	1.34	1.25
2	B	372	GLU	CD-OE2	7.73	1.34	1.25
2	H	301	GLU	CD-OE2	7.69	1.34	1.25
1	G	676	GLU	CD-OE2	7.67	1.34	1.25
1	E	673	GLU	CD-OE2	7.62	1.34	1.25
1	C	478	GLU	CD-OE2	7.60	1.34	1.25
1	C	219	GLU	CD-OE2	7.60	1.34	1.25
1	E	876	GLU	CD-OE2	7.57	1.33	1.25
2	H	372	GLU	CD-OE2	7.53	1.33	1.25
1	E	535	GLU	CD-OE2	7.53	1.33	1.25
1	E	703	GLU	CD-OE2	7.53	1.33	1.25
1	E	550	GLU	CD-OE2	7.52	1.33	1.25
2	D	166	GLU	CD-OE2	7.50	1.33	1.25
1	C	804	GLU	CD-OE2	7.46	1.33	1.25
1	A	217	GLU	CD-OE2	7.41	1.33	1.25
1	A	473	GLU	CD-OE2	7.41	1.33	1.25
2	D	301	GLU	CD-OE2	7.40	1.33	1.25
1	C	707	GLU	CD-OE2	7.40	1.33	1.25
2	D	70	GLU	CD-OE2	7.39	1.33	1.25
1	E	1024	GLU	CD-OE2	7.35	1.33	1.25
1	E	1009	GLU	CD-OE2	7.35	1.33	1.25
1	A	707	GLU	CD-OE2	7.32	1.33	1.25
1	G	955	GLU	CD-OE2	7.30	1.33	1.25
1	A	109	GLU	CD-OE2	7.29	1.33	1.25
2	B	375	GLU	CD-OE2	7.26	1.33	1.25
2	B	187	GLU	CD-OE2	7.23	1.33	1.25
1	A	731	GLU	CD-OE2	7.21	1.33	1.25
1	A	699	GLU	CD-OE2	7.21	1.33	1.25
2	B	355	GLU	CD-OE2	7.17	1.33	1.25
1	C	683	GLU	CD-OE2	7.16	1.33	1.25
1	E	427	GLU	CD-OE2	7.15	1.33	1.25
1	G	876	GLU	CD-OE2	7.15	1.33	1.25
1	G	783	GLU	CD-OE2	7.14	1.33	1.25
1	C	109	GLU	CD-OE2	7.12	1.33	1.25
2	B	145	GLU	CD-OE2	7.08	1.33	1.25
2	F	372	GLU	CD-OE2	7.07	1.33	1.25
1	E	819	GLU	CD-OE2	7.04	1.33	1.25
1	G	419	GLU	CD-OE2	7.03	1.33	1.25
1	G	804	GLU	CD-OE2	7.03	1.33	1.25
1	E	699	GLU	CD-OE2	7.02	1.33	1.25
2	H	355	GLU	CD-OE2	7.01	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	910	GLU	CD-OE2	6.97	1.33	1.25
1	A	299	GLU	CD-OE2	6.95	1.33	1.25
1	A	365	GLU	CD-OE2	6.94	1.33	1.25
2	H	375	GLU	CD-OE2	6.94	1.33	1.25
2	B	301	GLU	CD-OE2	6.93	1.33	1.25
1	A	783	GLU	CD-OE2	6.92	1.33	1.25
1	G	110	GLU	CD-OE2	6.90	1.33	1.25
1	E	393	GLU	CD-OE2	6.90	1.33	1.25
2	F	301	GLU	CD-OE2	6.90	1.33	1.25
1	C	334	GLU	CD-OE2	6.88	1.33	1.25
1	A	1060	GLU	CD-OE2	6.88	1.33	1.25
1	E	676	GLU	CD-OE2	6.88	1.33	1.25
1	C	72	GLU	CD-OE2	6.88	1.33	1.25
1	C	876	GLU	CD-OE2	6.82	1.33	1.25
2	D	375	GLU	CD-OE2	6.81	1.33	1.25
1	G	892	GLU	CD-OE2	6.81	1.33	1.25
1	E	731	GLU	CD-OE2	6.81	1.33	1.25
1	A	427	GLU	CD-OE2	6.79	1.33	1.25
1	E	951	GLU	CD-OE2	6.78	1.33	1.25
1	A	186	GLU	CD-OE2	6.77	1.33	1.25
1	G	535	GLU	CD-OE2	6.77	1.33	1.25
2	F	355	GLU	CD-OE2	6.76	1.33	1.25
2	H	70	GLU	CD-OE2	6.75	1.33	1.25
1	E	103	GLU	CD-OE2	6.72	1.33	1.25
1	A	383	GLU	CD-OE2	6.71	1.33	1.25
1	G	683	GLU	CD-OE2	6.71	1.33	1.25
2	F	318	GLU	CD-OE2	6.70	1.33	1.25
2	H	145	GLU	CD-OE2	6.69	1.33	1.25
1	C	910	GLU	CD-OE2	6.68	1.33	1.25
1	G	655	GLU	CD-OE2	6.67	1.32	1.25
1	C	655	GLU	CD-OE2	6.67	1.32	1.25
1	G	190	GLU	CD-OE2	6.65	1.32	1.25
1	E	761	GLU	CD-OE2	6.63	1.32	1.25
1	E	771	GLU	CD-OE2	6.63	1.32	1.25
1	A	478	GLU	CD-OE2	6.63	1.32	1.25
1	C	731	GLU	CD-OE2	6.62	1.32	1.25
2	D	189	GLU	CD-OE2	6.61	1.32	1.25
1	A	633	GLU	CD-OE2	6.60	1.32	1.25
2	D	145	GLU	CD-OE2	6.59	1.32	1.25
1	C	349	GLU	CD-OE2	6.58	1.32	1.25
2	H	318	GLU	CD-OE2	6.58	1.32	1.25
1	C	474	GLU	CD-OE2	6.57	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	577	GLU	CD-OE2	6.57	1.32	1.25
1	G	699	GLU	CD-OE2	6.57	1.32	1.25
1	A	468	GLU	CD-OE2	6.54	1.32	1.25
2	D	187	GLU	CD-OE2	6.53	1.32	1.25
1	A	1009	GLU	CD-OE2	6.53	1.32	1.25
1	A	103	GLU	CD-OE2	6.52	1.32	1.25
1	C	59	GLU	CD-OE2	6.52	1.32	1.25
2	F	96	GLU	CD-OE2	6.51	1.32	1.25
1	E	190	GLU	CD-OE2	6.50	1.32	1.25
2	F	375	GLU	CD-OE2	6.50	1.32	1.25
2	D	124	GLU	CD-OE2	6.50	1.32	1.25
1	G	478	GLU	CD-OE2	6.49	1.32	1.25
1	E	334	GLU	CD-OE2	6.49	1.32	1.25
1	A	761	GLU	CD-OE2	6.48	1.32	1.25
2	D	71	GLU	CD-OE2	6.48	1.32	1.25
1	A	577	GLU	CD-OE2	6.46	1.32	1.25
1	A	59[A]	GLU	CD-OE2	6.46	1.32	1.25
1	A	59[B]	GLU	CD-OE2	6.46	1.32	1.25
1	A	726	GLU	CD-OE2	6.45	1.32	1.25
1	E	683	GLU	CD-OE2	6.44	1.32	1.25
2	H	10	GLU	CD-OE2	6.44	1.32	1.25
1	G	186	GLU	CD-OE2	6.43	1.32	1.25
1	C	419	GLU	CD-OE2	6.43	1.32	1.25
1	A	208	GLU	CD-OE2	6.42	1.32	1.25
1	C	1024	GLU	CD-OE2	6.42	1.32	1.25
1	G	703	GLU	CD-OE2	6.42	1.32	1.25
1	G	1024	GLU	CD-OE2	6.42	1.32	1.25
1	A	25	GLU	CD-OE2	6.42	1.32	1.25
1	G	219	GLU	CD-OE2	6.41	1.32	1.25
1	C	591	GLU	CD-OE2	6.41	1.32	1.25
1	G	916	GLU	CD-OE2	6.40	1.32	1.25
1	C	189	GLU	CD-OE2	6.40	1.32	1.25
1	E	970	GLU	CD-OE2	6.40	1.32	1.25
1	A	512	GLU	CD-OE2	6.37	1.32	1.25
1	E	591	GLU	CD-OE2	6.37	1.32	1.25
1	C	473	GLU	CD-OE2	6.37	1.32	1.25
2	B	96	GLU	CD-OE2	6.37	1.32	1.25
1	G	970	GLU	CD-OE2	6.36	1.32	1.25
1	A	1024	GLU	CD-OE2	6.35	1.32	1.25
1	A	970	GLU	CD-OE2	6.35	1.32	1.25
1	A	334	GLU	CD-OE2	6.34	1.32	1.25
1	G	731	GLU	CD-OE2	6.34	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	208	GLU	CD-OE2	6.34	1.32	1.25
1	A	81	GLU	CD-OE2	6.33	1.32	1.25
1	A	836	GLU	CD-OE2	6.33	1.32	1.25
2	D	355	GLU	CD-OE2	6.32	1.32	1.25
1	G	560	GLU	CD-OE2	6.32	1.32	1.25
2	H	260	GLU	CD-OE2	6.30	1.32	1.25
2	H	41	GLU	CD-OE2	6.29	1.32	1.25
1	A	110	GLU	CD-OE2	6.29	1.32	1.25
1	A	703	GLU	CD-OE2	6.25	1.32	1.25
1	C	771	GLU	CD-OE2	6.25	1.32	1.25
1	E	187	GLU	CD-OE2	6.24	1.32	1.25
1	E	910	GLU	CD-OE2	6.24	1.32	1.25
1	A	260	GLU	CD-OE2	6.24	1.32	1.25
1	C	761	GLU	CD-OE2	6.23	1.32	1.25
1	E	655	GLU	CD-OE2	6.23	1.32	1.25
1	C	39	GLU	CD-OE2	6.22	1.32	1.25
1	G	189	GLU	CD-OE2	6.22	1.32	1.25
1	C	604	GLU	CD-OE2	6.22	1.32	1.25
1	G	473	GLU	CD-OE2	6.21	1.32	1.25
2	F	187	GLU	CD-OE2	6.21	1.32	1.25
1	E	39	GLU	CD-OE2	6.20	1.32	1.25
1	E	926	GLU	CD-OE2	6.20	1.32	1.25
1	E	109	GLU	CD-OE2	6.18	1.32	1.25
1	E	619	GLU	CD-OE2	6.18	1.32	1.25
2	H	187	GLU	CD-OE2	6.17	1.32	1.25
1	A	419	GLU	CD-OE2	6.17	1.32	1.25
1	A	153	GLU	CD-OE2	6.17	1.32	1.25
1	E	577	GLU	CD-OE2	6.17	1.32	1.25
1	C	190	GLU	CD-OE2	6.17	1.32	1.25
1	G	39	GLU	CD-OE2	6.15	1.32	1.25
1	G	278	GLU	CD-OE2	6.15	1.32	1.25
1	E	110	GLU	CD-OE2	6.14	1.32	1.25
1	G	673	GLU	CD-OE2	6.14	1.32	1.25
1	A	203	GLU	CD-OE2	6.12	1.32	1.25
1	E	707	GLU	CD-OE2	6.12	1.32	1.25
1	C	780	GLU	CD-OE2	6.12	1.32	1.25
1	E	983	GLU	CD-OE2	6.11	1.32	1.25
1	A	549	GLU	CD-OE2	6.11	1.32	1.25
1	C	103	GLU	CD-OE2	6.11	1.32	1.25
1	E	996	GLU	CD-OE2	6.10	1.32	1.25
2	F	226	GLU	CD-OE2	6.10	1.32	1.25
1	C	624	GLU	CD-OE2	6.09	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	468	GLU	CD-OE2	6.07	1.32	1.25
2	B	260	GLU	CD-OE2	6.06	1.32	1.25
2	H	161	GLU	CD-OE2	6.06	1.32	1.25
2	D	226	GLU	CD-OE2	6.05	1.32	1.25
1	A	467	GLU	CD-OE2	6.05	1.32	1.25
1	C	383	GLU	CD-OE2	6.05	1.32	1.25
1	G	510	GLU	CD-OE2	6.05	1.32	1.25
1	A	983	GLU	CD-OE2	6.05	1.32	1.25
1	E	836	GLU	CD-OE2	6.05	1.32	1.25
1	G	819	GLU	CD-OE2	6.05	1.32	1.25
1	G	771	GLU	CD-OE2	6.03	1.32	1.25
2	B	318	GLU	CD-OE2	6.03	1.32	1.25
1	C	983	GLU	CD-OE2	6.02	1.32	1.25
1	A	655	GLU	CD-OE2	6.01	1.32	1.25
1	A	951	GLU	CD-OE2	6.01	1.32	1.25
2	B	71	GLU	CD-OE2	6.00	1.32	1.25
1	A	560	GLU	CD-OE2	6.00	1.32	1.25
1	A	39	GLU	CD-OE2	5.99	1.32	1.25
1	G	951	GLU	CD-OE2	5.99	1.32	1.25
1	C	783	GLU	CD-OE2	5.99	1.32	1.25
1	E	40	GLU	CD-OE2	5.99	1.32	1.25
2	H	29	GLU	CD-OE2	5.98	1.32	1.25
1	C	703	GLU	CD-OE2	5.98	1.32	1.25
1	E	186	GLU	CD-OE2	5.97	1.32	1.25
1	C	110	GLU	CD-OE2	5.96	1.32	1.25
1	E	59	GLU	CD-OE2	5.96	1.32	1.25
2	D	41	GLU	CD-OE2	5.96	1.32	1.25
1	A	278	GLU	CD-OE2	5.95	1.32	1.25
1	G	365	GLU	CD-OE2	5.95	1.32	1.25
1	G	215	GLU	CD-OE2	5.94	1.32	1.25
1	G	836	GLU	CD-OE2	5.94	1.32	1.25
1	E	510	GLU	CD-OE2	5.93	1.32	1.25
2	B	189	GLU	CD-OE2	5.93	1.32	1.25
1	A	79	GLU	CD-OE2	5.91	1.32	1.25
1	C	819	GLU	CD-OE2	5.90	1.32	1.25
1	A	804	GLU	CD-OE2	5.90	1.32	1.25
2	F	41	GLU	CD-OE2	5.90	1.32	1.25
1	A	624	GLU	CD-OE2	5.90	1.32	1.25
1	E	552	GLU	CD-OE1	-5.89	1.19	1.25
1	A	474	GLU	CD-OE2	5.88	1.32	1.25
1	G	103	GLU	CD-OE2	5.86	1.32	1.25
1	C	40	GLU	CD-OE2	5.86	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	299	GLU	CD-OE2	5.85	1.32	1.25
1	E	153	GLU	CD-OE2	5.85	1.32	1.25
1	A	771	GLU	CD-OE2	5.84	1.32	1.25
1	C	892	GLU	CD-OE2	5.83	1.32	1.25
1	E	189	GLU	CD-OE2	5.82	1.32	1.25
1	A	189	GLU	CD-OE2	5.82	1.32	1.25
1	A	591	GLU	CD-OE2	5.81	1.32	1.25
1	G	403	GLU	CD-OE2	5.81	1.32	1.25
1	C	549	GLU	CD-OE2	5.80	1.32	1.25
1	E	783	GLU	CD-OE2	5.80	1.32	1.25
1	G	726	GLU	CD-OE2	5.79	1.32	1.25
1	G	109	GLU	CD-OE2	5.78	1.32	1.25
1	E	208	GLU	CD-OE2	5.77	1.31	1.25
2	B	70	GLU	CD-OE2	5.76	1.31	1.25
2	D	318	GLU	CD-OE2	5.76	1.31	1.25
2	B	29	GLU	CD-OE2	5.72	1.31	1.25
1	G	25	GLU	CD-OE2	5.72	1.31	1.25
1	G	203	GLU	CD-OE2	5.72	1.31	1.25
2	F	189	GLU	CD-OE2	5.72	1.31	1.25
1	E	467	GLU	CD-OE2	5.72	1.31	1.25
1	E	726	GLU	CD-OE2	5.71	1.31	1.25
1	A	996	GLU	CD-OE2	5.70	1.31	1.25
1	C	996	GLU	CD-OE2	5.70	1.31	1.25
1	E	67	GLU	CD-OE2	5.70	1.31	1.25
1	C	916	GLU	CD-OE2	5.70	1.31	1.25
1	G	40	GLU	CD-OE2	5.69	1.31	1.25
1	C	1060	GLU	CD-OE2	5.67	1.31	1.25
1	A	676[A]	GLU	CD-OE2	5.66	1.31	1.25
1	A	676[B]	GLU	CD-OE2	5.66	1.31	1.25
2	F	166	GLU	CD-OE2	5.66	1.31	1.25
1	G	1060	GLU	CD-OE2	5.66	1.31	1.25
1	G	552	GLU	CD-OE1	-5.65	1.19	1.25
1	G	427	GLU	CD-OE2	5.64	1.31	1.25
1	A	780	GLU	CD-OE1	-5.63	1.19	1.25
1	E	841	GLU	CD-OE2	5.63	1.31	1.25
1	G	187	GLU	CD-OE2	5.63	1.31	1.25
1	A	219	GLU	CD-OE2	5.63	1.31	1.25
2	B	226	GLU	CD-OE2	5.63	1.31	1.25
2	F	71	GLU	CD-OE2	5.63	1.31	1.25
1	C	548	GLU	CD-OE2	5.62	1.31	1.25
2	H	189	GLU	CD-OE2	5.62	1.31	1.25
1	C	726	GLU	CD-OE2	5.61	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	235	GLU	CD-OE2	5.61	1.31	1.25
2	B	41	GLU	CD-OE2	5.61	1.31	1.25
1	C	951	GLU	CD-OE2	5.61	1.31	1.25
1	C	926	GLU	CD-OE2	5.59	1.31	1.25
1	E	1060	GLU	CD-OE2	5.59	1.31	1.25
1	E	419	GLU	CD-OE2	5.59	1.31	1.25
1	C	970	GLU	CD-OE2	5.58	1.31	1.25
1	C	468	GLU	CD-OE2	5.58	1.31	1.25
1	C	550	GLU	CD-OE2	5.57	1.31	1.25
1	E	365	GLU	CD-OE2	5.57	1.31	1.25
2	B	161	GLU	CD-OE2	5.56	1.31	1.25
1	C	203	GLU	CD-OE2	5.56	1.31	1.25
1	C	79	GLU	CD-OE2	5.55	1.31	1.25
1	C	186	GLU	CD-OE2	5.55	1.31	1.25
1	G	882	GLU	CD-OE2	5.53	1.31	1.25
2	D	372	GLU	CD-OE2	5.51	1.31	1.25
1	C	365	GLU	CD-OE2	5.50	1.31	1.25
1	A	187	GLU	CD-OE2	5.49	1.31	1.25
1	G	841	GLU	CD-OE2	5.49	1.31	1.25
1	E	549	GLU	CD-OE2	5.49	1.31	1.25
1	G	512	GLU	CD-OE2	5.48	1.31	1.25
1	C	676	GLU	CD-OE2	5.48	1.31	1.25
1	G	474	GLU	CD-OE2	5.48	1.31	1.25
1	E	260	GLU	CD-OE2	5.47	1.31	1.25
1	A	101	GLU	CD-OE2	5.46	1.31	1.25
1	G	549	GLU	CD-OE2	5.44	1.31	1.25
1	C	101	GLU	CD-OE2	5.43	1.31	1.25
2	F	161	GLU	CD-OE2	5.43	1.31	1.25
1	G	154	GLU	CD-OE2	5.43	1.31	1.25
1	G	761	GLU	CD-OE2	5.42	1.31	1.25
2	H	96	GLU	CD-OE2	5.42	1.31	1.25
1	C	393	GLU	CD-OE2	5.42	1.31	1.25
1	C	467	GLU	CD-OE2	5.41	1.31	1.25
1	E	780	GLU	CD-OE2	5.41	1.31	1.25
1	G	1067	GLU	CD-OE2	5.41	1.31	1.25
1	E	560	GLU	CD-OE2	5.40	1.31	1.25
1	G	926	GLU	CD-OE2	5.40	1.31	1.25
1	A	550	GLU	CD-OE2	5.40	1.31	1.25
2	B	10	GLU	CD-OE2	5.40	1.31	1.25
1	C	278	GLU	CD-OE2	5.39	1.31	1.25
1	G	142	GLU	CD-OE2	5.38	1.31	1.25
1	G	127	GLU	CD-OE2	5.38	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	591	GLU	CD-OE2	5.37	1.31	1.25
1	C	595	GLU	CD-OE2	5.37	1.31	1.25
1	C	67	GLU	CD-OE2	5.36	1.31	1.25
1	E	468	GLU	CD-OE2	5.35	1.31	1.25
1	G	983	GLU	CD-OE2	5.34	1.31	1.25
2	F	124	GLU	CD-OE2	5.34	1.31	1.25
1	E	215	GLU	CD-OE2	5.33	1.31	1.25
1	G	628	GLU	CD-OE2	5.33	1.31	1.25
1	C	628	GLU	CD-OE2	5.33	1.31	1.25
2	D	29	GLU	CD-OE2	5.32	1.31	1.25
2	H	71	GLU	CD-OE2	5.32	1.31	1.25
1	E	217	GLU	CD-OE2	5.31	1.31	1.25
1	C	673	GLU	CD-OE2	5.31	1.31	1.25
1	G	548	GLU	CD-OE2	5.30	1.31	1.25
1	E	473	GLU	CD-OE2	5.29	1.31	1.25
2	F	260	GLU	CD-OE2	5.29	1.31	1.25
2	D	161	GLU	CD-OE2	5.29	1.31	1.25
1	A	190	GLU	CD-OE2	5.29	1.31	1.25
1	C	560	GLU	CD-OE2	5.28	1.31	1.25
1	C	260	GLU	CD-OE2	5.28	1.31	1.25
1	G	707	GLU	CD-OE2	5.26	1.31	1.25
1	E	274	GLU	CD-OE2	5.26	1.31	1.25
1	G	334	GLU	CD-OE2	5.26	1.31	1.25
1	G	624	GLU	CD-OE2	5.25	1.31	1.25
1	G	550	GLU	CD-OE2	5.25	1.31	1.25
1	C	510	GLU	CD-OE2	5.24	1.31	1.25
1	A	349	GLU	CD-OE2	5.22	1.31	1.25
1	E	512	GLU	CD-OE2	5.21	1.31	1.25
1	G	349	GLU	CD-OE2	5.20	1.31	1.25
1	A	628	GLU	CD-OE2	5.19	1.31	1.25
1	C	535	GLU	CD-OE2	5.19	1.31	1.25
1	A	1067	GLU	CD-OE2	5.18	1.31	1.25
1	C	217	GLU	CD-OE2	5.16	1.31	1.25
1	G	299	GLU	CD-OE2	5.16	1.31	1.25
1	C	187	GLU	CD-OE2	5.16	1.31	1.25
1	G	67	GLU	CD-OE2	5.14	1.31	1.25
1	G	393	GLU	CD-OE2	5.14	1.31	1.25
1	C	142	GLU	CD-OE2	5.13	1.31	1.25
1	A	552	GLU	CD-OE2	5.13	1.31	1.25
1	G	577	GLU	CD-OE2	5.12	1.31	1.25
1	A	819	GLU	CD-OE2	5.10	1.31	1.25
1	A	72	GLU	CD-OE2	5.08	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	GLU	CD-OE2	5.07	1.31	1.25
1	C	403	GLU	CD-OE2	5.06	1.31	1.25
1	A	673	GLU	CD-OE2	5.05	1.31	1.25
1	A	841	GLU	CD-OE1	-5.04	1.20	1.25
1	A	260	GLU	CD-OE1	-5.03	1.20	1.25
1	A	154	GLU	CD-OE2	5.02	1.31	1.25
1	A	926	GLU	CD-OE2	5.02	1.31	1.25
2	H	226	GLU	CD-OE2	5.02	1.31	1.25
1	E	72	GLU	CD-OE2	5.02	1.31	1.25
1	E	403	GLU	CD-OE2	5.01	1.31	1.25
1	A	535	GLU	CD-OE2	5.01	1.31	1.25
1	C	836	GLU	CD-OE2	5.01	1.31	1.25

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	490	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	C	517	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	E	185	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	G	43	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	G	579	ASP	CB-CG-OD2	-10.16	109.15	118.30
1	E	517	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	C	194	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	E	944	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	E	338	ASP	CB-CG-OD2	-9.75	109.53	118.30
2	D	18	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	A	43	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	C	867	ARG	NE-CZ-NH1	9.62	125.11	120.30
2	D	249	ASP	CB-CG-OD1	9.52	126.87	118.30
1	C	490	ARG	NE-CZ-NH2	-9.48	115.56	120.30
2	H	342	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	E	514	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	G	956	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	G	1004	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	C	6	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	C	517	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	E	471	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	G	490	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	G	75	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	C	514	ARG	NE-CZ-NH2	-9.09	115.75	120.30
2	D	234	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	A	944	ARG	NE-CZ-NH1	9.04	124.82	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	G	131	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	C	223	ASP	CB-CG-OD2	-8.96	110.23	118.30
2	B	211	ASP	CB-CG-OD2	-8.95	110.24	118.30
1	E	129	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	C	490	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	E	670	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	1004	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	E	104	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	128	ASP	CB-CG-OD1	8.78	126.20	118.30
1	G	131	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	G	736	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	E	579	ASP	CB-CG-OD2	-8.65	110.51	118.30
1	G	670	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	E	338	ASP	CB-CG-OD1	8.62	126.05	118.30
1	A	670	ASP	CB-CG-OD2	-8.61	110.55	118.30
2	F	317	ASP	CB-CG-OD2	-8.60	110.56	118.30
2	D	198	ASP	CB-CG-OD1	8.58	126.02	118.30
1	C	530	ASP	CB-CG-OD1	8.57	126.01	118.30
2	D	211	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	A	736	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	791	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	E	609	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	A	611	ASP	CB-CG-OD2	-8.43	110.72	118.30
2	F	112	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	G	904	ASP	CB-CG-OD1	8.41	125.87	118.30
1	G	222	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	E	82	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	C	530	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	C	161	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	G	124	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	E	558	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	G	410	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	C	912	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	G	460	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	223	ASP	CB-CG-OD1	8.27	125.75	118.30
2	F	211	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	E	579	ASP	CB-CG-OD1	8.22	125.69	118.30
1	A	128	ASP	CB-CG-OD1	8.20	125.68	118.30
1	E	625	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	C	571	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	609	ASP	CB-CG-OD2	-8.08	111.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	625	ASP	CB-CG-OD1	8.08	125.57	118.30
1	G	338	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	E	333	ASP	CB-CG-OD1	8.05	125.54	118.30
1	G	38	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	E	410	ASP	CB-CG-OD2	-8.01	111.09	118.30
2	D	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	590	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	194	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	E	223	ASP	CB-CG-OD1	7.88	125.39	118.30
1	E	667	ASP	CB-CG-OD1	7.87	125.38	118.30
2	H	139	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	C	338	ASP	CB-CG-OD1	7.86	125.37	118.30
2	D	262	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	C	6	ASP	CB-CG-OD1	7.84	125.35	118.30
1	C	128	ASP	CB-CG-OD2	-7.82	111.27	118.30
2	F	211	ASP	CB-CG-OD1	7.80	125.32	118.30
1	G	306	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	G	197	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	G	684	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	D	249	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	A	670	ASP	CB-CG-OD1	7.75	125.28	118.30
1	E	38	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	G	84	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	642	TYR	CB-CG-CD2	-7.71	116.37	121.00
1	E	38	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	B	198	ASP	CB-CG-OD1	7.68	125.21	118.30
2	H	188	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	C	867	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	416	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	E	494	ARG	NE-CZ-NH1	7.65	124.13	120.30
2	B	244	ASP	CB-CG-OD1	7.65	125.18	118.30
1	E	490	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	343	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	460	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	G	133	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	799	TYR	CB-CG-CD1	-7.62	116.42	121.00
1	A	459	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	38	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	G	667	ASP	CB-CG-OD1	7.56	125.10	118.30
2	B	227	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	E	333	ASP	CB-CG-OD2	-7.52	111.53	118.30
2	F	97	ASP	CB-CG-OD2	-7.51	111.54	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	ASP	CB-CG-OD1	7.50	125.05	118.30
1	G	667	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	E	487	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	C	609	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	E	389	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	H	211	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	E	128	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	G	904	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	E	82	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	614	ASP	CB-CG-OD1	7.42	124.98	118.30
1	C	197	ASP	CB-CG-OD2	-7.42	111.62	118.30
2	D	67	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	G	959	ASP	CB-CG-OD1	7.41	124.97	118.30
2	H	188	ASP	CB-CG-OD1	7.41	124.97	118.30
1	C	959	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	416	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	G	133	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	133	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	197	ASP	CB-CG-OD1	7.35	124.91	118.30
1	C	441	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	C	121	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	410	ASP	CB-CG-OD2	-7.33	111.70	118.30
2	B	136	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	H	112	ASP	CB-CG-OD1	7.32	124.89	118.30
2	D	136	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	C	426	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	C	426	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	G	410	ASP	CB-CG-OD1	7.28	124.86	118.30
2	H	114	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	G	57	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	H	139	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	338	ASP	CB-CG-OD2	-7.27	111.76	118.30
2	F	112	ASP	CB-CG-OD1	7.27	124.84	118.30
2	D	67	ASP	CB-CG-OD1	7.26	124.83	118.30
1	G	609	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	G	1041	ASP	CB-CG-OD2	-7.24	111.78	118.30
2	D	198	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	487	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	F	249	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	1041	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	G	791	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	E	223	ASP	CB-CG-OD2	-7.19	111.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	471	ARG	NE-CZ-NH1	7.19	123.90	120.30
2	B	216	LEU	CB-CA-C	-7.18	96.55	110.20
1	E	194	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	333	ASP	CB-CG-OD1	7.18	124.76	118.30
1	G	625	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	579	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	G	499	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	G	226	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	G	592	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	667	ASP	CB-CG-OD1	7.17	124.75	118.30
1	G	757	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	C	684	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	104	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	769	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	E	944	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	G	57	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	333	ASP	CB-CG-OD2	-7.11	111.90	118.30
2	D	136	ASP	CB-CG-OD1	7.10	124.69	118.30
1	E	753	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	736	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	G	579	ASP	CB-CG-OD1	7.06	124.66	118.30
1	G	373	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	E	434	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	E	487	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	161	ASP	CB-CG-OD2	-7.02	111.98	118.30
2	D	83	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	G	43	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	G	128	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	C	769	ASP	CB-CG-OD1	6.99	124.59	118.30
1	E	625	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	372	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	1003	ASP	CB-CG-OD2	-6.98	112.02	118.30
2	H	227	ASP	CB-CG-OD2	-6.98	112.02	118.30
2	F	136	ASP	CB-CG-OD1	6.97	124.57	118.30
1	E	372	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	G	609	ASP	CB-CG-OD1	6.95	124.55	118.30
2	B	262	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	E	667	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	G	161	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	G	434	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	128	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	753	ASP	CB-CG-OD2	-6.91	112.08	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	97	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	765	ASP	CB-CG-OD1	6.90	124.51	118.30
1	G	753	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	A	38	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	G	558	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	G	848	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	E	867	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	G	625	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	1021	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	H	84	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	1041	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	38	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	1021	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	1021	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	G	959	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	D	227	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	E	904	ASP	CB-CG-OD1	6.80	124.42	118.30
1	E	912	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	1003	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	E	671	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	D	212	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	246	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	C	373	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	1027	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	E	121	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	944	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	306	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	C	459	ASP	CB-CG-OD1	6.73	124.35	118.30
1	A	769	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	450	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	614	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	757	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	1041	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	471	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	642	TYR	CB-CG-CD1	6.69	125.01	121.00
1	C	194	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	769	ASP	CB-CG-OD1	6.64	124.28	118.30
2	H	97	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	H	378	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	C	670	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	G	6	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	E	559	ARG	CD-NE-CZ	6.62	132.87	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	959	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	C	434	ASP	CB-CG-OD2	-6.62	112.34	118.30
2	F	317	ASP	CB-CG-OD1	6.61	124.25	118.30
2	D	15	PHE	CB-CG-CD2	6.61	125.43	120.80
2	F	136	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	A	667	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	E	684	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	912	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	E	410	ASP	CB-CG-OD1	6.58	124.22	118.30
2	F	207	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	E	989	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	246	ASP	CB-CG-OD1	6.56	124.20	118.30
2	D	114	ASP	CB-CG-OD2	-6.56	112.39	118.30
2	F	157	ASP	CB-CG-OD1	6.55	124.20	118.30
1	G	1025	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	G	757	ASP	CB-CG-OD1	6.55	124.19	118.30
2	H	262	ASP	CB-CG-OD1	6.54	124.18	118.30
1	G	1030	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	G	425	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	434	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	E	684	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	C	133	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	E	1030	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	C	57	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	D	368	ASP	CB-CA-C	6.51	123.41	110.40
1	G	614	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	G	416	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	972	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	514	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	F	139	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	753	ASP	CB-CG-OD2	-6.48	112.47	118.30
2	F	50	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	G	27	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	460	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	G	807	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	D	188	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	521	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	B	211	ASP	CB-CG-OD1	6.41	124.07	118.30
2	F	262	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	303	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	H	93	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	H	198	ASP	CB-CG-OD1	6.40	124.06	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	518	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	867	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	530	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	E	222	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	757	ASP	CB-CG-OD1	6.38	124.04	118.30
1	E	416	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	671	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	G	438	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	G	27	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	G	758	ASP	CB-CG-OD1	6.37	124.03	118.30
1	G	1057	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	305	SER	N-CA-CB	-6.36	100.95	110.50
1	A	972	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	E	674	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	450	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	E	121	ASP	CB-CG-OD1	6.33	124.00	118.30
1	E	609	ASP	CB-CG-OD1	6.33	124.00	118.30
1	E	521	ASP	CB-CG-OD1	6.33	123.99	118.30
2	F	227	ASP	CB-CG-OD1	6.32	123.99	118.30
1	E	372	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A	765	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	E	434	ASP	CB-CG-OD1	6.29	123.97	118.30
2	F	227	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	D	262	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	353	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	1021	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	518	ASP	CB-CG-OD1	6.28	123.95	118.30
1	E	571	ARG	CB-CA-C	-6.27	97.85	110.40
1	A	223	ASP	CB-CG-OD1	6.27	123.94	118.30
1	E	904	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	758	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	E	670	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	671	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	G	490	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	H	216	LEU	N-CA-CB	6.25	122.90	110.40
2	F	114	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	204	LEU	CB-CA-C	-6.24	98.34	110.20
2	D	234	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	372	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	G	753	ASP	CB-CG-OD1	6.23	123.91	118.30
1	G	973	ALA	N-CA-CB	6.23	118.83	110.10
1	E	807	ASP	CB-CG-OD2	-6.22	112.70	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	400	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	H	97	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	736	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	84	ASP	CB-CG-OD1	6.21	123.89	118.30
1	G	1003	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	757	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	667	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	G	1025	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	226	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	733	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	B	198	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	E	133	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	E	1003	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	E	539	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	C	340	THR	CA-CB-CG2	-6.18	103.75	112.40
1	A	611	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	609	ASP	CB-CG-OD1	6.16	123.84	118.30
1	E	959	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	499	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	G	736	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	112	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	373	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	161	ASP	CB-CG-OD1	6.14	123.83	118.30
1	G	758	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	D	148	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	684	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	E	956	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	G	530	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	E	197	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	E	558	ASP	CB-CG-OD1	6.11	123.80	118.30
2	B	188	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	G	735	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	F	67	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	G	989	ARG	NE-CZ-NH1	-6.10	117.25	120.30
2	H	262	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	G	494	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	F	84	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	558	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	E	735	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	E	758	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	831	ALA	N-CA-CB	6.07	118.60	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	1021	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	G	441	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	736	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	G	416	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	121	ASP	CB-CG-OD2	-6.04	112.87	118.30
2	D	15	PHE	CB-CG-CD1	-6.03	116.58	120.80
2	F	197	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	6	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	674	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	625	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	518	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	1057	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	459	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	670	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	625	ASP	CB-CG-OD1	6.00	123.70	118.30
1	E	517	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	372	ASP	CB-CG-OD1	6.00	123.70	118.30
1	E	972	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	459	ASP	CB-CG-OD1	5.98	123.68	118.30
2	H	50	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	D	69	ASP	CB-CG-OD2	-5.97	112.93	118.30
2	H	211	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	642	TYR	CB-CG-CD1	5.96	124.58	121.00
1	A	715	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	611	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	736	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	807	ASP	CB-CG-OD2	-5.95	112.94	118.30
2	F	320	THR	CA-CB-CG2	-5.95	104.07	112.40
1	A	43	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	558	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	G	791	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	238	ASP	CB-CG-OD1	5.94	123.65	118.30
2	D	69	ASP	CB-CG-OD1	5.94	123.64	118.30
2	D	212	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	133	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	104	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	E	246	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	185	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	128	ASP	CB-CG-OD1	5.91	123.62	118.30
1	G	338	ASP	CB-CG-OD1	5.91	123.62	118.30
1	G	730	ASP	CB-CG-OD2	-5.91	112.98	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	H	45	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	539	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	G	807	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	161	ASP	CB-CG-OD1	5.87	123.59	118.30
1	G	226	ASP	CB-CG-OD1	5.87	123.59	118.30
2	H	136	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	E	1025	ASP	CB-CG-OD1	5.87	123.58	118.30
1	G	185	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	1025	ASP	CB-CG-OD1	5.87	123.58	118.30
1	G	361	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	161	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	131	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	1025	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	C	950	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	E	6	ASP	CB-CG-OD2	-5.85	113.04	118.30
2	F	70	GLU	CG-CD-OE2	-5.85	106.61	118.30
1	E	614	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	592	ASP	CB-CG-OD1	5.84	123.56	118.30
2	H	344	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	E	959	ASP	CB-CG-OD1	5.83	123.55	118.30
1	G	558	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	226	ASP	CB-CG-OD1	5.83	123.55	118.30
1	G	121	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	G	130	ARG	NE-CZ-NH1	5.83	123.21	120.30
2	F	157	ASP	CB-CG-OD2	-5.82	113.06	118.30
2	H	334	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	G	169	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	69	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	C	579	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	361	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	906	LEU	N-CA-CB	-5.80	98.80	110.40
2	B	136	ASP	CB-CG-OD1	5.80	123.52	118.30
1	G	6	ASP	CB-CG-OD1	5.80	123.52	118.30
1	E	185	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	6	ASP	CB-CG-OD1	5.79	123.52	118.30
1	C	1041	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	C	557	THR	CA-CB-CG2	-5.79	104.29	112.40
1	G	261	TYR	CB-CG-CD2	-5.79	117.53	121.00
2	B	250	TYR	CB-CG-CD1	5.78	124.47	121.00
1	C	238	ASP	CB-CG-OD1	5.78	123.50	118.30
2	B	97	ASP	CB-CG-OD1	5.77	123.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	344	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	1057	ASP	CB-CG-OD1	5.77	123.49	118.30
2	B	227	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	226	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	E	1041	ASP	CB-CG-OD1	5.75	123.48	118.30
2	F	123	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	G	104	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	514	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	579	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	G	426	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	197	ASP	CB-CG-OD1	5.75	123.47	118.30
1	E	84	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	E	133	ASP	CB-CG-OD1	5.74	123.47	118.30
2	B	368	ASP	CB-CG-OD1	5.74	123.47	118.30
2	H	67	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	E	353	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	1057	ASP	N-CA-CB	5.73	120.91	110.60
1	E	258	ASP	CB-CG-OD1	5.71	123.44	118.30
1	G	671	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	G	972	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	E	675	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	128	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	998	ARG	C-N-CD	-5.68	108.09	120.60
1	C	487	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	B	105	HIS	CA-CB-CG	-5.67	103.96	113.60
1	E	912	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	674	ASP	CB-CG-OD2	-5.65	113.21	118.30
2	D	132	ILE	CB-CA-C	-5.65	100.29	111.60
2	H	23	THR	CA-CB-CG2	-5.65	104.49	112.40
1	E	530	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	416	ASP	CB-CG-OD1	5.64	123.38	118.30
2	D	18	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	114	THR	CA-CB-CG2	-5.63	104.51	112.40
1	C	416	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	953	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	B	368	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	G	494	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	499	ASP	CB-CG-OD1	5.59	123.34	118.30
1	G	765	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	716	PRO	N-CA-CB	5.59	110.01	103.30
1	C	434	ASP	CB-CG-OD1	5.59	123.33	118.30
2	F	262	ASP	CB-CG-OD2	-5.58	113.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	ASP	CB-CG-OD1	5.58	123.32	118.30
2	H	215	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	B	299	ASP	CB-CG-OD2	-5.57	113.29	118.30
2	D	188	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	530	ASP	CB-CG-OD1	5.56	123.30	118.30
2	H	18	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	D	114	ASP	CB-CG-OD1	5.55	123.30	118.30
1	G	261	TYR	CB-CG-CD1	5.55	124.33	121.00
2	H	83	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	372	ASP	CB-CG-OD1	5.55	123.29	118.30
1	E	6	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	609	ASP	CB-CG-OD1	5.54	123.29	118.30
2	F	249	ASP	CB-CG-OD1	5.54	123.29	118.30
1	G	81	GLU	CG-CD-OE2	-5.53	107.23	118.30
1	G	372	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	361	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	B	342	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	D	342	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	E	611	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	G	223	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	614	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	C	611	ASP	CB-CG-OD1	5.51	123.26	118.30
1	E	757	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	223	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	G	121	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	996	GLU	C-N-CA	-5.51	110.74	122.30
2	F	84	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	944	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	499	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	615	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	E	996	GLU	C-N-CA	-5.49	110.77	122.30
1	G	161	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	999	PRO	N-CA-CB	5.49	109.88	103.30
1	A	504[A]	LYS	CA-CB-CG	5.49	125.47	113.40
1	A	504[B]	LYS	CA-CB-CG	5.49	125.47	113.40
1	G	389	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	H	112	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	B	97	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	G	1057	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	E	1027	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	G	173	THR	N-CA-CB	5.47	120.70	110.30
1	G	716	PRO	N-CA-CB	5.46	109.85	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	258	ASP	CB-CG-OD2	-5.45	113.39	118.30
2	B	157	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	E	1057	ASP	CB-CG-OD2	-5.44	113.40	118.30
2	F	198	ASP	CB-CG-OD1	5.44	123.20	118.30
1	G	438	TYR	CB-CG-CD1	5.44	124.26	121.00
1	E	521	ASP	CB-CG-OD2	-5.44	113.41	118.30
2	D	97	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	E	611	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	121	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	B	250	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	42	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	C	1069	HIS	CB-CA-C	5.42	121.24	110.40
1	C	1025	ASP	CB-CG-OD2	-5.42	113.43	118.30
2	D	166	GLU	N-CA-CB	5.41	120.34	110.60
1	A	273	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	1004	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	G	124	ASP	CB-CG-OD1	5.41	123.17	118.30
1	E	763	ASP	CB-CG-OD1	5.41	123.17	118.30
2	F	45	ASP	CB-CG-OD1	5.41	123.16	118.30
1	E	1020	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	207	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	F	116	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	B	69	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	518	ASP	CB-CG-OD1	5.39	123.15	118.30
2	B	114	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	557	THR	C-N-CA	5.38	135.16	121.70
1	E	571	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	1025	ASP	CB-CG-OD1	5.37	123.14	118.30
1	E	592	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	258	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	H	136	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	642	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	E	226	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	G	530	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	265	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	592	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	E	1010	TYR	CB-CG-CD1	-5.35	117.79	121.00
2	D	334	ASP	CB-CG-OD2	-5.34	113.49	118.30
2	D	344	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	E	420	ALA	CB-CA-C	5.34	118.11	110.10
1	G	361	ARG	NE-CZ-NH1	5.34	122.97	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	THR	CA-CB-CG2	-5.34	104.93	112.40
1	A	133	ASP	CB-CG-OD1	5.33	123.10	118.30
1	G	426	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	F	368	ASP	CB-CA-C	5.33	121.06	110.40
1	A	730	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	614	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	1057	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	677	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	139	ASP	CB-CG-OD2	-5.32	113.52	118.30
2	D	227	ASP	CB-CG-OD1	5.31	123.08	118.30
1	G	867	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	84	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	D	216	LEU	CB-CA-C	-5.30	100.14	110.20
1	G	769	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	C	757	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	E	471	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	G	460	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	G	674	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	E	57	ASP	N-CA-CB	-5.28	101.09	110.60
2	H	104	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	F	83	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	A	1021	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	G	343	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	G	1036	TYR	CA-CB-CG	-5.28	103.38	113.40
1	C	1003	ASP	CB-CG-OD1	5.27	123.04	118.30
2	D	378	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	G	246	ASP	CB-CG-OD1	5.26	123.04	118.30
1	G	501	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	197	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	922	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	127	ALA	N-CA-CB	5.26	117.46	110.10
1	C	1020	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	807	ASP	CB-CG-OD1	5.25	123.02	118.30
1	E	735	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	G	1003	ASP	CB-CG-OD1	5.25	123.02	118.30
2	F	50	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	H	317	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	H	234	ASP	CB-CG-OD1	5.24	123.01	118.30
2	H	249	ASP	CB-CG-OD1	5.24	123.01	118.30
2	F	216	LEU	CA-C-N	-5.23	105.69	117.20
2	F	368	ASP	CB-CG-OD1	5.23	123.01	118.30
1	G	267	ALA	N-CA-CB	-5.23	102.78	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	459	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	410	ASP	CB-CG-OD1	5.22	123.00	118.30
2	H	217	THR	CA-CB-CG2	-5.22	105.09	112.40
1	C	972	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	400	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	953	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	B	83	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	H	317	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	763	ASP	CB-CG-OD1	5.20	122.98	118.30
2	H	344	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	487	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	157	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	611	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	G	670	ASP	CB-CG-OD1	5.19	122.97	118.30
2	F	198	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	E	104	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	E	1025	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	B	104	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	490	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	590	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	558	ASP	N-CA-CB	-5.16	101.31	110.60
1	C	1041	ASP	CB-CG-OD1	5.16	122.94	118.30
2	H	249	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	763	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	C	558	ASP	CB-CG-OD1	5.15	122.93	118.30
2	F	199	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	G	539	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	E	425	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	234	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	G	258	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	674	ASP	CB-CG-OD1	5.13	122.92	118.30
2	F	67	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	223	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	197	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	509	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	757	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	F	188	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	226	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	558	ASP	N-CA-CB	-5.10	101.42	110.60
1	A	4	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	118	ALA	N-CA-CB	5.09	117.23	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	188	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	758	ASP	CB-CG-OD1	5.09	122.88	118.30
1	E	361	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	G	870	ALA	CB-CA-C	5.09	117.73	110.10
1	C	343	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	528	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	807	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	807	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	753	ASP	CB-CG-OD1	5.07	122.86	118.30
1	G	1016	THR	CA-CB-CG2	-5.06	105.31	112.40
1	C	131	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	677	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	758	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	E	712	LEU	CB-CA-C	-5.04	100.61	110.20
2	B	244	ASP	CB-CG-OD2	-5.04	113.76	118.30
2	D	97	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	471	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	677	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	417	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	G	62	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	G	333	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	557	THR	C-N-CA	5.01	134.23	121.70
1	E	197	ASP	CB-CG-OD1	5.01	122.81	118.30
2	H	69	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	G	487	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	216	LEU	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	8190	0	8213	225	0
1	C	8196	0	8236	225	0
1	E	8189	0	8219	254	0
1	G	8197	0	8218	334	0
2	B	2871	0	2850	213	0
2	D	2877	0	2852	108	0
2	F	2880	0	2859	156	0
2	H	2871	0	2850	199	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	5	0	0	1	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
5	A	5	0	0	0	0
5	B	1	0	0	0	0
5	C	7	0	0	1	0
5	D	1	0	0	1	0
5	E	6	0	0	0	0
5	F	1	0	0	0	0
5	G	6	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	3	0
7	C	54	0	24	1	0
7	E	54	0	24	1	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	3	0
9	C	9	0	20	1	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	793	0	0	23	0
10	B	130	0	0	3	0
10	C	681	0	0	13	0
10	D	177	0	0	2	0
10	E	813	0	0	20	0
10	F	205	0	0	9	0
10	G	645	0	0	17	0
10	H	117	0	0	6	0
All	All	48206	0	44517	1694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1694) 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)
4:A:4009:K:K	10:A:4434:HOH:O	1.26	1.26
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.15
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.25	1.14
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.30	1.11
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.32	1.10
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.31	1.08
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.11	1.06
1:C:1:MET:HB2	1:C:224:LYS:HE3	1.29	1.06
2:B:261:THR:HG22	2:B:263:ILE:H	1.12	1.06
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.37	1.04
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.19	1.03
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.37	1.03
1:E:1:MET:HB2	1:E:224:LYS:HE3	1.43	1.00
2:D:324:ASN:HD22	2:D:324:ASN:H	1.07	1.00
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.45	0.98
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.27	0.98
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.29	0.96
2:B:324:ASN:H	2:B:324:ASN:HD22	1.14	0.96
2:B:324:ASN:N	2:B:324:ASN:HD22	1.58	0.96
1:E:784:GLN:HE21	1:E:784:GLN:H	0.96	0.95
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.32	0.95
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.49	0.94
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.49	0.94
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.31	0.94
2:H:354:PRO:HB3	2:H:363:ALA:HB1	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:698:ILE:HD12	1:G:698:ILE:H	1.31	0.93
1:A:784:GLN:HE21	1:A:784:GLN:H	0.93	0.93
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.48	0.92
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.85	0.92
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.84	0.92
2:F:196:ALA:HB3	2:F:218:ILE:HD12	1.50	0.92
2:H:261:THR:HG22	2:H:263:ILE:H	1.31	0.91
1:G:674:ASP:HB3	1:G:677:ARG:HB2	1.49	0.91
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.04	0.91
2:D:261:THR:HG23	2:D:263:ILE:H	1.35	0.90
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.54	0.90
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.02	0.89
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.53	0.89
2:D:187:GLU:HG2	2:D:215:ARG:CD	2.03	0.89
1:A:784:GLN:NE2	1:A:784:GLN:H	1.72	0.88
1:E:1:MET:HB2	1:E:224:LYS:CE	2.02	0.88
1:E:57:ASP:HB3	1:E:59:GLU:OE1	1.74	0.88
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.03	0.88
2:H:228:VAL:HA	2:H:231:MET:HE2	1.54	0.87
1:E:784:GLN:NE2	1:E:784:GLN:H	1.73	0.87
2:H:228:VAL:HA	2:H:231:MET:CE	2.04	0.87
2:B:324:ASN:H	2:B:324:ASN:ND2	1.72	0.86
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.57	0.86
1:G:784:GLN:NE2	1:G:784:GLN:H	1.73	0.86
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.91	0.86
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.38	0.86
1:G:563:MET:CE	1:G:635:PRO:HG3	2.06	0.85
2:D:324:ASN:HD22	2:D:324:ASN:N	1.72	0.85
1:C:728:VAL:CG1	1:C:733:ASP:HB3	2.04	0.85
1:A:698:ILE:H	1:A:698:ILE:HD12	1.42	0.84
2:H:324:ASN:HD22	2:H:324:ASN:N	1.73	0.83
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.14	0.83
1:A:339:ILE:HD12	1:A:530:ASP:HA	1.59	0.83
2:B:261:THR:HG22	2:B:263:ILE:N	1.94	0.82
2:D:324:ASN:ND2	2:D:324:ASN:H	1.77	0.82
1:G:828:VAL:HG13	1:G:842:VAL:HG22	1.61	0.82
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.94	0.82
1:E:698:ILE:H	1:E:698:ILE:HD12	1.41	0.82
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.15	0.82
2:F:261:THR:CG2	2:F:263:ILE:HG13	2.09	0.82
2:H:236:ILE:HB	2:H:265:VAL:CG2	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.61	0.81
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.16	0.81
1:G:784:GLN:HE21	1:G:784:GLN:H	1.28	0.81
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.11	0.81
1:G:726:GLU:HG3	1:G:727:ILE:N	1.95	0.81
2:F:324:ASN:H	2:F:324:ASN:HD22	1.29	0.80
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.64	0.80
1:E:343:ARG:HG3	1:E:344:THR:HG23	1.62	0.80
2:F:354:PRO:HB3	2:F:363:ALA:CB	2.12	0.80
1:G:831:ALA:HB2	1:G:840:ILE:HD11	1.62	0.80
1:A:726:GLU:HG3	1:A:727:ILE:N	1.97	0.79
2:F:170:TRP:HB3	2:F:216:LEU:HD12	1.62	0.79
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.12	0.79
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.63	0.79
1:C:1:MET:HB2	1:C:224:LYS:CE	2.11	0.79
1:G:686:LYS:O	1:G:687:LEU:HD23	1.82	0.78
1:E:38:ARG:HG3	1:E:38:ARG:HH11	1.48	0.78
2:H:234:ASP:OD1	2:H:378:ARG:HD2	1.82	0.78
2:D:261:THR:CG2	2:D:263:ILE:H	1.95	0.78
1:C:726:GLU:HG3	1:C:727:ILE:N	1.98	0.78
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.65	0.78
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.65	0.78
2:B:226:GLU:O	2:B:230:LYS:HG3	1.84	0.77
1:E:698:ILE:O	1:E:702:VAL:HG23	1.84	0.77
1:E:559:ARG:HH21	1:E:559:ARG:HG3	1.49	0.77
2:F:354:PRO:HB3	2:F:363:ALA:HB2	1.66	0.77
2:H:228:VAL:O	2:H:231:MET:HG3	1.84	0.77
1:A:710:TYR:HA	1:A:712:LEU:HD13	1.66	0.77
1:E:563[A]:MET:CE	1:E:635:PRO:HG3	2.15	0.77
1:E:103:GLU:HG3	1:E:104:ARG:N	2.00	0.77
1:C:772:MET:SD	1:C:880:THR:HG22	2.25	0.77
2:H:227:ASP:HA	2:H:230[B]:LYS:HD3	1.67	0.76
2:B:201:ALA:HB2	2:B:239:SER:CB	2.16	0.76
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.67	0.76
1:C:698:ILE:H	1:C:698:ILE:HD12	1.50	0.76
2:H:201:ALA:HB2	2:H:239:SER:CB	2.16	0.76
2:H:291:HIS:HA	2:H:310:GLN:O	1.85	0.76
2:H:150:PHE:CD2	2:H:151:PRO:HD2	2.20	0.76
2:B:196:ALA:HB3	2:B:218:ILE:HD12	1.66	0.76
1:C:822:VAL:O	1:C:823:ARG:HD3	1.86	0.76
2:H:324:ASN:O	2:H:342:ARG:HD2	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.68	0.75
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.68	0.75
1:C:963:LYS:HA	1:C:966:LYS:HE3	1.68	0.75
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.02	0.75
2:F:261:THR:HG22	2:F:263:ILE:H	1.51	0.75
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.68	0.75
1:C:675:ARG:CD	1:C:675:ARG:H	2.01	0.74
1:G:130:ARG:O	1:G:134:VAL:HG23	1.86	0.74
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.69	0.74
2:H:259:LEU:HD13	2:H:342:ARG:NH1	2.01	0.74
1:E:941:LYS:NZ	10:E:2769:HOH:O	2.21	0.74
1:G:343:ARG:HG2	1:G:344:THR:HG23	1.69	0.74
2:D:71:GLU:O	2:D:203:ARG:HG3	1.88	0.74
2:F:272:HIS:HB2	2:F:349:SER:HB2	1.69	0.74
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.70	0.74
1:A:959:ASP:O	1:A:963:LYS:HG3	1.86	0.74
1:A:489:LEU:HD22	1:A:516:LEU:HD23	1.69	0.74
1:A:944:ARG:N	10:A:4490:HOH:O	2.20	0.74
1:C:973:ALA:O	1:C:991:VAL:HG12	1.88	0.74
1:A:1:MET:HB2	1:A:224:LYS:HE3	1.70	0.74
2:B:357:SER:H	2:B:358:PRO:HA	1.52	0.74
2:F:196:ALA:HB3	2:F:218:ILE:CD1	2.16	0.74
2:H:261:THR:CG2	2:H:263:ILE:HG13	2.18	0.74
1:E:646:THR:HB	1:E:647:PRO:HD3	1.70	0.73
2:F:334:ASP:OD2	2:F:336:THR:HG23	1.87	0.73
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.00	0.73
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.16	0.73
1:C:950:ARG:HD2	1:C:1018:SER:HB2	1.67	0.73
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.88	0.73
1:G:872:LYS:HD3	1:G:877:GLN:HG2	1.70	0.73
1:G:873:SER:O	1:G:877:GLN:HG3	1.88	0.73
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.71	0.73
2:F:261:THR:CG2	2:F:263:ILE:H	2.01	0.73
2:F:364:ALA:HB3	2:F:365:PRO:HD3	1.71	0.73
2:B:232:ASN:N	2:B:233:PRO:HD3	2.03	0.73
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.04	0.73
1:A:804:GLU:HB2	10:A:4642:HOH:O	1.88	0.73
1:G:525:VAL:HG22	1:G:548:GLU:H	1.53	0.73
2:B:324:ASN:O	2:B:342:ARG:HD2	1.89	0.72
2:F:228:VAL:O	2:F:231:MET:HG3	1.89	0.72
2:B:376:GLN:HA	2:B:379:LYS:HZ3	1.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:MET:CE	1:C:880:THR:HG22	2.19	0.72
1:A:697:ALA:O	1:A:700:MET:HB3	1.90	0.72
1:E:873:SER:O	1:E:877:GLN:HG3	1.89	0.72
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.70	0.72
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.88	0.72
2:D:357:SER:N	2:D:358:PRO:HA	2.04	0.72
2:H:236:ILE:HB	2:H:265:VAL:HG23	1.71	0.72
1:E:710:TYR:HB3	1:E:711:PRO:HA	1.71	0.72
2:F:228:VAL:HA	2:F:231:MET:CE	2.18	0.72
1:G:679:GLN:O	1:G:683:GLU:HG3	1.90	0.71
1:G:698:ILE:CD1	1:G:698:ILE:H	2.02	0.71
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.24	0.71
1:C:679:GLN:O	1:C:683:GLU:HG3	1.91	0.71
2:B:354:PRO:HB3	2:B:363:ALA:HA	1.71	0.71
1:E:726:GLU:HG3	1:E:727:ILE:N	2.05	0.71
1:G:343:ARG:CG	1:G:344:THR:HG23	2.19	0.71
2:H:376:GLN:HA	2:H:379:LYS:NZ	2.04	0.71
1:E:930:LYS:HE3	10:E:1236:HOH:O	1.91	0.71
2:F:194:VAL:HG13	2:F:235:GLY:O	1.90	0.71
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.05	0.71
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.25	0.71
2:B:357:SER:HB3	2:B:358:PRO:C	2.11	0.70
2:B:376:GLN:HA	2:B:379:LYS:NZ	2.04	0.70
2:D:170:TRP:HA	5:D:4043:CL:CL	2.27	0.70
1:A:946:LEU:C	1:A:947:LEU:HD12	2.10	0.70
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.27	0.70
1:E:8[B]:LYS:HD3	1:E:84:ASP:OD1	1.91	0.70
2:D:255:ILE:HA	2:D:258:PHE:CD2	2.26	0.70
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.91	0.70
2:B:354:PRO:HG2	2:B:367:PHE:HE2	1.56	0.70
2:B:376:GLN:HG2	2:B:377:TYR:N	2.04	0.70
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.26	0.70
1:C:702:VAL:HG11	1:C:735:ARG:HH21	1.57	0.70
1:C:784:GLN:H	1:C:784:GLN:HE21	1.37	0.70
2:H:196:ALA:HA	2:H:237:PHE:O	1.91	0.70
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.74	0.70
1:G:517:ARG:HB3	1:G:522:LEU:HB3	1.72	0.70
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.19	0.70
1:E:806:GLN:HA	1:E:809:MET:HE3	1.73	0.69
1:G:930:LYS:HE3	10:G:4146:HOH:O	1.91	0.69
2:D:201:ALA:HB2	2:D:239:SER:CB	2.23	0.69

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	2.01	0.69
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.74	0.69
2:H:251:ALA:O	2:H:255:ILE:HG13	1.93	0.69
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.40	0.69
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.21	0.69
1:A:65:TYR:OH	1:A:80:LYS:HE3	1.91	0.69
1:A:273:ARG:HD2	10:A:4130:HOH:O	1.93	0.69
2:H:254:ALA:O	2:H:257:LYS:HB2	1.93	0.69
1:A:130:ARG:HB2	1:A:148:ILE:HG13	1.73	0.69
2:B:357:SER:N	2:B:358:PRO:HA	2.05	0.69
2:D:2:ILE:HG23	10:D:2901:HOH:O	1.92	0.69
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.75	0.69
2:F:204:ASN:ND2	2:F:205:ILE:HG12	2.08	0.69
1:A:675:ARG:O	1:A:679:GLN:HG3	1.93	0.68
2:B:259:LEU:O	2:B:345:LYS:HD2	1.93	0.68
1:C:804:GLU:O	1:C:808:VAL:HG23	1.93	0.68
1:E:680:HIS:O	1:E:683:GLU:HB2	1.94	0.68
2:B:202:LYS:HE2	2:B:204:ASN:HD21	1.59	0.68
1:C:1061:LYS:HD3	10:C:4615:HOH:O	1.93	0.68
1:C:772:MET:HE2	1:C:880:THR:HA	1.76	0.68
2:F:357:SER:N	2:F:358:PRO:HA	2.08	0.68
2:H:272:HIS:CB	2:H:349:SER:HB2	2.22	0.68
1:A:339:ILE:CD1	1:A:530:ASP:HA	2.24	0.68
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.12	0.68
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.67
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.73	0.67
1:C:1064:SER:O	1:C:1068:MET:HG3	1.94	0.67
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.58	0.67
1:G:951:GLU:OE1	1:G:954:LYS:HD2	1.94	0.67
9:A:4012:NET:H42	9:A:4012:NET:H22	1.77	0.67
2:D:298:LYS:HB2	2:D:332:LEU:HD11	1.76	0.67
1:E:222:ARG:NH1	1:E:278[B]:GLU:HG2	2.09	0.67
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.93	0.67
1:E:76:LYS:HE3	10:E:2548:HOH:O	1.94	0.67
2:F:199:PHE:O	2:F:241:GLY:HA3	1.94	0.67
2:H:357:SER:N	2:H:358:PRO:HA	2.09	0.67
2:H:273:GLN:O	2:H:276:ALA:HB3	1.94	0.67
2:H:370:PHE:O	2:H:373:LEU:HB2	1.93	0.67
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.59	0.67
2:H:199:PHE:O	2:H:241:GLY:HA3	1.94	0.67
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.21	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:VAL:HG22	2:D:110:ILE:CG2	2.25	0.66
2:D:199:PHE:O	2:D:241:GLY:HA3	1.94	0.66
1:E:730:ASP:OD2	1:E:733:ASP:HB2	1.95	0.66
1:E:738:PHE:O	1:E:741:ALA:HB3	1.95	0.66
2:H:354:PRO:HB3	2:H:363:ALA:CB	2.24	0.66
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.18	0.66
2:H:286:MET:HE3	2:H:289:GLY:HA2	1.78	0.66
1:C:32:GLN:OE1	1:C:320:ALA:HB3	1.96	0.66
1:E:563[A]:MET:HE3	1:E:635:PRO:HG3	1.75	0.66
1:A:58:PRO:HD2	1:A:59[A]:GLU:OE2	1.96	0.66
2:H:170:TRP:HA	10:H:3185:HOH:O	1.96	0.66
1:E:222:ARG:CZ	1:E:278[B]:GLU:HG2	2.26	0.66
1:E:417:ASP:OD1	1:E:423:LYS:NZ	2.29	0.66
1:E:784:GLN:HE21	1:E:784:GLN:N	1.81	0.66
1:A:930:LYS:HE3	10:A:4080:HOH:O	1.96	0.66
2:F:224:SER:OG	2:F:227:ASP:HB2	1.95	0.66
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.29	0.66
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.96	0.66
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.78	0.66
1:C:1020:ARG:O	1:C:1024:GLU:HG3	1.95	0.66
1:C:38:ARG:NH1	1:C:38:ARG:HG3	1.99	0.66
1:A:1069:HIS:HA	1:A:1072:ILE:HD12	1.78	0.65
2:B:219:VAL:HG23	2:B:220:PRO:O	1.95	0.65
2:F:324:ASN:HD22	2:F:324:ASN:N	1.94	0.65
2:H:164:THR:HG21	2:H:168:TYR:HE1	1.61	0.65
1:A:1073:LYS:N	1:A:1073:LYS:HD3	2.12	0.65
2:B:71:GLU:O	2:B:203:ARG:HG3	1.95	0.65
2:F:261:THR:HG21	2:F:263:ILE:HG13	1.76	0.65
2:H:274:LEU:HD23	2:H:277:LEU:HD12	1.79	0.65
1:A:715:ARG:NH2	7:A:4007:ADP:O1A	2.30	0.65
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.17	0.65
2:D:120:ARG:HB2	10:D:1026:HOH:O	1.96	0.65
1:E:845:ARG:NH1	1:E:846:ALA:O	2.30	0.65
2:D:357:SER:H	2:D:358:PRO:HA	1.61	0.65
2:F:154:ASN:HD22	2:F:155:GLY:N	1.94	0.65
2:F:258:PHE:O	2:F:261:THR:HB	1.97	0.65
2:F:133:ILE:HD12	2:F:143:ALA:HB2	1.78	0.65
1:G:735:ARG:O	1:G:738:PHE:N	2.30	0.65
2:B:201:ALA:HB2	2:B:239:SER:OG	1.97	0.65
2:F:228:VAL:HA	2:F:231:MET:HE2	1.79	0.65
1:C:726:GLU:HG3	1:C:727:ILE:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:218:ILE:N	2:H:218:ILE:HD13	2.12	0.65
1:E:4:ARG:HD3	1:E:7:ILE:HD12	1.79	0.64
2:B:168:TYR:O	2:B:218:ILE:N	2.29	0.64
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.79	0.64
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.32	0.64
1:A:735:ARG:O	1:A:738:PHE:N	2.30	0.64
2:F:205:ILE:HG22	2:F:367:PHE:HZ	1.62	0.64
2:H:324:ASN:HA	2:H:343:THR:OG1	1.97	0.64
2:H:324:ASN:HB2	2:H:344:ASP:OD2	1.94	0.64
2:B:205:ILE:O	2:B:208:MET:HB2	1.96	0.64
1:C:79:GLU:HA	1:C:111:PHE:CE2	2.33	0.64
2:D:290:HIS:HB3	2:D:310:GLN:HB3	1.80	0.64
2:F:363:ALA:O	2:F:366:LEU:N	2.30	0.64
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.27	0.64
1:G:709:GLY:O	1:G:754:HIS:ND1	2.29	0.64
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.97	0.64
1:G:704:LYS:O	1:G:707:GLU:HB2	1.97	0.64
2:H:261:THR:HG21	2:H:263:ILE:HG13	1.78	0.64
2:B:135:GLY:O	2:B:138:PRO:HD3	1.98	0.64
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.79	0.64
2:H:160:LYS:HE3	2:H:161:GLU:OE2	1.97	0.64
1:E:688:LYS:HD3	1:E:838:TYR:CE1	2.32	0.64
1:E:698:ILE:N	1:E:698:ILE:HD12	2.13	0.64
2:H:258:PHE:O	2:H:261:THR:HB	1.97	0.64
2:H:103:LYS:O	2:H:106:ASN:N	2.30	0.64
2:H:195:VAL:HG22	2:H:217:THR:HB	1.79	0.64
2:H:324:ASN:HD22	2:H:324:ASN:H	1.45	0.64
1:A:563:MET:CE	1:A:635:PRO:HG3	2.27	0.64
2:D:255:ILE:HA	2:D:258:PHE:HD2	1.62	0.64
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.80	0.64
1:C:1037:LYS:HA	10:C:4613:HOH:O	1.98	0.64
1:C:698:ILE:H	1:C:698:ILE:CD1	2.11	0.64
1:C:734:LEU:HD22	1:C:738:PHE:CD2	2.32	0.64
2:F:318:GLU:O	2:F:321:LEU:HB2	1.98	0.64
1:G:1014:ILE:HD12	1:G:1015:ASN:N	2.13	0.64
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.44	0.63
2:D:228:VAL:HG12	2:D:229:LEU:N	2.13	0.63
1:E:315:THR:O	1:E:531:THR:HG22	1.98	0.63
1:E:686:LYS:O	1:E:687:LEU:HD23	1.97	0.63
1:G:1061:LYS:NZ	10:G:4665:HOH:O	2.31	0.63
2:H:324:ASN:N	2:H:324:ASN:ND2	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ALA:O	2:D:255:ILE:HG13	1.99	0.63
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.16	0.63
1:C:946:LEU:C	1:C:947:LEU:HD12	2.19	0.63
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.80	0.63
2:H:106:ASN:C	2:H:107:ILE:HD13	2.17	0.63
1:G:100:LEU:HD12	1:G:100:LEU:N	2.14	0.63
1:G:527:LYS:HD2	2:H:116:ARG:HD3	1.80	0.63
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.34	0.63
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.30	0.63
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.81	0.63
1:E:726:GLU:OE1	1:E:1020:ARG:NE	2.29	0.63
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.33	0.63
1:G:490:ARG:NH2	10:G:4419:HOH:O	2.31	0.63
1:G:993:LYS:NZ	10:G:4520:HOH:O	2.30	0.63
2:B:157:ASP:OD1	2:B:160:LYS:HG2	1.99	0.63
1:G:340:THR:O	1:G:343:ARG:NE	2.29	0.63
1:G:734:LEU:HD22	1:G:738:PHE:CE2	2.33	0.63
2:H:83:ARG:O	2:H:83:ARG:HD2	1.99	0.63
1:C:509:ARG:HD3	10:C:4385:HOH:O	1.99	0.62
1:G:702:VAL:O	1:G:706:LYS:HD3	1.98	0.62
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.80	0.62
1:E:930:LYS:NZ	1:E:1058:ALA:O	2.33	0.62
1:G:588:ALA:O	1:G:591:GLU:HB3	1.98	0.62
1:A:947:LEU:N	1:A:947:LEU:HD12	2.14	0.62
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.45	0.62
2:H:364:ALA:N	2:H:365:PRO:HD2	2.14	0.62
2:F:196:ALA:CB	2:F:218:ILE:HD12	2.28	0.62
2:H:228:VAL:HA	2:H:231:MET:HE3	1.82	0.62
1:G:695:VAL:HG22	1:G:700:MET:HG2	1.82	0.62
2:H:357:SER:H	2:H:358:PRO:HA	1.62	0.62
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.15	0.62
1:C:681:ALA:O	1:C:684:ARG:HB3	1.99	0.62
1:E:645:GLN:HG3	1:E:649:LYS:HE3	1.82	0.62
1:E:806:GLN:HA	1:E:809:MET:CE	2.30	0.62
1:G:668:ALA:O	1:G:671:ARG:HB2	2.00	0.62
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.80	0.62
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.82	0.62
1:C:947:LEU:N	1:C:947:LEU:HD12	2.15	0.62
1:E:340:THR:O	1:E:343:ARG:NE	2.31	0.62
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.80	0.62
2:B:186:LYS:O	2:B:189:GLU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:LEU:HD12	2:B:7:LEU:N	2.15	0.62
1:C:906:LEU:HD13	1:C:1030:ARG:NE	2.14	0.62
2:B:218:ILE:N	2:B:218:ILE:HD13	2.15	0.62
1:C:715:ARG:NH2	7:C:4027:ADP:O1A	2.29	0.62
1:E:478:GLU:HB3	1:E:479:VAL:HG13	1.81	0.62
2:F:187:GLU:HG2	2:F:215:ARG:HD3	1.81	0.62
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.30	0.61
1:A:166:CYS:C	1:A:167:ILE:HD12	2.19	0.61
1:E:959:ASP:O	1:E:963:LYS:HG3	2.00	0.61
2:F:376:GLN:HA	2:F:379[A]:LYS:NZ	2.15	0.61
1:G:905:PRO:HB2	1:G:1040:TYR:OH	2.00	0.61
1:E:125:LYS:NZ	10:E:1268:HOH:O	2.32	0.61
2:F:74:GLN:NE2	10:F:3611:HOH:O	2.32	0.61
2:H:364:ALA:O	2:H:368:ASP:N	2.30	0.61
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.81	0.61
2:B:375:GLU:O	2:B:376:GLN:C	2.38	0.61
1:E:282:SER:OG	1:E:302:PRO:HA	2.00	0.61
1:C:959:ASP:O	1:C:962:ALA:HB3	2.01	0.61
1:E:267:ALA:O	1:E:271:VAL:HG23	2.01	0.61
1:G:1000:HIS:NE2	1:G:1003:ASP:OD1	2.33	0.61
1:C:259:LYS:HD3	2:D:175:TRP:CE3	2.36	0.61
2:D:324:ASN:N	2:D:324:ASN:ND2	2.44	0.61
2:F:306:MET:CE	2:F:329:HIS:HD2	2.14	0.61
1:G:874:LEU:HB3	1:G:879:VAL:O	2.01	0.61
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.83	0.61
2:F:232:ASN:N	2:F:233:PRO:HD3	2.15	0.61
1:A:734:LEU:HD22	1:A:738:PHE:CE2	2.35	0.61
2:B:375:GLU:O	2:B:377:TYR:N	2.34	0.61
1:C:671:ARG:HG2	1:C:677:ARG:HD2	1.83	0.61
2:F:225:ALA:O	2:F:229:LEU:HG	2.01	0.61
1:G:680:HIS:O	1:G:683:GLU:HB2	2.01	0.61
2:H:232:ASN:N	2:H:233:PRO:HD3	2.15	0.61
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.66	0.61
1:A:784:GLN:N	1:A:784:GLN:HE21	1.79	0.60
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.29	0.60
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.60
1:G:1017:THR:HG22	1:G:1023:ILE:HG13	1.82	0.60
2:H:199:PHE:HB3	2:H:270:LEU:HD23	1.83	0.60
1:C:951:GLU:O	1:C:954:LYS:HB2	2.00	0.60
2:F:342:ARG:NH2	2:F:344:ASP:OD1	2.32	0.60
2:F:364:ALA:HB3	2:F:365:PRO:CD	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:O	2:B:120:ARG:HG3	2.01	0.60
1:C:950:ARG:HG2	1:C:1016:THR:OG1	2.01	0.60
2:D:274:LEU:O	2:D:275:LEU:C	2.37	0.60
2:F:228:VAL:HA	2:F:231:MET:HE3	1.83	0.60
1:G:64:THR:O	1:G:1065:VAL:HG23	2.01	0.60
1:G:784:GLN:N	1:G:784:GLN:HE21	1.98	0.60
1:A:709:GLY:O	1:A:754:HIS:ND1	2.29	0.60
1:C:751:LEU:O	1:C:752:LEU:HD12	2.02	0.60
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.83	0.60
2:F:253:THR:O	2:F:256:GLN:HB2	2.02	0.60
1:E:714:VAL:HG13	1:E:752:LEU:CD1	2.32	0.60
2:H:225:ALA:HB3	2:H:257:LYS:HG2	1.83	0.60
2:B:261:THR:HG21	2:B:263:ILE:HD12	1.84	0.60
1:E:679:GLN:HG3	1:E:689:GLN:HE22	1.66	0.60
2:F:261:THR:HG23	2:F:263:ILE:HG13	1.84	0.60
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.28	0.60
2:H:107:ILE:HD13	2:H:107:ILE:N	2.16	0.60
2:H:227:ASP:O	2:H:230[A]:LYS:HB2	2.02	0.60
1:A:583:VAL:O	1:A:587:LEU:HG	2.01	0.60
2:B:172:GLN:O	2:B:207:ARG:HA	2.02	0.60
2:B:324:ASN:HA	2:B:343:THR:OG1	2.02	0.60
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.32	0.60
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.15	0.60
1:A:730:ASP:OD2	1:A:733:ASP:HB2	2.02	0.60
1:C:907:LEU:HD11	8:C:4031:ORN:HD3	1.83	0.60
2:D:26:ALA:O	2:D:131:CYS:HA	2.02	0.60
2:D:364:ALA:N	2:D:365:PRO:HD3	2.17	0.60
1:A:150:HIS:N	1:A:154:GLU:OE1	2.30	0.59
1:A:504[B]:LYS:HB3	10:A:4325:HOH:O	2.01	0.59
1:E:591:GLU:HG3	1:E:591:GLU:O	2.02	0.59
2:F:306:MET:HE2	2:F:329:HIS:HD2	1.66	0.59
1:G:646:THR:HB	1:G:647:PRO:HD3	1.84	0.59
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.84	0.59
1:G:711:PRO:HG2	1:G:755:PHE:HD2	1.66	0.59
1:E:478:GLU:HA	10:E:1520:HOH:O	2.00	0.59
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.51	0.59
1:A:65:TYR:CG	1:A:77:ILE:HD13	2.38	0.59
2:B:183:GLN:HE21	2:B:183:GLN:HA	1.68	0.59
2:B:63:VAL:O	2:B:94:ASN:HB2	2.02	0.59
2:H:23:THR:HG23	2:H:134:ALA:O	2.01	0.59
1:A:1026:SER:HB2	1:A:1030:ARG:HH12	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLY:O	1:G:205:LEU:HD12	2.01	0.59
1:G:419:GLU:HB2	1:G:423:LYS:HE3	1.83	0.59
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.37	0.59
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.84	0.59
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.83	0.59
1:G:973:ALA:O	1:G:990:LEU:HD12	2.02	0.59
1:A:420:ALA:HA	1:A:423:LYS:HD2	1.83	0.59
1:E:734:LEU:HD22	1:E:738:PHE:CD2	2.38	0.59
2:H:184:ALA:N	10:H:2978:HOH:O	2.31	0.59
1:A:698:ILE:CD1	1:A:698:ILE:H	2.13	0.59
2:B:258:PHE:O	2:B:261:THR:HB	2.02	0.59
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.17	0.59
1:G:726:GLU:HG3	1:G:727:ILE:H	1.68	0.59
2:H:142:LEU:O	2:H:146:LYS:HG3	2.01	0.59
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.03	0.59
2:H:274:LEU:O	2:H:275:LEU:C	2.39	0.59
2:B:363:ALA:O	2:B:366:LEU:HB2	2.03	0.59
1:E:209:SER:OG	1:E:211:ILE:HG13	2.01	0.59
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.33	0.59
1:A:477:ALA:HB3	10:A:4355:HOH:O	2.01	0.58
1:C:698:ILE:N	1:C:698:ILE:HD12	2.15	0.58
1:E:59:GLU:OE1	10:E:1581:HOH:O	2.16	0.58
2:B:378:ARG:C	2:B:380:THR:H	2.06	0.58
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.38	0.58
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.84	0.58
2:H:48:TYR:HA	2:H:51:GLN:NE2	2.18	0.58
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.04	0.58
1:A:698:ILE:O	1:A:701:ALA:HB3	2.04	0.58
2:F:254:ALA:O	2:F:257:LYS:HB2	2.03	0.58
2:H:193:HIS:N	2:H:234:ASP:OD2	2.37	0.58
1:C:710:TYR:HB3	1:C:711:PRO:HA	1.85	0.58
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.85	0.58
2:F:298:LYS:NZ	10:F:2619:HOH:O	2.32	0.58
1:G:901:PRO:HD2	5:G:4083:CL:CL	2.39	0.58
1:G:678:PHE:O	1:G:682:VAL:HG23	2.03	0.58
1:A:1061:LYS:NZ	10:A:4658:HOH:O	2.35	0.58
2:B:228:VAL:HG12	2:B:229:LEU:N	2.19	0.58
1:G:150:HIS:N	1:G:154:GLU:OE1	2.35	0.58
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.03	0.58
1:C:873:SER:O	1:C:877:GLN:HG3	2.04	0.58
1:G:1041:ASP:HA	8:G:4076:ORN:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:HD11	1:E:141:LEU:HD12	1.86	0.58
1:C:421:LEU:HB3	1:G:421:LEU:HB3	1.84	0.58
2:D:196:ALA:HA	2:D:237:PHE:O	2.03	0.58
2:D:298:LYS:HB2	2:D:332:LEU:CD1	2.33	0.58
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.39	0.58
1:A:710:TYR:HA	1:A:712:LEU:CD1	2.33	0.58
2:B:160:LYS:HE3	2:B:161:GLU:OE2	2.04	0.58
1:C:953:ASP:CB	1:C:1044:LEU:HD22	2.34	0.58
1:C:906:LEU:HD13	1:C:1030:ARG:CD	2.33	0.58
2:D:228:VAL:O	2:D:231:MET:HG3	2.04	0.58
1:C:677:ARG:O	1:C:680:HIS:HB2	2.04	0.58
1:C:993:LYS:HD2	1:C:996:GLU:OE2	2.03	0.58
1:G:101:GLU:OE2	1:G:104:ARG:NH2	2.30	0.58
1:G:872:LYS:O	1:G:877:GLN:NE2	2.29	0.58
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.39	0.57
1:G:561:LYS:HE2	10:G:4453:HOH:O	2.03	0.57
1:C:703:GLU:O	1:C:706:LYS:HB2	2.04	0.57
1:C:9:SER:O	1:C:84:ASP:HB2	2.04	0.57
2:F:117:LYS:HE3	10:F:1560:HOH:O	2.03	0.57
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.39	0.57
1:A:1031:ARG:HB2	10:A:4508:HOH:O	2.04	0.57
1:A:904:ASP:OD2	1:A:905:PRO:HD2	2.04	0.57
1:C:781:HIS:HE1	1:C:789:SER:HB3	1.70	0.57
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.03	0.57
2:H:318:GLU:HA	2:H:321:LEU:HD13	1.86	0.57
1:E:976:GLY:O	1:E:980:VAL:HG23	2.04	0.57
1:G:224:LYS:HE2	1:G:329:GLY:O	2.05	0.57
2:D:6:LEU:O	2:D:133:ILE:N	2.35	0.57
2:H:255:ILE:HA	2:H:258:PHE:CD2	2.40	0.57
2:B:170:TRP:HA	10:B:4092:HOH:O	2.03	0.57
2:D:286:MET:HE1	2:D:314:PHE:O	2.05	0.57
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.22	0.57
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.85	0.57
1:E:27:ASP:OD2	1:E:55:MET:HB3	2.05	0.57
1:E:783:GLU:OE1	8:E:4054:ORN:NE	2.38	0.57
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.84	0.57
1:G:697:ALA:O	1:G:700:MET:HB3	2.05	0.57
1:C:1067:GLU:O	1:C:1070:ALA:HB3	2.05	0.57
1:E:27:ASP:OD2	1:E:53:THR:HB	2.04	0.57
2:H:253:THR:O	2:H:256:GLN:HB2	2.04	0.57
1:E:736:ARG:O	1:E:739:GLN:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ALA:HA	10:G:4315:HOH:O	2.04	0.57
1:G:1:MET:HB3	1:G:2:PRO:HD2	1.86	0.57
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.69	0.57
1:C:784:GLN:H	1:C:784:GLN:NE2	2.02	0.57
1:E:503:ALA:HB1	1:E:508:VAL:O	2.05	0.57
1:E:714:VAL:HG13	1:E:752:LEU:HD11	1.87	0.57
2:D:6:LEU:HD12	2:D:7:LEU:H	1.69	0.57
2:F:223:THR:CG2	2:F:228:VAL:HG23	2.35	0.57
2:F:286[A]:MET:CE	2:F:289:GLY:HA2	2.35	0.57
2:D:208:MET:O	2:D:211:ASP:HB2	2.04	0.56
2:F:279:SER:HB2	2:F:325:LEU:HD11	1.86	0.56
2:H:286:MET:HB2	2:H:313:GLY:O	2.05	0.56
1:A:70:HIS:O	1:A:74:VAL:HG23	2.05	0.56
1:C:482:THR:HG22	10:C:4369:HOH:O	2.04	0.56
2:H:190:LEU:HD23	2:H:213:GLY:HA2	1.87	0.56
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.86	0.56
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.06	0.56
1:A:467:GLU:O	1:A:471:ARG:HG2	2.05	0.56
1:E:258:ASP:O	1:E:262:GLN:HG2	2.04	0.56
1:E:59:GLU:H	1:E:59:GLU:CD	2.07	0.56
2:F:354:PRO:CB	2:F:363:ALA:HB2	2.34	0.56
1:G:806:GLN:HA	1:G:809:MET:HE2	1.87	0.56
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.86	0.56
1:A:89:THR:O	1:A:304:VAL:HG22	2.05	0.56
1:A:951:GLU:OE1	1:A:951:GLU:HA	2.04	0.56
1:C:622:THR:O	1:C:626:VAL:HG23	2.04	0.56
1:E:110:GLU:HG2	1:E:111:PHE:CE1	2.40	0.56
1:A:252:PRO:O	1:A:254:GLN:NE2	2.38	0.56
1:A:831:ALA:HB2	1:A:840:ILE:HD11	1.88	0.56
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.86	0.56
1:G:891:LYS:HG2	1:G:892:GLU:N	2.16	0.56
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.88	0.56
2:B:144:LEU:O	2:B:148:ARG:HG3	2.06	0.56
2:B:234:ASP:OD1	2:B:378:ARG:HD2	2.05	0.56
1:E:349:GLU:O	2:F:294:ASN:HB2	2.06	0.56
1:A:728:VAL:HG12	1:A:733:ASP:HB3	1.84	0.56
1:A:972:ASP:OD1	1:A:989:ARG:HB3	2.05	0.56
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.04	0.56
1:G:481:ILE:HD12	1:G:508:VAL:HG11	1.88	0.56
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.38	0.56
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:LEU:O	2:D:345:LYS:HE3	2.05	0.56
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.86	0.56
1:E:1026:SER:CB	1:E:1030:ARG:HH12	2.18	0.56
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.23	0.56
2:H:261:THR:HG22	2:H:263:ILE:N	2.13	0.56
2:H:286:MET:CE	2:H:289:GLY:HA2	2.36	0.56
1:C:343:ARG:HG3	1:C:344:THR:HG23	1.88	0.56
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.87	0.55
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.40	0.55
1:C:417:ASP:OD2	1:C:419:GLU:HB2	2.05	0.55
2:F:322:PRO:HD2	2:F:325:LEU:HD12	1.88	0.55
1:G:470:VAL:O	1:G:474:GLU:HG3	2.06	0.55
2:H:261:THR:HG22	2:H:262:ASP:N	2.20	0.55
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.38	0.55
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.30	0.55
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.88	0.55
1:C:770:GLY:HA3	1:C:823:ARG:CZ	2.36	0.55
2:D:174:SER:O	2:D:182:PRO:HD3	2.05	0.55
2:B:104:ARG:HG2	2:B:105:HIS:CD2	2.40	0.55
1:C:860:PRO:HB2	1:C:863:LYS:HB2	1.87	0.55
2:F:286[A]:MET:HE3	2:F:289:GLY:HA2	1.89	0.55
1:G:412:LYS:HE3	1:G:434:ASP:OD2	2.07	0.55
2:H:306:MET:HE1	2:H:350:PHE:CE1	2.41	0.55
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.42	0.55
1:A:805:ILE:HD12	1:A:835:ASN:ND2	2.21	0.55
1:E:146:SER:HB2	1:E:206:ILE:O	2.07	0.55
1:G:995:HIS:CD2	1:G:995:HIS:H	2.24	0.55
1:C:142:GLU:HG2	1:C:296:ILE:HG12	1.89	0.55
1:E:667:ASP:OD2	1:E:677:ARG:NH2	2.30	0.55
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.37	0.55
1:A:958:VAL:HG22	1:A:981:LEU:HD23	1.88	0.55
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.21	0.55
1:E:967[A]:GLN:HG3	1:E:1054:LEU:HB3	1.89	0.55
1:G:148:ILE:HD13	1:G:204:LEU:O	2.07	0.55
1:C:904:ASP:HB2	1:C:1027:ARG:NH1	2.22	0.55
1:E:688:LYS:HD3	1:E:838:TYR:CZ	2.42	0.55
2:F:317:ASP:OD1	2:F:320:THR:HG23	2.06	0.55
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.88	0.55
1:C:158:VAL:O	1:C:161:ASP:HB3	2.07	0.55
2:D:285:LYS:HB2	2:D:314:PHE:CE1	2.41	0.55
2:D:48:TYR:HA	2:D:51:GLN:NE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:324:ASN:HA	2:F:343:THR:OG1	2.06	0.55
1:G:586:SER:O	1:G:587:LEU:C	2.45	0.55
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.43	0.54
2:B:41:GLU:HG3	2:B:69:ASP:O	2.08	0.54
1:C:714:VAL:HG21	1:C:728:VAL:HG21	1.88	0.54
2:D:6:LEU:HD12	2:D:15:PHE:O	2.07	0.54
1:G:384:VAL:HG22	1:G:385:MET:N	2.22	0.54
1:A:523:HIS:HB3	1:A:524:PRO:HD2	1.89	0.54
1:C:734:LEU:HD22	1:C:738:PHE:CE2	2.43	0.54
1:E:1026:SER:HB2	1:E:1030:ARG:HH12	1.73	0.54
2:F:334:ASP:CG	2:F:336:THR:HG23	2.28	0.54
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.42	0.54
2:B:334:ASP:OD2	2:B:336:THR:HG23	2.08	0.54
1:G:358:LYS:HG2	1:G:359:ILE:N	2.22	0.54
1:A:220:VAL:O	1:A:281:GLY:HA2	2.07	0.54
2:B:175:TRP:HA	2:B:180:GLY:O	2.07	0.54
2:B:202:LYS:HE2	2:B:204:ASN:ND2	2.22	0.54
1:E:906:LEU:CD2	1:E:1023:ILE:HG23	2.38	0.54
1:G:164:PHE:HB3	1:G:165:PRO:HA	1.89	0.54
2:H:201:ALA:HB2	2:H:239:SER:HB2	1.89	0.54
1:E:479:VAL:CG2	1:E:483:GLY:HA3	2.37	0.54
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.43	0.54
2:D:212:ARG:HH21	2:D:364:ALA:CB	2.21	0.54
1:E:726:GLU:OE2	1:E:736:ARG:NH2	2.41	0.54
2:H:298:LYS:NZ	10:H:3040:HOH:O	2.30	0.54
1:C:58:PRO:HD2	1:C:59:GLU:OE2	2.08	0.54
2:F:234:ASP:HB3	2:F:374:ILE:CG2	2.38	0.54
1:G:738:PHE:O	1:G:741:ALA:HB3	2.08	0.54
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.18	0.54
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.90	0.54
2:H:345:LYS:HB3	2:H:346:PRO:CD	2.38	0.54
2:B:249:ASP:OD1	2:B:250:TYR:N	2.40	0.54
2:D:290:HIS:HB2	2:D:312:HIS:CD2	2.44	0.54
2:D:318:GLU:O	2:D:321:LEU:HB2	2.08	0.54
1:E:110:GLU:HG2	1:E:111:PHE:CD1	2.43	0.54
1:E:998:ARG:CB	1:E:999:PRO:HA	2.38	0.54
2:F:376:GLN:HA	2:F:379[A]:LYS:HZ2	1.71	0.54
2:F:46:PRO:O	2:F:242:PRO:HG3	2.08	0.54
1:G:892:GLU:OE1	8:G:4076:ORN:NE	2.41	0.54
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.86	0.54
2:H:376:GLN:HA	2:H:379:LYS:HZ3	1.74	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:TYR:OH	1:A:734:LEU:HD12	2.08	0.53
2:B:272:HIS:HB2	2:B:349:SER:HB2	1.89	0.53
2:D:286:MET:HE1	2:D:312:HIS:ND1	2.23	0.53
1:E:679:GLN:O	1:E:683:GLU:HG3	2.09	0.53
1:G:1017:THR:CG2	1:G:1023:ILE:HG13	2.37	0.53
1:G:73:VAL:O	1:G:77:ILE:HG13	2.08	0.53
1:E:702:VAL:HG13	1:E:731:GLU:HG2	1.89	0.53
2:F:139:ASP:HB3	2:F:142:LEU:HB3	1.90	0.53
1:G:1001:ILE:HG22	1:G:1002:GLN:N	2.24	0.53
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.34	0.53
2:B:39:TYR:CZ	2:B:61:GLY:HA2	2.44	0.53
1:E:417:ASP:HB3	1:E:420:ALA:CB	2.39	0.53
1:E:59:GLU:OE2	1:E:59:GLU:N	2.40	0.53
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.08	0.53
2:B:191:PRO:HD2	2:B:213:GLY:O	2.08	0.53
1:G:645[B]:GLN:HG3	1:G:649:LYS:HE3	1.91	0.53
1:G:685:LEU:HD13	1:G:815:LYS:HB3	1.90	0.53
2:H:259:LEU:HD13	2:H:342:ARG:HH12	1.72	0.53
2:F:203:ARG:NH2	10:F:3236:HOH:O	2.28	0.53
2:F:193:HIS:N	2:F:234:ASP:OD2	2.30	0.53
2:F:252:ILE:HG23	2:F:278:ALA:HA	1.89	0.53
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.91	0.53
2:B:45:ASP:O	2:B:76:HIS:HB2	2.08	0.53
2:B:46:PRO:O	2:B:242:PRO:HG3	2.08	0.53
2:F:272:HIS:CB	2:F:349:SER:HB2	2.37	0.53
1:G:693:ALA:HB3	1:G:708:ILE:HD11	1.91	0.53
1:A:734:LEU:HD22	1:A:738:PHE:HE2	1.72	0.53
2:B:86:PRO:HA	10:B:4038:HOH:O	2.09	0.53
2:B:222:GLN:H	2:B:222:GLN:HE21	1.55	0.53
1:C:511:ALA:O	1:C:515:LYS:HG3	2.08	0.53
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.90	0.53
2:F:125:LYS:HD3	10:F:3194:HOH:O	2.09	0.53
2:H:277:LEU:HD21	2:H:283:THR:HG23	1.89	0.53
2:H:34:THR:HA	2:H:56:THR:OG1	2.08	0.53
1:E:526:TYR:CE1	1:E:545:SER:HB3	2.43	0.53
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.28	0.53
1:G:426:ARG:HD3	1:G:426:ARG:C	2.29	0.53
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.43	0.53
2:H:363:ALA:O	2:H:367:PHE:N	2.39	0.53
1:A:417:ASP:OD2	1:A:418:PRO:HD2	2.08	0.52
1:C:11:LEU:HA	1:C:45:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:286[A]:MET:HE1	2:F:312:HIS:O	2.09	0.52
2:H:254:ALA:O	2:H:255:ILE:C	2.45	0.52
1:C:561:LYS:O	1:C:562:ILE:HD13	2.09	0.52
1:E:967[B]:GLN:OE1	1:E:1055:ASN:ND2	2.43	0.52
1:A:421:LEU:HB3	1:E:421:LEU:HB3	1.91	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.38	0.52
1:G:663:GLY:O	1:G:664:THR:C	2.47	0.52
1:G:686:LYS:C	1:G:687:LEU:HD23	2.30	0.52
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.90	0.52
1:A:1027:ARG:HA	1:A:1030:ARG:NH2	2.24	0.52
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.92	0.52
1:C:1031:ARG:NH2	10:C:4611:HOH:O	2.43	0.52
2:D:222:GLN:O	2:D:223:THR:C	2.45	0.52
1:E:967[B]:GLN:HG2	1:E:1054:LEU:HB3	1.91	0.52
1:G:579:ASP:O	1:G:583:VAL:HG23	2.10	0.52
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.12	0.52
2:H:369:HIS:O	2:H:370:PHE:C	2.45	0.52
1:A:103:GLU:HG3	1:A:104:ARG:N	2.16	0.52
1:C:78:ILE:O	1:C:82:ARG:N	2.31	0.52
1:E:912:ARG:NH2	10:E:3602:HOH:O	2.38	0.52
2:F:259:LEU:O	2:F:345:LYS:HD2	2.10	0.52
2:H:366:LEU:O	2:H:369:HIS:HB3	2.09	0.52
1:C:809:MET:O	1:C:813:VAL:HG23	2.09	0.52
1:G:223:ASP:OD2	1:G:227:ASN:HB2	2.09	0.52
1:G:343:ARG:HG3	1:G:344:THR:HG23	1.88	0.52
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.09	0.52
2:H:376:GLN:HA	2:H:379:LYS:HZ2	1.74	0.52
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.15	0.52
1:A:59[B]:GLU:HG3	1:A:60:MET:HE1	1.92	0.52
1:A:702:VAL:HG13	1:A:731:GLU:HG2	1.91	0.52
2:B:284:VAL:O	2:B:314:PHE:HB3	2.10	0.52
1:C:126:ALA:HB3	1:C:302:PRO:HG3	1.92	0.52
1:C:571:ARG:HD3	1:C:574:GLN:HB2	1.92	0.52
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.39	0.52
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.75	0.52
1:G:164:PHE:CB	1:G:165:PRO:HA	2.38	0.52
1:G:308:SER:HB3	10:G:4280:HOH:O	2.09	0.52
1:A:1006:LYS:O	1:A:1006:LYS:HG3	2.09	0.52
2:B:327:VAL:HG13	2:B:337:LEU:CD1	2.39	0.52
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.91	0.52
1:E:130:ARG:O	1:E:134:VAL:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:246:ALA:N	2:F:247:PRO:HD2	2.24	0.52
2:H:272:HIS:HA	2:H:349:SER:CB	2.39	0.52
1:A:1063:ILE:HD13	1:A:1068:MET:HG3	1.92	0.52
2:D:261:THR:HG23	2:D:262:ASP:N	2.24	0.52
2:D:375:GLU:O	2:D:376:GLN:C	2.48	0.52
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.39	0.52
1:G:679:GLN:HG3	1:G:689:GLN:HE22	1.75	0.52
1:E:726:GLU:HG3	1:E:727:ILE:H	1.70	0.52
1:E:998:ARG:HA	1:E:999:PRO:C	2.27	0.52
1:G:690:PRO:HG3	1:G:756:LEU:HD11	1.91	0.52
2:H:173:GLY:O	2:H:207:ARG:HG2	2.10	0.52
2:H:324:ASN:H	2:H:324:ASN:ND2	2.06	0.52
1:C:224:LYS:HE2	1:C:329:GLY:O	2.10	0.52
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.45	0.52
1:E:944:ARG:HG2	1:E:1010:TYR:HD1	1.74	0.52
1:G:828:VAL:HG13	1:G:842:VAL:CG2	2.37	0.52
1:G:954:LYS:O	1:G:980:VAL:HG11	2.10	0.52
2:H:226:GLU:O	2:H:230[A]:LYS:HG3	2.09	0.52
2:B:249:ASP:HA	2:B:252:ILE:HG13	1.91	0.51
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.75	0.51
1:G:69:ILE:O	1:G:69:ILE:HG22	2.11	0.51
1:A:675:ARG:H	1:A:675:ARG:HD3	1.74	0.51
2:B:254:ALA:O	2:B:257[B]:LYS:HB2	2.09	0.51
1:E:734:LEU:HD22	1:E:738:PHE:CE2	2.44	0.51
1:E:648:LEU:CD2	1:E:845:ARG:HD3	2.40	0.51
1:G:1063:ILE:HG13	1:G:1067:GLU:OE2	2.11	0.51
2:H:71:GLU:O	2:H:203:ARG:HG3	2.10	0.51
2:H:369:HIS:CE1	2:H:373:LEU:HG	2.45	0.51
9:A:4012:NET:H42	9:A:4012:NET:C2	2.40	0.51
1:C:674:ASP:OD2	1:C:677:ARG:HB2	2.11	0.51
1:E:101:GLU:OE2	1:E:104:ARG:NH2	2.30	0.51
1:E:164:PHE:HA	1:E:165:PRO:C	2.30	0.51
1:G:950:ARG:HG3	1:G:1016:THR:OG1	2.09	0.51
2:B:51:GLN:O	2:B:78:GLN:N	2.42	0.51
1:C:500:ALA:O	1:C:504:LYS:HG3	2.09	0.51
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.93	0.51
2:H:265:VAL:O	2:H:347:ALA:HA	2.10	0.51
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.31	0.51
1:A:426:ARG:C	1:A:426:ARG:HD3	2.31	0.51
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.75	0.51
2:H:306:MET:HE2	2:H:329:HIS:HD2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:VAL:HG22	1:A:548:GLU:H	1.76	0.51
1:A:733:ASP:O	1:A:736:ARG:HB3	2.10	0.51
2:B:228:VAL:O	2:B:231:MET:HG3	2.10	0.51
2:B:317:ASP:O	2:B:321:LEU:HD13	2.09	0.51
1:E:509:ARG:HH11	1:E:512:GLU:HG3	1.75	0.51
1:G:561:LYS:O	1:G:562:ILE:HD13	2.11	0.51
1:G:974:THR:O	1:G:975:HIS:C	2.49	0.51
2:H:222:GLN:O	2:H:223:THR:O	2.29	0.51
2:H:214:CYS:SG	2:H:371:ILE:HD11	2.50	0.51
2:F:218:ILE:HD13	2:F:218:ILE:N	2.25	0.51
1:G:333:ASP:N	1:G:333:ASP:OD1	2.43	0.51
2:H:169:SER:HA	2:H:216:LEU:O	2.11	0.51
1:E:464:VAL:HG11	2:F:88:ILE:HD13	1.93	0.51
1:G:947:LEU:HA	1:G:1014:ILE:CG2	2.41	0.51
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.26	0.51
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.10	0.51
2:B:10:GLU:HG3	2:B:129:ASN:O	2.11	0.51
1:E:475:LYS:HD3	1:E:488:PHE:CZ	2.46	0.51
1:A:737:TYR:CZ	1:A:741:ALA:HB2	2.46	0.50
2:B:13:THR:HG22	2:B:15:PHE:CE2	2.46	0.50
1:E:1021:ARG:O	1:E:1025:ASP:OD2	2.29	0.50
1:E:1026:SER:O	1:E:1027:ARG:C	2.47	0.50
1:E:6:ASP:N	1:E:6:ASP:OD2	2.44	0.50
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.93	0.50
1:E:840:ILE:O	1:E:841:GLU:HB3	2.11	0.50
1:A:504[A]:LYS:HB3	10:A:4325:HOH:O	2.11	0.50
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.24	0.50
1:G:135:ALA:HB1	1:G:274:GLU:HG3	1.93	0.50
1:A:361:ARG:CZ	1:A:404:VAL:HG12	2.41	0.50
2:B:236:ILE:HB	2:B:265:VAL:HG22	1.94	0.50
2:B:334:ASP:CG	2:B:336:THR:HG23	2.32	0.50
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.11	0.50
1:E:755:PHE:CE1	7:E:4050:ADP:C2	2.99	0.50
1:G:713:VAL:O	1:G:713:VAL:HG12	2.11	0.50
1:G:734:LEU:HD22	1:G:738:PHE:CD2	2.46	0.50
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.40	0.50
1:A:775:ILE:HG13	1:A:810:ARG:HG2	1.94	0.50
1:C:340:THR:O	1:C:343:ARG:HG2	2.12	0.50
1:C:6:ASP:N	1:C:6:ASP:OD2	2.45	0.50
1:E:8[A]:LYS:NZ	10:E:2527:HOH:O	2.43	0.50
2:F:234:ASP:HB3	2:F:374:ILE:HG23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:235:GLY:HA2	2:H:264:PRO:HD2	1.93	0.50
1:A:167:ILE:N	1:A:167:ILE:HD12	2.25	0.50
1:A:165:PRO:HA	1:A:182:ALA:O	2.12	0.50
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.11	0.50
1:G:711:PRO:O	1:G:712:LEU:HD12	2.11	0.50
2:B:231:MET:O	2:B:232:ASN:O	2.30	0.50
2:B:255:ILE:HG22	2:B:278:ALA:CB	2.42	0.50
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.47	0.50
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.29	0.50
1:G:731:GLU:O	1:G:735:ARG:HG3	2.12	0.50
1:C:343:ARG:HD2	1:C:536:PHE:HB3	1.93	0.50
1:G:220:VAL:O	1:G:281:GLY:HA2	2.11	0.50
2:B:222:GLN:HG3	2:B:250:TYR:CD1	2.47	0.49
2:B:254:ALA:O	2:B:257[A]:LYS:HB2	2.11	0.49
1:C:130:ARG:HD2	10:C:4522:HOH:O	2.11	0.49
1:G:461:TRP:O	1:G:465:GLN:HG3	2.11	0.49
1:G:695:VAL:HG21	1:G:701:ALA:CA	2.36	0.49
1:A:751:LEU:O	1:A:752:LEU:HD12	2.12	0.49
2:B:176:THR:O	2:B:180:GLY:N	2.37	0.49
2:B:324:ASN:HB2	2:B:342:ARG:HE	1.77	0.49
1:C:475:LYS:O	1:C:479:VAL:HG22	2.13	0.49
1:E:809:MET:O	1:E:813:VAL:HG23	2.12	0.49
1:G:495:LYS:NZ	10:G:4624:HOH:O	2.25	0.49
1:G:597:ILE:HG12	1:G:615:ARG:HB2	1.93	0.49
1:G:738:PHE:O	1:G:739:GLN:C	2.50	0.49
1:G:802:SER:OG	1:G:805:ILE:HB	2.12	0.49
1:G:873:SER:OG	1:G:876:GLU:HG3	2.12	0.49
10:G:4302:HOH:O	2:H:37:THR:HG22	2.13	0.49
2:B:158:LEU:HD12	2:B:243:GLY:CA	2.42	0.49
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.12	0.49
1:A:560:GLU:OE1	1:A:636:LYS:HE3	2.11	0.49
1:E:442:ALA:O	1:E:447:LEU:HB2	2.13	0.49
1:G:757:ASP:O	1:G:833:LYS:HE3	2.11	0.49
1:A:548:GLU:OE2	2:B:83:ARG:NE	2.43	0.49
1:A:993:LYS:HB2	1:A:996:GLU:OE1	2.12	0.49
1:C:262:GLN:OE1	1:C:262:GLN:HA	2.11	0.49
1:C:344:THR:HB	1:C:345:PRO:HD2	1.95	0.49
1:E:339:ILE:HD11	1:E:531:THR:HG23	1.94	0.49
2:H:201:ALA:HB2	2:H:239:SER:OG	2.12	0.49
1:E:805:ILE:O	1:E:809:MET:HE2	2.12	0.49
2:F:46:PRO:HA	2:F:76:HIS:CG	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:GLU:HG2	1:G:111:PHE:CZ	2.48	0.49
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.95	0.49
2:H:184:ALA:O	2:H:185:LYS:O	2.29	0.49
2:H:227:ASP:O	2:H:230[B]:LYS:HB2	2.11	0.49
1:A:11:LEU:HA	1:A:45:ILE:O	2.13	0.49
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.47	0.49
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.42	0.49
1:C:324:ALA:O	1:C:327:ALA:HB3	2.12	0.49
1:C:554:ASN:N	1:C:555:PRO:HD3	2.27	0.49
1:G:1014:ILE:HD12	1:G:1014:ILE:C	2.31	0.49
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.92	0.49
1:A:698:ILE:N	1:A:698:ILE:HD12	2.19	0.49
1:A:814:GLN:NE2	10:A:4443:HOH:O	2.45	0.49
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.94	0.49
2:D:290:HIS:HB2	2:D:312:HIS:NE2	2.28	0.49
2:D:290:HIS:HB3	2:D:310:GLN:CB	2.42	0.49
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.48	0.49
2:H:186:LYS:O	2:H:189:GLU:HB2	2.13	0.49
2:B:263:ILE:HG23	2:B:264:PRO:HD2	1.93	0.49
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.95	0.49
1:E:808:VAL:HA	10:E:1628:HOH:O	2.13	0.49
2:F:350:PHE:HB2	2:F:366:LEU:HD13	1.94	0.49
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.94	0.49
2:H:350:PHE:CG	2:H:366:LEU:HD11	2.48	0.49
2:H:63:VAL:HG12	2:H:91:ASN:HB2	1.94	0.49
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.32	0.49
1:A:501:ARG:NH1	10:A:4325:HOH:O	2.43	0.49
1:C:665:SER:O	1:C:666:PRO:C	2.51	0.49
1:E:1:MET:O	1:E:329:GLY:O	2.30	0.49
2:F:125:LYS:HB2	10:F:3196:HOH:O	2.12	0.49
1:G:698:ILE:O	1:G:701:ALA:HB3	2.13	0.49
1:A:954:LYS:O	1:A:957:VAL:HG12	2.13	0.48
1:C:180:GLY:HA2	1:C:376:THR:OG1	2.13	0.48
1:E:224:LYS:HE2	1:E:329:GLY:O	2.14	0.48
1:E:563[A]:MET:HE2	1:E:563[A]:MET:HB2	1.68	0.48
1:E:708:ILE:HD12	1:E:752:LEU:HB3	1.94	0.48
1:E:944:ARG:HG2	1:E:1010:TYR:CD1	2.46	0.48
2:H:264:PRO:HA	2:H:346:PRO:O	2.14	0.48
1:A:534:ALA:O	2:B:123:ARG:NH1	2.36	0.48
1:A:692:ASN:HA	1:A:752:LEU:O	2.13	0.48
2:B:371:ILE:O	2:B:374:ILE:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.94	0.48
2:F:251:ALA:O	2:F:252:ILE:C	2.49	0.48
1:G:167:ILE:HD12	1:G:167:ILE:N	2.28	0.48
1:G:1:MET:O	1:G:334:GLU:OE1	2.31	0.48
2:H:25:SER:HB2	2:H:133:ILE:HG12	1.95	0.48
2:B:166:GLU:O	2:B:167:ALA:O	2.32	0.48
2:B:285:LYS:HB2	2:B:314:PHE:CD1	2.49	0.48
1:C:615:ARG:NE	1:C:633:GLU:OE1	2.45	0.48
2:H:131:CYS:SG	2:H:133:ILE:HG13	2.53	0.48
1:A:222:ARG:HD3	1:A:277:VAL:O	2.13	0.48
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.94	0.48
2:B:249:ASP:CA	2:B:252:ILE:HG13	2.44	0.48
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.48	0.48
2:B:341:HIS:CG	2:B:348:PHE:HB3	2.49	0.48
1:C:145[A]:ARG:HB3	1:C:208:GLU:HG2	1.96	0.48
1:C:953:ASP:OD1	1:C:1016:THR:OG1	2.29	0.48
1:E:417:ASP:OD2	1:E:418:PRO:HD2	2.13	0.48
1:E:343:ARG:HD2	1:E:536:PHE:HB3	1.95	0.48
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.96	0.48
2:H:150:PHE:CG	2:H:151:PRO:HD2	2.48	0.48
1:A:1072:ILE:C	1:A:1073:LYS:HD3	2.34	0.48
2:B:203:ARG:O	2:B:207:ARG:HG3	2.14	0.48
1:C:1017[B]:THR:HG21	1:C:1023:ILE:HA	1.95	0.48
1:C:712:LEU:O	1:C:727:ILE:HA	2.12	0.48
1:G:598:MET:HG3	1:G:599:VAL:N	2.27	0.48
1:G:796:LEU:HD23	1:G:796:LEU:C	2.34	0.48
2:H:23:THR:HG22	2:H:24:GLY:N	2.28	0.48
2:H:323:ALA:C	2:H:325:LEU:H	2.17	0.48
1:A:473:GLU:HG2	1:A:497:PHE:CE1	2.48	0.48
2:B:174:SER:O	2:B:182:PRO:HD3	2.13	0.48
2:B:364:ALA:O	2:B:365:PRO:C	2.52	0.48
1:C:950:ARG:CD	1:C:1018:SER:HB2	2.40	0.48
1:E:1017:THR:HG21	1:E:1023:ILE:CA	2.44	0.48
1:E:698:ILE:CD1	1:E:698:ILE:H	2.14	0.48
1:E:750:VAL:HG12	1:E:752:LEU:HD13	1.95	0.48
2:F:324:ASN:ND2	2:F:324:ASN:H	2.05	0.48
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.48	0.48
1:G:336:MET:HB3	1:G:342:GLY:HA2	1.96	0.48
1:G:805:ILE:HD13	1:G:832:VAL:HG11	1.96	0.48
2:H:255:ILE:HA	2:H:258:PHE:HD2	1.77	0.48
1:A:133:ASP:HB2	10:A:4119:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:OE2	1:A:294:ARG:NH2	2.46	0.48
1:A:315:THR:O	1:A:531:THR:HG22	2.13	0.48
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.14	0.48
1:G:814[B]:GLN:HG2	1:G:818:PHE:CE2	2.49	0.48
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.13	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.14	0.48
1:A:951:GLU:HA	1:A:954:LYS:HD2	1.95	0.48
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.96	0.48
2:B:350:PHE:CG	2:B:366:LEU:HD11	2.48	0.48
1:C:697:ALA:O	1:C:700:MET:HB3	2.14	0.48
2:D:206:LEU:O	2:D:210:VAL:HG23	2.12	0.48
2:F:272:HIS:HA	2:F:349:SER:HB2	1.96	0.48
2:F:354:PRO:HB3	2:F:363:ALA:HB1	1.90	0.48
1:G:6:ASP:N	1:G:6:ASP:OD2	2.45	0.48
1:A:128:ASP:CG	1:A:131:ARG:HG3	2.34	0.48
1:A:143:THR:HA	1:A:296:ILE:HG23	1.96	0.48
9:A:4012:NET:C4	9:A:4012:NET:H22	2.41	0.48
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.48
1:C:946:LEU:HB3	1:C:1013:ILE:HG12	1.96	0.48
2:H:324:ASN:O	2:H:342:ARG:HA	2.14	0.48
1:C:1052:MET:HG3	10:C:4606:HOH:O	2.13	0.47
2:H:272:HIS:HA	2:H:349:SER:HB2	1.95	0.47
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.67	0.47
1:A:947:LEU:HG	1:A:1014:ILE:CG2	2.44	0.47
1:C:710:TYR:HA	1:C:712:LEU:CD1	2.44	0.47
2:D:172:GLN:HG2	2:D:173:GLY:N	2.28	0.47
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.50	0.47
1:A:528:ARG:HG2	1:A:543:MET:HG2	1.96	0.47
1:A:710:TYR:CB	1:A:711:PRO:HA	2.43	0.47
1:A:730:ASP:H	1:A:733:ASP:HB2	1.79	0.47
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.95	0.47
1:G:734:LEU:HD22	1:G:738:PHE:HE2	1.77	0.47
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.96	0.47
1:G:1017:THR:HG21	1:G:1023:ILE:CA	2.40	0.47
2:H:225:ALA:CB	2:H:257:LYS:HG2	2.44	0.47
1:A:101:GLU:OE2	1:A:104:ARG:NH1	2.43	0.47
1:A:972:ASP:HA	1:A:989:ARG:O	2.14	0.47
2:B:286:MET:HE3	2:B:286:MET:HB2	1.70	0.47
2:B:331:SER:O	2:B:335:GLY:N	2.46	0.47
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.50	0.47
2:D:116:ARG:O	2:D:120:ARG:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:692:ASN:HA	1:E:752:LEU:O	2.13	0.47
1:E:779:MET:HA	1:E:795:SER:O	2.14	0.47
2:F:244:ASP:O	2:F:247:PRO:HD2	2.14	0.47
1:G:936:ASN:HB2	10:G:4102:HOH:O	2.13	0.47
2:H:46:PRO:HA	2:H:76:HIS:CG	2.49	0.47
1:A:240:MET:HE3	7:A:4001:ADP:C4	2.49	0.47
2:B:75:VAL:HG11	2:B:107:ILE:HG13	1.96	0.47
2:B:290:HIS:HB3	2:B:310:GLN:HB3	1.96	0.47
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.50	0.47
2:D:6:LEU:O	2:D:132:ILE:HA	2.14	0.47
2:D:261:THR:CG2	2:D:263:ILE:HG13	2.45	0.47
1:G:479:VAL:HB	1:G:483:GLY:HA3	1.95	0.47
1:G:646:THR:HB	1:G:647:PRO:CD	2.44	0.47
1:G:892:GLU:HG3	1:G:893:VAL:N	2.29	0.47
1:A:755:PHE:CE1	7:A:4007:ADP:C2	3.03	0.47
1:A:812:GLN:NE2	10:A:4621:HOH:O	2.30	0.47
2:B:201:ALA:HA	2:B:240:ASN:OD1	2.14	0.47
2:D:317:ASP:OD1	2:D:320:THR:HG23	2.14	0.47
1:E:400:ARG:HD3	10:E:1472:HOH:O	2.15	0.47
1:E:646:THR:HB	1:E:647:PRO:CD	2.42	0.47
1:A:731:GLU:O	1:A:735:ARG:HG3	2.14	0.47
2:B:157:ASP:CG	2:B:160:LYS:HG2	2.34	0.47
1:C:358:LYS:HE3	10:C:4075:HOH:O	2.14	0.47
1:C:796:LEU:HD23	1:C:796:LEU:C	2.35	0.47
2:F:201:ALA:HB2	2:F:239:SER:CB	2.44	0.47
1:G:170:PRO:HA	1:G:204:LEU:HD23	1.97	0.47
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.15	0.47
2:H:297:VAL:HG11	2:H:306:MET:HE3	1.96	0.47
1:A:337:ASN:N	1:A:344:THR:O	2.32	0.47
1:C:167:ILE:HD12	1:C:167:ILE:N	2.30	0.47
1:E:534:ALA:O	2:F:123:ARG:HD3	2.15	0.47
1:G:29:SER:CB	1:G:304:VAL:HG21	2.45	0.47
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.30	0.47
1:G:98:CYS:O	1:G:99:ALA:C	2.51	0.47
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.39	0.47
1:E:157:ALA:O	1:E:160:ALA:HB3	2.15	0.47
1:E:648:LEU:HD22	1:E:845:ARG:HD3	1.97	0.47
2:F:170:TRP:CH2	2:F:203:ARG:HG2	2.50	0.47
2:H:45:ASP:CG	2:H:202:LYS:HD2	2.36	0.47
2:H:254:ALA:O	2:H:257:LYS:N	2.45	0.47
2:H:320:THR:OG1	2:H:320:THR:O	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:HG2	1:C:359:ILE:N	2.29	0.47
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.96	0.47
1:C:683:GLU:O	1:C:686:LYS:N	2.42	0.47
1:C:802:SER:O	1:C:805:ILE:HG22	2.15	0.47
2:H:133:ILE:CG2	2:H:138:PRO:HB3	2.45	0.47
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.78	0.47
1:E:676:GLU:O	1:E:680:HIS:ND1	2.48	0.46
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.97	0.46
2:F:324:ASN:O	2:F:343:THR:N	2.39	0.46
2:F:50:ARG:HD2	2:F:50:ARG:HA	1.57	0.46
1:G:3:LYS:HG3	1:G:3:LYS:O	2.13	0.46
1:C:891:LYS:HB3	1:C:891:LYS:HE2	1.76	0.46
1:E:54:ILE:O	1:E:57:ASP:HB2	2.15	0.46
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.80	0.46
2:F:160:LYS:HG3	2:F:161:GLU:HG2	1.96	0.46
1:G:222:ARG:CZ	1:G:273:ARG:HG2	2.46	0.46
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.80	0.46
1:G:642:TYR:OH	1:G:865:ALA:HB3	2.15	0.46
2:H:181:LEU:HD23	2:H:181:LEU:HA	1.74	0.46
2:B:197:TYR:HA	2:B:219:VAL:HG22	1.97	0.46
2:B:268:ILE:HA	2:B:268:ILE:HD13	1.73	0.46
2:B:273:GLN:O	2:B:276:ALA:HB3	2.14	0.46
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.44	0.46
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.50	0.46
1:E:51:PRO:HG3	1:E:918:MET:HB2	1.97	0.46
2:F:322:PRO:HG2	2:F:325:LEU:HD12	1.96	0.46
1:G:1030:ARG:NH1	1:G:1030:ARG:HG3	2.30	0.46
1:G:28:TYR:O	1:G:32:GLN:HG3	2.15	0.46
2:H:331:SER:O	2:H:335:GLY:N	2.46	0.46
1:A:680:HIS:O	1:A:683:GLU:HB2	2.15	0.46
1:A:957:VAL:O	1:A:958:VAL:C	2.52	0.46
2:B:285:LYS:HB2	2:B:314:PHE:CE1	2.50	0.46
1:C:940:LYS:HG3	1:C:1011:THR:HB	1.98	0.46
2:D:23:THR:HG22	2:D:24:GLY:N	2.30	0.46
2:D:286:MET:HB2	2:D:313:GLY:O	2.15	0.46
2:D:324:ASN:O	2:D:342:ARG:HA	2.15	0.46
1:E:950:ARG:HD3	10:E:1679:HOH:O	2.15	0.46
2:F:306:MET:CE	2:F:329:HIS:CD2	2.98	0.46
2:F:35:SER:HB3	2:F:37:THR:O	2.15	0.46
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.50	0.46
1:G:139:ILE:HG21	1:G:274:GLU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:GLU:CB	1:G:423:LYS:HE3	2.46	0.46
1:G:710:TYR:HA	1:G:711:PRO:C	2.34	0.46
1:G:735:ARG:O	1:G:736:ARG:C	2.54	0.46
1:G:807:ASP:HA	1:G:810:ARG:HG3	1.97	0.46
2:H:286:MET:N	2:H:313:GLY:O	2.42	0.46
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.97	0.46
1:A:278:GLU:HG2	10:A:4221:HOH:O	2.16	0.46
2:B:46:PRO:HA	2:B:76:HIS:CG	2.51	0.46
1:C:698:ILE:O	1:C:702:VAL:HG23	2.15	0.46
1:C:737:TYR:O	1:C:739:GLN:N	2.48	0.46
1:C:75:ARG:HD3	10:C:4110:HOH:O	2.14	0.46
2:F:227:ASP:O	2:F:230:LYS:HB2	2.14	0.46
2:F:236:ILE:HD13	2:F:258:PHE:CG	2.50	0.46
2:F:272:HIS:HA	2:F:349:SER:CB	2.45	0.46
1:G:955:GLU:HB2	10:G:4683:HOH:O	2.15	0.46
1:A:154:GLU:HA	10:A:4721:HOH:O	2.15	0.46
1:C:644:GLY:O	1:C:647:PRO:HD2	2.16	0.46
1:G:259:LYS:HE2	2:H:69:ASP:OD2	2.16	0.46
1:G:231:VAL:HG11	1:G:319:ILE:HD11	1.98	0.46
2:H:268:ILE:O	2:H:269:CYS:HB3	2.15	0.46
1:A:146:SER:HB2	1:A:206:ILE:O	2.15	0.46
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.97	0.46
2:B:192:PHE:HZ	2:B:375:GLU:OE2	1.99	0.46
2:F:59:HIS:ND1	2:F:84:ASP:OD2	2.44	0.46
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.51	0.46
1:G:479:VAL:CB	1:G:483:GLY:HA3	2.46	0.46
1:A:654:LEU:O	1:A:659:VAL:HG23	2.16	0.46
2:B:221:ALA:HB1	2:B:250:TYR:HE1	1.80	0.46
1:C:764:VAL:HG11	1:C:813:VAL:HG21	1.97	0.46
2:D:187:GLU:CG	2:D:215:ARG:HD2	2.18	0.46
1:E:953:ASP:O	1:E:955:GLU:N	2.49	0.46
1:G:24:CYS:O	1:G:25:GLU:C	2.51	0.46
1:G:344:THR:HB	1:G:345:PRO:HD2	1.98	0.46
2:B:286:MET:HE3	2:B:289:GLY:HA2	1.98	0.46
2:B:34:THR:HA	2:B:56:THR:OG1	2.16	0.46
1:C:119:THR:O	1:C:123:ILE:HG13	2.15	0.46
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.46
2:D:81:VAL:HG22	2:D:110:ILE:HG22	1.97	0.46
1:G:479:VAL:HG21	1:G:483:GLY:HA3	1.96	0.46
1:G:493:LYS:HD2	1:G:493:LYS:HA	1.73	0.46
1:G:516:LEU:HD12	1:G:516:LEU:HA	1.68	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:698:ILE:N	1:G:698:ILE:HD12	2.14	0.46
2:H:25:SER:HA	2:H:132:ILE:O	2.15	0.46
2:H:299:ASP:OD2	2:H:301:GLU:HB2	2.16	0.46
2:B:255:ILE:HG22	2:B:278:ALA:HB1	1.98	0.46
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.46	0.46
1:C:145[B]:ARG:HB3	1:C:208:GLU:HG2	1.98	0.46
1:C:343:ARG:HG3	1:C:344:THR:CG2	2.45	0.46
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.96	0.46
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.80	0.46
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.76	0.46
1:G:757:ASP:O	1:G:758:ASP:C	2.55	0.46
2:H:364:ALA:N	2:H:365:PRO:CD	2.79	0.46
1:A:29[B]:SER:OG	1:A:30:GLY:N	2.48	0.45
1:E:340:THR:O	1:E:343:ARG:HG2	2.15	0.45
1:G:763:ASP:O	1:G:779:MET:HE3	2.16	0.45
1:G:954:LYS:O	1:G:957:VAL:HG12	2.15	0.45
2:H:261:THR:CG2	2:H:262:ASP:N	2.79	0.45
1:A:642:TYR:OH	1:A:865:ALA:HB3	2.15	0.45
2:B:332:LEU:HA	2:B:332:LEU:HD12	1.69	0.45
1:C:315:THR:O	1:C:531:THR:HG22	2.16	0.45
1:C:734:LEU:CD2	1:C:738:PHE:CE2	2.99	0.45
2:D:222:GLN:HG3	2:D:250:TYR:CD1	2.51	0.45
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.15	0.45
1:G:247:SER:O	1:G:358:LYS:HE2	2.17	0.45
1:G:619:GLU:HB3	1:G:620:PRO:HD2	1.97	0.45
1:G:702:VAL:O	1:G:705:ALA:HB3	2.16	0.45
2:H:85:LEU:HD12	2:H:86:PRO:HD2	1.99	0.45
2:B:173:GLY:C	2:B:207:ARG:HB3	2.36	0.45
2:B:224:SER:O	2:B:225:ALA:C	2.54	0.45
2:B:273:GLN:O	2:B:277:LEU:HG	2.17	0.45
2:B:286:MET:CE	2:B:289:GLY:HA2	2.47	0.45
2:B:306:MET:CE	2:B:350:PHE:CZ	3.00	0.45
2:F:252:ILE:CG2	2:F:278:ALA:HA	2.47	0.45
1:G:730:ASP:OD2	1:G:733:ASP:HB2	2.17	0.45
1:G:865:ALA:O	1:G:869:MET:HG3	2.17	0.45
1:G:956:ARG:HB2	1:G:1044:LEU:CD2	2.47	0.45
2:B:167:ALA:HA	2:B:218:ILE:O	2.15	0.45
2:B:270:LEU:HD12	2:B:273:GLN:OE1	2.16	0.45
2:B:366:LEU:HD23	2:B:366:LEU:HA	1.86	0.45
2:B:57:TYR:O	2:B:60:ILE:HD11	2.16	0.45
2:D:227:ASP:O	2:D:230:LYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:MET:HE2	2:D:313:GLY:C	2.36	0.45
1:E:157:ALA:HA	10:E:1310:HOH:O	2.15	0.45
1:E:695:VAL:CG1	1:E:696:THR:N	2.79	0.45
1:E:765:ASP:O	1:E:776:GLY:N	2.49	0.45
2:F:274:LEU:HA	2:F:274:LEU:HD23	1.81	0.45
2:F:285:LYS:HB2	2:F:314:PHE:CE1	2.52	0.45
2:B:285:LYS:CG	2:B:314:PHE:CE1	2.99	0.45
1:C:101:GLU:O	1:C:105:GLN:HG2	2.16	0.45
1:C:554:ASN:N	1:C:555:PRO:CD	2.80	0.45
1:C:701:ALA:O	1:C:705:ALA:HB2	2.16	0.45
2:F:324:ASN:O	2:F:342:ARG:HA	2.16	0.45
1:G:782:ILE:N	1:G:782:ILE:HD12	2.31	0.45
2:H:227:ASP:HA	2:H:230[A]:LYS:HD2	1.98	0.45
1:A:479:VAL:HG23	1:A:480:GLY:N	2.31	0.45
2:B:261:THR:CG2	2:B:263:ILE:HG13	2.47	0.45
1:C:314:ALA:HB1	1:C:356:VAL:HG21	1.97	0.45
1:C:499:ASP:HA	1:C:513:ILE:HG21	1.99	0.45
2:D:153:LEU:N	2:D:153:LEU:CD1	2.80	0.45
1:E:1026:SER:HB2	1:E:1030:ARG:NH1	2.30	0.45
1:E:353:ASP:OD1	2:F:116:ARG:HD2	2.17	0.45
2:F:157:ASP:HB2	2:F:247:PRO:HB2	1.99	0.45
2:F:269:CYS:SG	2:F:270:LEU:N	2.90	0.45
1:G:738:PHE:O	1:G:739:GLN:O	2.35	0.45
1:A:947:LEU:N	1:A:947:LEU:CD1	2.80	0.45
2:B:229:LEU:HA	2:B:229:LEU:HD23	1.67	0.45
2:B:199:PHE:O	2:B:241:GLY:HA3	2.17	0.45
2:B:228:VAL:CG1	2:B:258:PHE:CE1	3.00	0.45
1:E:403:GLU:OE1	1:E:646:THR:HG23	2.16	0.45
1:E:854:SER:O	1:E:858:GLY:N	2.48	0.45
1:G:156:LEU:HB3	10:G:4217:HOH:O	2.16	0.45
1:G:704:LYS:HD2	1:G:704:LYS:HA	1.63	0.45
1:A:734:LEU:CD2	1:A:738:PHE:HE2	2.30	0.45
1:A:965:LEU:HA	1:A:965:LEU:HD23	1.77	0.45
2:B:222:GLN:O	2:B:223:THR:C	2.55	0.45
1:C:237:PHE:HB3	1:C:248:ILE:O	2.16	0.45
1:C:516:LEU:HA	1:C:516:LEU:HD12	1.73	0.45
2:F:286[A]:MET:HE3	2:F:286[A]:MET:HB2	1.85	0.45
1:G:903:VAL:HG12	1:G:904:ASP:N	2.30	0.45
2:H:164:THR:HG21	2:H:168:TYR:CE1	2.47	0.45
2:H:186:LYS:O	2:H:189:GLU:N	2.41	0.45
1:A:358:LYS:HE3	10:A:4053:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:CD2	1:A:738:PHE:CE2	3.00	0.45
1:A:740:THR:H	1:A:740:THR:HG23	1.41	0.45
2:B:120:ARG:HH21	2:B:120:ARG:HD3	1.61	0.45
2:B:246:ALA:N	2:B:247:PRO:CD	2.80	0.45
1:C:704:LYS:O	1:C:707:GLU:HB2	2.17	0.45
1:C:729:TYR:CD1	1:C:729:TYR:N	2.85	0.45
1:C:734:LEU:HD22	1:C:738:PHE:HD2	1.80	0.45
2:D:285:LYS:HB2	2:D:314:PHE:CD1	2.52	0.45
2:D:291:HIS:HA	2:D:310:GLN:O	2.17	0.45
1:E:165:PRO:HB3	1:E:183:TYR:CD1	2.51	0.45
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.52	0.45
1:E:436:ILE:CG2	1:E:437:TRP:CE3	3.00	0.45
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.51	0.45
2:F:154:ASN:HD22	2:F:154:ASN:C	2.19	0.45
2:F:261:THR:CG2	2:F:262:ASP:N	2.80	0.45
1:G:472:LEU:O	1:G:476:VAL:HG23	2.16	0.45
2:H:251:ALA:O	2:H:252:ILE:C	2.55	0.45
2:H:306:MET:CE	2:H:329:HIS:CD2	3.00	0.45
2:B:300:VAL:HG23	2:B:301:GLU:N	2.32	0.45
1:C:223:ASP:CG	1:C:227:ASN:HB2	2.37	0.45
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.70	0.45
1:E:259:LYS:HD3	2:F:175:TRP:CE3	2.52	0.45
1:G:734:LEU:CD2	1:G:738:PHE:CE2	2.99	0.45
2:H:194:VAL:CG1	2:H:195:VAL:N	2.79	0.45
2:B:245:PRO:C	2:B:247:PRO:HD2	2.37	0.44
1:C:1020:ARG:O	1:C:1020:ARG:HG3	2.16	0.44
2:D:154:ASN:HA	2:D:154:ASN:HD22	1.38	0.44
1:E:246:ASP:OD1	1:E:379:LYS:N	2.42	0.44
1:E:563[A]:MET:HE1	1:E:635:PRO:HG3	1.97	0.44
2:F:279:SER:O	2:F:322:PRO:HG3	2.17	0.44
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.46	0.44
1:G:471:ARG:HH21	1:G:474:GLU:CD	2.21	0.44
1:G:993:LYS:NZ	10:G:4681:HOH:O	2.49	0.44
2:H:326:ARG:O	2:H:340:ILE:HA	2.16	0.44
2:H:357:SER:N	2:H:358:PRO:CA	2.79	0.44
1:A:347:SER:O	2:B:296:PRO:HB3	2.17	0.44
2:B:71:GLU:HG3	2:B:202:LYS:HE3	1.98	0.44
2:B:226:GLU:HG2	2:B:226:GLU:H	1.52	0.44
2:D:261:THR:CG2	2:D:262:ASP:N	2.80	0.44
1:E:998:ARG:HB3	1:E:999:PRO:HA	2.00	0.44
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:259:LEU:HD23	2:H:259:LEU:HA	1.84	0.44
1:A:167:ILE:CD1	1:A:167:ILE:N	2.80	0.44
2:B:228:VAL:HG11	2:B:258:PHE:HE1	1.81	0.44
2:B:286:MET:CE	2:B:312:HIS:ND1	2.80	0.44
2:B:285:LYS:CB	2:B:314:PHE:CD1	3.00	0.44
2:B:375:GLU:O	2:B:378:ARG:N	2.44	0.44
1:C:930:LYS:NZ	1:C:1058:ALA:O	2.45	0.44
1:C:420:ALA:O	1:C:421:LEU:C	2.55	0.44
2:D:268:ILE:HD13	2:D:268:ILE:HA	1.44	0.44
1:E:67:GLU:HB3	1:E:68:PRO:HD2	1.99	0.44
2:F:291:HIS:HA	2:F:310:GLN:O	2.17	0.44
1:G:651:ALA:O	1:G:652:ARG:C	2.54	0.44
2:H:277:LEU:O	2:H:280:GLY:N	2.37	0.44
2:H:295:HIS:HA	2:H:296:PRO:HD3	1.94	0.44
1:A:990:LEU:HD23	1:G:979:ILE:CG1	2.41	0.44
1:C:235:GLU:HB2	1:C:253:ALA:HA	1.98	0.44
2:D:254:ALA:O	2:D:257:LYS:HB2	2.18	0.44
2:D:286:MET:CE	2:D:312:HIS:ND1	2.80	0.44
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.66	0.44
1:E:936:ASN:HB2	10:E:1189:HOH:O	2.17	0.44
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.98	0.44
2:F:204:ASN:ND2	2:F:205:ILE:N	2.65	0.44
1:G:710:TYR:HB3	1:G:729:TYR:O	2.16	0.44
1:A:896:PRO:HG3	1:A:914:THR:HG23	1.99	0.44
1:C:503:ALA:HB1	1:C:508:VAL:O	2.17	0.44
1:C:645:GLN:HG3	1:C:649:LYS:NZ	2.33	0.44
1:C:912:ARG:NH1	10:C:4459:HOH:O	2.51	0.44
2:D:133:ILE:HG22	2:D:134:ALA:N	2.33	0.44
2:D:6:LEU:HD12	2:D:7:LEU:N	2.32	0.44
1:E:289:ASN:O	1:E:293:GLY:N	2.46	0.44
1:E:686:LYS:C	1:E:687:LEU:HD23	2.37	0.44
1:E:956:ARG:HA	10:E:2746:HOH:O	2.17	0.44
2:F:222[A]:GLN:HG2	2:F:250:TYR:CG	2.52	0.44
1:G:65:TYR:OH	1:G:80:LYS:HE3	2.17	0.44
2:B:231:MET:O	2:B:232:ASN:C	2.54	0.44
2:B:249:ASP:O	2:B:252:ILE:HG13	2.17	0.44
1:C:229:ILE:O	1:C:229:ILE:HG13	2.18	0.44
1:C:18:ILE:HG23	1:C:23:ALA:HA	1.99	0.44
1:E:1032:SER:O	1:E:1036:TYR:HD1	2.00	0.44
1:G:905:PRO:HG2	1:G:1030:ARG:HB3	1.99	0.44
1:G:294:ARG:NH1	10:G:4546:HOH:O	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:475:LYS:CD	1:G:488:PHE:CZ	3.00	0.44
2:B:201:ALA:HB2	2:B:239:SER:HB2	1.94	0.44
2:B:228:VAL:CG1	2:B:258:PHE:HE1	2.31	0.44
1:E:150:HIS:N	1:E:154:GLU:OE1	2.48	0.44
1:E:756:LEU:HD23	1:E:756:LEU:HA	1.81	0.44
2:F:25:SER:HA	2:F:132:ILE:O	2.18	0.44
1:G:780:GLU:HB3	1:G:798:ALA:HA	1.98	0.44
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.36	0.44
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.18	0.44
1:A:704:LYS:HD2	1:A:704:LYS:HA	1.66	0.44
1:A:992:ASN:HB2	1:A:999:PRO:O	2.17	0.44
2:B:208:MET:O	2:B:211:ASP:HB2	2.17	0.44
1:C:145[B]:ARG:HB3	1:C:208:GLU:CD	2.37	0.44
1:C:784:GLN:O	1:C:784:GLN:HG2	2.18	0.44
1:C:992:ASN:ND2	1:E:975:HIS:NE2	2.66	0.44
1:E:1001:ILE:HG21	1:E:1029:ILE:HG12	2.00	0.44
1:E:559:ARG:NH2	1:E:559:ARG:HG3	2.26	0.44
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.99	0.44
2:F:268:ILE:O	2:F:269:CYS:HB3	2.18	0.44
1:G:272:LEU:HD12	1:G:272:LEU:N	2.31	0.44
1:G:729:TYR:N	1:G:729:TYR:CD1	2.86	0.44
2:H:223:THR:CG2	2:H:228:VAL:HG23	2.47	0.44
1:A:267:ALA:O	1:A:271:VAL:HG23	2.17	0.44
1:A:419:GLU:HG3	10:A:4778:HOH:O	2.18	0.44
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.18	0.44
1:C:57:ASP:HB3	1:C:59:GLU:OE1	2.18	0.44
1:E:456:THR:O	1:E:457:ASN:HB2	2.18	0.44
1:G:202:LYS:HG2	1:G:202:LYS:O	2.17	0.44
2:B:354:PRO:HB3	2:B:363:ALA:CA	2.46	0.43
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.88	0.43
2:D:193:HIS:ND1	2:D:215:ARG:NH2	2.66	0.43
2:D:226:GLU:O	2:D:230:LYS:HG3	2.17	0.43
2:D:23:THR:CG2	2:D:24:GLY:N	2.81	0.43
1:E:981:LEU:HD12	1:E:988:PRO:HG3	2.00	0.43
2:F:263:ILE:HG12	2:F:377:TYR:OH	2.17	0.43
2:B:379:LYS:HZ3	2:B:379:LYS:HB3	1.83	0.43
1:C:622:THR:OG1	1:C:625:ASP:OD1	2.30	0.43
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.18	0.43
1:E:623:LEU:HD11	1:E:627:LEU:HD11	2.00	0.43
1:E:641:GLN:N	1:E:641:GLN:OE1	2.51	0.43
1:E:704:LYS:O	1:E:707:GLU:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:363:ALA:C	2:F:365:PRO:HD2	2.38	0.43
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.83	0.43
1:A:85:ALA:HA	1:A:114:THR:O	2.18	0.43
1:C:1065:VAL:O	1:C:1069:HIS:HB2	2.18	0.43
1:C:424:ILE:O	1:C:425:ARG:C	2.56	0.43
2:F:172:GLN:HG2	2:F:173:GLY:N	2.33	0.43
1:G:257:THR:O	1:G:258:ASP:C	2.56	0.43
1:G:597:ILE:HA	1:G:615:ARG:O	2.18	0.43
1:G:967:GLN:HG3	1:G:1054:LEU:HB3	1.99	0.43
1:G:986:ILE:HG22	1:G:988:PRO:HD3	2.00	0.43
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.32	0.43
1:A:159:ALA:HB2	1:A:188:PHE:CZ	2.54	0.43
1:A:735:ARG:O	1:A:736:ARG:C	2.56	0.43
1:E:87:LEU:HA	1:E:88:PRO:HD3	1.84	0.43
2:F:205:ILE:H	2:F:205:ILE:HG12	1.40	0.43
2:F:263:ILE:HG23	2:F:264:PRO:HD2	1.99	0.43
2:F:363:ALA:O	2:F:364:ALA:C	2.57	0.43
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.84	0.43
1:G:417:ASP:OD2	1:G:418:PRO:HD2	2.18	0.43
2:H:102:LEU:HA	2:H:102:LEU:HD23	1.84	0.43
2:H:107:ILE:CD1	2:H:107:ILE:N	2.82	0.43
2:H:175:TRP:HA	2:H:180:GLY:O	2.17	0.43
2:H:222:GLN:H	2:H:222:GLN:HE21	1.64	0.43
2:H:273:GLN:NE2	2:H:351:GLN:HE22	2.17	0.43
2:H:351:GLN:NE2	10:H:3174:HOH:O	2.34	0.43
2:B:297:VAL:O	2:B:306:MET:HG3	2.18	0.43
1:C:698:ILE:N	1:C:698:ILE:CD1	2.80	0.43
1:C:991:VAL:HB	1:C:1004[B]:ARG:NH1	2.33	0.43
1:E:669:ILE:HA	1:E:844:PRO:HG2	2.00	0.43
1:E:940:LYS:HG3	1:E:1011:THR:HB	2.01	0.43
1:G:148:ILE:CG2	1:G:149:ALA:N	2.80	0.43
1:G:727:ILE:HD12	1:G:909:PRO:HG3	1.99	0.43
1:G:950:ARG:HG3	1:G:950:ARG:H	1.58	0.43
1:G:9:SER:OG	1:G:83:PRO:HA	2.17	0.43
1:G:347:SER:O	2:H:296:PRO:HB3	2.18	0.43
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.19	0.43
2:B:367:PHE:O	2:B:368:ASP:C	2.55	0.43
1:C:145[A]:ARG:HB3	1:C:208:GLU:CD	2.38	0.43
1:C:604:GLU:HG2	10:C:4550:HOH:O	2.18	0.43
1:C:772:MET:HE2	1:C:880:THR:HG22	1.98	0.43
1:C:947:LEU:N	1:C:947:LEU:CD1	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:ALA:N	1:E:708:ILE:HD11	2.33	0.43
1:G:645[A]:GLN:HG3	1:G:649:LYS:HE3	2.00	0.43
1:E:208:GLU:HG3	1:E:208:GLU:O	2.18	0.43
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.43
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.65	0.43
1:G:237:PHE:HB3	1:G:248:ILE:HB	2.01	0.43
1:G:3:LYS:HB3	1:G:330:TYR:CE1	2.54	0.43
1:G:58:PRO:HD2	1:G:59:GLU:OE2	2.18	0.43
1:G:992:ASN:HB2	1:G:999:PRO:O	2.18	0.43
2:H:261:THR:HG21	2:H:263:ILE:CG1	2.48	0.43
1:A:679:GLN:HG2	10:A:4614:HOH:O	2.17	0.43
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.43
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.43
1:C:892:GLU:OE1	8:C:4031:ORN:NE	2.52	0.43
2:F:116:ARG:O	2:F:120:ARG:HG3	2.19	0.43
2:F:252:ILE:HG23	2:F:278:ALA:CA	2.48	0.43
1:G:158:VAL:HG11	1:G:206:ILE:HB	2.01	0.43
1:G:423:LYS:HB3	10:G:4377:HOH:O	2.19	0.43
1:G:735:ARG:O	1:G:738:PHE:HB2	2.18	0.43
1:G:973:ALA:O	1:G:990:LEU:HA	2.18	0.43
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.49	0.43
1:A:409:PHE:CE1	1:A:469:LEU:HD12	2.54	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.84	0.43
2:B:300:VAL:HG22	2:B:328:THR:O	2.19	0.43
2:B:371:ILE:HD13	2:B:371:ILE:HA	1.81	0.43
1:E:220:VAL:O	1:E:281:GLY:HA2	2.19	0.43
1:E:726:GLU:CD	1:E:736:ARG:HH22	2.21	0.43
2:F:204:ASN:HD21	2:F:205:ILE:CD1	2.31	0.43
1:G:420:ALA:HA	1:G:423:LYS:HD2	2.00	0.43
1:G:625:ASP:O	1:G:629:ILE:HG13	2.18	0.43
1:G:534:ALA:O	2:H:123:ARG:HD3	2.19	0.43
2:H:194:VAL:HG13	2:H:195:VAL:N	2.34	0.43
2:H:201:ALA:CB	2:H:239:SER:HB2	2.49	0.43
1:A:726:GLU:HG3	1:A:727:ILE:H	1.81	0.43
1:A:9:SER:OG	1:A:83:PRO:HA	2.19	0.43
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.83	0.43
1:C:294:ARG:HD2	5:C:4038:CL:CL	2.56	0.43
2:D:194:VAL:HB	2:D:216:LEU:HD23	2.01	0.43
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.84	0.43
1:E:773[A]:VAL:HG21	1:E:814:GLN:HA	2.00	0.43
1:E:805:ILE:HD12	1:E:832:VAL:HG11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:TYR:HA	2:F:51:GLN:NE2	2.30	0.43
1:G:1063:ILE:HG12	1:G:1064:SER:N	2.33	0.43
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.92	0.42
2:B:261:THR:CG2	2:B:262:ASP:N	2.81	0.42
1:C:456:THR:O	1:C:457:ASN:HB2	2.18	0.42
1:C:563:MET:CE	1:C:635:PRO:HG3	2.49	0.42
2:F:236:ILE:HB	2:F:265:VAL:HG22	2.01	0.42
1:G:417:ASP:HB3	1:G:420:ALA:HB2	2.00	0.42
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.23	0.42
2:H:209:LEU:O	2:H:212:ARG:N	2.52	0.42
1:A:358:LYS:HG2	1:A:359:ILE:N	2.33	0.42
2:B:190:LEU:HB2	2:B:215:ARG:HB2	2.02	0.42
2:B:259:LEU:HA	2:B:259:LEU:HD23	1.77	0.42
1:C:306:ARG:NH1	1:C:306:ARG:HG2	2.33	0.42
1:C:375:THR:OG1	1:C:376:THR:N	2.51	0.42
1:C:561:LYS:HE2	10:C:4424:HOH:O	2.19	0.42
1:C:839:LEU:HD12	1:C:839:LEU:HA	1.81	0.42
1:C:974:THR:O	1:C:975:HIS:C	2.57	0.42
1:E:213:TRP:CH2	1:E:289:ASN:HB2	2.54	0.42
1:E:331:THR:OG1	1:E:334:GLU:HG3	2.18	0.42
1:E:479:VAL:HG23	1:E:483:GLY:HA3	2.00	0.42
1:E:568:GLY:O	1:E:602:ASN:HB2	2.18	0.42
2:F:378:ARG:NH2	10:F:3310:HOH:O	2.51	0.42
1:G:343:ARG:HG3	1:G:344:THR:CG2	2.49	0.42
2:H:236:ILE:O	2:H:265:VAL:HG22	2.19	0.42
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.53	0.42
1:A:10:ILE:HD13	1:A:37:LEU:HD13	2.01	0.42
1:A:703:GLU:O	1:A:704:LYS:C	2.57	0.42
1:A:936:ASN:HB2	10:A:4034:HOH:O	2.18	0.42
2:B:144:LEU:HD11	2:B:148:ARG:NE	2.34	0.42
1:C:523:HIS:HB3	1:C:524:PRO:HD2	2.01	0.42
1:C:704:LYS:HD2	1:C:707:GLU:OE2	2.19	0.42
2:D:71:GLU:C	2:D:203:ARG:HG3	2.39	0.42
2:D:258:PHE:O	2:D:261:THR:HB	2.19	0.42
1:E:1067:GLU:O	1:E:1068:MET:C	2.56	0.42
1:E:339:ILE:HG21	1:E:339:ILE:HD13	1.83	0.42
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.43	0.42
1:G:860:PRO:O	1:G:861:LEU:C	2.57	0.42
2:H:132:ILE:HG22	2:H:133:ILE:N	2.33	0.42
2:H:150:PHE:CE1	2:H:152:GLY:HA2	2.54	0.42
2:B:137:ASN:O	2:B:138:PRO:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:LEU:O	2:D:145:GLU:C	2.56	0.42
2:F:206:LEU:O	2:F:209:LEU:N	2.48	0.42
2:F:214:CYS:SG	2:F:371:ILE:HD11	2.60	0.42
1:G:854:SER:HA	1:G:859:VAL:O	2.19	0.42
1:G:938:THR:HB	10:G:4673:HOH:O	2.18	0.42
2:H:198:ASP:C	2:H:200:GLY:H	2.23	0.42
1:A:139:ILE:HG13	1:A:141:LEU:HG	2.00	0.42
1:A:76:LYS:HA	1:A:76:LYS:HD2	1.70	0.42
2:B:162:VAL:HG21	2:B:200:GLY:HA3	2.01	0.42
2:B:48:TYR:HA	2:B:51:GLN:NE2	2.34	0.42
1:C:671:ARG:NH2	1:C:819:GLU:O	2.52	0.42
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.00	0.42
1:E:766:ALA:HB1	1:E:774:LEU:O	2.19	0.42
1:E:773[B]:VAL:HG12	1:E:818:PHE:CZ	2.55	0.42
1:E:904:ASP:O	1:E:906:LEU:N	2.48	0.42
2:F:328:THR:HG21	2:F:341:HIS:HB2	2.02	0.42
1:G:85:ALA:HB1	1:G:114:THR:O	2.19	0.42
1:G:514:ARG:HD3	10:G:4409:HOH:O	2.20	0.42
1:A:17:PRO:HB2	1:A:894:VAL:HG21	2.01	0.42
1:A:820:LEU:O	1:A:821:GLN:HB2	2.19	0.42
1:A:946:LEU:HB3	1:A:1013:ILE:HG12	2.01	0.42
1:C:529:VAL:HB	1:C:542:TYR:CD2	2.54	0.42
2:F:357:SER:N	2:F:358:PRO:CA	2.79	0.42
2:F:63:VAL:O	2:F:94:ASN:HB2	2.19	0.42
1:G:669:ILE:HA	1:G:844:PRO:HG2	2.02	0.42
2:B:261:THR:HG21	2:B:263:ILE:CD1	2.49	0.42
2:B:279:SER:HB2	2:B:325:LEU:HD11	2.02	0.42
1:C:953:ASP:CG	1:C:1044:LEU:HD22	2.40	0.42
1:C:363:ASN:ND2	1:C:365:GLU:OE1	2.40	0.42
2:D:224:SER:OG	2:D:227:ASP:HB2	2.20	0.42
2:D:267:GLY:O	2:D:349:SER:HB2	2.19	0.42
1:E:796:LEU:HA	1:E:797:PRO:HA	1.79	0.42
2:F:78:GLN:NE2	10:F:3227:HOH:O	2.48	0.42
1:G:763:ASP:HB3	1:G:779:MET:CE	2.50	0.42
1:G:891:LYS:HE3	1:G:893:VAL:HG12	2.01	0.42
2:H:170:TRP:HB3	2:H:216:LEU:HD12	2.01	0.42
2:H:342:ARG:HA	2:H:342:ARG:HD2	1.85	0.42
1:A:1021:ARG:O	1:A:1025:ASP:OD2	2.37	0.42
2:B:306:MET:HE1	2:B:350:PHE:CZ	2.55	0.42
1:C:375:THR:HG23	1:C:377:GLN:H	1.84	0.42
1:C:470:VAL:O	1:C:474:GLU:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:HD3	1:C:675:ARG:H	1.83	0.42
2:D:158:LEU:O	2:D:161:GLU:HB2	2.20	0.42
2:D:228:VAL:O	2:D:229:LEU:C	2.57	0.42
1:E:503:ALA:HB2	1:E:510:GLU:HA	2.01	0.42
1:E:734:LEU:HA	1:E:734:LEU:HD23	1.82	0.42
1:G:1031:ARG:HB3	1:G:1031:ARG:HE	1.41	0.42
1:G:764:VAL:O	1:G:827:ASN:HA	2.19	0.42
2:H:219:VAL:HG23	2:H:220:PRO:O	2.20	0.42
1:A:237:PHE:HB3	1:A:248:ILE:O	2.19	0.42
1:A:353:ASP:OD1	2:B:116:ARG:HD2	2.19	0.42
2:B:298:LYS:O	2:B:329:HIS:HA	2.19	0.42
1:C:695:VAL:HG12	1:C:696:THR:N	2.35	0.42
1:E:471:ARG:O	1:E:474:GLU:HB2	2.20	0.42
1:G:407:THR:HG21	1:G:504:LYS:HE3	2.00	0.42
2:H:60:ILE:O	2:H:86:PRO:HD2	2.19	0.42
2:B:71:GLU:C	2:B:203:ARG:HG3	2.39	0.42
2:B:209:LEU:O	2:B:214:CYS:HB2	2.19	0.42
2:B:169:SER:HA	2:B:216:LEU:O	2.20	0.42
2:B:221:ALA:HB1	2:B:250:TYR:CE1	2.55	0.42
2:B:348:PHE:HE1	2:B:366:LEU:HD22	1.84	0.42
1:C:145[A]:ARG:HB3	1:C:208:GLU:CG	2.50	0.42
9:C:4032:NET:H31	9:C:4032:NET:H63	1.90	0.42
2:D:188:ASP:N	2:D:188:ASP:OD2	2.29	0.42
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.50	0.42
1:E:308:SER:HB3	10:E:1376:HOH:O	2.19	0.42
1:E:504:LYS:NZ	10:E:3574:HOH:O	2.52	0.42
1:E:750:VAL:O	1:E:750:VAL:HG12	2.19	0.42
1:G:560:GLU:HB3	1:G:636:LYS:HD2	2.00	0.42
1:A:435:ARG:O	1:A:439:ILE:HG13	2.20	0.41
1:A:504[B]:LYS:HG2	10:A:4325:HOH:O	2.19	0.41
2:B:33:ASN:HB3	2:B:55:LEU:CD2	2.50	0.41
1:C:1041:ASP:OD1	1:C:1047:GLY:HA2	2.20	0.41
1:E:781:HIS:CE1	1:E:789:SER:HA	2.55	0.41
1:G:1063:ILE:O	1:G:1063:ILE:HG23	2.20	0.41
1:G:275:ILE:HD12	1:G:275:ILE:HA	1.74	0.41
2:H:222:GLN:O	2:H:223:THR:C	2.58	0.41
2:H:252:ILE:O	2:H:253:THR:C	2.58	0.41
2:H:274:LEU:HD23	2:H:274:LEU:HA	1.74	0.41
1:A:701:ALA:O	1:A:705:ALA:N	2.32	0.41
2:B:138:PRO:HA	10:B:4125:HOH:O	2.19	0.41
1:E:275:ILE:HD12	1:E:275:ILE:HA	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:LYS:NZ	1:E:611:ASP:OD1	2.46	0.41
1:A:136:MET:HA	1:A:139:ILE:HG12	2.02	0.41
1:A:843:ASN:HA	1:A:844:PRO:HD3	1.76	0.41
2:B:340:ILE:O	2:B:340:ILE:HG13	2.18	0.41
2:D:6:LEU:N	2:D:133:ILE:O	2.47	0.41
1:E:58:PRO:HD2	1:E:59:GLU:OE2	2.19	0.41
1:E:648:LEU:HD13	10:E:1595:HOH:O	2.20	0.41
1:E:734:LEU:CD2	1:E:738:PHE:CE2	3.03	0.41
1:E:805:ILE:HD12	1:E:832:VAL:CG1	2.51	0.41
1:G:3:LYS:HB3	1:G:330:TYR:CZ	2.54	0.41
1:G:472:LEU:O	1:G:473:GLU:C	2.55	0.41
1:G:734:LEU:HD23	1:G:734:LEU:HA	1.80	0.41
1:G:818:PHE:O	1:G:819:GLU:C	2.57	0.41
2:H:363:ALA:O	2:H:366:LEU:HB2	2.20	0.41
1:A:534:ALA:HB2	2:B:116:ARG:NH1	2.35	0.41
2:B:342:ARG:HD2	2:B:342:ARG:HA	1.88	0.41
1:C:421:LEU:HD23	1:C:421:LEU:HA	1.84	0.41
1:E:417:ASP:OD2	1:E:419:GLU:N	2.47	0.41
1:E:781:HIS:HE1	1:E:789:SER:HB3	1.85	0.41
2:F:154:ASN:HD22	2:F:155:GLY:H	1.69	0.41
1:G:1051:ALA:HA	1:G:1054:LEU:HD12	2.01	0.41
1:G:423:LYS:HG3	1:G:423:LYS:H	1.68	0.41
2:B:144:LEU:O	2:B:147:ALA:HB3	2.20	0.41
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.90	0.41
1:E:101:GLU:OE2	1:E:101:GLU:HA	2.20	0.41
1:E:1061:LYS:HD3	10:E:3549:HOH:O	2.20	0.41
1:E:516:LEU:HD12	1:E:516:LEU:HA	1.85	0.41
1:E:628:GLU:O	1:E:631:ARG:HB3	2.21	0.41
1:E:710:TYR:CB	1:E:711:PRO:HA	2.43	0.41
2:F:150:PHE:CG	2:F:151:PRO:HD2	2.52	0.41
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.86	0.41
1:G:11:LEU:O	1:G:86:VAL:HA	2.19	0.41
1:G:421:LEU:HA	1:G:421:LEU:HD23	1.89	0.41
1:G:752:LEU:HA	1:G:752:LEU:HD12	1.68	0.41
1:G:4:ARG:HD3	1:G:7:ILE:HD12	2.00	0.41
1:G:947:LEU:N	1:G:947:LEU:HD12	2.34	0.41
1:A:318:PRO:HB2	1:A:321:LYS:HB2	2.02	0.41
1:A:943:GLY:C	10:A:4490:HOH:O	2.56	0.41
2:B:256:GLN:O	2:B:259:LEU:HB2	2.21	0.41
2:B:321:LEU:HA	2:B:321:LEU:HD12	1.67	0.41
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:ILE:CG2	2:D:134:ALA:N	2.84	0.41
1:E:186:GLU:HB2	10:E:1334:HOH:O	2.21	0.41
1:E:18:ILE:HD12	1:E:23:ALA:C	2.40	0.41
2:F:207:ARG:NH2	10:F:3234:HOH:O	2.54	0.41
1:G:1044:LEU:HD12	1:G:1044:LEU:HA	1.87	0.41
1:G:647:PRO:O	1:G:648:LEU:C	2.58	0.41
1:G:734:LEU:CD2	1:G:738:PHE:HE2	2.32	0.41
1:G:259:LYS:HD3	2:H:175:TRP:CD2	2.56	0.41
2:H:263:ILE:HG23	2:H:264:PRO:HD2	2.03	0.41
2:H:267:GLY:O	2:H:268:ILE:HD13	2.21	0.41
1:A:223:ASP:OD2	1:A:227:ASN:HB2	2.21	0.41
1:A:534:ALA:O	2:B:123:ARG:HD3	2.21	0.41
2:B:283:THR:HA	2:B:315:ALA:O	2.20	0.41
2:B:46:PRO:O	2:B:47:SER:C	2.58	0.41
1:C:1071:GLN:HE21	1:C:1071:GLN:HB3	1.54	0.41
1:C:166:CYS:C	1:C:167:ILE:HD12	2.41	0.41
1:C:475:LYS:O	1:C:476:VAL:C	2.58	0.41
1:C:59:GLU:HG2	1:C:60:MET:HE2	2.02	0.41
1:E:735:ARG:O	1:E:736:ARG:C	2.58	0.41
2:F:321:LEU:HA	2:F:321:LEU:HD12	1.82	0.41
1:G:1057:ASP:HB3	1:G:1060:GLU:HB2	2.02	0.41
1:G:596:THR:O	1:G:614:ASP:HB2	2.21	0.41
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.56	0.41
1:A:367:PHE:CE1	1:A:912:ARG:HG2	2.56	0.41
1:A:860:PRO:O	1:A:864:VAL:HG23	2.21	0.41
2:B:153:LEU:O	2:B:156:MET:HB2	2.20	0.41
2:B:265:VAL:O	2:B:347:ALA:HA	2.20	0.41
2:B:6:LEU:HD11	2:B:8:VAL:HG22	2.02	0.41
1:C:992:ASN:O	1:C:1000:HIS:HB2	2.20	0.41
1:C:1001:ILE:HG22	1:C:1002:GLN:N	2.34	0.41
1:C:130:ARG:HG3	1:C:148:ILE:HG13	2.03	0.41
1:C:525:VAL:HG12	1:C:551:CYS:HB2	2.01	0.41
1:C:783:GLU:OE2	1:C:783:GLU:N	2.51	0.41
2:D:153:LEU:N	2:D:153:LEU:HD12	2.34	0.41
1:E:809:MET:HG2	1:E:830:PHE:CD2	2.55	0.41
2:F:219:VAL:HG11	2:F:231:MET:HE1	2.03	0.41
2:F:306:MET:HE1	2:F:329:HIS:CD2	2.55	0.41
1:G:194:ARG:HD3	1:G:194:ARG:HH11	1.76	0.41
2:H:66:ASN:OD1	2:H:68:ALA:N	2.54	0.41
1:A:322:VAL:O	1:A:326:LEU:HD13	2.21	0.41
1:A:689:GLN:HG2	1:A:690:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ASN:HB3	2:B:55:LEU:HD23	2.03	0.41
1:C:695:VAL:CG1	1:C:696:THR:N	2.83	0.41
1:E:509:ARG:NH1	1:E:515:LYS:NZ	2.68	0.41
1:E:695:VAL:HG13	1:E:696:THR:N	2.36	0.41
1:E:948:SER:O	1:E:1015:ASN:HA	2.21	0.41
2:F:299:ASP:O	2:F:303:ASN:N	2.47	0.41
1:G:1034:LEU:HD12	1:G:1034:LEU:HA	1.85	0.41
1:G:392:GLN:O	1:G:396:GLN:HG3	2.21	0.41
1:G:671:ARG:HH22	1:G:819:GLU:HG3	1.84	0.41
1:A:509:ARG:O	1:A:510:GLU:C	2.57	0.41
1:A:527:LYS:HB2	1:A:544:TYR:CE2	2.55	0.41
2:B:373:LEU:HA	2:B:373:LEU:HD23	1.64	0.41
1:C:427:GLU:HG3	1:C:438:TYR:CE1	2.56	0.41
2:D:191:PRO:HD2	2:D:213:GLY:O	2.21	0.41
1:E:1073:LYS:N	1:E:1073:LYS:HD3	2.36	0.41
1:E:854:SER:HA	1:E:859:VAL:O	2.20	0.41
1:E:891:LYS:HE2	1:E:891:LYS:HB3	1.71	0.41
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.42	0.41
2:H:45:ASP:OD1	2:H:202:LYS:HD2	2.19	0.41
2:H:8:VAL:HG12	2:H:9:LEU:N	2.35	0.41
1:A:259:LYS:HD3	2:B:175:TRP:CZ3	2.57	0.41
1:A:425:ARG:HG2	10:A:4337:HOH:O	2.20	0.41
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.49	0.41
1:E:141:LEU:HA	1:E:141:LEU:HD23	1.82	0.41
1:E:236:ASN:HA	1:E:249:THR:HG22	2.03	0.41
1:E:3:LYS:HB2	1:E:42:TYR:OH	2.21	0.41
1:E:490:ARG:HA	1:E:522:LEU:HD21	2.02	0.41
1:E:731:GLU:O	1:E:735:ARG:HG3	2.21	0.41
1:G:100:LEU:O	1:G:104:ARG:HB2	2.21	0.41
1:G:427:GLU:HG3	1:G:438:TYR:CD1	2.56	0.41
1:G:472:LEU:HD23	1:G:472:LEU:HA	1.90	0.41
1:G:475:LYS:HG2	1:G:488:PHE:CZ	2.56	0.41
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.56	0.41
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.86	0.41
1:A:1044:LEU:HA	1:A:1044:LEU:HD12	1.70	0.40
1:A:375:THR:OG1	1:A:376:THR:N	2.52	0.40
1:A:57:ASP:HA	1:A:58:PRO:HD3	1.67	0.40
2:B:73:SER:HA	2:B:203:ARG:NH2	2.36	0.40
1:C:553:ALA:HB3	10:C:4403:HOH:O	2.21	0.40
2:D:266:PHE:HB2	2:D:370:PHE:CE1	2.56	0.40
1:E:735:ARG:O	1:E:738:PHE:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:249:ASP:OD1	2:F:250:TYR:N	2.52	0.40
1:G:223:ASP:OD1	1:G:227:ASN:HB2	2.21	0.40
1:G:262:GLN:HA	1:G:262:GLN:OE1	2.19	0.40
1:G:293:GLY:O	1:G:294:ARG:C	2.57	0.40
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.02	0.40
1:G:9:SER:HA	1:G:43:ARG:O	2.21	0.40
1:G:674:ASP:HB3	1:G:677:ARG:CB	2.35	0.40
1:G:795:SER:OG	1:G:797:PRO:O	2.39	0.40
2:H:153:LEU:HD12	2:H:153:LEU:HA	1.66	0.40
2:H:153:LEU:HD12	2:H:156:MET:SD	2.60	0.40
2:H:261:THR:HG22	2:H:263:ILE:HG13	2.00	0.40
2:H:33:ASN:OD1	2:H:292:GLY:HA2	2.21	0.40
2:H:371:ILE:HA	2:H:371:ILE:HD13	1.92	0.40
1:A:163:GLY:O	1:A:166:CYS:HB3	2.22	0.40
2:B:81:VAL:HG22	2:B:110:ILE:CG2	2.51	0.40
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.83	0.40
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.51	0.40
2:D:261:THR:HG21	2:D:263:ILE:HG13	2.03	0.40
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.21	0.40
1:G:349:GLU:O	2:H:294:ASN:HB2	2.21	0.40
2:H:46:PRO:O	2:H:48:TYR:N	2.53	0.40
2:B:191:PRO:HD2	2:B:213:GLY:CA	2.52	0.40
1:C:43:ARG:HD2	1:C:43:ARG:HH11	1.73	0.40
1:C:562:ILE:HA	1:C:562:ILE:HD13	1.92	0.40
2:D:257:LYS:O	2:D:258:PHE:C	2.59	0.40
1:E:884:ILE:HA	1:E:885:PRO:HD3	1.65	0.40
1:E:8[A]:LYS:HG3	10:E:2527:HOH:O	2.21	0.40
2:F:268:ILE:HA	2:F:268:ILE:HD13	1.82	0.40
1:G:1021:ARG:O	1:G:1022:ALA:C	2.60	0.40
1:G:1073:LYS:HD3	1:G:1073:LYS:HA	1.65	0.40
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.90	0.40
1:G:168:ILE:HG22	1:G:204:LEU:HD22	2.03	0.40
1:G:688:LYS:HZ3	1:G:836:GLU:HG2	1.87	0.40
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.99	0.40
2:H:264:PRO:HA	2:H:346:PRO:HB2	2.02	0.40
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.77	0.40
1:A:998:ARG:HA	1:A:999:PRO:HA	1.68	0.40
2:B:164:THR:HG23	2:B:220:PRO:HG3	2.04	0.40
2:B:326:ARG:CZ	2:B:341:HIS:HB3	2.51	0.40
1:C:85:ALA:HB1	1:C:114:THR:O	2.21	0.40
1:C:867:ARG:O	1:C:868:VAL:C	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:374:ILE:O	2:D:377:TYR:HB3	2.21	0.40
1:E:47:VAL:HA	1:E:65:TYR:O	2.22	0.40
1:E:979:ILE:O	1:E:983:GLU:HG3	2.21	0.40
2:F:273:GLN:NE2	2:F:314:PHE:O	2.54	0.40
2:F:364:ALA:N	2:F:365:PRO:HD2	2.35	0.40
2:F:376:GLN:HA	2:F:379[A]:LYS:HZ3	1.87	0.40
1:G:622:THR:O	1:G:623:LEU:C	2.59	0.40
1:G:671:ARG:NH2	1:G:819:GLU:O	2.54	0.40
1:G:819:GLU:O	1:G:821:GLN:HG2	2.21	0.40
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.76	0.40
2:H:289:GLY:N	10:H:3157:HOH:O	2.47	0.40
2:H:354:PRO:CB	2:H:363:ALA:CB	2.98	0.40
1:A:86:VAL:HG13	1:A:86:VAL:O	2.20	0.40
1:C:780:GLU:HB3	1:C:798:ALA:HA	2.02	0.40
1:E:109:GLU:O	1:E:110:GLU:C	2.57	0.40
1:E:358:LYS:HG2	1:E:359:ILE:N	2.36	0.40
1:E:712:LEU:N	1:E:728:VAL:O	2.42	0.40
1:G:165:PRO:HA	1:G:182:ALA:O	2.22	0.40
2:H:283:THR:OG1	10:H:3162:HOH:O	2.22	0.40
2:H:33:ASN:HA	2:H:291:HIS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1059/1073 (99%)	993 (94%)	63 (6%)	3 (0%)	44	44
1	C	1060/1073 (99%)	997 (94%)	59 (6%)	4 (0%)	38	35
1	E	1059/1073 (99%)	1008 (95%)	46 (4%)	5 (0%)	32	28
1	G	1060/1073 (99%)	989 (93%)	64 (6%)	7 (1%)	25	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	372/382 (97%)	334 (90%)	31 (8%)	7 (2%)	9	4
2	D	373/382 (98%)	351 (94%)	21 (6%)	1 (0%)	44	44
2	F	374/382 (98%)	360 (96%)	11 (3%)	3 (1%)	22	17
2	H	372/382 (97%)	324 (87%)	40 (11%)	8 (2%)	8	3
All	All	5729/5820 (98%)	5356 (94%)	335 (6%)	38 (1%)	28	20

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	ALA
1	G	558	ASP
1	G	739	GLN
2	H	185	LYS
2	H	223	THR
2	B	336	THR
1	C	738	PHE
1	C	739	GLN
1	E	954	LYS
2	B	127	ALA
2	B	376	GLN
1	E	478	GLU
1	E	975	HIS
2	H	47	SER
2	H	253	THR
1	A	342	GLY
1	A	716	PRO
1	A	975	HIS
2	B	145	GLU
1	C	1020	ARG
1	E	675	ARG
2	F	165	ALA
2	F	364	ALA
1	G	586	SER
1	G	736	ARG
1	G	975	HIS
2	D	364	ALA
2	F	243	GLY
1	G	740	THR
2	H	230[A]	LYS
2	H	230[B]	LYS
2	H	366	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	652	ARG
2	B	191	PRO
2	B	233	PRO
1	C	2	PRO
1	E	2	PRO
2	H	138	PRO

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	871/878 (99%)	810 (93%)	61 (7%)	18	14
1	C	872/878 (99%)	820 (94%)	52 (6%)	22	19
1	E	871/878 (99%)	807 (93%)	64 (7%)	16	13
1	G	872/878 (99%)	798 (92%)	74 (8%)	12	8
2	B	306/311 (98%)	267 (87%)	39 (13%)	5	2
2	D	307/311 (99%)	288 (94%)	19 (6%)	21	18
2	F	308/311 (99%)	279 (91%)	29 (9%)	10	6
2	H	306/311 (98%)	270 (88%)	36 (12%)	6	3
All	All	4713/4756 (99%)	4339 (92%)	374 (8%)	14	10

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	LYS
1	A	38	ARG
1	A	103	GLU
1	A	137	LYS
1	A	174	MET
1	A	185	ARG
1	A	202	LYS
1	A	220	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	236	ASN
1	A	338	ASP
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	416	ASP
1	A	426	ARG
1	A	429	LYS
1	A	459	ASP
1	A	471	ARG
1	A	481	ILE
1	A	542	TYR
1	A	548	GLU
1	A	559	ARG
1	A	562	ILE
1	A	571	ARG
1	A	591	GLU
1	A	636	LYS
1	A	645	GLN
1	A	671	ARG
1	A	675	ARG
1	A	696	THR
1	A	704	LYS
1	A	706	LYS
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	736	ARG
1	A	753	ASP
1	A	757	ASP
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	835	ASN
1	A	839	LEU
1	A	855	LYS
1	A	912	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	963	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	966	LYS
1	A	967	GLN
1	A	992	ASN
1	A	1006	LYS
1	A	1014	ILE
1	A	1018	SER
1	A	1020	ARG
1	A	1026	SER
1	A	1032	SER
1	A	1063	ILE
2	B	6	LEU
2	B	18	ARG
2	B	25	SER
2	B	49	SER
2	B	78	GLN
2	B	87	LEU
2	B	104	ARG
2	B	113	ILE
2	B	118	LEU
2	B	154	ASN
2	B	156	MET
2	B	166	GLU
2	B	169	SER
2	B	186	LYS
2	B	192	PHE
2	B	204	ASN
2	B	215	ARG
2	B	218	ILE
2	B	219	VAL
2	B	222	GLN
2	B	226	GLU
2	B	228	VAL
2	B	231	MET
2	B	252	ILE
2	B	257[A]	LYS
2	B	257[B]	LYS
2	B	268	ILE
2	B	282	LYS
2	B	284	VAL
2	B	304	VAL
2	B	306	MET
2	B	321	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	324	ASN
2	B	326	ARG
2	B	332	LEU
2	B	333	PHE
2	B	336	THR
2	B	373	LEU
2	B	376	GLN
1	C	4	ARG
1	C	38	ARG
1	C	44	VAL
1	C	46	ASN
1	C	76	LYS
1	C	145[A]	ARG
1	C	145[B]	ARG
1	C	174	MET
1	C	185	ARG
1	C	207	ASP
1	C	279	THR
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	416	ASP
1	C	548	GLU
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	645	GLN
1	C	655	GLU
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	677	ARG
1	C	680	HIS
1	C	688	LYS
1	C	696	THR
1	C	706	LYS
1	C	707	GLU
1	C	728	VAL
1	C	733	ASP
1	C	734	LEU
1	C	735	ARG
1	C	751	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	763	ASP
1	C	784	GLN
1	C	805	ILE
1	C	811	GLN
1	C	835	ASN
1	C	845	ARG
1	C	849	THR
1	C	855	LYS
1	C	912	ARG
1	C	940	LYS
1	C	998	ARG
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1028	VAL
1	C	1031	ARG
2	D	18	ARG
2	D	104	ARG
2	D	142	LEU
2	D	154	ASN
2	D	166	GLU
2	D	169	SER
2	D	185	LYS
2	D	204	ASN
2	D	222	GLN
2	D	257	LYS
2	D	261	THR
2	D	306	MET
2	D	324	ASN
2	D	326	ARG
2	D	355	GLU
2	D	357	SER
2	D	372	GLU
2	D	376	GLN
2	D	379	LYS
1	E	5	THR
1	E	8[A]	LYS
1	E	8[B]	LYS
1	E	38	ARG
1	E	55	MET
1	E	59	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	103	GLU
1	E	119	THR
1	E	174	MET
1	E	185	ARG
1	E	202	LYS
1	E	217	GLU
1	E	236	ASN
1	E	275	ILE
1	E	363	ASN
1	E	414	SER
1	E	416	ASP
1	E	479	VAL
1	E	509	ARG
1	E	515	LYS
1	E	518	ASP
1	E	542	TYR
1	E	548	GLU
1	E	556	SER
1	E	558	ASP
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	645	GLN
1	E	675	ARG
1	E	684	ARG
1	E	688	LYS
1	E	689	GLN
1	E	695	VAL
1	E	703	GLU
1	E	706	LYS
1	E	715	ARG
1	E	731	GLU
1	E	733	ASP
1	E	734	LEU
1	E	751	LEU
1	E	763	ASP
1	E	774	LEU
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	839	LEU
1	E	849	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	891	LYS
1	E	912	ARG
1	E	940	LYS
1	E	941	LYS
1	E	950	ARG
1	E	951	GLU
1	E	966	LYS
1	E	967[A]	GLN
1	E	967[B]	GLN
1	E	980	VAL
1	E	1006	LYS
1	E	1014	ILE
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1032	SER
2	F	6	LEU
2	F	10	GLU
2	F	18	ARG
2	F	104	ARG
2	F	113	ILE
2	F	154	ASN
2	F	166	GLU
2	F	178	THR
2	F	186	LYS
2	F	192	PHE
2	F	204	ASN
2	F	205	ILE
2	F	212	ARG
2	F	215	ARG
2	F	216	LEU
2	F	226	GLU
2	F	231	MET
2	F	257	LYS
2	F	261	THR
2	F	282	LYS
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	333	PHE
2	F	343	THR
2	F	354	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	376	GLN
2	F	379[A]	LYS
2	F	379[B]	LYS
1	G	3	LYS
1	G	8	LYS
1	G	24	CYS
1	G	55	MET
1	G	79	GLU
1	G	103	GLU
1	G	148	ILE
1	G	174	MET
1	G	185	ARG
1	G	217	GLU
1	G	275	ILE
1	G	300	MET
1	G	321	LYS
1	G	331	THR
1	G	338	ASP
1	G	358	LYS
1	G	363	ASN
1	G	412	LYS
1	G	416	ASP
1	G	422	THR
1	G	426	ARG
1	G	428	LEU
1	G	475	LYS
1	G	509	ARG
1	G	519	GLN
1	G	542	TYR
1	G	548	GLU
1	G	558	ASP
1	G	559	ARG
1	G	571	ARG
1	G	591	GLU
1	G	645[A]	GLN
1	G	645[B]	GLN
1	G	665	SER
1	G	670	ASP
1	G	675	ARG
1	G	684	ARG
1	G	688	LYS
1	G	692	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	704	LYS
1	G	706	LYS
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	753	ASP
1	G	763	ASP
1	G	774	LEU
1	G	780	GLU
1	G	784	GLN
1	G	795	SER
1	G	800	THR
1	G	811	GLN
1	G	815	LYS
1	G	821	GLN
1	G	836	GLU
1	G	849	THR
1	G	855	LYS
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	951	GLU
1	G	955	GLU
1	G	967	GLN
1	G	991	VAL
1	G	992	ASN
1	G	1006	LYS
1	G	1014	ILE
1	G	1018	SER
1	G	1020	ARG
1	G	1031	ARG
1	G	1037	LYS
2	H	6	LEU
2	H	18	ARG
2	H	25	SER
2	H	73	SER
2	H	78	GLN
2	H	97	ASP
2	H	104	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	107	ILE
2	H	153	LEU
2	H	154	ASN
2	H	166	GLU
2	H	178	THR
2	H	192	PHE
2	H	205	ILE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	226	GLU
2	H	231	MET
2	H	239	SER
2	H	252	ILE
2	H	265	VAL
2	H	268	ILE
2	H	272	HIS
2	H	279	SER
2	H	282	LYS
2	H	291	HIS
2	H	300	VAL
2	H	306	MET
2	H	311	ASN
2	H	324	ASN
2	H	326	ARG
2	H	332	LEU
2	H	369	HIS
2	H	372	GLU
2	H	376	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	679	GLN
1	A	784	GLN
1	A	803	GLN
1	A	814	GLN
1	A	834	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	835	ASN
1	A	936	ASN
1	A	942	HIS
1	A	967	GLN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1039	HIS
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	183	GLN
2	B	193	HIS
2	B	204	ASN
2	B	222	GLN
2	B	324	ASN
1	C	46	ASN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN
1	C	811	GLN
1	C	812	GLN
1	C	936	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	14	GLN
2	D	51	GLN
2	D	154	ASN
2	D	222	GLN
2	D	324	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	351	GLN
1	E	105	GLN
1	E	266	ASN
1	E	454	ASN
1	E	457	ASN
1	E	679	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	814	GLN
1	E	834	ASN
1	E	942	HIS
1	E	987	ASN
1	E	992	ASN
1	E	1000	HIS
1	E	1007	ASN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	78	GLN
2	F	105	HIS
2	F	154	ASN
2	F	204	ASN
2	F	324	ASN
1	G	105	GLN
1	G	679	GLN
1	G	689	GLN
1	G	784	GLN
1	G	803	GLN
1	G	812	GLN
1	G	967	GLN
1	G	987	ASN
1	G	992	ASN
1	G	995	HIS
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	105	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	154	ASN
2	H	204	ASN
2	H	222	GLN
2	H	232	ASN
2	H	273	GLN
2	H	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 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	$\# Z > 2$
7	ADP	A	4001	3	25,29,29	1.12	3 (12%)	24,45,45	1.48	2 (8%)
6	PO4	A	4006	3	4,4,4	1.78	1 (25%)	6,6,6	1.22	1 (16%)
7	ADP	A	4007	3,4	25,29,29	1.01	2 (8%)	24,45,45	1.11	1 (4%)
8	ORN	A	4011	-	3,8,8	0.52	0	2,9,9	0.47	0
9	NET	A	4012	-	8,8,8	0.54	0	10,10,10	0.69	0
7	ADP	C	4021	3	25,29,29	1.53	5 (20%)	24,45,45	1.37	4 (16%)
6	PO4	C	4026	3	4,4,4	2.28	3 (75%)	6,6,6	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	C	4027	3,4	25,29,29	1.49	4 (16%)	24,45,45	1.11	1 (4%)
8	ORN	C	4031	-	3,8,8	0.45	0	2,9,9	0.41	0
9	NET	C	4032	-	8,8,8	0.55	0	10,10,10	0.67	0
7	ADP	E	4044	3	25,29,29	1.00	1 (4%)	24,45,45	1.13	2 (8%)
6	PO4	E	4049	3	4,4,4	2.05	2 (50%)	6,6,6	0.66	0
7	ADP	E	4050	3,4	25,29,29	1.28	4 (16%)	24,45,45	1.09	2 (8%)
8	ORN	E	4054	-	3,8,8	0.69	0	2,9,9	0.94	0
9	NET	E	4055	-	8,8,8	0.63	0	10,10,10	0.60	0
7	ADP	G	4066	3	25,29,29	1.43	5 (20%)	24,45,45	1.38	4 (16%)
6	PO4	G	4071	3	4,4,4	1.94	1 (25%)	6,6,6	0.95	0
7	ADP	G	4072	3,4	25,29,29	1.58	4 (16%)	24,45,45	1.17	1 (4%)
8	ORN	G	4076	-	3,8,8	0.46	0	2,9,9	0.30	0
9	NET	G	4077	-	8,8,8	0.63	0	10,10,10	0.64	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
7	ADP	A	4001	3	-	0/12/32/32	0/3/3/3
6	PO4	A	4006	3	-	0/0/0/0	0/0/0/0
7	ADP	A	4007	3,4	-	0/12/32/32	0/3/3/3
8	ORN	A	4011	-	-	0/4/8/8	0/0/0/0
9	NET	A	4012	-	-	0/12/12/12	0/0/0/0
7	ADP	C	4021	3	-	0/12/32/32	0/3/3/3
6	PO4	C	4026	3	-	0/0/0/0	0/0/0/0
7	ADP	C	4027	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	4031	-	-	0/4/8/8	0/0/0/0
9	NET	C	4032	-	-	0/12/12/12	0/0/0/0
7	ADP	E	4044	3	-	0/12/32/32	0/3/3/3
6	PO4	E	4049	3	-	0/0/0/0	0/0/0/0
7	ADP	E	4050	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	4054	-	-	0/4/8/8	0/0/0/0
9	NET	E	4055	-	-	0/12/12/12	0/0/0/0
7	ADP	G	4066	3	-	0/12/32/32	0/3/3/3
6	PO4	G	4071	3	-	0/0/0/0	0/0/0/0
7	ADP	G	4072	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	4076	-	-	0/4/8/8	0/0/0/0
9	NET	G	4077	-	-	0/12/12/12	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	4072	ADP	O4'-C1'	-3.37	1.36	1.41
6	C	4026	PO4	P-O2	-3.13	1.43	1.54
7	C	4021	ADP	O4'-C1'	-2.85	1.37	1.41
7	G	4066	ADP	O4'-C1'	-2.75	1.37	1.41
6	G	4071	PO4	P-O2	-2.74	1.44	1.54
6	E	4049	PO4	P-O3	-2.67	1.44	1.54
6	A	4006	PO4	P-O2	-2.39	1.46	1.54
6	E	4049	PO4	P-O2	-2.29	1.46	1.54
6	C	4026	PO4	P-O3	-2.28	1.46	1.54
6	C	4026	PO4	P-O4	-2.22	1.46	1.54
7	E	4050	ADP	O4'-C1'	-2.09	1.38	1.41
7	A	4001	ADP	C2-N1	2.00	1.37	1.33
7	A	4007	ADP	C2-N1	2.01	1.37	1.33
7	C	4027	ADP	C2-N1	2.03	1.37	1.33
7	A	4007	ADP	O3'-C3'	2.07	1.47	1.43
7	E	4044	ADP	O3'-C3'	2.08	1.47	1.43
7	E	4050	ADP	O3'-C3'	2.15	1.47	1.43
7	A	4001	ADP	O3'-C3'	2.29	1.48	1.43
7	C	4021	ADP	O3'-C3'	2.56	1.48	1.43
7	G	4066	ADP	C2-N1	2.59	1.38	1.33
7	C	4021	ADP	C2-N1	2.62	1.38	1.33
7	A	4001	ADP	O2'-C2'	2.69	1.49	1.43
7	E	4050	ADP	O2'-C2'	2.70	1.49	1.43
7	G	4066	ADP	O3'-C3'	2.75	1.49	1.43
7	G	4072	ADP	O2'-C2'	2.94	1.49	1.43
7	G	4066	ADP	O2'-C2'	2.99	1.49	1.43
7	G	4066	ADP	PB-O3A	3.34	1.65	1.60
7	C	4021	ADP	O2'-C2'	3.41	1.50	1.43
7	C	4027	ADP	O3'-C3'	3.50	1.51	1.43
7	E	4050	ADP	PB-O3A	3.53	1.65	1.60
7	C	4027	ADP	PB-O3A	3.63	1.65	1.60
7	G	4072	ADP	O3'-C3'	3.71	1.51	1.43
7	C	4027	ADP	O2'-C2'	3.92	1.52	1.43
7	G	4072	ADP	PB-O3A	4.08	1.66	1.60
7	C	4021	ADP	PB-O3A	4.09	1.66	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	4066	ADP	C1'-N9-C4	-2.57	122.20	126.64
7	A	4001	ADP	N6-C6-N1	-2.47	113.86	118.77
6	A	4006	PO4	O2-P-O1	-2.34	101.01	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	4021	ADP	N6-C6-N1	-2.30	114.21	118.77
7	E	4044	ADP	O3'-C3'-C2'	2.05	118.39	111.83
7	E	4050	ADP	C4-C5-N7	2.23	111.56	109.41
7	C	4021	ADP	O2'-C2'-C3'	2.24	119.01	111.83
7	G	4072	ADP	C5-C6-N6	2.39	125.34	120.47
7	G	4066	ADP	O3'-C3'-C2'	2.52	119.91	111.83
7	E	4050	ADP	O3'-C3'-C2'	2.53	119.94	111.83
7	E	4044	ADP	C5-C6-N6	2.71	125.99	120.47
7	C	4021	ADP	O3'-C3'-C2'	2.77	120.69	111.83
7	C	4027	ADP	O2'-C2'-C3'	2.80	120.81	111.83
7	A	4007	ADP	C5-C6-N6	2.81	126.20	120.47
7	G	4066	ADP	O2'-C2'-C3'	2.91	121.14	111.83
7	G	4066	ADP	C5-C6-N6	3.16	126.91	120.47
7	C	4021	ADP	C5-C6-N6	4.05	128.72	120.47
7	A	4001	ADP	C5-C6-N6	5.16	131.00	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4001	ADP	1	0
7	A	4007	ADP	2	0
9	A	4012	NET	3	0
7	C	4027	ADP	1	0
8	C	4031	ORN	2	0
9	C	4032	NET	1	0
7	E	4050	ADP	1	0
8	E	4054	ORN	1	0
8	G	4076	ORN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1059/1073 (98%)	-0.56	14 (1%) 77 81	14, 29, 71, 100	0
1	C	1059/1073 (98%)	-0.51	19 (1%) 69 73	14, 31, 76, 100	0
1	E	1059/1073 (98%)	-0.57	19 (1%) 69 73	13, 27, 75, 100	0
1	G	1059/1073 (98%)	-0.38	23 (2%) 62 67	17, 36, 81, 100	0
2	B	375/382 (98%)	-0.09	9 (2%) 59 64	21, 48, 84, 100	0
2	D	375/382 (98%)	-0.40	5 (1%) 77 81	17, 33, 71, 100	0
2	F	375/382 (98%)	-0.34	7 (1%) 67 71	16, 36, 76, 100	0
2	H	375/382 (98%)	0.04	15 (4%) 39 46	26, 52, 90, 100	0
All	All	5736/5820 (98%)	-0.42	111 (1%) 67 71	13, 33, 79, 100	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.7
1	C	1	MET	7.4
1	E	1	MET	7.0
1	G	1	MET	6.9
2	D	358	PRO	6.8
2	B	358	PRO	6.6
2	F	363	ALA	5.9
2	B	2	ILE	5.7
2	B	363	ALA	5.5
1	G	741	ALA	5.5
2	F	358	PRO	5.5
1	A	739	GLN	5.5
2	H	363	ALA	5.4
1	A	717	SER	5.3
1	C	696	THR	5.0
2	F	2	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	716	PRO	4.5
2	H	380	THR	4.4
1	C	740	THR	4.4
2	H	358	PRO	4.3
2	H	2	ILE	4.2
1	G	738	PHE	4.2
1	G	740	THR	4.2
1	A	750	VAL	4.1
2	D	364	ALA	4.0
2	B	379	LYS	3.9
2	D	357	SER	3.9
2	D	2	ILE	3.9
1	G	739	GLN	3.9
1	E	741	ALA	3.9
1	A	740	THR	3.9
2	F	379[A]	LYS	3.8
1	E	740	THR	3.7
1	C	739	GLN	3.7
2	H	188	ASP	3.4
2	F	380	THR	3.4
2	D	379	LYS	3.4
2	H	379	LYS	3.3
1	G	1021	ARG	3.3
2	F	364	ALA	3.3
1	C	716	PRO	3.2
1	G	680	HIS	3.1
1	G	717	SER	3.1
2	H	364	ALA	3.0
1	C	675	ARG	3.0
1	C	695	VAL	2.9
1	G	368	ALA	2.9
1	G	751	LEU	2.9
1	C	1022	ALA	2.9
1	E	739	GLN	2.8
1	C	741	ALA	2.8
1	C	751	LEU	2.8
1	E	716	PRO	2.7
1	C	1073	LYS	2.7
1	G	683	GLU	2.7
1	C	717	SER	2.7
1	C	724	ALA	2.6
1	E	1020	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	717	SER	2.6
1	A	342	GLY	2.6
1	E	1073	LYS	2.6
1	E	1021	ARG	2.6
1	E	697	ALA	2.6
1	G	737	TYR	2.5
1	E	703	GLU	2.5
2	B	364	ALA	2.5
1	A	1073	LYS	2.5
1	G	1020	ARG	2.5
2	B	376	GLN	2.5
1	G	733	ASP	2.5
1	E	680	HIS	2.5
1	A	1021	ARG	2.5
1	G	675	ARG	2.5
1	G	716	PRO	2.5
1	E	368	ALA	2.5
1	C	1021	ARG	2.4
1	E	700	MET	2.4
1	G	729	TYR	2.4
2	F	186	LYS	2.3
1	A	675	ARG	2.3
2	H	165	ALA	2.3
1	G	708	ILE	2.3
2	H	265	VAL	2.3
1	C	736	ARG	2.3
1	A	712	LEU	2.3
1	G	700	MET	2.3
1	G	1073	LYS	2.3
1	C	703	GLU	2.3
2	H	186	LYS	2.3
1	G	732	ALA	2.3
1	C	1070	ALA	2.2
1	E	416	ASP	2.2
1	A	738	PHE	2.2
2	B	226	GLU	2.2
1	E	696	THR	2.2
1	E	706	LYS	2.2
2	H	232	ASN	2.2
1	A	341	GLY	2.1
1	G	734	LEU	2.1
1	C	738	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	188	ASP	2.1
2	H	166	GLU	2.1
1	G	676	GLU	2.0
2	H	236	ILE	2.0
1	A	1024	GLU	2.0
2	B	380	THR	2.0
2	H	187	GLU	2.0
2	H	372	GLU	2.0
1	C	1025	ASP	2.0
1	E	707	GLU	2.0
1	E	947	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	ORN	E	4054	9/9	0.95	0.14	6.10	17,28,35,38	0
8	ORN	G	4076	9/9	0.96	0.12	4.03	22,30,47,60	0
8	ORN	C	4031	9/9	0.96	0.12	2.40	19,26,46,57	0
9	NET	G	4077	9/9	0.96	0.10	2.34	23,28,36,42	0
8	ORN	A	4011	9/9	0.97	0.10	2.30	15,23,32,38	0
9	NET	E	4055	9/9	0.98	0.07	1.88	12,19,31,35	0
9	NET	A	4012	9/9	0.98	0.08	1.56	12,19,26,28	0
9	NET	C	4032	9/9	0.98	0.07	0.52	15,21,28,30	0
4	K	C	4034	1/1	0.96	0.10	0.12	51,51,51,51	0
7	ADP	G	4066	27/27	0.98	0.08	0.09	9,22,31,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	H	4085	1/1	0.98	0.09	0.04	52,52,52,52	0
5	CL	G	4083	1/1	0.98	0.10	-0.05	58,58,58,58	0
7	ADP	C	4021	27/27	0.99	0.07	-0.16	12,19,24,45	0
6	PO4	A	4006	5/5	0.99	0.07	-0.40	16,22,28,30	0
7	ADP	A	4001	27/27	0.99	0.07	-0.42	12,22,32,38	0
7	ADP	G	4072	27/27	0.96	0.08	-0.52	30,43,80,95	0
7	ADP	C	4027	27/27	0.98	0.08	-0.57	16,33,62,83	0
7	ADP	E	4050	27/27	0.97	0.08	-0.59	19,33,50,58	0
6	PO4	C	4026	5/5	0.99	0.07	-0.64	14,15,19,24	0
7	ADP	E	4044	27/27	0.99	0.07	-0.67	8,20,25,28	0
6	PO4	G	4071	5/5	0.99	0.06	-0.85	15,16,17,32	0
7	ADP	A	4007	27/27	0.99	0.06	-0.87	14,28,48,77	0
5	CL	A	4017	1/1	0.99	0.05	-1.34	39,39,39,39	0
5	CL	E	4062	1/1	0.98	0.05	-1.44	48,48,48,48	0
6	PO4	E	4049	5/5	0.99	0.05	-1.83	17,17,21,25	0
4	K	E	4048	1/1	1.00	0.07	-1.91	23,23,23,23	0
3	MN	G	4067	1/1	1.00	0.04	-1.92	25,25,25,25	0
3	MN	E	4045	1/1	1.00	0.05	-2.16	24,24,24,24	0
4	K	G	4070	1/1	0.99	0.06	-2.38	30,30,30,30	0
5	CL	C	4039	1/1	0.98	0.04	-2.40	45,45,45,45	0
4	K	G	4069	1/1	0.99	0.04	-2.40	24,24,24,24	0
4	K	A	4005	1/1	1.00	0.05	-2.43	25,25,25,25	0
5	CL	F	4064	1/1	1.00	0.04	-2.45	33,33,33,33	0
3	MN	A	4002	1/1	1.00	0.04	-2.75	21,21,21,21	0
4	K	G	4075	1/1	1.00	0.04	-2.89	37,37,37,37	0
4	K	C	4025	1/1	0.98	0.05	-3.29	25,25,25,25	0
5	CL	B	4019	1/1	0.99	0.03	-3.37	33,33,33,33	0
4	K	A	4010	1/1	1.00	0.04	-3.91	21,21,21,21	0
4	K	E	4047	1/1	1.00	0.03	-3.99	19,19,19,19	0
4	K	A	4004	1/1	1.00	0.03	-4.02	20,20,20,20	0
4	K	E	4053	1/1	1.00	0.02	-4.37	23,23,23,23	0
4	K	C	4030	1/1	0.99	0.03	-4.44	26,26,26,26	0
4	K	C	4024	1/1	1.00	0.02	-4.71	19,19,19,19	0
3	MN	C	4022	1/1	1.00	0.04	-4.86	21,21,21,21	0
5	CL	G	4084	1/1	0.97	0.10	-	76,76,76,76	0
5	CL	A	4020	1/1	0.97	0.06	-	45,45,45,45	0
3	MN	C	4028	1/1	0.99	0.03	-	39,39,39,39	0
3	MN	C	4023	1/1	1.00	0.04	-	24,24,24,24	0
5	CL	A	4018	1/1	0.88	0.10	-	58,58,58,58	0
4	K	A	4009	1/1	0.99	0.06	-	80,80,80,80	0
3	MN	E	4046	1/1	1.00	0.03	-	21,21,21,21	0
5	CL	G	4081	1/1	0.93	0.20	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	G	4086	1/1	0.98	0.05	-	47,47,47,47	0
4	K	F	4058	1/1	0.99	0.04	-	39,39,39,39	0
5	CL	G	4082	1/1	0.99	0.06	-	39,39,39,39	0
3	MN	E	4051	1/1	0.99	0.02	-	36,36,36,36	0
5	CL	A	4015	1/1	1.00	0.03	-	23,23,23,23	0
5	CL	C	4040	1/1	0.94	0.08	-	59,59,59,59	0
5	CL	G	4080	1/1	1.00	0.03	-	23,23,23,23	0
5	CL	D	4043	1/1	0.75	0.15	-	80,80,80,80	0
4	K	G	4074	1/1	0.90	0.10	-	86,86,86,86	0
5	CL	E	4065	1/1	0.99	0.11	-	46,46,46,46	0
4	K	G	4078	1/1	0.97	0.07	-	53,53,53,53	0
4	K	D	4035	1/1	0.98	0.04	-	34,34,34,34	0
5	CL	E	4061	1/1	0.99	0.05	-	41,41,41,41	0
4	K	C	4033	1/1	0.98	0.06	-	55,55,55,55	0
4	K	A	4013	1/1	0.96	0.05	-	55,55,55,55	0
5	CL	E	4059	1/1	1.00	0.04	-	24,24,24,24	0
5	CL	C	4041	1/1	0.99	0.04	-	27,27,27,27	0
3	MN	A	4003	1/1	1.00	0.04	-	21,21,21,21	0
5	CL	C	4037	1/1	0.66	0.18	-	81,81,81,81	0
5	CL	C	4036	1/1	0.99	0.04	-	26,26,26,26	0
4	K	C	4029	1/1	0.97	0.05	-	76,76,76,76	0
5	CL	E	4060	1/1	0.95	0.11	-	56,56,56,56	0
5	CL	C	4042	1/1	0.98	0.07	-	45,45,45,45	0
3	MN	A	4008	1/1	1.00	0.02	-	28,28,28,28	0
5	CL	A	4016	1/1	0.98	0.04	-	39,39,39,39	0
4	K	B	4014	1/1	0.97	0.07	-	42,42,42,42	0
4	K	E	4056	1/1	0.98	0.05	-	42,42,42,42	0
4	K	E	4052	1/1	0.98	0.04	-	61,61,61,61	0
3	MN	G	4073	1/1	1.00	0.02	-	49,49,49,49	0
5	CL	C	4038	1/1	0.99	0.03	-	33,33,33,33	0
5	CL	E	4063	1/1	0.97	0.08	-	59,59,59,59	0
3	MN	G	4068	1/1	1.00	0.03	-	22,22,22,22	0
4	K	G	4079	1/1	0.99	0.12	-	49,49,49,49	0
4	K	E	4057	1/1	0.95	0.06	-	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.