



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 2PJR / pdb_00002pjr
Title : HELICASE PRODUCT COMPLEX
Authors : Velankar, S.S.; Soultanas, P.; Dillingham, M.S.; Subramanya, H.S.; Wigley, D.B.
Deposited on : 1999-03-12
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

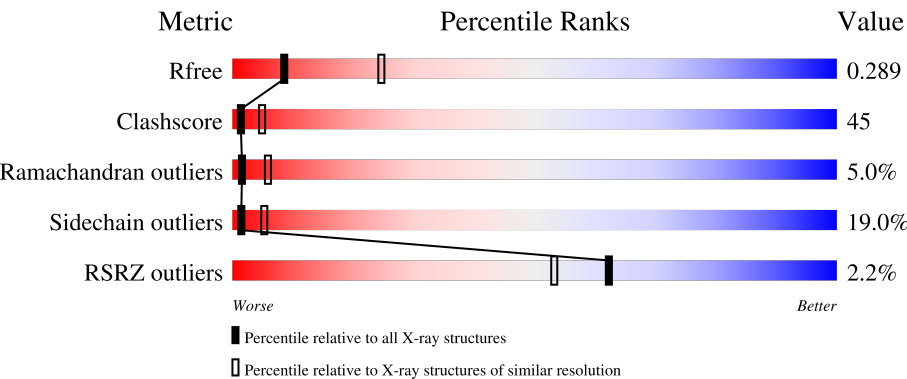
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	C	5	100%
1	D	5	100%
2	H	2	50%50%
3	I	5	40%40%20%
4	A	548	2%36%50%11%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	548	3% 36% 45% 15% • •
5	B	95	3% 28% 49% 16% 6%
5	G	95	2% 28% 45% 22% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10671 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 DNA chain called DNA (5'-D(*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			
1	D	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	P	0	0	0
			98	48	18	28	4			

- Molecule 4 is a protein called PROTEIN (HELICASE PCRA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	542	Total	C	N	O	S	0	0	0
			4409	2792	775	829	13			
4	F	544	Total	C	N	O	S	0	0	0
			4424	2802	777	832	13			

- Molecule 5 is a protein called PROTEIN (HELICASE PCRA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	95	Total	C	N	O	S	0	0	0
			749	471	125	147	6			
5	G	95	Total	C	N	O	S	0	0	0
			749	471	125	147	6			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

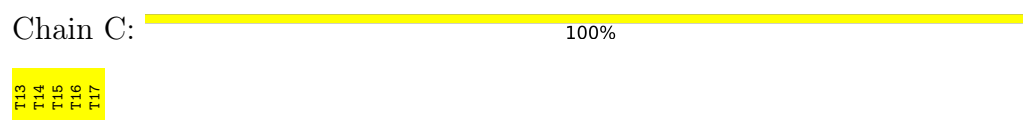


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

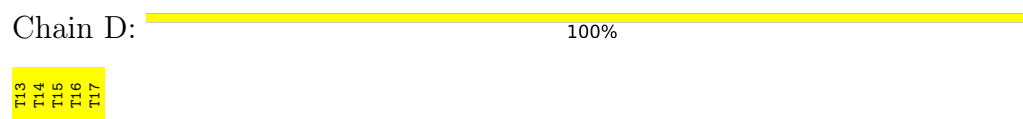
3 Residue-property plots

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

- Molecule 1: DNA (5'-D(*TP*TP*TP*TP*T)-3')



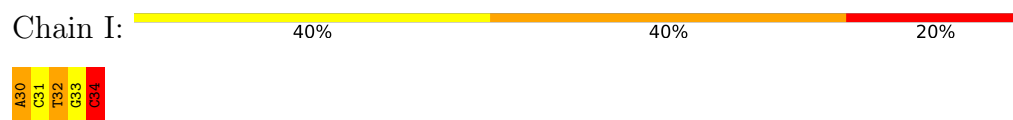
- Molecule 1: DNA (5'-D(*TP*TP*TP*TP*T)-3')



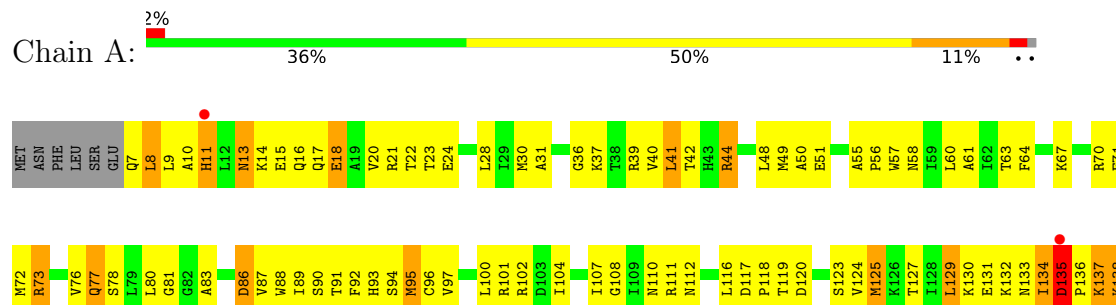
- Molecule 2: DNA (5'-D(*GP*C)-3')

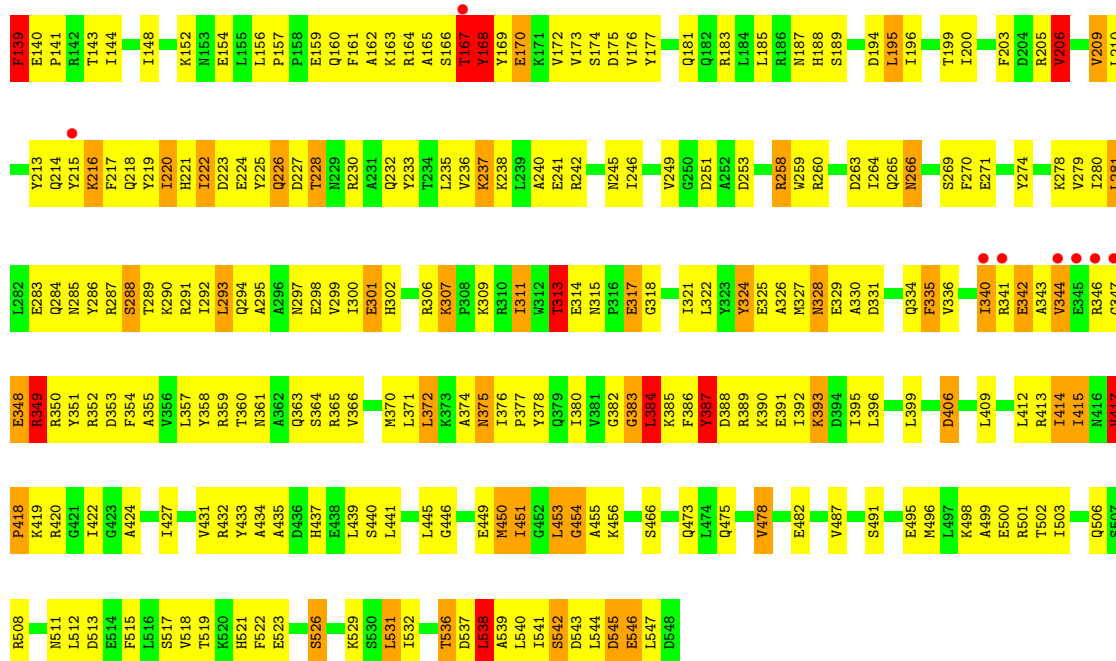


- Molecule 3: DNA (5'-D(*AP*CP*TP*GP*C)-3')

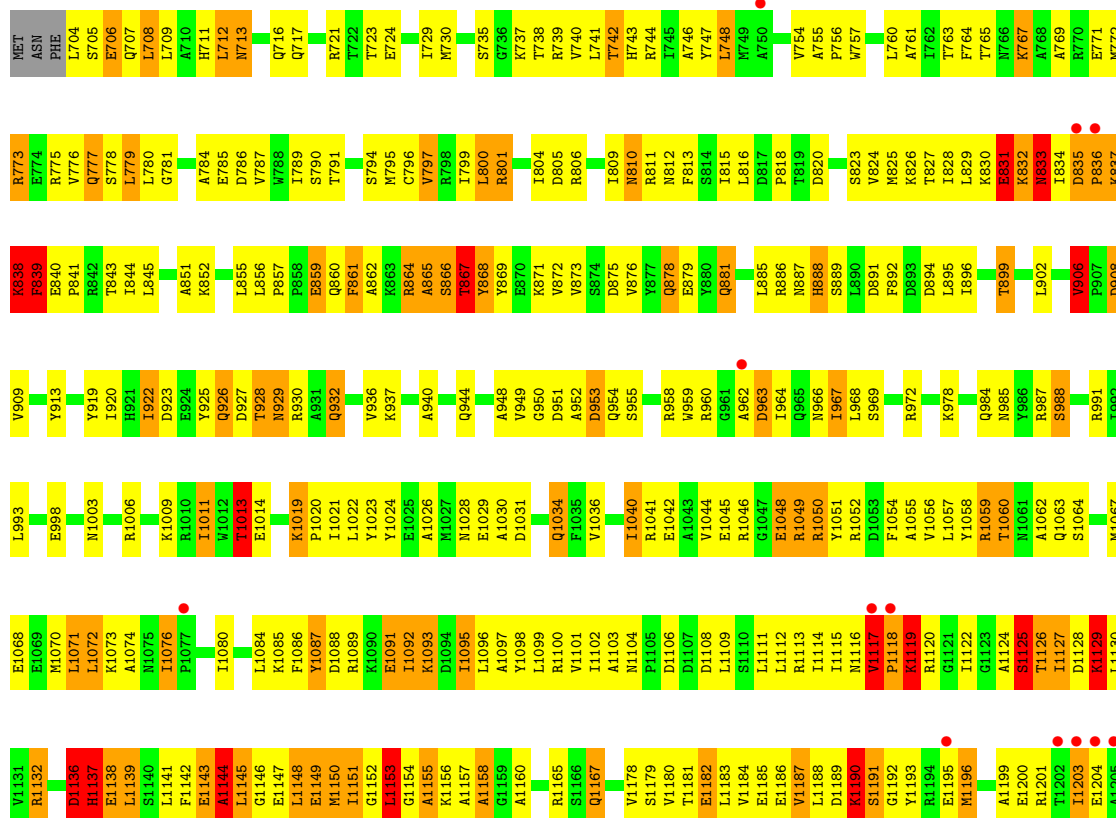


- Molecule 4: PROTEIN (HELICASE PCRA)



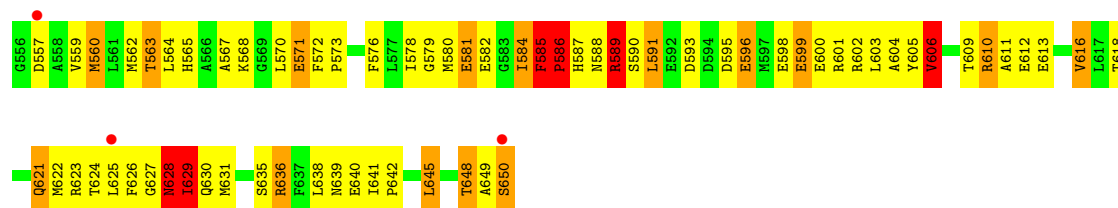


• Molecule 4: PROTEIN (HELICASE PCRA)

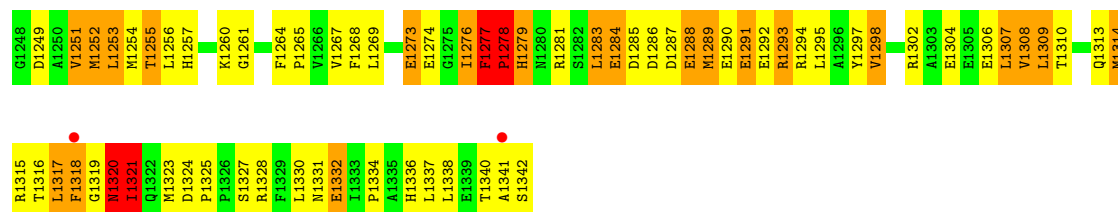




• Molecule 5: PROTEIN (HELICASE PCRA)



• Molecule 5: PROTEIN (HELICASE PCRA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.05Å 62.60Å 141.83Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.90) 97.0 (15.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.296 0.240 , 0.289	Depositor DCC
R_{free} test set	1644 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10671	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 3.57% 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: SO4

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	C	0.41	0/106	0.98	0/162
1	D	0.39	0/106	1.21	1/162 (0.6%)
2	H	1.07	0/42	1.41	1/63 (1.6%)
3	I	1.34	1/109 (0.9%)	1.94	5/166 (3.0%)
4	A	0.65	3/4485 (0.1%)	1.16	33/6059 (0.5%)
4	F	0.61	0/4500	1.16	39/6079 (0.6%)
5	B	0.75	2/762 (0.3%)	1.17	6/1028 (0.6%)
5	G	0.69	0/762	1.26	12/1028 (1.2%)
All	All	0.65	6/10872 (0.1%)	1.18	97/14747 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
4	A	0	1
4	F	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	32	DT	O3'-P	-8.51	1.48	1.61
5	B	606	VAL	CA-CB	6.38	1.62	1.54
4	A	157	PRO	CA-C	5.62	1.54	1.51
5	B	650	SER	CA-CB	5.16	1.63	1.53
4	A	209	VAL	CA-CB	5.16	1.61	1.54
4	A	125	MET	SD-CE	-5.07	1.66	1.79

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1151	ILE	N-CA-C	-15.19	94.00	112.98
4	A	417	VAL	CA-C-N	-14.45	103.22	119.98
4	A	417	VAL	C-N-CA	-14.45	103.22	119.98
3	I	30	DA	O5'-C5'-C4'	12.06	128.89	110.80
4	A	133	ASN	N-CA-C	10.36	125.57	109.52
4	F	1117	VAL	CA-C-N	-10.12	107.18	119.84
4	F	1117	VAL	C-N-CA	-10.12	107.18	119.84
4	A	216	LYS	N-CA-C	-9.60	101.93	114.31
4	F	1224	ASN	N-CA-C	-9.41	101.36	113.12
4	F	833	ASN	N-CA-C	8.96	124.00	109.94
4	A	161	PHE	N-CA-C	-8.68	101.75	111.82
4	F	1227	ASP	N-CA-C	-8.24	101.35	111.40
5	B	585	PHE	CA-C-N	-8.16	109.64	119.84
5	B	585	PHE	C-N-CA	-8.16	109.64	119.84
4	A	206	VAL	CA-C-N	8.07	129.92	119.84
4	A	206	VAL	C-N-CA	8.07	129.92	119.84
5	G	1287	ASP	N-CA-C	-8.06	103.42	113.18
5	G	1320	ASN	N-CA-C	8.05	121.47	108.76
4	A	545	ASP	N-CA-C	-7.88	104.55	114.56
4	A	335	PHE	N-CA-C	-7.81	104.35	114.04
4	F	1190	LYS	N-CA-C	-7.67	94.46	110.80
5	G	1341	ALA	N-CA-C	7.59	121.83	109.76
4	F	769	ALA	N-CA-C	-7.57	102.69	112.23
5	G	1278	PRO	N-CA-C	-7.56	96.89	112.47
4	A	546	GLU	N-CA-C	-7.28	104.21	113.23
4	F	906	VAL	CA-C-N	7.12	128.74	119.84
4	F	906	VAL	C-N-CA	7.12	128.74	119.84
4	A	288	SER	N-CA-C	7.10	119.69	110.53
4	F	1207	SER	N-CA-C	-7.10	95.68	110.80
4	F	861	PHE	N-CA-C	-7.06	103.63	111.82
4	F	1238	LEU	N-CA-C	-6.99	95.91	110.80
4	F	864	ARG	N-CA-C	-6.96	98.69	109.76
4	F	747	TYR	N-CA-C	-6.96	105.41	114.04
4	F	1137	HIS	N-CA-C	-6.90	96.09	110.80
4	F	1013	THR	N-CA-C	6.87	119.30	108.79
5	B	610	ARG	N-CA-C	-6.86	105.19	113.97
4	A	91	THR	N-CA-C	-6.77	99.93	110.42
4	A	418	PRO	N-CA-C	-6.76	99.99	110.95
4	F	786	ASP	N-CA-C	-6.73	103.26	113.89
4	F	1118	PRO	N-CA-C	-6.64	98.80	112.47
4	A	313	THR	N-CA-C	6.63	119.15	109.07
5	G	1332	GLU	N-CA-C	-6.61	104.44	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	868	TYR	N-CA-C	-6.47	107.24	114.62
4	F	706	GLU	N-CA-C	-6.47	105.52	113.41
4	F	866	SER	N-CA-C	-6.38	97.21	110.80
4	A	390	LYS	N-CA-C	6.30	121.69	111.37
4	A	414	ILE	N-CA-C	6.29	118.22	112.43
3	I	30	DA	C5'-C4'-O4'	6.23	118.75	109.40
4	F	1132	ARG	N-CA-C	-6.14	104.70	111.82
5	B	586	PRO	N-CA-C	-6.10	99.90	112.47
4	A	135	ASP	CA-C-N	-6.09	112.22	119.84
4	A	135	ASP	C-N-CA	-6.09	112.22	119.84
5	G	1277	PHE	CA-C-N	-6.09	112.22	119.84
5	G	1277	PHE	C-N-CA	-6.09	112.22	119.84
4	F	1156	LYS	N-CA-C	-6.07	104.78	111.82
2	H	1	DG	O5'-C5'-C4'	6.05	119.87	110.80
4	A	220	ILE	N-CA-C	6.02	116.52	107.80
4	A	50	ALA	N-CA-C	5.95	119.01	111.69
4	F	724	GLU	N-CA-C	5.90	119.25	109.46
4	F	1155	ALA	N-CA-C	-5.87	98.30	110.80
4	F	1242	SER	N-CA-C	5.82	120.50	113.17
4	F	845	LEU	N-CA-C	-5.81	104.95	111.28
4	F	1129	LYS	N-CA-C	-5.80	104.96	111.28
4	A	307	LYS	N-CA-C	-5.78	102.13	110.40
5	G	1279	HIS	N-CA-C	5.75	118.17	110.35
4	A	78	SER	N-CA-C	-5.70	106.32	113.28
4	F	1217	SER	N-CA-C	-5.70	104.68	111.69
4	F	1231	LEU	N-CA-C	-5.70	104.07	111.02
4	F	1136	ASP	N-CA-C	-5.68	104.52	112.25
3	I	30	DA	N9-C1'-C2'	5.62	121.92	113.50
4	F	1191	SER	N-CA-C	-5.59	98.89	110.80
3	I	34	DC	O5'-C5'-C4'	-5.56	102.46	110.80
4	A	435	ALA	N-CA-C	-5.53	105.26	111.28
3	I	34	DC	C2'-C3'-O3'	-5.52	103.22	111.50
5	G	1321	ILE	N-CA-C	5.52	120.82	109.34
1	D	17	DT	C2'-C3'-O3'	5.49	119.73	111.50
4	F	831	GLU	N-CA-C	-5.45	99.19	110.80
4	F	1144	ALA	N-CA-C	-5.43	99.23	110.80
4	A	138	LYS	CB-CA-C	-5.40	108.77	115.89
4	F	1019	LYS	CA-C-N	5.36	125.30	119.78
4	F	1019	LYS	C-N-CA	5.36	125.30	119.78
4	A	199	THR	N-CA-C	-5.33	105.47	111.28
5	B	560	MET	N-CA-C	5.33	117.65	109.07
4	A	340	ILE	N-CA-C	-5.32	106.08	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1293	ARG	N-CA-C	-5.30	105.58	111.36
5	G	1292	GLU	N-CA-C	-5.24	105.17	112.45
4	F	1142	PHE	N-CA-C	-5.23	106.75	113.23
4	A	301	GLU	N-CA-C	-5.22	106.88	113.20
4	A	317	GLU	N-CA-C	-5.22	105.27	111.69
4	A	83	ALA	N-CA-C	-5.21	106.88	113.18
4	A	446	GLY	N-CA-C	-5.20	106.20	112.49
4	A	265	GLN	N-CA-C	-5.13	107.31	113.21
5	B	629	ILE	N-CA-C	5.11	119.97	109.34
4	F	1014	GLU	N-CA-C	-5.10	106.81	112.57
4	A	108	GLY	N-CA-C	5.08	122.91	113.76
5	G	1289	MET	N-CA-C	-5.02	106.67	112.89
4	A	440	SER	N-CA-C	-5.00	103.80	110.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	387	TYR	Sidechain
4	F	1193	TYR	Sidechain
3	I	34	DC	Sidechain

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	C	97	0	62	10	0
1	D	97	0	62	9	0
2	H	38	0	24	0	0
3	I	98	0	58	11	0
4	A	4409	0	4432	369	0
4	F	4424	0	4450	460	0
5	B	749	0	731	107	0
5	G	749	0	731	92	0
6	A	5	0	0	1	0
6	F	5	0	0	0	0
All	All	10671	0	10550	956	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 45.

All (956) 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:F:1096:LEU:HD21	4:F:1238:LEU:HD23	1.23	1.15
5:G:1316:THR:HG23	5:G:1320:ASN:HA	1.24	1.14
4:A:326:ALA:O	5:B:621:GLN:HG2	1.55	1.06
4:A:327:MET:HA	5:B:621:GLN:HG3	1.33	1.05
4:A:396:LEU:HD11	4:A:538:LEU:HD23	1.38	1.04
5:G:1256:LEU:HD21	5:G:1269:LEU:HD21	1.37	1.03
5:B:605:TYR:O	5:B:609:THR:HG22	1.61	1.00
4:F:1232:ILE:HD12	4:F:1232:ILE:H	1.25	0.99
4:F:1041:ARG:HB2	4:F:1076:ILE:HD11	1.45	0.98
4:F:780:LEU:HD12	4:F:784:ALA:HB2	1.43	0.98
4:F:1190:LYS:C	4:F:1192:GLY:H	1.72	0.98
5:B:585:PHE:O	5:B:587:HIS:N	1.97	0.97
4:F:825:MET:HE1	4:F:876:VAL:HG11	1.44	0.97
4:F:832:LYS:HB3	4:F:833:ASN:ND2	1.80	0.96
4:F:713:ASN:HD21	4:F:716:GLN:HG3	1.31	0.96
4:F:1231:LEU:HD22	4:F:1235:LEU:HD11	1.48	0.96
1:D:16:DT:H2"	4:F:765:THR:HG22	1.48	0.95
4:A:298:GLU:HG2	5:B:642:PRO:HD3	1.46	0.94
4:F:929:ASN:HD22	4:F:929:ASN:N	1.66	0.94
4:F:1011:ILE:HD12	4:F:1011:ILE:H	1.31	0.93
5:B:642:PRO:HB2	5:B:645:LEU:HD12	1.51	0.93
4:A:73:ARG:HG3	4:A:73:ARG:HH11	1.33	0.93
4:F:929:ASN:H	4:F:929:ASN:ND2	1.57	0.93
4:F:929:ASN:HD21	4:F:932:GLN:CD	1.76	0.93
4:A:293:LEU:HG	4:A:311:ILE:HG13	1.50	0.91
4:A:49:MET:HE3	4:A:56:PRO:HG3	1.51	0.91
4:F:834:ILE:HG12	4:F:836:PRO:HD2	1.50	0.91
4:A:112:ASN:OD1	4:A:532:ILE:HG12	1.71	0.90
4:A:374:ALA:O	4:A:375:ASN:HB2	1.69	0.90
4:A:13:ASN:HD22	4:A:13:ASN:H	0.92	0.89
4:F:833:ASN:N	4:F:833:ASN:HD22	1.70	0.89
4:F:1050:ARG:NH1	5:G:1249:ASP:CG	2.29	0.89
5:G:1298:VAL:O	5:G:1302:ARG:HG2	1.72	0.89
4:A:100:LEU:HD22	4:A:104:ILE:HD13	1.54	0.89
5:B:564:LEU:HB3	5:B:603:LEU:HD22	1.55	0.89
4:A:13:ASN:HD21	4:A:16:GLN:CD	1.80	0.88
4:A:139:PHE:HD1	4:A:139:PHE:H	1.17	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:215:TYR:HB3	4:A:242:ARG:HD3	1.55	0.87
4:F:742:THR:HG22	4:F:743:HIS:HD2	1.38	0.87
4:A:328:ASN:ND2	4:A:331:ASP:H	1.72	0.87
5:G:1277:PHE:HB3	5:G:1278:PRO:HD3	1.57	0.87
4:A:13:ASN:H	4:A:13:ASN:ND2	1.64	0.86
4:F:1087:TYR:HA	4:F:1092:ILE:HG21	1.58	0.86
4:F:1114:ILE:HA	4:F:1117:VAL:HG23	1.57	0.85
5:G:1277:PHE:O	5:G:1279:HIS:N	2.08	0.85
4:A:13:ASN:HD22	4:A:13:ASN:N	1.76	0.84
4:F:959:TRP:H	4:F:959:TRP:CD1	1.93	0.84
4:F:746:ALA:HB1	4:F:780:LEU:HD21	1.60	0.83
4:A:328:ASN:HD22	4:A:330:ALA:H	1.25	0.83
4:A:449:GLU:O	4:A:450:MET:HG2	1.79	0.83
4:F:761:ALA:HB1	4:F:772:MET:HE1	1.59	0.82
4:A:287:ARG:HD3	5:B:571:GLU:HB3	1.62	0.82
4:A:359:ARG:HH12	5:B:600:GLU:CD	1.87	0.82
5:B:636:ARG:HG2	5:B:636:ARG:HH11	1.45	0.82
4:F:1238:LEU:O	4:F:1240:LEU:N	2.13	0.82
4:A:336:VAL:HG12	4:A:340:ILE:HD11	1.61	0.81
4:F:1021:ILE:HG23	5:G:1307:LEU:HD23	1.62	0.81
4:A:73:ARG:HG3	4:A:73:ARG:NH1	1.92	0.81
4:A:336:VAL:O	4:A:340:ILE:HG13	1.81	0.81
4:F:833:ASN:ND2	4:F:833:ASN:N	2.27	0.81
4:F:988:SER:HB2	4:F:993:LEU:HD12	1.60	0.80
4:F:1157:ALA:O	4:F:1160:ALA:N	2.14	0.80
4:F:1091:GLU:CD	4:F:1091:GLU:H	1.90	0.79
4:A:298:GLU:HG2	5:B:642:PRO:CD	2.13	0.79
4:F:929:ASN:HD22	4:F:929:ASN:H	0.83	0.79
4:F:1150:MET:C	4:F:1152:GLY:H	1.83	0.78
4:F:1178:VAL:CG1	4:F:1182:GLU:HB2	2.13	0.78
4:A:285:ASN:O	4:A:313:THR:HG23	1.82	0.78
4:F:1041:ARG:CB	4:F:1076:ILE:HD11	2.14	0.78
4:F:790:SER:OG	4:F:794:SER:HB3	1.84	0.78
4:A:163:LYS:HB2	4:F:1150:MET:CE	2.14	0.77
5:B:606:VAL:O	5:B:610:ARG:HG2	1.84	0.77
1:D:15:DT:OP1	5:G:1255:THR:HG21	1.84	0.77
4:F:1050:ARG:HH12	5:G:1249:ASP:CG	1.92	0.76
4:A:263:ASP:O	4:A:266:ASN:HB2	1.84	0.76
4:F:730:MET:HE1	4:F:967:ILE:HD11	1.67	0.76
4:F:1049:ARG:HH22	5:G:1306:GLU:CD	1.92	0.76
4:F:1049:ARG:HD3	4:F:1049:ARG:N	2.00	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1099:LEU:HD23	4:F:1231:LEU:HD21	1.68	0.76
4:F:709:LEU:HA	4:F:712:LEU:HD12	1.68	0.75
4:A:13:ASN:ND2	4:A:16:GLN:CD	2.43	0.75
4:F:711:HIS:NE2	4:F:739:ARG:NH2	2.33	0.75
5:G:1289:MET:HE2	5:G:1328:ARG:HD2	1.67	0.75
4:A:137:LYS:HD2	4:A:138:LYS:NZ	2.02	0.75
4:A:154:GLU:HA	4:A:230:ARG:HB3	1.67	0.75
4:A:230:ARG:NH2	4:F:1139:LEU:HD21	2.01	0.75
4:F:1048:GLU:CB	4:F:1049:ARG:HD3	2.17	0.75
4:F:1114:ILE:HA	4:F:1117:VAL:CG2	2.16	0.74
4:A:139:PHE:HD1	4:A:139:PHE:N	1.85	0.74
4:F:1125:SER:O	4:F:1128:ASP:N	2.20	0.74
4:F:969:SER:HB2	4:F:972:ARG:HD2	1.70	0.74
4:F:1050:ARG:HG2	4:F:1050:ARG:HH11	1.50	0.74
5:B:628:ASN:N	5:B:628:ASN:HD22	1.83	0.74
4:A:23:THR:HB	4:A:48:LEU:HD21	1.69	0.74
4:A:165:ALA:HA	4:A:170:GLU:OE1	1.88	0.74
5:B:585:PHE:HB3	5:B:586:PRO:HD3	1.67	0.74
4:A:327:MET:HA	5:B:621:GLN:CG	2.14	0.74
4:A:352:ARG:HD2	4:A:352:ARG:O	1.87	0.74
4:F:1021:ILE:CG2	5:G:1307:LEU:HD23	2.18	0.74
4:F:1232:ILE:H	4:F:1232:ILE:CD1	1.97	0.73
5:B:606:VAL:O	5:B:610:ARG:CG	2.36	0.73
4:F:742:THR:HG22	4:F:743:HIS:CD2	2.23	0.73
4:F:985:ASN:ND2	4:F:987:ARG:H	1.87	0.73
4:F:1150:MET:C	4:F:1152:GLY:N	2.46	0.73
4:A:125:MET:HE1	4:A:176:VAL:HG11	1.69	0.73
5:B:564:LEU:CB	5:B:603:LEU:HD22	2.19	0.73
4:F:1086:PHE:CE1	4:F:1244:LEU:HD13	2.24	0.73
4:A:139:PHE:HA	4:A:144:ILE:HD11	1.71	0.73
4:F:1003:ASN:OD1	5:G:1290:GLU:HG2	1.87	0.73
4:F:1221:HIS:O	4:F:1224:ASN:HB2	1.89	0.73
4:A:20:VAL:HA	4:A:44:ARG:HG3	1.69	0.73
4:A:44:ARG:HE	4:A:221:HIS:HE1	1.36	0.73
4:F:832:LYS:HB3	4:F:833:ASN:HD22	1.52	0.73
4:F:746:ALA:CB	4:F:780:LEU:HD21	2.18	0.72
4:F:1048:GLU:HB3	4:F:1049:ARG:HD3	1.71	0.72
4:F:1178:VAL:HG13	4:F:1182:GLU:HB2	1.70	0.72
5:G:1307:LEU:HD21	5:G:1309:LEU:HD21	1.71	0.72
4:F:1056:VAL:HB	5:G:1253:LEU:HD12	1.71	0.72
4:F:713:ASN:N	4:F:713:ASN:HD22	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:164:ARG:HB2	4:F:1150:MET:SD	2.30	0.72
5:G:1334:PRO:HB3	5:G:1336:HIS:NE2	2.05	0.72
4:A:230:ARG:HH22	4:F:1139:LEU:HD21	1.55	0.71
3:I:32:DT:H2''	3:I:33:DG:O5'	1.90	0.71
4:A:139:PHE:N	4:A:139:PHE:CD1	2.54	0.71
5:B:579:GLY:HA2	5:B:623:ARG:NH2	2.05	0.71
4:F:991:ARG:HG2	5:G:1337:LEU:CD2	2.19	0.71
4:F:1095:ILE:O	4:F:1099:LEU:HD12	1.89	0.71
4:A:13:ASN:ND2	4:A:16:GLN:OE1	2.23	0.71
4:F:713:ASN:HD21	4:F:716:GLN:CG	2.03	0.71
4:F:1096:LEU:HD21	4:F:1238:LEU:CD2	2.12	0.71
4:A:139:PHE:CZ	4:A:172:VAL:HG21	2.24	0.71
4:F:805:ASP:OD2	4:F:811:ARG:HD3	1.90	0.71
4:A:544:LEU:O	4:A:544:LEU:HG	1.91	0.71
5:G:1265:PRO:HA	5:G:1304:GLU:HB2	1.72	0.71
4:F:712:LEU:HB3	4:F:716:GLN:HB2	1.73	0.71
4:F:926:GLN:H	4:F:926:GLN:NE2	1.88	0.71
4:F:1149:GLU:O	4:F:1150:MET:HG3	1.91	0.71
4:A:313:THR:HG21	4:A:315:ASN:ND2	2.05	0.70
4:F:773:ARG:NH1	4:F:789:ILE:HD12	2.05	0.70
4:A:537:ASP:HB2	4:A:541:ILE:HD12	1.73	0.70
4:F:834:ILE:CG1	4:F:836:PRO:HD2	2.21	0.70
4:F:902:LEU:O	4:F:906:VAL:HG13	1.91	0.70
4:A:125:MET:HE1	4:A:176:VAL:CG1	2.21	0.70
4:F:993:LEU:HD22	4:F:1013:THR:HG22	1.72	0.70
4:A:328:ASN:HD22	4:A:330:ALA:N	1.89	0.70
5:B:584:ILE:HG22	5:B:585:PHE:N	2.05	0.70
4:A:237:LYS:HZ1	4:F:1138:GLU:HB2	1.54	0.70
4:A:125:MET:CE	4:A:129:LEU:HD13	2.22	0.69
4:A:196:ILE:O	4:A:200:ILE:HD12	1.92	0.69
4:F:1044:VAL:HG21	4:F:1051:TYR:CE1	2.27	0.69
4:F:1068:GLU:O	4:F:1072:LEU:HB2	1.92	0.69
4:F:1057:LEU:HD22	5:G:1254:MET:HG2	1.73	0.69
4:A:44:ARG:HE	4:A:221:HIS:CE1	2.10	0.69
4:F:795:MET:O	4:F:799:ILE:HG13	1.92	0.69
4:F:1044:VAL:HG21	4:F:1051:TYR:CD1	2.27	0.69
4:F:1150:MET:CE	4:F:1152:GLY:HA2	2.23	0.69
4:F:1226:SER:O	4:F:1229:LYS:HE2	1.93	0.69
4:A:226:GLN:HG2	4:A:251:ASP:O	1.92	0.69
4:F:865:ALA:HB1	4:F:871:LYS:HG3	1.74	0.69
4:F:1054:PHE:HB2	5:G:1251:VAL:HG22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:865:ALA:O	4:F:871:LYS:HE2	1.92	0.69
4:F:1235:LEU:N	4:F:1235:LEU:HD12	2.08	0.69
5:G:1257:HIS:HE1	5:G:1295:LEU:HD11	1.58	0.69
5:B:636:ARG:HG2	5:B:636:ARG:NH1	2.06	0.69
5:B:626:PHE:CD1	5:B:627:GLY:N	2.61	0.68
4:A:388:ASP:HA	4:A:393:LYS:HD2	1.75	0.68
4:F:928:THR:HG22	4:F:932:GLN:HB3	1.74	0.68
4:F:1095:ILE:CD1	4:F:1187:VAL:HG11	2.24	0.68
5:G:1291:GLU:HG3	5:G:1294:ARG:NH2	2.08	0.68
4:F:834:ILE:HG12	4:F:836:PRO:CD	2.21	0.68
4:F:1058:TYR:CZ	4:F:1064:SER:HB3	2.29	0.68
4:A:298:GLU:CG	5:B:642:PRO:HD3	2.23	0.68
4:A:340:ILE:O	4:A:344:VAL:HG11	1.94	0.68
4:F:748:LEU:O	4:F:754:VAL:HG22	1.94	0.68
4:F:1099:LEU:CD2	4:F:1231:LEU:HD21	2.24	0.67
4:F:1139:LEU:HB2	4:F:1143:GLU:HB3	1.76	0.67
4:A:139:PHE:CE2	4:A:172:VAL:HG11	2.28	0.67
5:G:1252:MET:HG3	5:G:1264:PHE:CE2	2.30	0.67
4:A:258:ARG:NH2	5:B:595:ASP:HB2	2.10	0.67
4:A:417:VAL:O	4:A:419:LYS:N	2.27	0.67
4:A:386:PHE:CD1	4:A:544:LEU:HD22	2.30	0.67
4:F:729:ILE:HD13	4:F:740:VAL:HG11	1.77	0.67
4:F:859:GLU:O	4:F:862:ALA:HB3	1.94	0.67
4:A:478:VAL:HG13	4:A:482:GLU:HB2	1.76	0.67
4:F:1048:GLU:C	4:F:1049:ARG:HD3	2.19	0.67
4:A:125:MET:HE2	4:A:129:LEU:HD13	1.76	0.67
5:B:648:THR:HG23	5:B:650:SER:H	1.59	0.67
3:I:31:DC:H5'	3:I:31:DC:C6	2.30	0.67
4:A:116:LEU:HD13	4:A:189:SER:HB3	1.77	0.66
4:F:988:SER:HB2	4:F:993:LEU:CD1	2.25	0.66
4:A:127:THR:O	4:A:131:GLU:HG3	1.94	0.66
4:F:1050:ARG:NH1	4:F:1050:ARG:HG2	2.08	0.66
5:B:629:ILE:HD12	5:B:629:ILE:H	1.60	0.66
4:A:420:ARG:HG3	4:A:422:ILE:HD12	1.78	0.66
4:F:844:ILE:HG23	4:F:873:VAL:HG13	1.77	0.66
4:A:96:CYS:SG	4:A:196:ILE:HD13	2.36	0.66
4:F:922:ILE:O	4:F:922:ILE:HG13	1.96	0.65
4:A:138:LYS:O	4:A:140:GLU:N	2.29	0.65
4:F:837:LYS:O	4:F:838:LYS:HB2	1.96	0.65
4:F:1114:ILE:HG22	4:F:1117:VAL:HG21	1.77	0.65
4:A:253:ASP:OD1	4:A:306:ARG:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:837:LYS:C	4:F:838:LYS:HD2	2.21	0.65
4:F:985:ASN:HD21	4:F:988:SER:H	1.43	0.65
4:F:1011:ILE:HD12	4:F:1011:ILE:N	2.09	0.65
4:F:928:THR:HG22	4:F:932:GLN:CB	2.26	0.65
4:F:1060:THR:HG23	4:F:1062:ALA:H	1.61	0.65
4:A:88:TRP:HE1	4:A:95:MET:HB2	1.62	0.64
4:F:741:LEU:HD13	4:F:949:VAL:HG21	1.79	0.64
4:F:742:THR:CG2	4:F:743:HIS:HD2	2.09	0.64
4:A:73:ARG:HE	4:A:89:ILE:HD12	1.61	0.64
4:F:1231:LEU:CD2	4:F:1235:LEU:HD11	2.26	0.64
4:F:906:VAL:HG22	4:F:909:VAL:HG23	1.79	0.64
4:A:526:SER:O	4:A:529:LYS:NZ	2.31	0.64
4:A:70:ARG:NH1	4:A:546:GLU:OE2	2.31	0.64
4:A:291:ARG:HB2	4:A:317:GLU:O	1.97	0.64
5:B:590:SER:HB2	5:B:596:GLU:HB3	1.79	0.64
4:F:972:ARG:HH11	4:F:972:ARG:HG2	1.60	0.64
4:A:238:LYS:O	4:A:241:GLU:HB2	1.98	0.64
4:F:833:ASN:ND2	4:F:833:ASN:H	1.94	0.64
4:F:1030:ALA:O	4:F:1034:GLN:HB2	1.98	0.64
4:A:352:ARG:CD	5:B:560:MET:HE2	2.28	0.64
4:F:810:ASN:OD1	4:F:812:ASN:ND2	2.31	0.64
4:F:816:LEU:HD13	4:F:889:SER:HB3	1.78	0.64
4:F:861:PHE:O	4:F:864:ARG:O	2.15	0.63
4:F:1148:LEU:O	4:F:1149:GLU:C	2.41	0.63
4:F:1150:MET:HE3	4:F:1152:GLY:HA2	1.80	0.63
4:A:328:ASN:ND2	4:A:331:ASP:N	2.44	0.63
4:A:386:PHE:CE1	4:A:544:LEU:HD22	2.33	0.63
4:A:101:ARG:O	4:A:111:ARG:HG2	1.98	0.63
5:B:585:PHE:O	5:B:586:PRO:C	2.41	0.63
4:F:1190:LYS:C	4:F:1192:GLY:N	2.45	0.63
4:F:1120:ARG:HH22	4:F:1191:SER:HA	1.63	0.63
4:F:1181:THR:O	4:F:1185:GLU:HB2	1.98	0.63
4:F:1087:TYR:HA	4:F:1092:ILE:CG2	2.28	0.63
5:G:1319:GLY:C	5:G:1320:ASN:HD22	2.06	0.63
4:A:134:ILE:HG13	4:A:136:PRO:HD2	1.80	0.63
4:A:160:GLN:HA	4:F:1150:MET:HE1	1.81	0.63
4:F:1138:GLU:O	4:F:1138:GLU:HG3	1.98	0.63
4:A:285:ASN:HB3	4:A:293:LEU:HD21	1.81	0.63
4:F:1125:SER:O	4:F:1127:ILE:N	2.32	0.63
4:A:417:VAL:O	4:A:418:PRO:C	2.37	0.62
4:A:206:VAL:HG22	4:A:206:VAL:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:167:THR:O	4:A:168:TYR:O	2.18	0.62
4:F:1231:LEU:HD22	4:F:1235:LEU:CD1	2.27	0.62
4:F:1151:ILE:HB	4:F:1153:LEU:HD22	1.81	0.62
5:G:1277:PHE:HB3	5:G:1278:PRO:CD	2.27	0.62
4:A:7:GLN:O	4:A:9:LEU:N	2.33	0.62
4:F:1091:GLU:O	4:F:1095:ILE:HG22	2.00	0.61
5:G:1276:ILE:HG22	5:G:1277:PHE:N	2.14	0.61
4:F:857:PRO:HG2	4:F:860:GLN:HG3	1.81	0.61
5:G:1257:HIS:CE1	5:G:1295:LEU:HD11	2.34	0.61
4:A:67:LYS:O	4:A:71:GLU:HG3	2.00	0.61
4:A:96:CYS:HB3	4:A:195:LEU:O	1.99	0.61
4:F:1117:VAL:HG12	4:F:1118:PRO:CD	2.30	0.61
4:F:748:LEU:HD22	4:F:754:VAL:HG21	1.81	0.61
4:F:1021:ILE:HG12	5:G:1307:LEU:HD23	1.83	0.61
4:A:20:VAL:HG13	4:A:44:ARG:HA	1.81	0.61
5:B:625:LEU:HB3	5:B:630:GLN:NE2	2.15	0.61
4:F:773:ARG:O	4:F:777:GLN:HB2	2.01	0.61
1:C:14:DT:H2''	1:C:15:DT:H5'	1.82	0.61
4:F:713:ASN:HD22	4:F:713:ASN:H	1.47	0.61
4:F:835:ASP:N	4:F:836:PRO:HD2	2.15	0.61
4:F:1011:ILE:H	4:F:1011:ILE:CD1	2.06	0.61
4:A:290:LYS:HE3	4:A:315:ASN:O	1.99	0.61
5:B:623:ARG:O	5:B:630:GLN:HG2	2.01	0.61
4:F:797:VAL:HG23	4:F:895:LEU:HD22	1.82	0.61
4:F:1144:ALA:O	4:F:1146:GLY:N	2.34	0.60
4:A:313:THR:HG21	4:A:315:ASN:HD22	1.65	0.60
4:A:375:ASN:H	4:A:376:ILE:HD12	1.65	0.60
4:F:906:VAL:HG22	4:F:906:VAL:O	1.99	0.60
4:F:920:ILE:HD12	4:F:940:ALA:HB2	1.83	0.60
4:A:163:LYS:HB2	4:F:1150:MET:SD	2.41	0.60
4:A:357:LEU:HD22	5:B:567:ALA:HB2	1.82	0.60
4:F:991:ARG:HG2	5:G:1337:LEU:HD23	1.83	0.60
4:A:376:ILE:HD12	4:A:376:ILE:N	2.15	0.60
4:A:137:LYS:HD2	4:A:138:LYS:HZ2	1.66	0.60
4:A:358:TYR:CZ	4:A:364:SER:HB3	2.37	0.60
4:F:952:ALA:C	4:F:954:GLN:H	2.10	0.60
4:F:1091:GLU:CD	4:F:1208:ARG:HD3	2.27	0.60
1:C:13:DT:H5''	5:B:589:ARG:NH2	2.16	0.60
4:A:340:ILE:HG21	5:B:559:VAL:HG21	1.82	0.60
4:A:451:ILE:HB	4:A:453:LEU:HG	1.84	0.60
4:A:160:GLN:O	4:F:1150:MET:SD	2.60	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1235:LEU:HD12	4:F:1235:LEU:H	1.67	0.60
4:F:1144:ALA:O	4:F:1147:GLU:N	2.16	0.60
4:A:349:ARG:NH2	5:B:613:GLU:OE1	2.35	0.59
4:F:1184:VAL:O	4:F:1188:LEU:HG	2.02	0.59
5:B:587:HIS:CE1	5:B:589:ARG:HD3	2.37	0.59
4:A:253:ASP:OD2	4:A:309:LYS:NZ	2.35	0.59
4:F:743:HIS:CD2	4:F:779:LEU:HD21	2.37	0.59
4:A:206:VAL:O	4:A:206:VAL:CG2	2.49	0.59
4:A:227:ASP:OD2	5:B:568:LYS:NZ	2.35	0.59
4:F:742:THR:HG22	4:F:743:HIS:N	2.17	0.59
4:F:1144:ALA:O	4:F:1145:LEU:C	2.45	0.59
4:F:1024:TYR:O	5:G:1310:THR:HB	2.02	0.59
4:A:281:LEU:HD22	4:A:283:GLU:CG	2.32	0.59
4:F:1064:SER:O	4:F:1068:GLU:HG3	2.02	0.59
4:F:1234:PHE:O	4:F:1238:LEU:HB2	2.01	0.59
4:A:387:TYR:HA	4:A:392:ILE:HG21	1.85	0.59
4:F:1207:SER:O	4:F:1208:ARG:C	2.45	0.59
4:A:374:ALA:HB3	4:A:376:ILE:CD1	2.33	0.59
4:F:1070:MET:HE1	4:F:1073:LYS:HZ3	1.68	0.59
4:F:1127:ILE:HG22	4:F:1128:ASP:N	2.17	0.59
4:A:363:GLN:NE2	5:B:579:GLY:HA3	2.18	0.59
4:A:387:TYR:CZ	4:A:542:SER:HB3	2.37	0.59
4:A:427:ILE:O	4:A:431:VAL:HG23	2.03	0.59
5:G:1294:ARG:O	5:G:1297:TYR:HB3	2.03	0.58
4:A:334:GLN:HB2	4:A:370:MET:HE3	1.83	0.58
4:F:1049:ARG:N	4:F:1049:ARG:CD	2.66	0.58
4:A:348:GLU:HG2	4:A:349:ARG:HG2	1.85	0.58
4:A:359:ARG:NH1	5:B:600:GLU:OE2	2.30	0.58
4:F:1203:ILE:CG2	4:F:1203:ILE:O	2.51	0.58
4:A:328:ASN:HD21	4:A:331:ASP:N	2.01	0.58
4:F:1148:LEU:O	4:F:1150:MET:N	2.37	0.58
4:A:119:THR:HB	4:A:393:LYS:HE2	1.86	0.58
4:F:964:ILE:HG12	4:F:968:LEU:HD12	1.85	0.58
5:G:1314:MET:HB2	5:G:1323:MET:HG2	1.84	0.58
4:A:138:LYS:HB2	4:A:139:PHE:CD1	2.39	0.58
4:A:293:LEU:HD22	4:A:313:THR:OG1	2.02	0.58
4:F:810:ASN:HD22	4:F:888:HIS:CD2	2.22	0.58
4:A:363:GLN:HE22	5:B:579:GLY:HA3	1.67	0.57
3:I:31:DC:H5'	3:I:31:DC:H6	1.68	0.57
4:F:785:GLU:O	4:F:785:GLU:HG3	2.02	0.57
4:F:1122:ILE:HG23	4:F:1126:THR:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:125:MET:HE2	4:A:129:LEU:HD22	1.85	0.57
4:A:544:LEU:O	4:A:544:LEU:CG	2.52	0.57
4:A:259:TRP:CE3	4:A:260:ARG:HG2	2.40	0.57
4:F:1117:VAL:HG12	4:F:1118:PRO:N	2.19	0.57
5:G:1273:GLU:OE2	5:G:1315:ARG:NH1	2.38	0.57
4:A:300:ILE:HG13	4:A:300:ILE:O	2.04	0.57
4:A:334:GLN:O	4:A:334:GLN:HG2	2.03	0.57
4:A:328:ASN:ND2	4:A:330:ALA:HB3	2.19	0.57
4:F:704:LEU:C	4:F:706:GLU:H	2.13	0.57
4:F:1070:MET:HE1	4:F:1073:LYS:NZ	2.19	0.57
4:F:1120:ARG:HB2	4:F:1122:ILE:HD12	1.86	0.57
4:F:985:ASN:HB2	4:F:1011:ILE:HG22	1.87	0.57
4:A:23:THR:OG1	4:A:24:GLU:OE1	2.23	0.56
4:A:433:TYR:CD2	4:A:433:TYR:O	2.58	0.56
4:F:922:ILE:HG12	4:F:925:TYR:HD1	1.69	0.56
4:A:166:SER:O	4:A:167:THR:O	2.23	0.56
4:F:708:LEU:HD11	4:F:746:ALA:O	2.06	0.56
4:F:717:GLN:HE21	4:F:721:ARG:HH21	1.52	0.56
4:F:772:MET:HE2	4:F:789:ILE:HG23	1.85	0.56
4:F:804:ILE:HG12	4:F:809:ILE:HB	1.85	0.56
4:F:1139:LEU:CB	4:F:1143:GLU:HB3	2.35	0.56
5:B:570:LEU:HD12	5:B:570:LEU:N	2.19	0.56
4:F:881:GLN:HA	4:F:881:GLN:NE2	2.20	0.56
4:F:1054:PHE:O	5:G:1252:MET:HG2	2.05	0.56
4:A:164:ARG:O	4:A:164:ARG:HG2	2.05	0.56
4:A:437:HIS:O	4:A:439:LEU:HD13	2.06	0.56
4:F:713:ASN:ND2	4:F:716:GLN:H	2.03	0.56
5:G:1254:MET:HE1	5:G:1264:PHE:CZ	2.40	0.56
4:F:825:MET:HE2	4:F:844:ILE:HB	1.88	0.56
4:F:993:LEU:HD23	4:F:1011:ILE:O	2.05	0.56
4:F:1044:VAL:C	4:F:1046:ARG:H	2.14	0.56
4:A:72:MET:O	4:A:76:VAL:HG23	2.06	0.56
4:A:523:GLU:HG3	4:A:529:LYS:HE3	1.87	0.56
4:F:1120:ARG:NH2	4:F:1191:SER:HA	2.21	0.56
4:F:909:VAL:O	4:F:913:TYR:HD2	1.88	0.56
4:F:1137:HIS:O	4:F:1138:GLU:CB	2.54	0.56
4:F:713:ASN:ND2	4:F:716:GLN:CG	2.69	0.56
5:B:585:PHE:HB3	5:B:586:PRO:CD	2.33	0.55
4:F:763:THR:HG23	4:F:791:THR:HG22	1.87	0.55
4:F:790:SER:OG	4:F:794:SER:CB	2.54	0.55
4:F:881:GLN:CA	4:F:881:GLN:HE21	2.18	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1127:ILE:O	4:F:1130:LEU:HB3	2.05	0.55
4:A:295:ALA:HB2	4:A:321:ILE:CD1	2.36	0.55
4:F:801:ARG:HD3	4:F:811:ARG:O	2.07	0.55
1:C:17:DT:O3'	4:A:540:LEU:HD22	2.06	0.55
5:B:636:ARG:O	5:B:640:GLU:HG3	2.06	0.55
4:A:194:ASP:C	4:A:196:ILE:H	2.14	0.55
4:A:298:GLU:HG3	5:B:640:GLU:O	2.07	0.55
4:A:351:TYR:CE1	4:A:376:ILE:HG23	2.41	0.55
5:B:625:LEU:HB3	5:B:630:GLN:HE22	1.71	0.55
4:F:1067:MET:O	4:F:1071:LEU:HB2	2.06	0.55
4:F:820:ASP:O	4:F:824:VAL:HG23	2.07	0.55
4:F:1085:LYS:HB2	4:F:1088:ASP:OD2	2.07	0.55
4:F:1223:GLU:HG2	4:F:1229:LYS:HD3	1.89	0.55
4:F:1097:ALA:O	4:F:1101:VAL:HG23	2.06	0.55
4:A:431:VAL:HA	4:A:441:LEU:HD21	1.87	0.54
4:A:437:HIS:HB3	4:A:439:LEU:HD13	1.88	0.54
4:F:959:TRP:CZ3	4:F:960:ARG:HG3	2.41	0.54
4:A:13:ASN:ND2	4:A:13:ASN:N	2.38	0.54
4:A:288:SER:HB3	4:A:292:ILE:HB	1.89	0.54
4:A:288:SER:OG	5:B:611:ALA:O	2.20	0.54
4:A:325:GLU:HG2	5:B:621:GLN:OE1	2.07	0.54
4:F:830:LYS:O	4:F:830:LYS:HG2	2.07	0.54
5:G:1277:PHE:CD1	5:G:1277:PHE:C	2.85	0.54
4:A:73:ARG:HD2	4:A:89:ILE:HB	1.88	0.54
4:F:909:VAL:O	4:F:913:TYR:CD2	2.60	0.54
4:F:1125:SER:O	4:F:1126:THR:C	2.49	0.54
4:F:1203:ILE:O	4:F:1203:ILE:HG23	2.07	0.54
4:F:1238:LEU:O	4:F:1239:ALA:C	2.51	0.54
4:A:55:ALA:HB1	4:A:57:TRP:CE2	2.42	0.54
4:A:351:TYR:CZ	4:A:377:PRO:HD2	2.42	0.54
4:F:742:THR:HG23	4:F:779:LEU:HD22	1.89	0.54
4:A:264:ILE:C	4:A:266:ASN:H	2.15	0.54
4:A:532:ILE:HD12	4:A:532:ILE:H	1.73	0.54
5:B:628:ASN:HD22	5:B:628:ASN:H	1.56	0.54
4:F:869:TYR:O	4:F:873:VAL:HG23	2.08	0.54
4:A:383:GLY:O	4:A:384:LEU:HD12	2.07	0.54
5:G:1273:GLU:OE2	5:G:1315:ARG:HD2	2.08	0.54
4:F:713:ASN:ND2	4:F:716:GLN:HG3	2.12	0.54
4:F:756:PRO:O	4:F:787:VAL:HA	2.07	0.54
4:F:1050:ARG:HB3	4:F:1052:ARG:HG2	1.89	0.54
5:G:1277:PHE:C	5:G:1277:PHE:HD1	2.14	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1342:SER:OXT	5:G:1342:SER:OG	2.17	0.54
5:B:642:PRO:CB	5:B:645:LEU:HD12	2.32	0.53
4:F:878:GLN:HE21	4:F:878:GLN:HA	1.73	0.53
4:F:927:ASP:OD2	5:G:1260:LYS:NZ	2.40	0.53
4:A:228:THR:HA	4:A:232:GLN:OE1	2.08	0.53
4:A:329:GLU:CD	5:B:624:THR:H	2.15	0.53
4:A:341:ARG:O	4:A:344:VAL:HG22	2.06	0.53
4:F:1023:TYR:HA	5:G:1309:LEU:O	2.09	0.53
4:F:1060:THR:CG2	4:F:1062:ALA:H	2.21	0.53
4:F:922:ILE:HD12	4:F:923:ASP:O	2.08	0.53
4:A:508:ARG:HH11	4:A:508:ARG:HG2	1.74	0.53
5:B:626:PHE:CG	5:B:627:GLY:N	2.71	0.53
5:B:588:ASN:HA	5:B:591:LEU:HD22	1.91	0.53
4:F:1199:ALA:O	4:F:1201:ARG:HG3	2.08	0.53
1:D:14:DT:H72	1:D:15:DT:O4	2.09	0.53
4:A:163:LYS:HB2	4:F:1150:MET:HE1	1.88	0.53
4:A:168:TYR:O	4:A:170:GLU:N	2.42	0.53
4:F:1059:ARG:HG2	5:G:1277:PHE:HA	1.89	0.53
4:A:163:LYS:C	4:F:1150:MET:SD	2.92	0.53
5:G:1274:GLU:HB2	5:G:1325:PRO:HD2	1.91	0.53
4:A:194:ASP:C	4:A:196:ILE:N	2.66	0.53
4:A:536:THR:HG22	4:A:537:ASP:N	2.23	0.53
4:F:820:ASP:OD1	4:F:1093:LYS:HE2	2.08	0.53
5:G:1293:ARG:NH1	5:G:1332:GLU:OE2	2.42	0.53
4:A:42:THR:HG22	4:A:76:VAL:HG23	1.91	0.52
4:A:521:HIS:O	4:A:522:PHE:C	2.52	0.52
4:F:730:MET:CE	4:F:967:ILE:HD11	2.37	0.52
4:F:864:ARG:O	4:F:865:ALA:HB2	2.10	0.52
4:A:194:ASP:O	4:A:196:ILE:N	2.43	0.52
4:F:972:ARG:HG2	4:F:972:ARG:NH1	2.24	0.52
5:G:1268:PHE:CD1	5:G:1308:VAL:HG13	2.44	0.52
5:G:1285:ASP:HB3	5:G:1288:GLU:HB2	1.91	0.52
5:B:596:GLU:O	5:B:600:GLU:HG2	2.09	0.52
4:F:1116:ASN:ND2	4:F:1122:ILE:H	2.08	0.52
4:F:1150:MET:HE2	4:F:1152:GLY:HA2	1.90	0.52
4:A:41:LEU:HD13	4:A:249:VAL:HG21	1.92	0.52
4:A:487:VAL:O	4:A:491:SER:HB3	2.09	0.52
4:F:825:MET:HE1	4:F:876:VAL:CG1	2.30	0.52
4:F:855:LEU:HD12	4:F:930:ARG:NH2	2.25	0.52
4:A:258:ARG:NH2	5:B:595:ASP:CB	2.72	0.52
4:F:1049:ARG:NH2	5:G:1306:GLU:OE1	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:24:GLU:OE2	4:A:219:TYR:OH	2.25	0.52
5:B:564:LEU:HB3	5:B:603:LEU:CD2	2.34	0.52
4:F:987:ARG:HG2	4:F:988:SER:N	2.24	0.52
4:A:210:LEU:O	4:A:214:GLN:HG3	2.09	0.52
4:A:495:GLU:OE2	4:A:498:LYS:HE3	2.09	0.52
4:F:1055:ALA:HB3	5:G:1267:VAL:HG22	1.91	0.52
1:D:15:DT:H2''	1:D:16:DT:OP2	2.09	0.52
4:A:417:VAL:HG12	4:A:418:PRO:HD3	1.92	0.52
4:A:517:SER:O	4:A:518:VAL:C	2.52	0.52
5:B:584:ILE:CG2	5:B:585:PHE:N	2.73	0.52
4:F:908:ASP:OD1	4:F:908:ASP:N	2.43	0.52
4:F:1117:VAL:O	4:F:1119:LYS:N	2.43	0.52
4:F:1244:LEU:HA	4:F:1247:LEU:HD12	1.92	0.52
4:A:313:THR:HG22	4:A:315:ASN:H	1.74	0.52
4:A:543:ASP:OD1	4:A:545:ASP:HB2	2.10	0.52
4:F:835:ASP:O	4:F:840:GLU:HA	2.10	0.52
4:A:518:VAL:HG13	4:A:547:LEU:HB3	1.91	0.51
5:B:580:MET:C	5:B:581:GLU:HG3	2.33	0.51
5:B:587:HIS:ND1	5:B:589:ARG:HB2	2.25	0.51
4:F:1055:ALA:HB2	5:G:1264:PHE:CG	2.45	0.51
4:A:233:TYR:O	4:A:237:LYS:HB2	2.10	0.51
4:F:868:TYR:O	4:F:872:VAL:HG23	2.11	0.51
4:F:1167:GLN:OE1	4:F:1190:LYS:HG3	2.10	0.51
4:F:1221:HIS:O	4:F:1225:VAL:HG22	2.09	0.51
4:F:1231:LEU:O	4:F:1235:LEU:CD1	2.58	0.51
4:A:73:ARG:HH11	4:A:73:ARG:CG	2.10	0.51
5:B:601:ARG:NH1	5:B:640:GLU:OE2	2.43	0.51
4:F:748:LEU:HD21	4:F:919:TYR:CE2	2.45	0.51
4:F:756:PRO:O	4:F:787:VAL:HG22	2.10	0.51
5:B:602:ARG:O	5:B:605:TYR:HB3	2.10	0.51
4:F:1129:LYS:HD3	4:F:1151:ILE:CG2	2.40	0.51
5:G:1328:ARG:O	5:G:1332:GLU:HG3	2.10	0.51
4:F:1091:GLU:OE1	4:F:1208:ARG:HD3	2.10	0.51
4:F:1118:PRO:O	4:F:1119:LYS:C	2.53	0.51
5:G:1291:GLU:HG3	5:G:1294:ARG:HH21	1.76	0.51
5:B:629:ILE:HD12	5:B:629:ILE:N	2.25	0.51
4:F:730:MET:HE1	4:F:967:ILE:CD1	2.39	0.51
4:F:764:PHE:HE2	4:F:932:GLN:NE2	2.08	0.51
4:F:797:VAL:HG21	4:F:815:ILE:HD11	1.93	0.51
4:A:117:ASP:HB2	4:A:118:PRO:HD2	1.93	0.51
4:A:449:GLU:C	4:A:450:MET:HG2	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:224:GLU:HA	4:A:224:GLU:OE1	2.11	0.51
4:A:298:GLU:HG2	5:B:642:PRO:CG	2.41	0.51
4:A:363:GLN:HE21	5:B:578:ILE:HD12	1.76	0.51
4:F:954:GLN:HG2	5:G:1298:VAL:HG12	1.93	0.51
4:F:1179:SER:H	4:F:1182:GLU:HG3	1.76	0.51
4:A:340:ILE:O	4:A:344:VAL:CG1	2.59	0.51
4:A:340:ILE:CG2	5:B:559:VAL:HG21	2.41	0.51
4:F:742:THR:CG2	4:F:743:HIS:N	2.74	0.51
4:F:824:VAL:HG22	4:F:1109:LEU:HD13	1.93	0.51
4:F:1092:ILE:O	4:F:1096:LEU:HB2	2.10	0.51
4:F:1108:ASP:O	4:F:1109:LEU:C	2.55	0.51
4:A:285:ASN:CB	4:A:293:LEU:HD21	2.40	0.50
4:A:342:GLU:O	4:A:346:ARG:HG3	2.12	0.50
4:A:414:ILE:HD12	4:A:414:ILE:C	2.35	0.50
4:F:713:ASN:N	4:F:713:ASN:ND2	2.58	0.50
4:F:985:ASN:CB	4:F:993:LEU:HD21	2.41	0.50
4:F:1087:TYR:C	4:F:1089:ARG:H	2.19	0.50
4:F:1095:ILE:HD13	4:F:1187:VAL:CG1	2.42	0.50
4:F:1112:LEU:HD13	4:F:1141:LEU:CD1	2.41	0.50
4:F:1115:ILE:HG23	4:F:1116:ASN:N	2.26	0.50
4:F:1120:ARG:HH12	4:F:1167:GLN:HE22	1.58	0.50
4:A:134:ILE:CG1	4:A:136:PRO:HD2	2.41	0.50
4:A:200:ILE:HD11	4:A:235:LEU:HB2	1.92	0.50
4:F:1024:TYR:HB3	5:G:1310:THR:HG22	1.93	0.50
4:F:1060:THR:HB	4:F:1063:GLN:HE21	1.76	0.50
4:A:28:LEU:HB3	4:A:279:VAL:HG22	1.92	0.50
4:A:216:LYS:O	4:A:216:LYS:HD3	2.11	0.50
4:F:881:GLN:HA	4:F:881:GLN:HE21	1.74	0.50
4:F:824:VAL:O	4:F:828:ILE:HG13	2.12	0.50
4:F:887:ASN:O	4:F:888:HIS:C	2.54	0.50
4:F:895:LEU:O	4:F:899:THR:CG2	2.60	0.50
4:F:929:ASN:ND2	4:F:932:GLN:CD	2.60	0.50
3:I:30:DA:H2"	3:I:31:DC:OP2	2.09	0.50
4:A:13:ASN:ND2	4:A:16:GLN:CG	2.75	0.50
4:A:187:ASN:HA	4:A:406:ASP:O	2.11	0.50
4:A:393:LYS:HZ2	4:A:393:LYS:HB3	1.77	0.50
4:F:926:GLN:H	4:F:926:GLN:HE21	1.60	0.50
4:F:998:GLU:HG3	5:G:1334:PRO:CG	2.42	0.50
4:F:1050:ARG:HH11	5:G:1249:ASP:CG	2.16	0.50
5:G:1314:MET:CB	5:G:1323:MET:HG2	2.41	0.50
4:A:295:ALA:O	4:A:299:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:628:ASN:N	5:B:628:ASN:ND2	2.54	0.50
4:F:834:ILE:O	4:F:834:ILE:HG23	2.12	0.50
4:F:929:ASN:HD21	4:F:932:GLN:NE2	2.10	0.50
4:F:1095:ILE:O	4:F:1098:TYR:HB2	2.11	0.50
4:A:77:GLN:O	4:A:81:GLY:HA2	2.12	0.50
4:A:137:LYS:HD2	4:A:138:LYS:HZ1	1.72	0.50
5:B:560:MET:HE3	5:B:572:PHE:CE2	2.46	0.50
4:F:1089:ARG:NH1	4:F:1211:ASN:HD21	2.10	0.50
4:F:1151:ILE:HB	4:F:1153:LEU:CD2	2.41	0.50
5:G:1277:PHE:O	5:G:1278:PRO:C	2.48	0.50
4:F:1003:ASN:CG	5:G:1290:GLU:HG2	2.37	0.50
4:F:1189:ASP:O	4:F:1190:LYS:CB	2.60	0.49
4:A:120:ASP:O	4:A:124:VAL:HG23	2.12	0.49
4:A:359:ARG:NH1	5:B:600:GLU:OE1	2.45	0.49
4:A:294:GLN:HG2	5:B:645:LEU:HD11	1.94	0.49
5:B:587:HIS:HE1	5:B:589:ARG:HD3	1.76	0.49
5:B:593:ASP:HB3	5:B:596:GLU:HB2	1.95	0.49
4:F:756:PRO:CB	4:F:787:VAL:HG23	2.42	0.49
4:F:952:ALA:O	4:F:954:GLN:N	2.45	0.49
4:F:985:ASN:ND2	4:F:988:SER:H	2.10	0.49
4:F:1199:ALA:O	4:F:1200:GLU:C	2.54	0.49
5:G:1256:LEU:HD21	5:G:1269:LEU:CD2	2.26	0.49
4:A:144:ILE:HD12	4:A:173:VAL:HG22	1.94	0.49
4:F:1122:ILE:HG23	4:F:1126:THR:CG2	2.42	0.49
4:A:119:THR:CB	4:A:393:LYS:HE2	2.42	0.49
4:A:291:ARG:HG2	5:B:645:LEU:HD23	1.95	0.49
4:F:796:CYS:HB3	4:F:895:LEU:O	2.13	0.49
3:I:31:DC:H2''	3:I:32:DT:H5'	1.94	0.49
3:I:31:DC:H2''	3:I:32:DT:C5'	2.43	0.49
4:A:37:LYS:NZ	4:A:223:ASP:OD2	2.46	0.49
4:A:97:VAL:HG21	4:A:540:LEU:HD11	1.94	0.49
4:A:396:LEU:CD1	4:A:538:LEU:HD23	2.27	0.49
4:F:1137:HIS:O	4:F:1138:GLU:HB2	2.13	0.49
4:F:1223:GLU:O	4:F:1229:LYS:NZ	2.43	0.49
4:F:839:PHE:HD1	4:F:869:TYR:HD1	1.61	0.49
4:F:851:ALA:O	4:F:856:LEU:HB2	2.12	0.49
4:A:313:THR:HG22	4:A:314:GLU:N	2.28	0.49
4:A:328:ASN:ND2	4:A:328:ASN:C	2.71	0.49
4:A:295:ALA:HB2	4:A:321:ILE:HD11	1.95	0.49
4:F:929:ASN:N	4:F:929:ASN:ND2	2.34	0.49
4:A:138:LYS:O	4:A:139:PHE:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:866:SER:O	4:F:867:THR:C	2.53	0.49
4:F:1139:LEU:HB3	4:F:1143:GLU:HG2	1.94	0.49
4:F:835:ASP:N	4:F:836:PRO:CD	2.75	0.48
4:F:886:ARG:C	4:F:888:HIS:H	2.21	0.48
4:A:64:PHE:CD1	4:A:224:GLU:HB2	2.48	0.48
4:A:222:ILE:HD11	4:A:228:THR:HG21	1.95	0.48
4:A:290:LYS:HB2	4:A:317:GLU:HA	1.95	0.48
4:A:375:ASN:N	4:A:376:ILE:HD12	2.27	0.48
4:A:437:HIS:CB	4:A:439:LEU:HD13	2.43	0.48
4:F:712:LEU:HB3	4:F:716:GLN:CB	2.42	0.48
4:A:343:ALA:O	4:A:348:GLU:O	2.32	0.48
4:A:432:ARG:C	4:A:434:ALA:H	2.22	0.48
4:F:713:ASN:H	4:F:713:ASN:ND2	2.10	0.48
4:F:985:ASN:ND2	4:F:987:ARG:N	2.59	0.48
4:A:226:GLN:HG2	4:A:251:ASP:C	2.39	0.48
4:A:399:LEU:HB3	4:A:531:LEU:HD21	1.95	0.48
4:F:838:LYS:HD2	4:F:838:LYS:N	2.28	0.48
4:F:1028:ASN:O	4:F:1031:ASP:HB3	2.14	0.48
4:F:1050:ARG:NH1	5:G:1249:ASP:OD2	2.38	0.48
4:F:1095:ILE:HD13	4:F:1187:VAL:HG11	1.95	0.48
4:F:1148:LEU:HD12	4:F:1151:ILE:HD12	1.95	0.48
5:G:1273:GLU:HB2	5:G:1324:ASP:HB2	1.94	0.48
1:C:15:DT:OP1	5:B:563:THR:HG21	2.13	0.48
4:A:271:GLU:OE2	4:A:279:VAL:HG21	2.12	0.48
4:A:353:ASP:HA	5:B:573:PRO:HD2	1.95	0.48
5:B:565:HIS:CE1	5:B:603:LEU:HD11	2.49	0.48
4:F:711:HIS:ND1	4:F:743:HIS:HE1	2.12	0.48
4:F:737:LYS:HB2	4:F:949:VAL:HG11	1.95	0.48
4:F:771:GLU:O	4:F:775:ARG:HG3	2.14	0.48
4:F:818:PRO:HD3	4:F:892:PHE:HE2	1.77	0.48
4:F:951:ASP:OD2	4:F:954:GLN:OE1	2.31	0.48
4:A:328:ASN:HD21	4:A:330:ALA:HB3	1.79	0.48
4:F:895:LEU:O	4:F:899:THR:HG22	2.13	0.48
4:F:1051:TYR:O	5:G:1251:VAL:HA	2.13	0.48
4:F:1213:ASP:HA	4:F:1216:LEU:HD12	1.95	0.48
4:A:230:ARG:HH22	4:F:1139:LEU:CD2	2.25	0.48
4:F:1120:ARG:NH1	4:F:1167:GLN:HE22	2.12	0.48
4:A:9:LEU:HD21	4:A:21:ARG:HG2	1.95	0.48
4:A:284:GLN:NE2	4:A:286:TYR:CZ	2.82	0.48
4:F:1003:ASN:OD1	5:G:1293:ARG:HD2	2.14	0.48
4:F:1117:VAL:HG12	4:F:1118:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:30:DA:H1'	3:I:31:DC:H5''	1.95	0.48
4:A:538:LEU:O	4:A:540:LEU:N	2.35	0.48
4:F:746:ALA:CB	4:F:779:LEU:HD23	2.44	0.48
4:A:134:ILE:O	4:A:136:PRO:O	2.32	0.47
4:A:387:TYR:CD1	4:A:387:TYR:C	2.92	0.47
4:A:396:LEU:HD21	4:A:538:LEU:HD22	1.96	0.47
4:A:437:HIS:O	4:A:439:LEU:CD1	2.62	0.47
4:A:499:ALA:O	4:A:501:ARG:HG3	2.14	0.47
4:F:838:LYS:O	4:F:840:GLU:N	2.47	0.47
4:F:1118:PRO:HA	4:F:1196:MET:HE3	1.96	0.47
4:A:13:ASN:HD21	4:A:16:GLN:CG	2.27	0.47
4:A:125:MET:HE3	4:A:125:MET:O	2.15	0.47
5:B:571:GLU:HA	5:B:610:ARG:O	2.14	0.47
4:F:839:PHE:CD1	4:F:839:PHE:N	2.78	0.47
4:F:925:TYR:CG	4:F:948:ALA:HB1	2.49	0.47
4:F:1021:ILE:O	5:G:1338:LEU:HA	2.14	0.47
4:A:41:LEU:CD1	4:A:249:VAL:HG21	2.44	0.47
4:A:293:LEU:CD2	4:A:313:THR:OG1	2.62	0.47
4:A:454:GLY:O	4:A:456:LYS:N	2.47	0.47
4:F:711:HIS:O	4:F:711:HIS:CD2	2.66	0.47
4:A:391:GLU:HG2	4:A:392:ILE:HD12	1.96	0.47
4:A:417:VAL:HG12	4:A:418:PRO:CD	2.45	0.47
5:B:582:GLU:OE2	5:B:636:ARG:HG2	2.15	0.47
4:A:125:MET:HE2	4:A:129:LEU:CD1	2.44	0.47
4:A:137:LYS:HD3	4:A:137:LYS:HA	1.59	0.47
4:A:518:VAL:CG1	4:A:547:LEU:HB3	2.43	0.47
4:F:1040:ILE:HG22	4:F:1041:ARG:N	2.29	0.47
4:F:1190:LYS:O	4:F:1191:SER:CB	2.62	0.47
4:A:351:TYR:CE1	4:A:377:PRO:HD2	2.50	0.47
4:F:953:ASP:C	5:G:1294:ARG:HG2	2.39	0.47
3:I:31:DC:H1'	3:I:32:DT:H5''	1.95	0.47
4:A:30:MET:HB2	4:A:281:LEU:HA	1.96	0.47
4:F:958:ARG:HB3	5:G:1291:GLU:OE2	2.14	0.47
4:F:1122:ILE:HG22	4:F:1127:ILE:HG13	1.97	0.47
4:A:328:ASN:HD22	4:A:328:ASN:C	2.23	0.47
4:F:1048:GLU:HB3	4:F:1049:ARG:CD	2.41	0.47
4:A:281:LEU:HD22	4:A:283:GLU:HG3	1.96	0.47
4:A:348:GLU:O	4:A:349:ARG:HB2	2.15	0.47
4:F:764:PHE:CE2	4:F:932:GLN:NE2	2.82	0.47
4:F:838:LYS:HB3	4:F:839:PHE:CD1	2.49	0.47
4:F:852:LYS:NZ	4:F:894:ASP:OD1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:835:ASP:HA	4:F:839:PHE:O	2.14	0.47
5:G:1286:ASP:OD1	5:G:1286:ASP:N	2.48	0.47
5:G:1289:MET:CE	5:G:1328:ARG:HD2	2.42	0.47
1:D:14:DT:H2"	5:G:1257:HIS:CG	2.50	0.46
4:A:451:ILE:HD13	4:A:451:ILE:N	2.30	0.46
4:A:515:PHE:HE1	4:A:538:LEU:HD21	1.80	0.46
5:B:641:ILE:O	5:B:642:PRO:C	2.58	0.46
4:F:891:ASP:O	4:F:894:ASP:HB2	2.14	0.46
4:F:1074:ALA:HB3	4:F:1076:ILE:HD12	1.97	0.46
4:F:1091:GLU:OE1	4:F:1091:GLU:N	2.42	0.46
4:F:1111:LEU:HD22	4:F:1141:LEU:HB3	1.98	0.46
4:F:1157:ALA:O	4:F:1158:ALA:C	2.58	0.46
4:A:361:ASN:C	4:A:363:GLN:H	2.24	0.46
4:A:450:MET:C	4:A:451:ILE:HD13	2.40	0.46
4:F:1145:LEU:C	4:F:1147:GLU:N	2.72	0.46
4:A:61:ALA:HB1	4:A:72:MET:HE1	1.97	0.46
4:A:117:ASP:OD1	4:A:119:THR:HB	2.16	0.46
4:A:313:THR:CG2	4:A:315:ASN:ND2	2.76	0.46
4:F:1116:ASN:ND2	4:F:1120:ARG:H	2.13	0.46
5:G:1295:LEU:O	5:G:1298:VAL:HG22	2.15	0.46
4:A:28:LEU:HB2	4:A:270:PHE:CD2	2.50	0.46
5:B:628:ASN:O	5:B:629:ILE:O	2.33	0.46
4:A:129:LEU:O	4:A:132:LYS:N	2.44	0.46
4:A:313:THR:HG22	4:A:314:GLU:H	1.81	0.46
4:F:835:ASP:HB2	4:F:841:PRO:HD3	1.97	0.46
5:G:1320:ASN:ND2	5:G:1320:ASN:N	2.63	0.46
1:D:13:DT:H5"	5:G:1318:PHE:HZ	1.81	0.46
4:A:93:HIS:O	4:A:97:VAL:HG23	2.15	0.46
4:A:326:ALA:O	5:B:621:GLN:CG	2.46	0.46
4:A:500:GLU:O	4:A:502:THR:HG23	2.16	0.46
4:F:1060:THR:CG2	4:F:1062:ALA:HB3	2.46	0.46
4:F:1098:TYR:O	4:F:1102:ILE:HG13	2.16	0.46
4:F:1232:ILE:HD12	4:F:1232:ILE:N	2.09	0.46
5:G:1256:LEU:HB3	5:G:1295:LEU:HD22	1.97	0.46
4:A:246:ILE:HG21	4:A:274:TYR:CE1	2.50	0.46
4:A:300:ILE:HG23	4:A:306:ARG:NH2	2.31	0.46
5:G:1281:ARG:HA	5:G:1281:ARG:HD3	1.82	0.46
5:B:578:ILE:HG22	5:B:618:THR:OG1	2.16	0.46
5:B:598:GLU:O	5:B:602:ARG:HG3	2.16	0.46
5:G:1317:LEU:HD23	5:G:1317:LEU:HA	1.72	0.46
4:A:37:LYS:NZ	4:A:223:ASP:OD1	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1187:VAL:HG12	4:F:1188:LEU:N	2.30	0.46
4:F:776:VAL:CG1	4:F:784:ALA:HB1	2.46	0.46
4:F:1092:ILE:HG22	4:F:1093:LYS:N	2.30	0.46
5:G:1327:SER:O	5:G:1330:LEU:HB2	2.16	0.46
4:F:755:ALA:HB1	4:F:757:TRP:CE2	2.50	0.45
4:A:328:ASN:ND2	4:A:330:ALA:H	2.04	0.45
4:F:887:ASN:N	4:F:887:ASN:HD22	2.13	0.45
4:A:290:LYS:CE	4:A:315:ASN:O	2.65	0.45
4:A:349:ARG:HB3	4:A:354:PHE:CE1	2.51	0.45
4:F:1087:TYR:CZ	4:F:1242:SER:HB3	2.51	0.45
4:F:1103:ALA:HB2	4:F:1231:LEU:HD13	1.99	0.45
4:A:215:TYR:HB3	4:A:242:ARG:CD	2.37	0.45
5:B:599:GLU:HG3	5:B:602:ARG:HH21	1.82	0.45
4:F:761:ALA:CB	4:F:772:MET:HE1	2.39	0.45
4:F:1091:GLU:CD	4:F:1091:GLU:N	2.67	0.45
4:A:42:THR:HG22	4:A:76:VAL:CG2	2.46	0.45
4:A:328:ASN:ND2	4:A:330:ALA:N	2.62	0.45
4:F:796:CYS:O	4:F:800:LEU:HD22	2.17	0.45
4:F:922:ILE:HG12	4:F:925:TYR:CD1	2.51	0.45
4:A:348:GLU:O	4:A:349:ARG:CB	2.64	0.45
4:A:60:LEU:HB2	4:A:217:PHE:CD1	2.52	0.45
5:B:626:PHE:CD1	5:B:626:PHE:C	2.95	0.45
4:F:832:LYS:C	4:F:833:ASN:HD22	2.24	0.45
4:A:119:THR:HG21	4:A:393:LYS:CE	2.47	0.45
4:A:324:TYR:CE1	4:A:326:ALA:HA	2.51	0.45
4:A:329:GLU:OE1	5:B:624:THR:N	2.47	0.45
4:A:392:ILE:O	4:A:396:LEU:HB2	2.16	0.45
4:A:511:ASN:O	4:A:515:PHE:N	2.49	0.45
4:A:522:PHE:O	4:A:526:SER:HB2	2.17	0.45
5:B:576:PHE:CE1	5:B:616:VAL:HG11	2.52	0.45
4:F:962:ALA:C	4:F:963:ASP:OD1	2.60	0.45
4:F:1087:TYR:O	4:F:1093:LYS:HG3	2.17	0.45
4:A:341:ARG:HD3	4:A:376:ILE:HD11	1.99	0.45
4:A:363:GLN:NE2	5:B:578:ILE:HD12	2.32	0.45
4:A:523:GLU:CG	4:A:523:GLU:O	2.64	0.45
4:F:852:LYS:NZ	4:F:881:GLN:OE1	2.47	0.45
4:A:281:LEU:HD22	4:A:283:GLU:HG2	1.98	0.45
4:A:393:LYS:HB2	4:A:413:ARG:NH2	2.32	0.45
4:A:433:TYR:O	4:A:433:TYR:CG	2.70	0.45
5:B:593:ASP:HB3	5:B:596:GLU:CB	2.46	0.45
4:F:820:ASP:O	4:F:823:SER:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1022:LEU:HB2	5:G:1308:VAL:HB	1.99	0.45
1:C:16:DT:O4	4:A:227:ASP:HB3	2.17	0.44
4:A:8:LEU:O	4:A:11:HIS:CE1	2.70	0.44
4:F:1120:ARG:CB	4:F:1122:ILE:HD12	2.46	0.44
4:A:154:GLU:HA	4:A:230:ARG:CB	2.42	0.44
4:A:266:ASN:HD22	4:A:266:ASN:HA	1.51	0.44
4:A:359:ARG:HA	4:A:359:ARG:HD2	1.71	0.44
4:F:953:ASP:OD1	4:F:1006:ARG:HD2	2.16	0.44
5:G:1284:GLU:CG	5:G:1285:ASP:N	2.80	0.44
4:A:112:ASN:HD21	4:A:532:ILE:HD11	1.83	0.44
4:A:137:LYS:C	4:A:138:LYS:HG3	2.42	0.44
4:A:413:ARG:O	4:A:417:VAL:HG23	2.17	0.44
4:F:711:HIS:HD1	4:F:743:HIS:HE1	1.66	0.44
4:F:834:ILE:HG12	4:F:836:PRO:CG	2.47	0.44
5:G:1249:ASP:CG	5:G:1249:ASP:O	2.60	0.44
5:G:1276:ILE:CD1	5:G:1315:ARG:HD3	2.47	0.44
4:A:351:TYR:HB2	5:B:557:ASP:O	2.17	0.44
4:F:816:LEU:CD1	4:F:889:SER:HB3	2.44	0.44
4:F:1190:LYS:HD2	4:F:1190:LYS:HA	1.76	0.44
4:A:220:ILE:HD12	4:A:240:ALA:HB2	2.00	0.44
4:A:347:GLY:O	4:A:348:GLU:CB	2.66	0.44
5:B:635:SER:O	5:B:638:LEU:HB2	2.18	0.44
4:F:704:LEU:C	4:F:706:GLU:N	2.76	0.44
4:F:707:GLN:O	4:F:708:LEU:C	2.60	0.44
4:A:11:HIS:CD2	4:A:39:ARG:HH21	2.35	0.44
4:A:412:LEU:HG	4:A:441:LEU:CD1	2.48	0.44
4:F:1118:PRO:O	4:F:1120:ARG:HG3	2.18	0.44
4:A:130:LYS:O	4:A:130:LYS:HG3	2.18	0.44
4:A:391:GLU:O	4:A:395:ILE:HG22	2.18	0.44
4:F:1021:ILE:HG12	5:G:1307:LEU:CD2	2.47	0.44
4:F:1085:LYS:HB2	4:F:1088:ASP:HB2	2.00	0.44
4:A:37:LYS:NZ	4:A:223:ASP:CG	2.76	0.44
5:B:573:PRO:HA	5:B:612:GLU:HB2	1.99	0.44
4:F:789:ILE:O	4:F:789:ILE:HG22	2.18	0.44
4:F:801:ARG:HG2	4:F:813:PHE:CE2	2.53	0.44
5:B:621:GLN:HG2	5:B:621:GLN:H	1.37	0.43
5:B:631:MET:HE3	5:B:631:MET:HB2	1.93	0.43
4:F:866:SER:OG	4:F:867:THR:N	2.49	0.43
4:A:18:GLU:HB3	4:A:280:ILE:HD13	2.00	0.43
4:A:162:ALA:HA	4:A:174:SER:OG	2.18	0.43
4:A:218:GLN:O	4:A:245:ASN:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:LEU:CD1	4:A:378:TYR:HE2	2.31	0.43
4:A:385:LYS:HG3	4:A:542:SER:HB2	2.00	0.43
4:F:1026:ALA:HB1	4:F:1031:ASP:HB3	1.99	0.43
4:F:1136:ASP:O	4:F:1137:HIS:CG	2.71	0.43
4:F:1178:VAL:HG12	4:F:1179:SER:N	2.33	0.43
4:A:342:GLU:C	4:A:344:VAL:H	2.27	0.43
4:F:1019:LYS:HA	4:F:1019:LYS:HD2	1.81	0.43
1:C:17:DT:H3'	4:A:540:LEU:O	2.19	0.43
4:F:964:ILE:HG12	4:F:968:LEU:CD1	2.47	0.43
4:F:1180:VAL:HG22	4:F:1231:LEU:HA	2.00	0.43
5:G:1257:HIS:CE1	5:G:1295:LEU:HD21	2.52	0.43
4:A:56:PRO:O	4:A:87:VAL:HA	2.17	0.43
4:A:285:ASN:ND2	4:A:293:LEU:HD11	2.34	0.43
5:B:587:HIS:HE1	5:B:589:ARG:CD	2.30	0.43
4:F:723:THR:HA	4:F:744:ARG:NH2	2.34	0.43
4:F:735:SER:HA	4:F:984:GLN:O	2.18	0.43
4:F:959:TRP:CD1	4:F:959:TRP:N	2.71	0.43
4:F:963:ASP:OD1	4:F:963:ASP:N	2.51	0.43
4:F:1113:ARG:O	4:F:1117:VAL:HG23	2.18	0.43
4:F:1208:ARG:O	4:F:1212:LEU:HD12	2.18	0.43
4:A:56:PRO:HB2	4:A:86:ASP:HB3	1.99	0.43
4:A:346:ARG:HB2	4:A:347:GLY:H	1.58	0.43
5:B:565:HIS:HE1	5:B:603:LEU:HD11	1.83	0.43
4:F:837:LYS:HB2	4:F:838:LYS:HD2	2.01	0.43
4:A:37:LYS:HZ3	4:A:223:ASP:CG	2.24	0.43
4:A:73:ARG:NE	4:A:89:ILE:HD12	2.30	0.43
4:A:396:LEU:HD21	4:A:538:LEU:CD2	2.49	0.43
4:F:878:GLN:HE21	4:F:878:GLN:CA	2.32	0.43
1:C:17:DT:H5'	4:A:64:PHE:O	2.19	0.43
4:A:104:ILE:HD12	4:A:107:ILE:HD11	2.00	0.43
4:A:138:LYS:C	4:A:140:GLU:N	2.76	0.43
4:A:164:ARG:HB2	4:F:1150:MET:HG3	2.01	0.43
4:A:203:PHE:HE1	4:A:209:VAL:HG12	1.84	0.43
4:A:512:LEU:HA	4:A:512:LEU:HD23	1.83	0.43
4:F:926:GLN:HE22	4:F:950:GLY:HA3	1.84	0.43
4:F:1042:GLU:HA	4:F:1045:GLU:HG2	2.01	0.43
4:A:225:TYR:O	4:A:228:THR:OG1	2.37	0.43
5:B:636:ARG:HH11	5:B:636:ARG:CG	2.20	0.43
4:F:824:VAL:HG12	4:F:828:ILE:HD11	2.01	0.43
4:A:102:ARG:HA	4:A:111:ARG:HD2	2.01	0.42
4:A:135:ASP:C	4:A:136:PRO:O	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:433:TYR:CD2	4:A:451:ILE:HD12	2.54	0.42
4:F:760:LEU:HD12	4:F:761:ALA:H	1.84	0.42
4:F:1036:VAL:HG22	5:G:1268:PHE:CD1	2.54	0.42
4:A:355:ALA:HB2	5:B:572:PHE:CG	2.54	0.42
5:B:602:ARG:O	5:B:606:VAL:HG13	2.19	0.42
4:F:764:PHE:HE2	4:F:932:GLN:HE22	1.66	0.42
4:F:797:VAL:HG11	4:F:1236:THR:CG2	2.49	0.42
4:F:866:SER:C	4:F:867:THR:O	2.62	0.42
4:F:887:ASN:N	4:F:887:ASN:ND2	2.64	0.42
4:F:1153:LEU:CD2	4:F:1153:LEU:N	2.83	0.42
5:G:1276:ILE:HD11	5:G:1317:LEU:CD1	2.49	0.42
4:A:360:THR:O	4:A:363:GLN:HB2	2.19	0.42
5:B:564:LEU:HD12	5:B:564:LEU:N	2.34	0.42
4:F:1226:SER:O	4:F:1229:LYS:HG3	2.19	0.42
4:F:1238:LEU:HD12	4:F:1238:LEU:HA	1.81	0.42
4:F:922:ILE:CG1	4:F:925:TYR:HD1	2.31	0.42
4:F:1228:ASP:OD2	4:F:1233:ALA:HB2	2.19	0.42
1:D:13:DT:C7	5:G:1281:ARG:NH1	2.83	0.42
4:F:761:ALA:HB1	4:F:772:MET:CE	2.40	0.42
4:F:827:THR:O	4:F:831:GLU:HG2	2.19	0.42
4:F:952:ALA:C	4:F:954:GLN:N	2.74	0.42
3:I:32:DT:H5'	3:I:32:DT:H6	1.83	0.42
4:A:56:PRO:HB3	4:A:87:VAL:HG23	2.02	0.42
4:A:148:ILE:HG23	4:A:177:TYR:CE1	2.54	0.42
4:F:776:VAL:HG12	4:F:784:ALA:CB	2.49	0.42
4:F:838:LYS:HB3	4:F:839:PHE:CE1	2.54	0.42
4:F:1138:GLU:O	4:F:1138:GLU:CG	2.66	0.42
4:A:152:LYS:HZ3	4:A:181:GLN:NE2	2.16	0.42
4:A:287:ARG:NH2	6:A:901:SO4:O2	2.52	0.42
4:F:832:LYS:HB3	4:F:833:ASN:HD21	1.78	0.42
4:F:1042:GLU:C	4:F:1044:VAL:N	2.78	0.42
4:F:1068:GLU:OE2	4:F:1080:ILE:HD11	2.20	0.42
4:F:1216:LEU:O	4:F:1220:LYS:HD2	2.20	0.42
4:A:9:LEU:O	4:A:17:GLN:NE2	2.50	0.42
4:A:387:TYR:C	4:A:387:TYR:HD1	2.28	0.42
4:A:519:THR:O	4:A:522:PHE:HB3	2.20	0.42
4:F:1084:LEU:HD23	4:F:1089:ARG:NH2	2.34	0.42
4:F:1186:GLU:O	4:F:1186:GLU:HG3	2.20	0.42
4:F:1203:ILE:HD12	4:F:1203:ILE:HA	1.85	0.42
5:G:1283:LEU:HD12	5:G:1283:LEU:HA	1.80	0.42
4:A:187:ASN:O	4:A:188:HIS:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:780:LEU:HB2	4:F:781:GLY:H	1.63	0.41
4:F:818:PRO:HD3	4:F:892:PHE:CE2	2.53	0.41
4:F:1052:ARG:HB3	5:G:1249:ASP:HA	2.01	0.41
4:F:1085:LYS:HD2	4:F:1242:SER:HB2	2.01	0.41
4:A:36:GLY:O	4:A:40:VAL:HG23	2.20	0.41
4:A:284:GLN:NE2	4:A:286:TYR:OH	2.53	0.41
4:A:387:TYR:O	4:A:393:LYS:HG2	2.21	0.41
4:A:409:LEU:H	4:A:409:LEU:HG	1.68	0.41
5:B:562:MET:SD	5:B:567:ALA:HA	2.60	0.41
4:F:729:ILE:HB	4:F:949:VAL:HG22	2.01	0.41
4:F:1041:ARG:O	4:F:1045:GLU:HG2	2.20	0.41
4:A:415:ILE:O	4:A:415:ILE:HG13	2.19	0.41
4:F:796:CYS:SG	4:F:899:THR:HG21	2.60	0.41
4:F:869:TYR:CZ	4:F:873:VAL:HG21	2.55	0.41
4:F:1060:THR:HB	4:F:1063:GLN:NE2	2.35	0.41
4:F:1218:VAL:HG12	4:F:1234:PHE:HE1	1.85	0.41
4:F:1231:LEU:O	4:F:1235:LEU:HD12	2.21	0.41
4:A:140:GLU:O	4:A:141:PRO:C	2.63	0.41
4:A:152:LYS:NZ	4:A:181:GLN:NE2	2.68	0.41
4:A:324:TYR:HB2	5:B:649:ALA:CB	2.50	0.41
4:F:1056:VAL:HB	5:G:1253:LEU:CD1	2.46	0.41
4:F:1157:ALA:O	4:F:1160:ALA:HB3	2.20	0.41
4:A:58:ASN:HA	4:A:216:LYS:O	2.20	0.41
4:A:58:ASN:HB3	4:A:218:GLN:HB2	2.02	0.41
4:A:213:TYR:HA	4:A:216:LYS:HB3	2.01	0.41
4:A:352:ARG:HD3	5:B:560:MET:HE2	2.03	0.41
4:A:378:TYR:HA	5:B:559:VAL:O	2.20	0.41
4:A:418:PRO:O	4:A:419:LYS:C	2.62	0.41
4:A:432:ARG:C	4:A:434:ALA:N	2.79	0.41
5:B:584:ILE:HG22	5:B:585:PHE:H	1.80	0.41
5:B:584:ILE:HD12	5:B:584:ILE:HA	1.88	0.41
5:B:601:ARG:O	5:B:604:ALA:HB3	2.21	0.41
4:F:1019:LYS:HA	4:F:1020:PRO:HD3	1.78	0.41
4:F:1216:LEU:C	4:F:1219:THR:HG1	2.26	0.41
5:G:1317:LEU:C	5:G:1319:GLY:N	2.78	0.41
4:A:160:GLN:HB3	4:F:1150:MET:HE2	2.03	0.41
4:F:829:LEU:HD12	4:F:829:LEU:HA	1.88	0.41
4:F:866:SER:O	4:F:867:THR:O	2.38	0.41
4:F:998:GLU:HG3	5:G:1334:PRO:HG3	2.02	0.41
4:F:1117:VAL:CG1	4:F:1118:PRO:HD3	2.50	0.41
1:C:15:DT:OP1	5:B:563:THR:CG2	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:DT:H72	1:D:15:DT:C4	2.56	0.41
4:A:351:TYR:HE1	4:A:376:ILE:HG23	1.82	0.41
4:F:1100:ARG:O	4:F:1104:ASN:N	2.48	0.41
4:F:1111:LEU:C	4:F:1111:LEU:HD23	2.46	0.41
4:F:1112:LEU:HD13	4:F:1141:LEU:HD11	2.01	0.41
4:F:1114:ILE:CG2	4:F:1117:VAL:HG21	2.48	0.41
4:F:1189:ASP:O	4:F:1190:LYS:HB2	2.21	0.41
1:C:14:DT:H6	1:C:14:DT:H2'	1.67	0.41
4:A:300:ILE:C	4:A:302:HIS:H	2.29	0.41
4:A:478:VAL:HG13	4:A:482:GLU:CB	2.48	0.41
5:B:560:MET:HE3	5:B:572:PHE:CD2	2.56	0.41
4:F:1092:ILE:HG23	4:F:1096:LEU:HD12	2.02	0.41
4:F:1225:VAL:HG23	4:F:1225:VAL:O	2.21	0.41
4:F:1234:PHE:CE2	4:F:1238:LEU:HD22	2.56	0.41
4:F:1237:ASP:C	4:F:1238:LEU:O	2.63	0.41
1:D:13:DT:H73	5:G:1281:ARG:NH1	2.36	0.41
4:A:371:LEU:CD2	4:A:376:ILE:HB	2.51	0.41
4:F:767:LYS:H	4:F:767:LYS:HG3	1.37	0.41
4:F:839:PHE:CD1	4:F:869:TYR:HD1	2.37	0.41
4:F:953:ASP:OD2	4:F:1009:LYS:HE3	2.21	0.41
4:F:1087:TYR:HD1	4:F:1088:ASP:N	2.19	0.41
4:F:1125:SER:C	4:F:1127:ILE:N	2.79	0.41
4:F:1150:MET:HE2	4:F:1150:MET:HB3	1.79	0.41
4:F:1152:GLY:O	4:F:1153:LEU:O	2.39	0.41
4:F:1157:ALA:O	4:F:1160:ALA:CB	2.69	0.41
1:C:14:DT:H2''	1:C:15:DT:C5'	2.48	0.41
4:A:125:MET:HE2	4:A:129:LEU:CD2	2.49	0.41
4:A:164:ARG:HB2	4:F:1150:MET:CG	2.50	0.41
4:A:508:ARG:HG2	4:A:508:ARG:NH1	2.36	0.41
4:A:537:ASP:O	4:A:541:ILE:HB	2.21	0.41
4:F:1095:ILE:CD1	4:F:1187:VAL:CG1	2.97	0.41
4:F:1104:ASN:HD21	4:F:1106:ASP:HB2	1.86	0.41
4:F:1200:GLU:O	4:F:1201:ARG:HB2	2.20	0.41
4:A:22:THR:O	4:A:44:ARG:NH1	2.54	0.40
4:A:289:THR:HG21	4:A:318:GLY:HA3	2.03	0.40
4:A:532:ILE:HD12	4:A:532:ILE:N	2.35	0.40
4:A:536:THR:O	4:A:540:LEU:HB2	2.21	0.40
4:F:800:LEU:HG	4:F:804:ILE:HD12	2.02	0.40
5:G:1261:GLY:H	5:G:1302:ARG:NH1	2.18	0.40
4:A:73:ARG:NH1	4:A:77:GLN:OE1	2.32	0.40
4:A:342:GLU:CG	4:A:346:ARG:HH21	2.34	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:964:ILE:HG12	4:F:964:ILE:O	2.21	0.40
3:I:31:DC:H2'	3:I:32:DT:H71	2.02	0.40
4:A:44:ARG:HH11	4:A:44:ARG:HD2	1.69	0.40
4:A:297:ASN:O	4:A:301:GLU:HB2	2.21	0.40
4:A:326:ALA:O	5:B:621:GLN:N	2.41	0.40
4:F:925:TYR:O	4:F:928:THR:OG1	2.39	0.40
4:F:1111:LEU:O	4:F:1115:ILE:HB	2.21	0.40
3:I:33:DG:H2''	3:I:34:DC:H5'	2.03	0.40
4:A:31:ALA:HB1	4:A:37:LYS:HB3	2.02	0.40
4:F:713:ASN:O	4:F:717:GLN:HG3	2.21	0.40
4:F:1111:LEU:HD22	4:F:1141:LEU:HD13	2.03	0.40
4:A:88:TRP:NE1	4:A:95:MET:HB2	2.32	0.40
4:A:342:GLU:HG3	4:A:346:ARG:NH2	2.37	0.40
4:A:375:ASN:C	4:A:376:ILE:HD12	2.47	0.40
4:A:417:VAL:CG1	4:A:418:PRO:HD3	2.51	0.40
4:A:511:ASN:C	4:A:513:ASP:N	2.79	0.40
4:F:1087:TYR:C	4:F:1089:ARG:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	540/548 (98%)	456 (84%)	60 (11%)	24 (4%)	2	8
4	F	542/548 (99%)	448 (83%)	63 (12%)	31 (6%)	1	4
5	B	93/95 (98%)	80 (86%)	8 (9%)	5 (5%)	1	5
5	G	93/95 (98%)	81 (87%)	8 (9%)	4 (4%)	2	8
All	All	1268/1286 (99%)	1065 (84%)	139 (11%)	64 (5%)	1	6

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	134	ILE
4	A	139	PHE
4	A	167	THR
4	A	168	TYR
4	A	348	GLU
4	A	375	ASN
4	A	424	ALA
4	A	539	ALA
5	B	628	ASN
5	B	629	ILE
4	F	831	GLU
4	F	836	PRO
4	F	839	PHE
4	F	865	ALA
4	F	953	ASP
4	F	1126	THR
4	F	1138	GLU
4	F	1144	ALA
4	F	1145	LEU
4	F	1149	GLU
4	F	1153	LEU
4	F	1154	GLY
4	F	1204	GLU
4	F	1208	ARG
4	F	1239	ALA
5	G	1321	ILE
4	A	342	GLU
4	A	350	ARG
4	A	382	GLY
4	A	384	LEU
4	A	454	GLY
4	A	538	LEU
4	F	838	LYS
4	F	867	THR
4	F	1048	GLU
4	F	1119	LYS
4	F	1124	ALA
4	F	1137	HIS
4	F	1158	ALA
4	F	1190	LYS
4	A	8	LEU
4	A	11	HIS
4	A	195	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	349	ARG
4	F	888	HIS
4	F	1155	ALA
4	A	10	ALA
4	A	169	TYR
4	A	383	GLY
5	B	589	ARG
4	F	832	LYS
4	F	1150	MET
4	F	1238	LEU
5	G	1318	PHE
4	A	455	ALA
5	B	585	PHE
4	F	1117	VAL
4	F	1125	SER
4	A	365	ARG
5	B	586	PRO
4	F	1232	ILE
5	G	1277	PHE
5	G	1278	PRO
4	A	417	VAL

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	
4	A	472/478 (99%)	394 (84%)	78 (16%)	2	8
4	F	474/478 (99%)	380 (80%)	94 (20%)	1	5
5	B	81/81 (100%)	64 (79%)	17 (21%)	1	4
5	G	81/81 (100%)	60 (74%)	21 (26%)	0	2
All	All	1108/1118 (99%)	898 (81%)	210 (19%)	1	5

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	13	ASN
4	A	14	LYS
4	A	15	GLU
4	A	18	GLU
4	A	41	LEU
4	A	44	ARG
4	A	51	GLU
4	A	63	THR
4	A	73	ARG
4	A	77	GLN
4	A	80	LEU
4	A	86	ASP
4	A	90	SER
4	A	92	PHE
4	A	94	SER
4	A	95	MET
4	A	110	ASN
4	A	123	SER
4	A	129	LEU
4	A	135	ASP
4	A	137	LYS
4	A	139	PHE
4	A	143	THR
4	A	156	LEU
4	A	159	GLU
4	A	167	THR
4	A	168	TYR
4	A	170	GLU
4	A	175	ASP
4	A	183	ARG
4	A	185	LEU
4	A	205	ARG
4	A	206	VAL
4	A	222	ILE
4	A	226	GLN
4	A	228	THR
4	A	236	VAL
4	A	237	LYS
4	A	258	ARG
4	A	266	ASN
4	A	269	SER
4	A	278	LYS
4	A	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	293	LEU
4	A	307	LYS
4	A	311	ILE
4	A	313	THR
4	A	322	LEU
4	A	324	TYR
4	A	328	ASN
4	A	335	PHE
4	A	344	VAL
4	A	349	ARG
4	A	366	VAL
4	A	372	LEU
4	A	380	ILE
4	A	384	LEU
4	A	387	TYR
4	A	389	ARG
4	A	393	LYS
4	A	406	ASP
4	A	415	ILE
4	A	445	LEU
4	A	450	MET
4	A	451	ILE
4	A	453	LEU
4	A	466	SER
4	A	473	GLN
4	A	475	GLN
4	A	478	VAL
4	A	496	MET
4	A	503	ILE
4	A	506	GLN
4	A	526	SER
4	A	531	LEU
4	A	536	THR
4	A	538	LEU
4	A	542	SER
5	B	563	THR
5	B	571	GLU
5	B	581	GLU
5	B	584	ILE
5	B	589	ARG
5	B	591	LEU
5	B	596	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	599	GLU
5	B	606	VAL
5	B	616	VAL
5	B	621	GLN
5	B	622	MET
5	B	628	ASN
5	B	636	ARG
5	B	639	ASN
5	B	645	LEU
5	B	648	THR
4	F	705	SER
4	F	708	LEU
4	F	712	LEU
4	F	713	ASN
4	F	738	THR
4	F	742	THR
4	F	748	LEU
4	F	767	LYS
4	F	773	ARG
4	F	777	GLN
4	F	778	SER
4	F	779	LEU
4	F	797	VAL
4	F	800	LEU
4	F	801	ARG
4	F	806	ARG
4	F	810	ASN
4	F	826	LYS
4	F	833	ASN
4	F	835	ASP
4	F	837	LYS
4	F	838	LYS
4	F	839	PHE
4	F	843	THR
4	F	859	GLU
4	F	867	THR
4	F	875	ASP
4	F	878	GLN
4	F	879	GLU
4	F	881	GLN
4	F	885	LEU
4	F	896	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	899	THR
4	F	906	VAL
4	F	908	ASP
4	F	922	ILE
4	F	926	GLN
4	F	928	THR
4	F	929	ASN
4	F	932	GLN
4	F	936	VAL
4	F	937	LYS
4	F	944	GLN
4	F	955	SER
4	F	963	ASP
4	F	966	ASN
4	F	967	ILE
4	F	978	LYS
4	F	988	SER
4	F	1011	ILE
4	F	1013	THR
4	F	1029	GLU
4	F	1034	GLN
4	F	1040	ILE
4	F	1049	ARG
4	F	1050	ARG
4	F	1059	ARG
4	F	1060	THR
4	F	1071	LEU
4	F	1072	LEU
4	F	1076	ILE
4	F	1087	TYR
4	F	1091	GLU
4	F	1092	ILE
4	F	1093	LYS
4	F	1095	ILE
4	F	1119	LYS
4	F	1125	SER
4	F	1127	ILE
4	F	1129	LYS
4	F	1132	ARG
4	F	1136	ASP
4	F	1139	LEU
4	F	1143	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	1148	LEU
4	F	1153	LEU
4	F	1165	ARG
4	F	1167	GLN
4	F	1182	GLU
4	F	1183	LEU
4	F	1187	VAL
4	F	1195	GLU
4	F	1196	MET
4	F	1203	ILE
4	F	1207	SER
4	F	1212	LEU
4	F	1214	GLU
4	F	1222	PHE
4	F	1223	GLU
4	F	1224	ASN
4	F	1227	ASP
4	F	1231	LEU
4	F	1232	ILE
4	F	1237	ASP
5	G	1251	VAL
5	G	1252	MET
5	G	1253	LEU
5	G	1255	THR
5	G	1273	GLU
5	G	1276	ILE
5	G	1283	LEU
5	G	1284	GLU
5	G	1288	GLU
5	G	1291	GLU
5	G	1298	VAL
5	G	1307	LEU
5	G	1308	VAL
5	G	1309	LEU
5	G	1313	GLN
5	G	1314	MET
5	G	1317	LEU
5	G	1320	ASN
5	G	1321	ILE
5	G	1331	ASN
5	G	1340	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

Mol	Chain	Res	Type
4	A	13	ASN
4	A	93	HIS
4	A	110	ASN
4	A	153	ASN
4	A	181	GLN
4	A	214	GLN
4	A	221	HIS
4	A	226	GLN
4	A	266	ASN
4	A	284	GLN
4	A	315	ASN
4	A	328	ASN
4	A	363	GLN
4	A	404	ASN
4	A	473	GLN
5	B	565	HIS
5	B	628	ASN
5	B	630	GLN
4	F	707	GLN
4	F	713	ASN
4	F	717	GLN
4	F	743	HIS
4	F	766	ASN
4	F	777	GLN
4	F	833	ASN
4	F	853	ASN
4	F	878	GLN
4	F	882	GLN
4	F	887	ASN
4	F	888	HIS
4	F	914	GLN
4	F	918	GLN
4	F	926	GLN
4	F	929	ASN
4	F	944	GLN
4	F	965	GLN
4	F	976	ASN
4	F	984	GLN
4	F	985	ASN
4	F	1015	ASN
4	F	1034	GLN
4	F	1063	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	1104	ASN
4	F	1116	ASN
4	F	1167	GLN
4	F	1170	GLN
4	F	1175	GLN
4	F	1206	GLN
4	F	1211	ASN
4	F	1224	ASN
5	G	1257	HIS
5	G	1280	ASN
5	G	1313	GLN
5	G	1320	ASN
5	G	1322	GLN
5	G	1331	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	901	-	4,4,4	0.62	0	6,6,6	0.52	0
6	SO4	F	1249	-	4,4,4	0.55	0	6,6,6	0.75	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	SO4	1	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	C	5/5 (100%)	-0.66	0 100 100	22, 25, 37, 37	0
1	D	5/5 (100%)	-0.45	0 100 100	29, 32, 41, 55	0
2	H	2/2 (100%)	0.89	0 100 100	53, 53, 53, 64	0
3	I	5/5 (100%)	-0.24	0 100 100	39, 39, 43, 47	0
4	A	542/548 (98%)	-0.23	10 (1%) 67 59	7, 31, 68, 100	0
4	F	544/548 (99%)	0.03	14 (2%) 57 48	16, 42, 74, 101	0
5	B	95/95 (100%)	0.03	3 (3%) 50 41	11, 39, 79, 91	0
5	G	95/95 (100%)	0.05	2 (2%) 63 54	19, 41, 79, 91	0
All	All	1293/1303 (99%)	-0.08	29 (2%) 62 53	7, 37, 74, 101	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	835	ASP	5.9
4	A	345	GLU	4.3
4	F	1203	ILE	3.4
4	A	167	THR	3.3
5	G	1318	PHE	3.2
4	A	346	ARG	3.1
4	F	1117	VAL	3.0
5	B	557	ASP	2.9
4	A	340	ILE	2.9
5	B	625	LEU	2.9
4	A	347	GLY	2.8
4	A	344	VAL	2.7
4	A	215	TYR	2.7
4	A	341	ARG	2.7
4	F	1077	PRO	2.6
4	F	1202	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	G	1341	ALA	2.5
4	F	836	PRO	2.5
4	A	11	HIS	2.4
4	F	1232	ILE	2.4
4	F	1207	SER	2.4
5	B	650	SER	2.3
4	F	750	ALA	2.2
4	A	135	ASP	2.2
4	F	1204	GLU	2.2
4	F	1118	PRO	2.2
4	F	962	ALA	2.2
4	F	1195	GLU	2.1
4	F	1205	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	901	5/5	0.95	0.08	44,49,52,52	0
6	SO4	F	1249	5/5	0.95	0.07	48,49,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.