



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 2E6K / pdb_00002e6k
Title : X-ray structure of Thermus thermophilus HB8 TT0505
Authors : Yoshida, H.; Kamitori, S.; Agari, Y.; Iino, H.; Kanagawa, M.; Nakagawa, N.; Ebihara, A.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-12-27
Resolution : 2.09 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

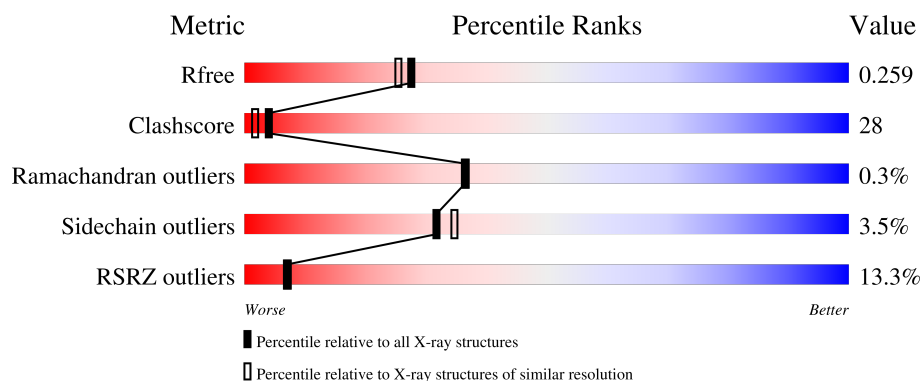
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	651	74% 23% ..
1	B	651	74% 23% ..
1	C	651	14% 57% 40% ..
1	D	651	36% 39% 55% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21768 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	B	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	C	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	D	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			

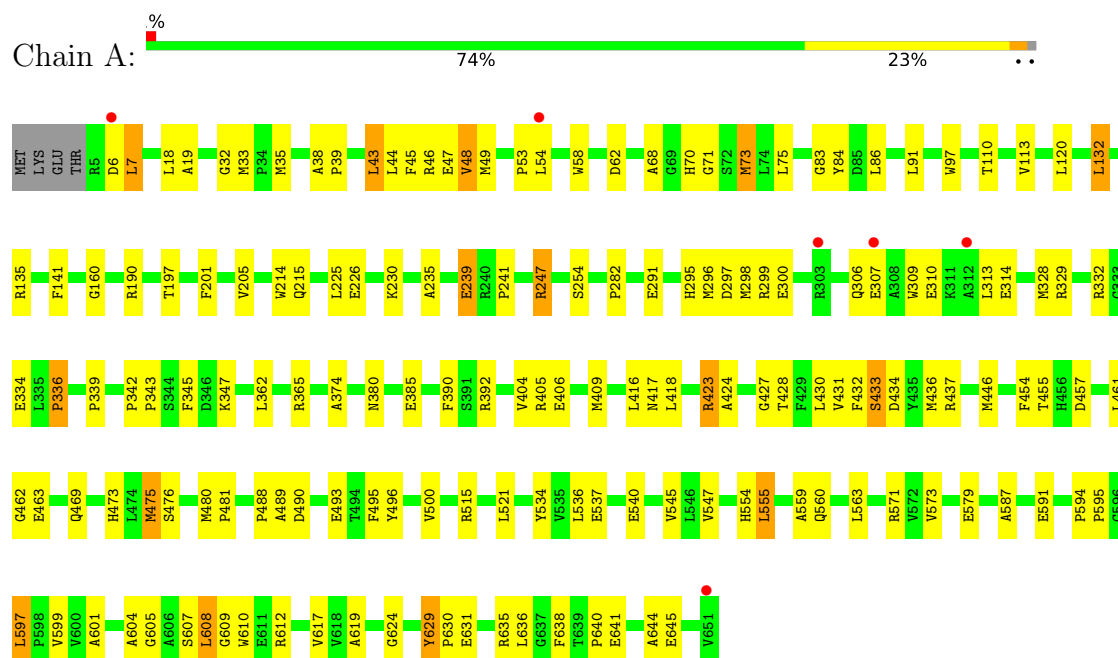
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	531	Total	O	0	0
			531	531		
2	B	496	Total	O	0	0
			496	496		
2	C	297	Total	O	0	0
			297	297		
2	D	288	Total	O	0	0
			288	288		

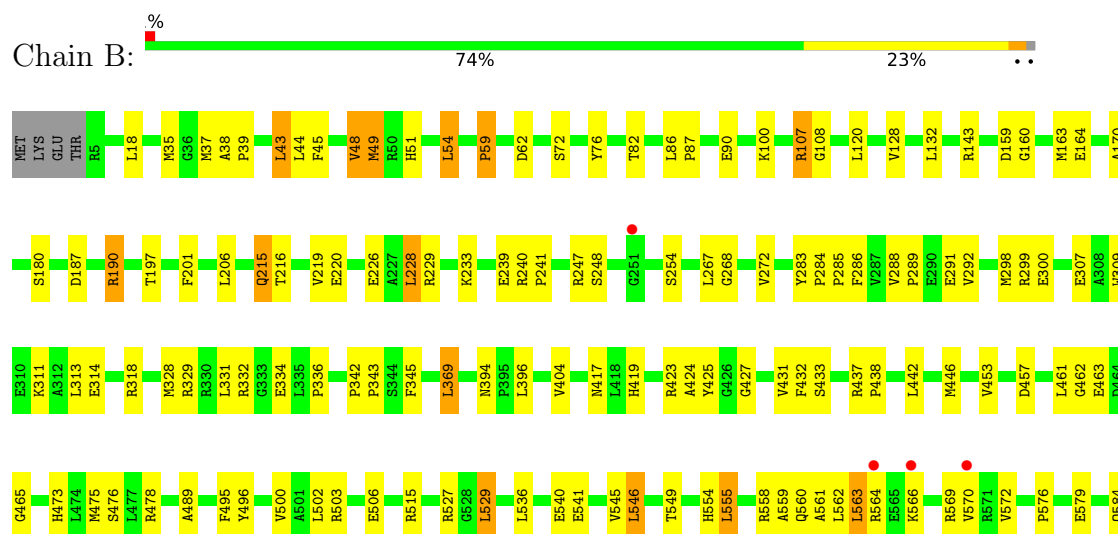
3 Residue-property plots

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: Transketolase

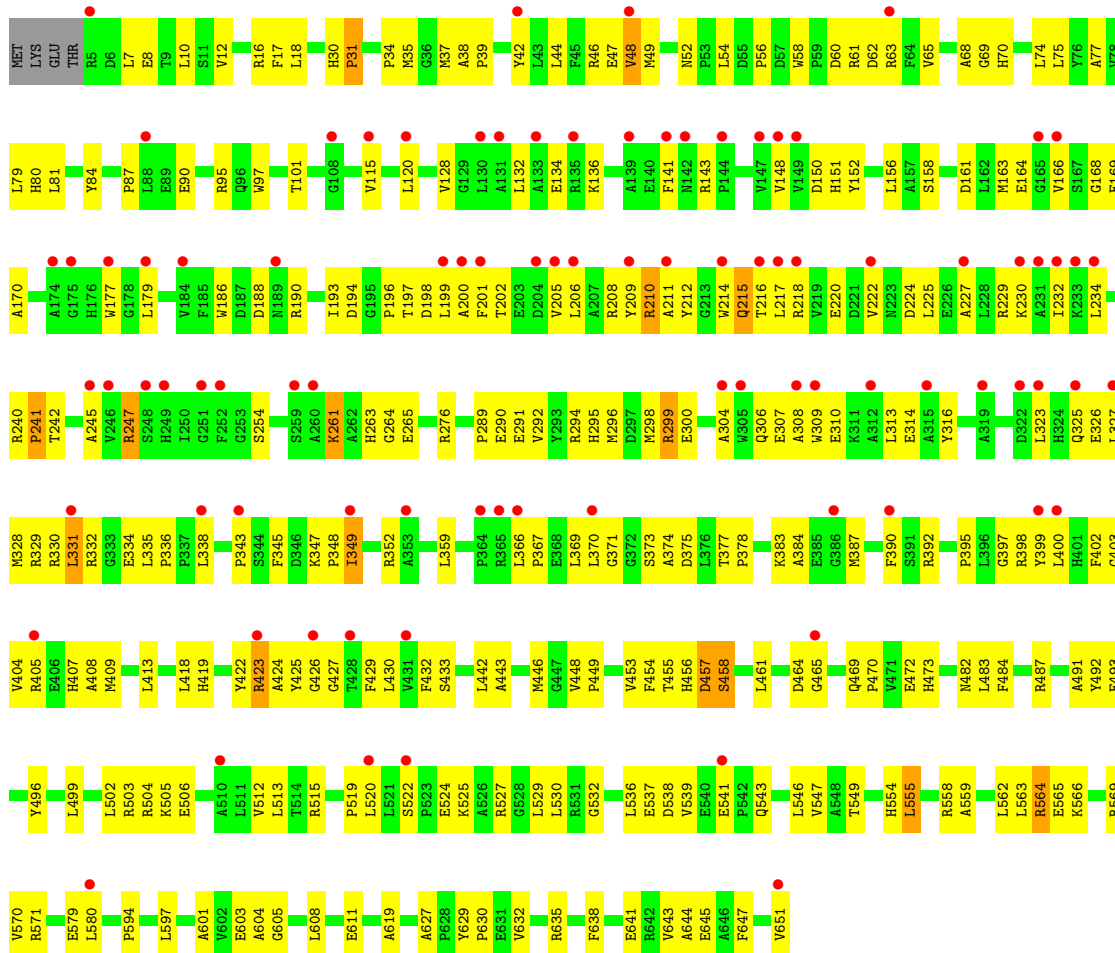


• Molecule 1: Transketolase

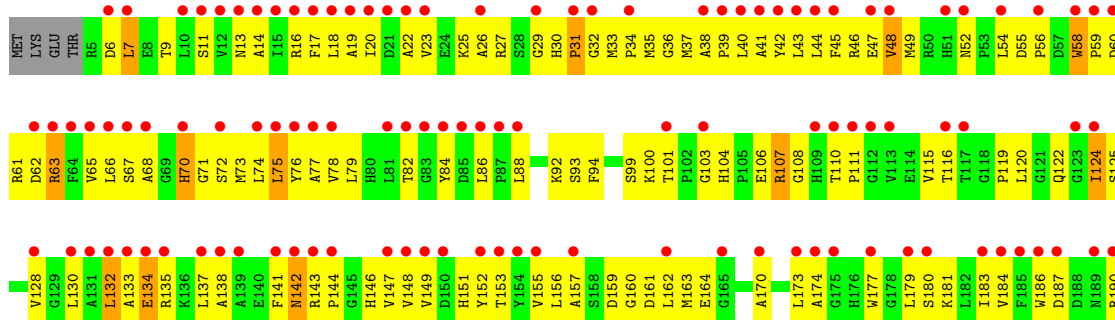


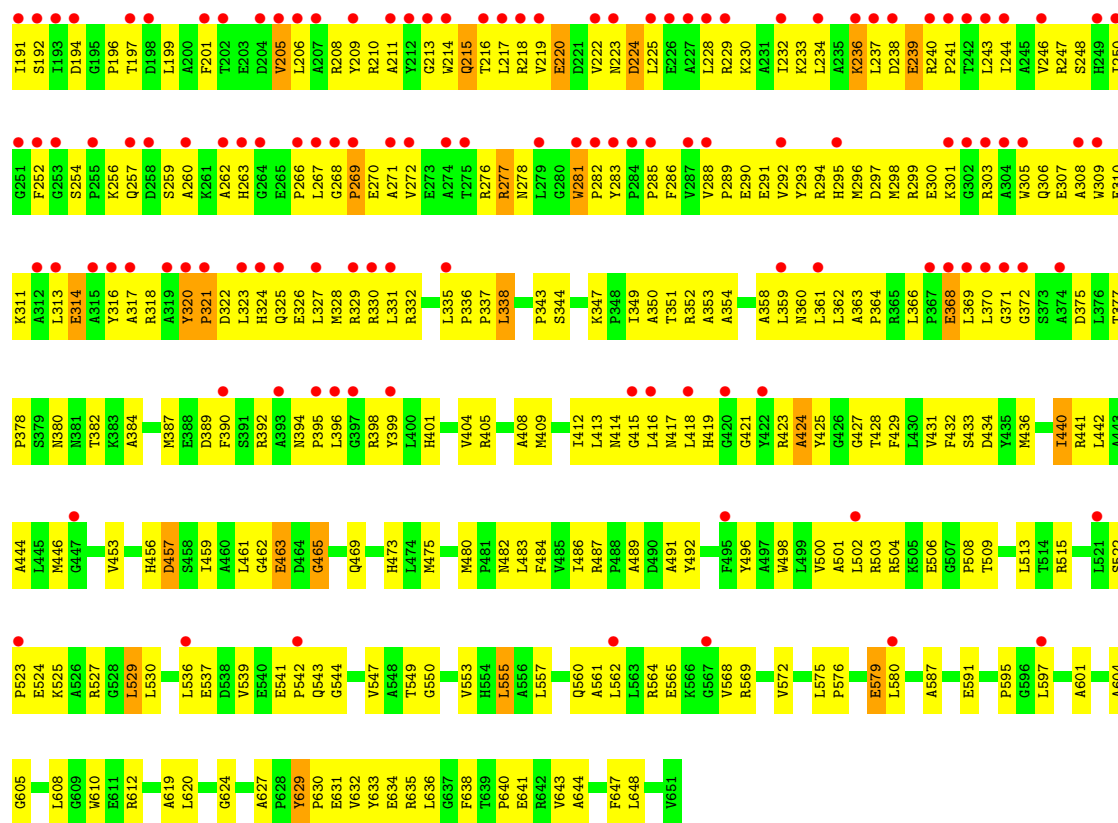


● Molecule 1: Transketolase



● Molecule 1: Transketolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.61Å 88.96Å 117.18Å 72.48° 89.13° 73.36°	Depositor
Resolution (Å)	38.59 – 2.09 38.59 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.59-2.09) 97.7 (38.59-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.259	Depositor DCC
R_{free} test set	15242 reflections (7.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21768	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/5159	0.96	19/6995 (0.3%)
1	B	0.42	0/5159	0.96	16/6995 (0.2%)
1	C	0.36	0/5159	0.91	13/6995 (0.2%)
1	D	0.34	0/5159	0.92	18/6995 (0.3%)
All	All	0.39	0/20636	0.94	66/27980 (0.2%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	VAL	N-CA-C	12.12	122.06	110.30
1	A	462	GLY	N-CA-C	9.53	125.44	111.24
1	B	462	GLY	N-CA-C	9.09	124.79	111.24
1	A	48	VAL	N-CA-C	8.89	119.44	110.82
1	D	48	VAL	N-CA-C	8.39	120.14	111.00
1	A	473	HIS	N-CA-C	8.35	120.00	111.07
1	B	463	GLU	N-CA-C	8.17	122.21	111.75
1	D	463	GLU	N-CA-C	8.02	122.02	111.75
1	C	473	HIS	N-CA-C	7.89	119.51	111.07
1	C	465	GLY	CA-C-N	7.84	127.75	119.05
1	C	465	GLY	C-N-CA	7.84	127.75	119.05
1	C	48	VAL	N-CA-C	7.79	117.90	110.42
1	C	263	HIS	N-CA-C	7.57	120.63	111.40
1	B	457	ASP	N-CA-C	7.51	122.12	113.19
1	B	473	HIS	N-CA-C	7.41	120.00	111.11
1	A	463	GLU	N-CA-C	7.36	121.91	112.34
1	D	465	GLY	CA-C-N	7.30	127.94	119.47
1	D	465	GLY	C-N-CA	7.30	127.94	119.47
1	A	433	SER	N-CA-C	-7.26	103.68	112.54
1	D	473	HIS	N-CA-C	6.60	119.03	111.11
1	B	629	TYR	N-CA-C	-6.59	101.19	110.29
1	A	457	ASP	N-CA-C	6.37	120.77	113.19
1	A	515	ARG	N-CA-C	-6.35	103.62	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	ARG	N-CA-C	-6.33	105.20	113.12
1	C	433	SER	N-CA-C	-6.29	104.86	112.54
1	D	457	ASP	N-CA-C	6.22	120.60	113.19
1	A	521	LEU	N-CA-C	-6.17	100.84	110.17
1	C	457	ASP	N-CA-C	6.06	120.40	113.19
1	A	141	PHE	N-CA-C	6.05	121.33	113.88
1	A	18	LEU	N-CA-C	-6.05	104.75	111.71
1	A	205	VAL	N-CA-C	6.03	116.69	110.36
1	B	49	MSE	N-CA-C	5.98	119.32	110.48
1	A	32	GLY	N-CA-C	5.92	119.80	112.64
1	D	47	GLU	N-CA-C	5.81	120.05	111.04
1	D	629	TYR	N-CA-C	-5.81	102.28	110.29
1	A	336	PRO	N-CA-C	-5.80	103.62	110.70
1	B	433	SER	N-CA-C	-5.78	105.06	111.71
1	A	362	LEU	N-CA-C	5.76	117.36	111.14
1	D	281	TRP	CA-C-N	5.69	125.31	119.56
1	D	281	TRP	C-N-CA	5.69	125.31	119.56
1	A	62	ASP	N-CA-C	-5.67	102.51	110.50
1	C	69	GLY	N-CA-C	5.66	120.80	113.27
1	C	215	GLN	N-CA-C	-5.64	100.50	109.59
1	A	347	LYS	N-CA-C	5.64	113.09	108.07
1	A	629	TYR	N-CA-C	-5.58	102.58	110.29
1	B	215	GLN	N-CA-C	-5.58	101.45	110.32
1	D	433	SER	N-CA-C	-5.50	105.68	112.38
1	A	423	ARG	N-CA-C	-5.49	99.14	108.26
1	B	18	LEU	N-CA-C	-5.48	105.30	111.28
1	C	241	PRO	N-CA-C	-5.39	102.81	111.38
1	B	241	PRO	N-CA-C	-5.38	102.83	111.38
1	D	320	TYR	CA-C-N	-5.34	113.17	119.84
1	D	320	TYR	C-N-CA	-5.34	113.17	119.84
1	D	424	ALA	N-CA-C	5.31	118.14	109.59
1	B	59	PRO	N-CA-C	5.30	120.73	113.84
1	C	18	LEU	N-CA-C	-5.28	105.53	111.28
1	C	458	SER	N-CA-C	5.19	115.39	108.38
1	B	465	GLY	N-CA-C	5.14	122.83	112.34
1	B	419	HIS	N-CA-C	5.14	116.88	111.28
1	D	58	TRP	CA-C-N	5.11	125.40	119.47
1	D	58	TRP	C-N-CA	5.11	125.40	119.47
1	D	132	LEU	N-CA-C	-5.11	105.84	111.71
1	B	62	ASP	N-CA-C	-5.09	103.32	110.50
1	D	440	ILE	N-CA-C	-5.09	105.74	110.53
1	C	210	ARG	N-CA-C	-5.09	105.73	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	PHE	N-CA-C	-5.04	103.02	110.48

There are no chirality outliers.

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	5039	0	5004	127	0
1	B	5039	0	5004	162	0
1	C	5039	0	5004	319	0
1	D	5039	0	5004	546	0
2	A	531	0	0	22	0
2	B	496	0	0	42	0
2	C	297	0	0	92	0
2	D	288	0	0	168	0
All	All	21768	0	20016	1119	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 28.

All (1119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:THR:HB	2:A:1149:HOH:O	1.51	1.08
1:C:405:ARG:NH1	1:D:163:MSE:HE2	1.74	1.03
1:D:76:TYR:HA	2:D:854:HOH:O	1.60	1.00
1:B:475:MSE:HE2	1:B:609:GLY:HA3	1.43	0.99
1:A:493:GLU:HB2	2:A:1175:HOH:O	1.62	0.97
1:A:405:ARG:NH2	1:B:163:MSE:HE2	1.78	0.96
1:C:543:GLN:HE21	1:C:569:ARG:H	1.04	0.95
1:C:487:ARG:HH21	1:C:549:THR:HG23	1.32	0.95
1:C:39:PRO:HG2	1:C:222:VAL:HG22	1.49	0.94
1:B:546:LEU:HD13	1:B:570:VAL:HG11	1.50	0.94
1:C:241:PRO:HD3	2:C:915:HOH:O	1.68	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:PRO:HG3	2:D:858:HOH:O	1.69	0.93
1:B:417:ASN:HD21	1:B:424:ALA:H	1.02	0.92
1:C:405:ARG:HH12	1:D:163:MSE:HE2	1.27	0.90
1:C:163:MSE:HE2	1:D:405:ARG:NH2	1.86	0.89
1:D:215:GLN:NE2	1:D:240:ARG:HB2	1.86	0.88
1:D:240:ARG:HA	2:D:846:HOH:O	1.74	0.88
1:B:546:LEU:HB2	2:B:1114:HOH:O	1.73	0.88
1:B:647:PHE:HB3	2:B:1146:HOH:O	1.74	0.87
1:C:205:VAL:HG23	1:C:206:LEU:HD12	1.56	0.87
1:A:417:ASN:HD21	1:A:424:ALA:H	1.15	0.87
1:D:399:TYR:HA	2:D:861:HOH:O	1.74	0.87
1:C:369:LEU:HD11	1:C:425:TYR:HE2	1.39	0.87
1:A:405:ARG:CZ	1:B:163:MSE:HE2	2.06	0.86
1:C:330:ARG:HD2	2:C:909:HOH:O	1.75	0.86
1:B:163:MSE:HE3	1:B:201:PHE:HB2	1.58	0.86
1:D:137:LEU:HB3	2:D:883:HOH:O	1.76	0.86
1:D:263:HIS:HA	2:D:860:HOH:O	1.77	0.85
1:A:332:ARG:HD3	2:A:1176:HOH:O	1.77	0.85
1:D:16:ARG:O	1:D:20:ILE:HG12	1.77	0.85
1:D:41:ALA:HB2	1:D:74:LEU:HD11	1.59	0.85
1:C:306:GLN:HB2	2:C:929:HOH:O	1.76	0.85
1:D:37:MSE:HB2	2:D:842:HOH:O	1.77	0.84
1:D:79:LEU:HD12	2:D:854:HOH:O	1.74	0.84
1:C:44:LEU:HB3	1:C:49:MSE:HE2	1.59	0.84
1:C:148:VAL:HG21	2:C:914:HOH:O	1.76	0.84
1:C:220:GLU:HA	2:C:903:HOH:O	1.79	0.83
1:A:428:THR:OG1	1:A:436:MSE:HE1	1.79	0.83
1:D:148:VAL:HG13	1:D:149:VAL:HG23	1.60	0.83
1:D:161:ASP:HB2	2:D:878:HOH:O	1.80	0.82
1:A:475:MSE:HG2	1:A:608:LEU:O	1.80	0.81
1:C:549:THR:HG21	1:C:603:GLU:OE2	1.80	0.81
1:D:153:THR:HG23	2:D:863:HOH:O	1.80	0.81
1:C:31:PRO:HD2	2:C:935:HOH:O	1.81	0.81
1:C:387:MSE:HE2	1:C:399:TYR:HB2	1.63	0.81
1:D:73:MSE:HG3	2:D:867:HOH:O	1.81	0.81
1:D:44:LEU:HB3	1:D:49:MSE:HE2	1.63	0.80
1:D:73:MSE:HB3	2:D:932:HOH:O	1.80	0.80
1:A:488:PRO:HB2	2:A:1175:HOH:O	1.80	0.80
1:D:326:GLU:HB2	2:D:805:HOH:O	1.81	0.80
1:A:405:ARG:HH22	1:B:163:MSE:HE2	1.47	0.79
1:C:30:HIS:HA	2:C:935:HOH:O	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD23	1:D:335:LEU:H	1.47	0.79
1:D:240:ARG:NE	1:D:392:ARG:HH22	1.79	0.79
1:D:244:ILE:HG13	2:D:889:HOH:O	1.83	0.79
1:B:59:PRO:HG2	1:B:309:TRP:CH2	2.18	0.79
1:D:236:LYS:HA	1:D:236:LYS:HZ3	1.48	0.78
1:C:46:ARG:HA	1:C:298:MSE:HE3	1.65	0.78
1:D:232:ILE:O	1:D:236:LYS:HG2	1.83	0.78
1:C:374:ALA:HA	2:C:928:HOH:O	1.82	0.78
1:D:210:ARG:HD2	2:D:790:HOH:O	1.83	0.78
1:D:22:ALA:HB3	2:D:867:HOH:O	1.83	0.78
1:D:29:GLY:HA3	2:D:853:HOH:O	1.83	0.78
1:D:74:LEU:HD13	2:D:829:HOH:O	1.81	0.78
1:B:417:ASN:HD21	1:B:424:ALA:N	1.81	0.77
1:C:543:GLN:NE2	1:C:569:ARG:H	1.82	0.77
1:D:457:ASP:HB3	2:D:929:HOH:O	1.84	0.77
1:B:309:TRP:CH2	1:B:313:LEU:HD11	2.18	0.77
1:B:576:PRO:HA	2:B:1117:HOH:O	1.83	0.77
1:C:424:ALA:HB1	2:C:894:HOH:O	1.83	0.77
1:B:37:MSE:HE1	1:B:248:SER:HB3	1.66	0.77
1:D:530:LEU:HG	2:D:896:HOH:O	1.85	0.76
1:C:594:PRO:HG2	1:C:597:LEU:HD12	1.66	0.76
1:D:134:GLU:HA	2:D:883:HOH:O	1.85	0.76
1:D:215:GLN:HE21	1:D:215:GLN:N	1.83	0.76
1:D:390:PHE:CE1	1:D:395:PRO:HA	2.20	0.76
1:D:115:VAL:HG22	2:D:872:HOH:O	1.86	0.76
1:D:267:LEU:N	2:D:858:HOH:O	2.18	0.76
1:B:442:LEU:HG	1:B:446:MSE:HE2	1.68	0.75
1:D:442:LEU:HG	1:D:446:MSE:HE3	1.67	0.75
1:B:163:MSE:HE3	1:B:201:PHE:CB	2.17	0.75
1:C:367:PRO:HG2	2:C:909:HOH:O	1.86	0.75
1:D:116:THR:H	1:D:446:MSE:HE2	1.51	0.75
1:D:191:ILE:HD12	2:D:887:HOH:O	1.87	0.75
1:D:250:ILE:HG21	2:D:937:HOH:O	1.85	0.74
1:C:81:LEU:HG	2:C:932:HOH:O	1.87	0.74
1:D:44:LEU:HA	1:D:48:VAL:CG1	2.16	0.74
1:D:361:LEU:HD23	2:D:870:HOH:O	1.88	0.74
1:A:476:SER:HB2	1:B:476:SER:HB2	1.70	0.74
1:D:192:SER:OG	1:D:197:THR:HG22	1.88	0.74
1:C:409:MSE:O	1:C:413:LEU:HG	1.88	0.74
1:C:569:ARG:HB2	1:C:569:ARG:NH2	2.02	0.74
2:C:910:HOH:O	1:D:199:LEU:HD22	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HD13	2:C:897:HOH:O	1.87	0.73
1:C:216:THR:HG23	2:C:902:HOH:O	1.89	0.73
1:D:25:LYS:HB3	2:D:926:HOH:O	1.89	0.73
1:D:73:MSE:HE3	2:D:932:HOH:O	1.89	0.73
1:B:54:LEU:HD13	1:B:299:ARG:HG2	1.71	0.73
1:C:564:ARG:HB2	1:C:564:ARG:HH11	1.54	0.72
1:D:128:VAL:HG21	1:D:170:ALA:HB1	1.71	0.72
1:D:68:ALA:HB1	1:D:70:HIS:NE2	2.04	0.72
1:B:417:ASN:ND2	1:B:424:ALA:H	1.82	0.72
1:B:563:LEU:HD11	2:B:1146:HOH:O	1.89	0.72
1:A:409:MSE:HE1	1:A:428:THR:HG23	1.72	0.72
1:D:191:ILE:HG21	2:D:937:HOH:O	1.86	0.72
1:D:484:PHE:HA	1:D:579:GLU:HG3	1.72	0.72
1:C:443:ALA:HB1	2:C:940:HOH:O	1.90	0.72
1:D:56:PRO:HD3	2:D:902:HOH:O	1.88	0.72
1:D:94:PHE:HA	1:D:101:THR:OG1	1.90	0.72
1:B:313:LEU:HD13	2:B:1132:HOH:O	1.90	0.72
1:D:369:LEU:HD23	1:D:423:ARG:O	1.89	0.72
1:D:27:ARG:HD2	2:D:928:HOH:O	1.89	0.71
1:C:402:PHE:CD2	1:C:409:MSE:HE3	2.26	0.71
1:C:409:MSE:HE2	1:C:426:GLY:HA3	1.70	0.71
1:C:569:ARG:HB2	1:C:569:ARG:HH21	1.54	0.71
1:D:79:LEU:HD23	2:D:888:HOH:O	1.90	0.71
1:A:43:LEU:HD22	1:A:48:VAL:HG23	1.72	0.71
1:B:549:THR:HB	2:B:1117:HOH:O	1.90	0.71
1:C:151:HIS:HB3	2:C:924:HOH:O	1.90	0.71
1:D:215:GLN:HG3	2:D:756:HOH:O	1.90	0.71
1:C:152:TYR:HB2	2:C:906:HOH:O	1.89	0.71
1:D:307:GLU:HG3	1:D:308:ALA:N	2.06	0.71
1:D:390:PHE:HE1	1:D:395:PRO:HA	1.56	0.71
1:D:220:GLU:HG3	2:D:662:HOH:O	1.88	0.71
1:D:34:PRO:HA	2:D:842:HOH:O	1.89	0.70
1:D:20:ILE:HG23	1:D:267:LEU:HD12	1.73	0.70
1:A:374:ALA:HB3	1:A:428:THR:HG22	1.72	0.70
1:C:513:LEU:HD12	2:C:907:HOH:O	1.91	0.70
1:D:306:GLN:O	1:D:310:GLU:HG2	1.90	0.70
1:D:20:ILE:HD11	1:D:35:MSE:HG2	1.73	0.70
1:D:162:LEU:HG	2:D:878:HOH:O	1.91	0.70
1:D:363:ALA:HB3	1:D:364:PRO:HD3	1.74	0.70
1:D:39:PRO:HG2	1:D:222:VAL:HG22	1.73	0.70
1:A:610:TRP:HB3	1:A:617:VAL:HG11	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:MSE:O	1:D:332:ARG:HG3	1.92	0.69
1:A:559:ALA:O	1:A:563:LEU:HD13	1.92	0.69
1:D:444:ALA:HA	2:D:874:HOH:O	1.92	0.69
1:D:184:VAL:HG13	2:D:824:HOH:O	1.91	0.69
1:D:366:LEU:HD11	1:D:502:LEU:HD21	1.73	0.69
1:D:215:GLN:NE2	1:D:215:GLN:N	2.40	0.69
1:C:329:ARG:HH22	1:C:336:PRO:HD3	1.57	0.69
1:C:329:ARG:NH2	1:C:336:PRO:HD3	2.07	0.69
1:D:217:LEU:HG	2:D:838:HOH:O	1.92	0.69
1:B:564:ARG:HH22	1:B:569:ARG:HG2	1.58	0.69
1:C:522:SER:OG	1:C:524:GLU:HG2	1.93	0.69
1:A:405:ARG:NH1	1:B:163:MSE:HE2	2.08	0.69
1:A:417:ASN:HD21	1:A:424:ALA:N	1.89	0.68
1:B:560:GLN:HG2	2:B:1144:HOH:O	1.93	0.68
1:C:194:ASP:OD2	1:D:375:ASP:HA	1.94	0.68
1:D:324:HIS:C	1:D:326:GLU:H	2.01	0.68
1:C:532:GLY:N	1:C:580:LEU:HD22	2.08	0.68
1:B:163:MSE:CE	1:B:201:PHE:HB2	2.23	0.68
1:D:482:ASN:ND2	1:D:504:ARG:HH12	1.92	0.68
1:D:543:GLN:NE2	1:D:569:ARG:H	1.90	0.68
1:C:310:GLU:O	1:C:314:GLU:HG2	1.93	0.68
1:D:298:MSE:HB2	2:D:903:HOH:O	1.94	0.68
1:D:133:ALA:HA	2:D:873:HOH:O	1.93	0.68
1:C:46:ARG:HD3	1:C:298:MSE:HE1	1.76	0.68
1:C:54:LEU:HD21	1:C:299:ARG:HG2	1.75	0.67
1:B:197:THR:HG22	1:B:201:PHE:HB3	1.76	0.67
1:D:23:VAL:HG23	2:D:867:HOH:O	1.94	0.67
1:D:240:ARG:HE	1:D:392:ARG:HH22	1.39	0.67
1:D:569:ARG:HD2	2:D:815:HOH:O	1.94	0.67
1:C:383:LYS:HD2	2:C:927:HOH:O	1.94	0.67
1:D:79:LEU:HA	2:D:888:HOH:O	1.93	0.67
1:D:371:GLY:C	2:D:861:HOH:O	2.37	0.67
1:B:159:ASP:HB2	2:B:1062:HOH:O	1.94	0.67
1:C:215:GLN:HG3	1:C:240:ARG:NH1	2.10	0.67
1:C:241:PRO:HA	2:C:946:HOH:O	1.95	0.67
1:C:295:HIS:CD2	1:C:296:MSE:HE3	2.30	0.67
1:C:336:PRO:O	1:C:338:LEU:HD22	1.95	0.67
1:C:316:TYR:OH	1:C:323:LEU:HB3	1.94	0.67
1:D:130:LEU:O	1:D:133:ALA:HB3	1.95	0.67
1:C:370:LEU:HA	2:C:917:HOH:O	1.95	0.66
1:D:311:LYS:HA	1:D:314:GLU:HG2	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLY:O	1:D:272:VAL:HG23	1.96	0.66
1:B:289:PRO:HD3	2:B:1076:HOH:O	1.95	0.66
1:C:409:MSE:HE2	1:C:426:GLY:CA	2.26	0.66
1:D:30:HIS:HB2	1:D:70:HIS:O	1.95	0.66
1:A:239:GLU:HG3	2:A:949:HOH:O	1.96	0.66
1:D:309:TRP:O	1:D:313:LEU:HG	1.95	0.66
1:D:605:GLY:O	1:D:619:ALA:HB1	1.96	0.66
1:D:157:ALA:HB1	2:D:878:HOH:O	1.95	0.66
1:C:247:ARG:HB2	2:C:903:HOH:O	1.95	0.66
1:B:37:MSE:CE	1:B:248:SER:HB3	2.26	0.66
1:B:298:MSE:HG3	2:B:1087:HOH:O	1.95	0.66
1:D:587:ALA:O	1:D:591:GLU:HG3	1.96	0.66
1:A:73:MSE:HE1	1:A:91:LEU:HD22	1.78	0.65
1:B:229:ARG:O	1:B:233:LYS:HG3	1.96	0.65
1:D:63:ARG:HH21	1:D:63:ARG:HG3	1.62	0.65
1:D:416:LEU:H	1:D:416:LEU:HD22	1.61	0.65
1:A:640:PRO:HA	2:A:1113:HOH:O	1.97	0.65
1:D:543:GLN:HE21	1:D:569:ARG:H	1.44	0.65
1:D:327:LEU:O	1:D:331:LEU:HB2	1.96	0.65
1:A:555:LEU:HD22	2:A:1113:HOH:O	1.95	0.65
1:C:166:VAL:HG23	2:C:904:HOH:O	1.95	0.65
1:C:403:GLY:N	2:C:928:HOH:O	2.28	0.65
1:D:18:LEU:HB2	2:D:907:HOH:O	1.96	0.65
1:D:52:ASN:OD1	1:D:54:LEU:HB3	1.97	0.65
1:D:289:PRO:HG2	1:D:292:VAL:CG2	2.27	0.65
1:D:487:ARG:HG2	1:D:550:GLY:HA3	1.78	0.65
1:C:329:ARG:O	1:C:334:GLU:HB2	1.97	0.65
1:C:163:MSE:HE2	1:D:405:ARG:HH22	1.58	0.65
1:C:217:LEU:HD11	2:C:916:HOH:O	1.95	0.64
1:D:94:PHE:HB3	2:D:891:HOH:O	1.97	0.64
1:D:219:VAL:O	1:D:247:ARG:HG2	1.96	0.64
1:D:405:ARG:HD2	2:D:855:HOH:O	1.96	0.64
1:C:242:THR:HG22	2:C:939:HOH:O	1.97	0.64
1:D:20:ILE:HD12	1:D:267:LEU:HD11	1.79	0.64
1:D:370:LEU:HB2	1:D:424:ALA:HB2	1.79	0.64
1:C:563:LEU:HD11	1:C:644:ALA:HA	1.79	0.64
1:C:423:ARG:HH21	1:C:449:PRO:HB2	1.63	0.64
1:D:289:PRO:HG2	1:D:292:VAL:HG23	1.79	0.64
1:A:608:LEU:HD12	1:B:475:MSE:HE1	1.78	0.64
1:B:288:VAL:HA	2:B:1076:HOH:O	1.97	0.64
1:B:605:GLY:O	1:B:619:ALA:HB1	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:HA	2:D:926:HOH:O	1.97	0.64
1:D:384:ALA:HB3	1:D:387:MSE:SE	2.48	0.64
1:D:37:MSE:HE2	1:D:156:LEU:HD11	1.79	0.64
1:B:475:MSE:CE	1:B:609:GLY:HA3	2.22	0.64
1:D:368:GLU:CD	1:D:368:GLU:H	2.06	0.64
1:B:478:ARG:HB3	2:B:1088:HOH:O	1.97	0.64
1:D:384:ALA:HA	2:D:840:HOH:O	1.98	0.64
1:D:138:ALA:O	1:D:142:ASN:HB2	1.99	0.63
1:D:416:LEU:HD22	2:D:923:HOH:O	1.98	0.63
1:D:115:VAL:HG13	1:D:446:MSE:HE1	1.79	0.63
1:D:148:VAL:HG23	1:D:313:LEU:CD2	2.27	0.63
1:A:46:ARG:HE	1:A:295:HIS:CE1	2.17	0.63
1:D:267:LEU:HG	2:D:858:HOH:O	1.97	0.63
1:D:604:ALA:HA	1:D:638:PHE:CZ	2.33	0.63
1:A:579:GLU:CD	1:A:579:GLU:H	2.06	0.63
1:D:9:THR:HG22	2:D:798:HOH:O	1.98	0.63
1:D:612:ARG:HG2	2:D:885:HOH:O	1.98	0.63
1:A:19:ALA:HA	1:A:73:MSE:HG3	1.81	0.63
1:B:564:ARG:NH2	1:B:569:ARG:HG2	2.13	0.63
1:C:327:LEU:HB2	2:C:870:HOH:O	1.98	0.63
1:D:88:LEU:HD11	2:D:905:HOH:O	1.98	0.62
1:D:124:ILE:HG21	2:D:844:HOH:O	1.99	0.62
1:D:187:ASP:OD1	1:D:248:SER:HB3	1.99	0.62
1:D:66:LEU:HD11	2:D:892:HOH:O	1.98	0.62
1:D:323:LEU:HB3	2:D:801:HOH:O	1.99	0.62
1:C:101:THR:HG22	2:C:913:HOH:O	1.98	0.62
1:D:180:SER:HB3	1:D:239:GLU:C	2.24	0.62
1:C:169:GLU:CA	1:C:405:ARG:HD3	2.30	0.62
1:D:7:LEU:HG	2:D:879:HOH:O	2.00	0.62
1:D:163:MSE:HE3	1:D:201:PHE:HB2	1.80	0.62
1:D:222:VAL:HG23	2:D:894:HOH:O	1.99	0.62
1:A:433:SER:HA	1:A:436:MSE:HE3	1.81	0.62
1:B:44:LEU:HB3	1:B:49:MSE:HE2	1.80	0.62
1:B:309:TRP:CZ2	1:B:313:LEU:HD11	2.34	0.62
1:D:88:LEU:O	1:D:92:LYS:HG3	2.00	0.62
1:D:416:LEU:HA	2:D:849:HOH:O	1.99	0.62
1:A:83:GLY:HA3	1:A:299:ARG:HD2	1.81	0.62
1:C:261:LYS:NZ	1:C:261:LYS:HB3	2.15	0.62
1:C:327:LEU:HG	1:C:331:LEU:HD22	1.81	0.62
1:D:63:ARG:HE	1:D:151:HIS:CD2	2.17	0.62
1:C:369:LEU:HD11	1:C:425:TYR:CE2	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLY:O	1:D:74:LEU:HB3	1.98	0.62
1:D:94:PHE:HD1	1:D:101:THR:HB	1.65	0.62
1:C:143:ARG:HH11	1:C:143:ARG:HG3	1.65	0.61
1:C:647:PHE:O	1:C:651:VAL:HG23	1.99	0.61
1:D:384:ALA:O	1:D:387:MSE:HB2	2.00	0.61
1:D:409:MSE:SE	2:D:809:HOH:O	2.68	0.61
1:C:169:GLU:HA	1:C:405:ARG:HD3	1.83	0.61
1:D:252:PHE:HA	1:D:257:GLN:NE2	2.16	0.61
1:D:366:LEU:HB3	1:D:368:GLU:OE2	2.01	0.61
1:A:197:THR:HG22	1:A:201:PHE:HB3	1.81	0.61
1:C:163:MSE:HE2	1:D:405:ARG:CZ	2.29	0.61
1:D:26:ALA:HB2	2:D:891:HOH:O	2.01	0.61
1:D:45:PHE:CD1	1:D:78:VAL:HG21	2.35	0.61
1:D:225:LEU:HB3	1:D:229:ARG:NH1	2.15	0.61
1:A:608:LEU:HD22	1:B:612:ARG:CZ	2.30	0.61
1:C:143:ARG:HB3	2:C:918:HOH:O	2.00	0.61
1:C:605:GLY:O	1:C:619:ALA:HB1	2.01	0.61
1:D:394:ASN:HD21	1:D:396:LEU:HB2	1.63	0.61
1:C:579:GLU:H	1:C:579:GLU:CD	2.09	0.61
1:D:483:LEU:HD23	1:D:508:PRO:HG2	1.83	0.61
1:A:297:ASP:O	1:A:298:MSE:HE2	2.00	0.61
1:B:54:LEU:CD1	1:B:299:ARG:HG2	2.31	0.61
1:D:116:THR:N	1:D:446:MSE:HE2	2.14	0.61
1:D:82:THR:HB	2:D:903:HOH:O	2.00	0.61
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.64	0.61
1:C:449:PRO:HB3	1:C:505:LYS:HA	1.83	0.61
1:D:66:LEU:HD21	2:D:892:HOH:O	2.00	0.60
1:D:133:ALA:HB1	1:D:419:HIS:CG	2.36	0.60
1:D:149:VAL:HA	2:D:868:HOH:O	2.00	0.60
1:D:636:LEU:HD13	2:D:847:HOH:O	1.99	0.60
1:B:37:MSE:HE3	1:B:187:ASP:OD1	2.00	0.60
1:C:555:LEU:HD22	1:C:643:VAL:HG21	1.84	0.60
1:C:522:SER:HB3	1:C:525:LYS:CG	2.31	0.60
1:D:277:ARG:O	1:D:277:ARG:HD3	2.01	0.60
1:D:215:GLN:HE22	1:D:240:ARG:HB2	1.64	0.60
1:B:437:ARG:HB3	1:B:438:PRO:HD3	1.83	0.60
1:D:225:LEU:HA	2:D:884:HOH:O	2.01	0.60
1:B:394:ASN:ND2	2:B:1057:HOH:O	2.34	0.60
1:C:487:ARG:HD3	1:C:549:THR:HG23	1.83	0.60
1:D:197:THR:HB	2:D:839:HOH:O	2.02	0.60
1:D:236:LYS:HA	1:D:236:LYS:NZ	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HB3	1:A:49:MSE:HE2	1.84	0.59
1:C:46:ARG:HG3	1:C:296:MSE:HE1	1.84	0.59
1:C:56:PRO:HA	2:C:930:HOH:O	2.02	0.59
1:D:13:ASN:O	1:D:17:PHE:HD1	1.85	0.59
1:D:543:GLN:HE22	1:D:568:VAL:HA	1.66	0.59
1:C:37:MSE:HG2	2:C:922:HOH:O	2.01	0.59
1:A:385:GLU:HB3	2:A:790:HOH:O	2.02	0.59
1:B:190:ARG:N	1:B:190:ARG:HD2	2.17	0.59
1:B:506:GLU:CD	1:B:506:GLU:H	2.10	0.59
1:D:228:LEU:HD22	2:D:884:HOH:O	2.02	0.59
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.67	0.59
1:D:629:TYR:CD1	1:D:630:PRO:HA	2.37	0.59
1:A:608:LEU:HD22	1:B:612:ARG:NH2	2.18	0.59
1:D:7:LEU:CD2	1:D:7:LEU:H	2.15	0.59
1:D:67:SER:HB2	2:D:837:HOH:O	2.03	0.59
1:D:252:PHE:HA	1:D:257:GLN:HE21	1.67	0.59
1:A:417:ASN:ND2	1:A:424:ALA:H	1.94	0.59
1:C:387:MSE:HE2	1:C:399:TYR:CB	2.31	0.59
1:C:538:ASP:HA	2:C:853:HOH:O	2.02	0.59
1:C:289:PRO:HB2	1:C:291:GLU:OE2	2.02	0.59
1:C:349:ILE:HD13	1:C:349:ILE:N	2.16	0.59
1:D:132:LEU:HD23	1:D:132:LEU:O	2.02	0.59
1:D:303:ARG:HB3	2:D:788:HOH:O	2.03	0.59
1:C:306:GLN:O	1:C:310:GLU:HG3	2.03	0.59
1:A:427:GLY:O	1:A:428:THR:HG23	2.02	0.59
1:B:247:ARG:HG2	2:B:1103:HOH:O	2.02	0.59
1:C:327:LEU:HD22	2:C:897:HOH:O	2.02	0.59
1:D:76:TYR:HD1	2:D:854:HOH:O	1.85	0.59
1:C:569:ARG:HH21	1:C:569:ARG:CB	2.16	0.59
1:D:272:VAL:O	1:D:276:ARG:HG3	2.03	0.59
1:C:136:LYS:HG3	1:C:422:TYR:OH	2.03	0.58
1:D:120:LEU:HD22	1:D:120:LEU:H	1.68	0.58
1:D:297:ASP:HB2	2:D:901:HOH:O	2.01	0.58
1:D:413:LEU:C	1:D:415:GLY:H	2.11	0.58
1:C:348:PRO:HA	1:C:520:LEU:CD2	2.33	0.58
1:A:328:MSE:O	1:A:332:ARG:HD2	2.03	0.58
1:C:347:LYS:O	1:C:349:ILE:HG23	2.02	0.58
1:D:31:PRO:O	1:D:34:PRO:HG2	2.02	0.58
1:C:169:GLU:CB	1:C:405:ARG:HD3	2.33	0.58
1:C:538:ASP:OD1	1:C:539:VAL:N	2.37	0.58
1:D:94:PHE:HE2	2:D:853:HOH:O	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ARG:HB3	1:D:421:GLY:HA2	1.85	0.58
1:D:415:GLY:HA2	2:D:856:HOH:O	2.03	0.58
1:D:417:ASN:HB2	2:D:808:HOH:O	2.03	0.58
1:D:529:LEU:HG	2:D:933:HOH:O	2.02	0.58
1:C:193:ILE:HD13	1:D:375:ASP:OD2	2.03	0.58
1:B:43:LEU:HD13	1:B:48:VAL:HG23	1.85	0.58
1:D:52:ASN:C	1:D:54:LEU:H	2.12	0.58
1:D:163:MSE:HE3	1:D:201:PHE:CB	2.33	0.58
1:D:46:ARG:HG2	1:D:46:ARG:HH11	1.68	0.58
1:D:250:ILE:HD11	2:D:860:HOH:O	2.03	0.58
1:B:594:PRO:HG2	1:B:597:LEU:HD11	1.86	0.58
1:C:562:LEU:O	1:C:565:GLU:HB3	2.03	0.58
1:A:7:LEU:HD11	1:A:291:GLU:HG2	1.84	0.58
1:C:487:ARG:HH21	1:C:549:THR:CG2	2.12	0.58
1:D:224:ASP:O	1:D:228:LEU:HD13	2.04	0.58
1:B:240:ARG:HB2	2:B:1134:HOH:O	2.04	0.57
2:C:849:HOH:O	1:D:104:HIS:HE1	1.86	0.57
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.86	0.57
1:C:546:LEU:HG	1:C:570:VAL:HG21	1.86	0.57
2:C:901:HOH:O	1:D:480:MSE:HG3	2.03	0.57
1:D:135:ARG:NH2	1:D:181:LYS:HG3	2.19	0.57
1:B:627:ALA:HB3	1:B:632:VAL:HB	1.87	0.57
1:D:119:PRO:HB2	1:D:122:GLN:CG	2.34	0.57
1:A:631:GLU:O	1:A:635:ARG:HG3	2.05	0.57
1:D:151:HIS:HB2	2:D:852:HOH:O	2.05	0.57
1:D:527:ARG:HA	2:D:896:HOH:O	2.04	0.57
2:C:901:HOH:O	1:D:441:ARG:HG3	2.04	0.57
1:D:290:GLU:O	1:D:294:ARG:HG3	2.05	0.57
1:D:336:PRO:HD3	2:D:916:HOH:O	2.03	0.57
1:D:483:LEU:C	1:D:483:LEU:HD13	2.30	0.57
1:A:537:GLU:HB3	2:A:1170:HOH:O	2.05	0.57
1:C:559:ALA:O	1:C:563:LEU:HD13	2.04	0.57
1:D:32:GLY:HA3	2:D:860:HOH:O	2.05	0.57
1:D:130:LEU:HD12	2:D:856:HOH:O	2.04	0.57
1:D:366:LEU:CD1	1:D:502:LEU:HD21	2.34	0.57
1:A:343:PRO:HG2	1:A:345:PHE:CE2	2.39	0.57
1:C:461:LEU:CD1	1:C:464:ASP:HB2	2.35	0.57
1:D:179:LEU:N	1:D:179:LEU:HD22	2.20	0.57
1:D:360:ASN:C	2:D:886:HOH:O	2.48	0.57
1:A:300:GLU:HG3	2:A:1128:HOH:O	2.03	0.57
1:D:292:VAL:HG21	2:D:871:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:PHE:HA	1:C:579:GLU:HG3	1.86	0.56
1:D:522:SER:HB2	1:D:525:LYS:CG	2.35	0.56
1:B:107:ARG:HD2	1:B:108:GLY:N	2.20	0.56
1:D:86:LEU:HD21	1:D:110:THR:HG23	1.87	0.56
1:D:522:SER:HB3	2:D:890:HOH:O	2.05	0.56
1:B:219:VAL:HG11	1:B:228:LEU:HD13	1.86	0.56
1:C:46:ARG:HD3	1:C:46:ARG:O	2.04	0.56
1:C:205:VAL:HG23	1:C:206:LEU:N	2.20	0.56
1:C:289:PRO:HG2	1:C:292:VAL:HG23	1.87	0.56
1:D:177:TRP:O	1:D:392:ARG:HB3	2.04	0.56
1:A:489:ALA:O	1:A:554:HIS:HE1	1.88	0.56
1:D:416:LEU:HD13	2:D:849:HOH:O	2.04	0.56
1:C:132:LEU:CD2	1:C:136:LYS:HD2	2.35	0.56
1:C:349:ILE:HD11	1:C:520:LEU:HD11	1.86	0.56
1:C:7:LEU:HG	1:C:295:HIS:CD2	2.40	0.56
1:C:37:MSE:HE2	1:C:156:LEU:HD11	1.88	0.56
1:D:215:GLN:CD	1:D:240:ARG:HB2	2.30	0.56
1:C:164:GLU:HB3	1:C:166:VAL:HG12	1.87	0.56
1:D:579:GLU:CD	1:D:579:GLU:H	2.12	0.56
1:A:563:LEU:HD11	1:A:644:ALA:HA	1.87	0.56
1:D:278:ASN:HB3	2:D:687:HOH:O	2.06	0.56
1:C:338:LEU:HD11	1:C:366:LEU:HD21	1.87	0.55
1:D:116:THR:HB	1:D:446:MSE:HE2	1.87	0.55
1:D:343:PRO:HD3	2:D:870:HOH:O	2.06	0.55
1:B:594:PRO:HG2	1:B:597:LEU:HD21	1.88	0.55
1:D:359:LEU:HD12	2:D:877:HOH:O	2.07	0.55
1:D:414:ASN:C	2:D:808:HOH:O	2.49	0.55
1:B:307:GLU:HB2	2:B:1039:HOH:O	2.06	0.55
1:C:198:ASP:HA	2:C:908:HOH:O	2.06	0.55
1:C:201:PHE:N	2:C:908:HOH:O	2.35	0.55
1:C:506:GLU:N	1:C:506:GLU:OE1	2.39	0.55
1:D:124:ILE:HD13	1:D:124:ILE:O	2.06	0.55
1:D:141:PHE:HE1	2:D:805:HOH:O	1.90	0.55
1:D:155:VAL:HG12	2:D:824:HOH:O	2.06	0.55
1:D:557:LEU:O	1:D:560:GLN:HG2	2.06	0.55
1:B:37:MSE:CE	1:B:248:SER:CB	2.83	0.55
1:C:218:ARG:NH1	1:C:245:ALA:HB1	2.21	0.55
1:D:465:GLY:O	1:D:469:GLN:HG3	2.07	0.55
1:D:536:LEU:HD23	1:D:536:LEU:C	2.30	0.55
1:A:215:GLN:HE22	1:A:235:ALA:HA	1.71	0.55
1:C:304:ALA:HA	1:C:307:GLU:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ASP:HA	2:D:798:HOH:O	2.05	0.55
1:D:201:PHE:HB3	2:D:839:HOH:O	2.06	0.55
1:B:220:GLU:CD	1:B:247:ARG:HH11	2.14	0.55
1:C:571:ARG:HG3	2:C:853:HOH:O	2.07	0.55
1:D:475:MSE:HE3	1:D:608:LEU:O	2.07	0.55
1:B:314:GLU:O	1:B:318:ARG:HG3	2.06	0.55
1:C:209:TYR:HA	1:C:212:TYR:HD2	1.72	0.55
1:C:369:LEU:C	1:C:369:LEU:HD13	2.32	0.55
1:D:215:GLN:HE22	1:D:240:ARG:CB	2.20	0.55
1:A:197:THR:CG2	1:A:201:PHE:HB3	2.37	0.55
1:C:65:VAL:HG13	1:C:115:VAL:CG1	2.36	0.55
1:C:408:ALA:N	2:C:904:HOH:O	2.40	0.55
1:B:82:THR:HG21	2:B:1087:HOH:O	2.06	0.55
1:C:404:VAL:H	1:D:163:MSE:SE	2.40	0.55
1:D:461:LEU:HA	1:D:515:ARG:HD3	1.87	0.55
1:C:54:LEU:HD11	1:C:299:ARG:HG2	1.89	0.55
1:C:77:ALA:HB1	2:C:905:HOH:O	2.07	0.55
1:D:547:VAL:O	1:D:601:ALA:HA	2.06	0.55
1:A:610:TRP:CB	1:A:617:VAL:HG11	2.37	0.54
1:C:17:PHE:CE2	1:C:276:ARG:HG2	2.42	0.54
1:C:218:ARG:HH11	1:C:245:ALA:CB	2.19	0.54
1:D:75:LEU:O	1:D:75:LEU:HD22	2.07	0.54
1:A:608:LEU:CD1	1:B:475:MSE:HE1	2.36	0.54
1:C:60:ASP:CG	2:C:924:HOH:O	2.49	0.54
1:C:218:ARG:HH11	1:C:245:ALA:C	2.14	0.54
1:D:236:LYS:HZ3	1:D:236:LYS:CA	2.20	0.54
1:C:120:LEU:HD22	1:C:120:LEU:H	1.73	0.54
1:D:174:ALA:HA	1:D:179:LEU:HD23	1.90	0.54
1:D:300:GLU:HA	2:D:788:HOH:O	2.08	0.54
1:B:601:ALA:HB3	1:B:617:VAL:HG13	1.90	0.54
1:C:54:LEU:HD21	1:C:299:ARG:CG	2.37	0.54
1:D:291:GLU:OE1	1:D:291:GLU:N	2.40	0.54
1:D:459:ILE:HD13	1:D:636:LEU:HD23	1.88	0.54
1:A:641:GLU:O	1:A:645:GLU:HG3	2.08	0.54
1:B:329:ARG:NH2	1:B:336:PRO:HD3	2.22	0.54
1:C:63:ARG:NH1	1:C:419:HIS:HA	2.22	0.54
1:A:247:ARG:NE	2:A:759:HOH:O	2.40	0.54
1:D:7:LEU:H	1:D:7:LEU:HD23	1.71	0.54
1:D:338:LEU:H	1:D:338:LEU:CD2	2.21	0.54
1:A:431:VAL:HG13	1:A:432:PHE:CD1	2.43	0.54
1:D:142:ASN:ND2	1:D:147:VAL:HG13	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ILE:HD13	1:C:349:ILE:H	1.73	0.54
1:C:461:LEU:C	1:C:461:LEU:HD12	2.33	0.54
1:C:493:GLU:HG2	1:C:529:LEU:HB2	1.90	0.54
1:D:119:PRO:HB2	1:D:122:GLN:HG2	1.89	0.54
1:D:214:TRP:C	1:D:215:GLN:NE2	2.65	0.54
1:A:342:PRO:HB3	1:A:495:PHE:CD2	2.43	0.54
1:C:294:ARG:HA	1:C:294:ARG:NE	2.23	0.54
1:D:134:GLU:HG3	2:D:685:HOH:O	2.07	0.54
1:D:213:GLY:HA3	2:D:876:HOH:O	2.07	0.54
1:C:461:LEU:HD13	1:C:464:ASP:HB2	1.90	0.53
1:D:45:PHE:HA	1:D:49:MSE:HE3	1.89	0.53
1:D:148:VAL:HG21	1:D:327:LEU:HD21	1.90	0.53
1:D:239:GLU:O	1:D:240:ARG:HD3	2.08	0.53
1:D:442:LEU:CG	1:D:446:MSE:HE3	2.36	0.53
1:C:193:ILE:HD12	1:C:193:ILE:H	1.74	0.53
1:C:225:LEU:O	1:C:229:ARG:HG3	2.08	0.53
1:D:138:ALA:HA	1:D:149:VAL:HB	1.91	0.53
1:C:566:LYS:NZ	2:C:695:HOH:O	2.42	0.53
1:C:594:PRO:CG	1:C:597:LEU:HD12	2.36	0.53
1:D:322:ASP:C	1:D:324:HIS:H	2.15	0.53
1:C:402:PHE:CE2	1:C:409:MSE:HE3	2.44	0.53
1:D:323:LEU:HD12	1:D:323:LEU:N	2.23	0.53
1:D:301:LYS:HE2	2:D:759:HOH:O	2.09	0.53
1:C:398:ARG:HB3	2:C:917:HOH:O	2.09	0.53
1:D:20:ILE:HD12	1:D:267:LEU:CD1	2.39	0.53
1:A:605:GLY:O	1:A:619:ALA:HB1	2.09	0.52
1:B:587:ALA:O	1:B:591:GLU:HG3	2.09	0.52
1:C:202:THR:HG23	2:C:908:HOH:O	2.08	0.52
1:C:423:ARG:CZ	2:C:850:HOH:O	2.55	0.52
1:D:529:LEU:HD23	1:D:576:PRO:CG	2.38	0.52
1:A:132:LEU:HD13	1:A:416:LEU:HD21	1.91	0.52
1:B:332:ARG:NH2	1:B:334:GLU:OE1	2.42	0.52
1:C:179:LEU:N	2:C:915:HOH:O	2.41	0.52
1:D:215:GLN:NE2	1:D:240:ARG:CB	2.66	0.52
1:B:309:TRP:CZ3	1:B:313:LEU:HD11	2.44	0.52
1:B:328:MSE:HB3	1:B:332:ARG:NH1	2.25	0.52
1:D:338:LEU:H	1:D:338:LEU:HD23	1.73	0.52
1:D:529:LEU:HD23	1:D:576:PRO:HB2	1.92	0.52
1:D:635:ARG:HD2	2:D:831:HOH:O	2.09	0.52
1:B:43:LEU:HD13	1:B:48:VAL:CG2	2.39	0.52
1:D:74:LEU:O	1:D:78:VAL:HG12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:THR:CB	1:D:446:MSE:HE2	2.40	0.52
1:D:562:LEU:O	1:D:565:GLU:HG2	2.09	0.52
1:A:35:MSE:HE1	1:A:254:SER:HB3	1.90	0.52
1:C:329:ARG:NH1	2:C:909:HOH:O	2.41	0.52
1:D:459:ILE:CD1	1:D:636:LEU:HD23	2.39	0.52
1:D:529:LEU:O	1:D:529:LEU:HD22	2.09	0.52
1:A:83:GLY:HA3	1:A:299:ARG:CD	2.40	0.52
1:B:343:PRO:HG2	1:B:345:PHE:CE1	2.45	0.52
1:A:406:GLU:HB3	1:A:436:MSE:HE2	1.90	0.52
1:B:579:GLU:CD	1:B:579:GLU:H	2.17	0.52
1:C:214:TRP:CG	1:C:241:PRO:HG2	2.45	0.52
1:C:373:SER:N	1:C:409:MSE:HE1	2.24	0.52
1:D:19:ALA:HB2	2:D:932:HOH:O	2.10	0.52
1:D:55:ASP:HB2	2:D:825:HOH:O	2.10	0.52
1:D:179:LEU:N	2:D:846:HOH:O	2.43	0.52
1:D:252:PHE:HB2	2:D:848:HOH:O	2.10	0.52
1:D:529:LEU:HD23	1:D:576:PRO:CB	2.40	0.52
1:C:377:THR:N	1:C:378:PRO:HD2	2.25	0.52
1:B:431:VAL:HG13	1:B:432:PHE:CD1	2.45	0.52
1:B:529:LEU:HD22	1:B:576:PRO:CG	2.40	0.52
1:D:173:LEU:HD13	1:D:177:TRP:CH2	2.45	0.52
1:C:58:TRP:HB2	1:C:306:GLN:OE1	2.10	0.51
1:D:11:SER:HB3	2:D:909:HOH:O	2.09	0.51
1:C:115:VAL:HG23	1:C:446:MSE:SE	2.61	0.51
1:D:156:LEU:HB2	2:D:881:HOH:O	2.10	0.51
1:D:183:ILE:HD11	1:D:236:LYS:NZ	2.26	0.51
1:D:527:ARG:HE	1:D:530:LEU:CD1	2.23	0.51
1:C:151:HIS:NE2	1:C:419:HIS:NE2	2.57	0.51
1:D:41:ALA:CB	1:D:74:LEU:HD11	2.35	0.51
1:C:387:MSE:HE3	2:C:917:HOH:O	2.10	0.51
1:C:442:LEU:HG	1:C:446:MSE:HE2	1.91	0.51
1:C:492:TYR:HB2	2:C:925:HOH:O	2.10	0.51
1:C:604:ALA:HA	1:C:638:PHE:CZ	2.46	0.51
1:D:323:LEU:HD12	1:D:323:LEU:H	1.76	0.51
1:A:405:ARG:HH22	1:B:163:MSE:CE	2.21	0.51
1:D:372:GLY:C	2:D:809:HOH:O	2.53	0.51
1:B:215:GLN:CB	2:B:1134:HOH:O	2.57	0.51
1:C:48:VAL:HG21	1:C:232:ILE:HD13	1.92	0.51
1:D:31:PRO:O	1:D:35:MSE:HG3	2.11	0.51
1:D:354:ALA:HB1	1:D:491:ALA:HA	1.93	0.51
1:B:107:ARG:HD2	1:B:107:ARG:C	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HA	1:C:48:VAL:HB	1.93	0.51
1:D:11:SER:O	1:D:14:ALA:HB3	2.11	0.51
1:D:501:ALA:HB2	1:D:509:THR:HG21	1.92	0.51
1:D:358:ALA:O	1:D:362:LEU:HG	2.11	0.51
1:C:63:ARG:HG2	2:C:941:HOH:O	2.11	0.51
1:C:163:MSE:HE3	1:C:201:PHE:HB2	1.93	0.51
1:D:157:ALA:N	2:D:824:HOH:O	2.44	0.51
1:D:344:SER:HA	2:D:845:HOH:O	2.11	0.51
1:D:7:LEU:HG	1:D:295:HIS:CE1	2.46	0.51
1:D:321:PRO:HG2	1:D:322:ASP:H	1.76	0.51
1:C:35:MSE:HE1	1:C:254:SER:HB3	1.93	0.50
1:C:31:PRO:C	1:C:34:PRO:HD2	2.36	0.50
1:C:325:GLN:HG3	1:C:326:GLU:N	2.26	0.50
1:C:343:PRO:HG2	1:C:345:PHE:CE1	2.46	0.50
1:D:107:ARG:HD3	1:D:108:GLY:N	2.25	0.50
1:D:636:LEU:HB2	2:D:847:HOH:O	2.10	0.50
1:A:247:ARG:HH21	1:A:247:ARG:HG3	1.76	0.50
1:C:325:GLN:HG3	1:C:326:GLU:H	1.76	0.50
1:B:313:LEU:HB3	2:B:1132:HOH:O	2.12	0.50
1:B:570:VAL:HG12	2:B:1114:HOH:O	2.11	0.50
1:D:246:VAL:HG13	2:D:898:HOH:O	2.10	0.50
1:B:190:ARG:HG3	1:B:190:ARG:NH1	2.27	0.50
1:C:61:ARG:NE	2:C:941:HOH:O	2.43	0.50
1:C:332:ARG:HD2	1:C:334:GLU:OE2	2.12	0.50
1:D:267:LEU:HD13	2:D:789:HOH:O	2.11	0.50
1:D:414:ASN:O	1:D:418:LEU:HD12	2.10	0.50
1:D:423:ARG:HH11	1:D:423:ARG:HG2	1.76	0.50
1:D:456:HIS:CD2	1:D:515:ARG:HD2	2.47	0.50
1:B:143:ARG:NH2	2:B:1129:HOH:O	2.45	0.50
1:C:218:ARG:HH11	1:C:245:ALA:HB1	1.75	0.50
1:D:484:PHE:CD2	1:D:579:GLU:HG3	2.46	0.50
1:C:522:SER:HB3	1:C:525:LYS:HG2	1.92	0.50
1:A:392:ARG:HG3	2:A:716:HOH:O	2.11	0.50
1:B:651:VAL:HG22	1:B:651:VAL:OXT	2.12	0.50
1:C:265:GLU:N	2:C:935:HOH:O	2.44	0.50
1:B:284:PRO:HG3	2:B:1145:HOH:O	2.10	0.50
1:C:413:LEU:CD2	2:C:894:HOH:O	2.59	0.50
1:D:46:ARG:HG3	1:D:298:MSE:CE	2.41	0.50
1:D:163:MSE:HE3	1:D:201:PHE:CD1	2.46	0.50
1:A:120:LEU:HD12	1:B:404:VAL:HG11	1.94	0.49
1:B:226:GLU:OE2	1:B:229:ARG:NH2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD13	1:A:160:GLY:HA3	1.93	0.49
1:A:554:HIS:HD2	2:A:945:HOH:O	1.94	0.49
1:C:496:TYR:CZ	1:C:527:ARG:HG2	2.48	0.49
1:D:18:LEU:HD12	1:D:77:ALA:HB1	1.94	0.49
1:D:42:TYR:HD1	1:D:296:MSE:HE1	1.77	0.49
1:D:208:ARG:O	1:D:211:ALA:HB3	2.12	0.49
1:D:311:LYS:CA	1:D:314:GLU:HG2	2.43	0.49
1:D:543:GLN:NE2	1:D:568:VAL:HA	2.26	0.49
1:D:631:GLU:HG3	1:D:635:ARG:HD2	1.94	0.49
1:D:23:VAL:HG22	2:D:853:HOH:O	2.12	0.49
1:D:33:MSE:N	1:D:34:PRO:HD2	2.28	0.49
1:D:36:GLY:HA2	2:D:848:HOH:O	2.10	0.49
1:D:259:SER:C	2:D:937:HOH:O	2.55	0.49
1:A:601:ALA:HB3	1:A:617:VAL:HG12	1.94	0.49
1:C:166:VAL:HA	2:C:904:HOH:O	2.12	0.49
1:C:205:VAL:HG23	1:C:206:LEU:H	1.78	0.49
1:D:119:PRO:O	1:D:122:GLN:HG2	2.13	0.49
1:D:163:MSE:CE	1:D:201:PHE:HB2	2.42	0.49
1:D:318:ARG:HH21	1:D:318:ARG:HG2	1.78	0.49
1:D:496:TYR:HB3	1:D:529:LEU:HD12	1.94	0.49
1:B:128:VAL:HG21	1:B:170:ALA:HB1	1.95	0.49
1:D:23:VAL:N	2:D:867:HOH:O	2.45	0.49
1:C:455:THR:HB	2:C:907:HOH:O	2.13	0.49
1:D:219:VAL:HG11	1:D:228:LEU:HD12	1.93	0.49
1:D:415:GLY:HA2	2:D:841:HOH:O	2.13	0.49
1:D:549:THR:HG22	1:D:575:LEU:O	2.13	0.49
1:C:61:ARG:HG3	2:C:941:HOH:O	2.13	0.49
1:C:327:LEU:CD1	1:C:331:LEU:HD13	2.43	0.49
1:C:499:LEU:HB3	1:C:503:ARG:HH21	1.77	0.49
1:C:541:GLU:O	1:C:569:ARG:NH2	2.45	0.49
1:D:285:PRO:O	1:D:286:PHE:HB2	2.12	0.49
1:B:554:HIS:HD2	2:B:1072:HOH:O	1.95	0.49
1:C:143:ARG:HG3	1:C:143:ARG:NH1	2.27	0.49
1:C:456:HIS:CE1	1:C:515:ARG:HG3	2.48	0.49
1:C:482:ASN:ND2	1:C:504:ARG:HH22	2.10	0.49
1:D:267:LEU:O	1:D:271:ALA:HB3	2.12	0.49
1:D:364:PRO:CD	2:D:886:HOH:O	2.60	0.49
1:C:186:TRP:CZ3	1:C:205:VAL:HG21	2.48	0.48
1:D:39:PRO:O	1:D:43:LEU:HB2	2.13	0.48
1:A:97:TRP:HH2	1:B:636:LEU:HD13	1.78	0.48
1:B:644:ALA:HA	2:B:1146:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:CD	1:D:108:GLY:N	2.75	0.48
1:D:394:ASN:ND2	1:D:396:LEU:H	2.10	0.48
1:D:413:LEU:C	1:D:415:GLY:N	2.71	0.48
1:D:597:LEU:N	1:D:597:LEU:HD12	2.28	0.48
1:A:490:ASP:N	2:A:1175:HOH:O	2.20	0.48
1:A:629:TYR:CD2	1:A:630:PRO:HA	2.47	0.48
1:B:206:LEU:HG	1:B:216:THR:HB	1.95	0.48
1:D:37:MSE:HE2	1:D:156:LEU:CD1	2.43	0.48
1:D:52:ASN:C	1:D:54:LEU:N	2.71	0.48
1:D:206:LEU:HG	1:D:216:THR:HB	1.95	0.48
1:D:289:PRO:HB2	1:D:291:GLU:OE1	2.14	0.48
1:D:610:TRP:C	1:D:612:ARG:H	2.20	0.48
1:C:169:GLU:HB3	1:C:408:ALA:HB2	1.96	0.48
1:C:348:PRO:HA	1:C:520:LEU:HD21	1.95	0.48
1:C:423:ARG:HG3	1:C:423:ARG:HH11	1.78	0.48
1:D:277:ARG:HD3	1:D:277:ARG:C	2.39	0.48
1:D:569:ARG:NE	2:D:724:HOH:O	2.46	0.48
1:B:87:PRO:HG2	1:B:90:GLU:HG2	1.96	0.48
1:B:120:LEU:HD13	1:B:160:GLY:HA3	1.94	0.48
1:B:496:TYR:O	1:B:500:VAL:HG23	2.14	0.48
1:C:38:ALA:N	1:C:39:PRO:HD2	2.28	0.48
1:D:35:MSE:HE1	1:D:254:SER:HB3	1.95	0.48
1:D:135:ARG:NH2	1:D:181:LYS:HE3	2.28	0.48
1:D:363:ALA:N	2:D:886:HOH:O	2.46	0.48
1:B:545:VAL:HG23	1:B:597:LEU:HD13	1.96	0.48
1:A:33:MSE:HE2	2:A:1173:HOH:O	2.12	0.48
1:B:332:ARG:NH1	2:B:860:HOH:O	2.45	0.48
1:B:506:GLU:CD	1:B:506:GLU:N	2.72	0.48
1:C:218:ARG:HD2	1:C:245:ALA:O	2.13	0.48
1:D:186:TRP:CZ3	1:D:205:VAL:HG21	2.48	0.48
1:D:506:GLU:CD	1:D:506:GLU:H	2.21	0.48
1:A:310:GLU:O	1:A:314:GLU:HG2	2.14	0.48
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.96	0.48
1:B:570:VAL:HA	2:B:1138:HOH:O	2.13	0.48
1:C:31:PRO:CD	2:C:935:HOH:O	2.49	0.48
1:D:173:LEU:HD11	2:D:855:HOH:O	2.14	0.48
1:D:368:GLU:CD	1:D:368:GLU:N	2.72	0.48
1:B:369:LEU:HD11	1:B:425:TYR:HE2	1.78	0.48
1:B:635:ARG:HD3	2:B:1116:HOH:O	2.14	0.48
1:C:8:GLU:O	1:C:12:VAL:HG23	2.14	0.48
1:C:37:MSE:HE2	1:C:156:LEU:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ASN:OD1	1:C:54:LEU:HD23	2.14	0.48
1:C:97:TRP:HZ3	2:D:847:HOH:O	1.97	0.48
1:C:309:TRP:O	1:C:313:LEU:HD23	2.14	0.48
1:D:38:ALA:N	1:D:39:PRO:HD2	2.29	0.48
1:D:191:ILE:O	2:D:827:HOH:O	2.20	0.48
1:D:555:LEU:HD22	1:D:643:VAL:HG21	1.95	0.48
1:C:352:ARG:HH21	1:C:456:HIS:HE1	1.60	0.47
1:C:196:PRO:O	1:C:199:LEU:HD13	2.13	0.47
1:C:209:TYR:HA	1:C:212:TYR:CD2	2.47	0.47
1:C:327:LEU:HD12	1:C:331:LEU:HD13	1.96	0.47
1:D:79:LEU:O	1:D:84:TYR:HB2	2.14	0.47
1:D:252:PHE:HD2	1:D:257:GLN:HE22	1.62	0.47
1:D:459:ILE:HD13	1:D:620:LEU:HD22	1.96	0.47
1:C:310:GLU:HG2	2:C:723:HOH:O	2.13	0.47
1:D:370:LEU:O	1:D:424:ALA:HA	2.14	0.47
1:D:427:GLY:HA2	1:D:453:VAL:O	2.14	0.47
1:D:536:LEU:HD23	1:D:536:LEU:O	2.15	0.47
1:B:328:MSE:O	1:B:332:ARG:HG3	2.14	0.47
1:B:417:ASN:ND2	1:B:423:ARG:HA	2.29	0.47
1:B:558:ARG:NH2	2:B:666:HOH:O	2.46	0.47
1:C:390:PHE:CE1	1:C:395:PRO:HA	2.49	0.47
1:D:404:VAL:HG12	1:D:404:VAL:O	2.15	0.47
1:A:545:VAL:HG22	1:A:571:ARG:CG	2.43	0.47
1:B:180:SER:HB3	1:B:239:GLU:O	2.15	0.47
1:B:562:LEU:HD23	1:B:562:LEU:O	2.15	0.47
1:B:563:LEU:HD21	2:B:1146:HOH:O	2.15	0.47
1:C:264:GLY:CA	2:C:935:HOH:O	2.63	0.47
1:C:519:PRO:HB2	1:C:554:HIS:CD2	2.49	0.47
1:D:44:LEU:HD23	1:D:48:VAL:HG11	1.97	0.47
1:A:475:MSE:HE3	1:A:608:LEU:O	2.14	0.47
1:C:555:LEU:HD23	1:C:555:LEU:O	2.15	0.47
1:D:329:ARG:NH1	2:D:916:HOH:O	2.47	0.47
1:A:547:VAL:O	1:A:601:ALA:HA	2.15	0.47
1:C:46:ARG:CG	1:C:296:MSE:HE1	2.45	0.47
1:C:210:ARG:HA	2:C:902:HOH:O	2.15	0.47
1:C:210:ARG:HG3	2:C:902:HOH:O	2.14	0.47
1:C:448:VAL:HB	2:C:940:HOH:O	2.14	0.47
1:D:44:LEU:HA	1:D:48:VAL:HG12	1.95	0.47
1:D:223:ASN:O	1:D:225:LEU:HD12	2.15	0.47
1:D:311:LYS:HA	1:D:314:GLU:CG	2.44	0.47
1:B:328:MSE:HB3	1:B:332:ARG:HH12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:HD23	2:B:1057:HOH:O	2.14	0.47
1:B:475:MSE:HE2	1:B:608:LEU:O	2.15	0.47
1:C:352:ARG:NH2	1:C:456:HIS:HE1	2.12	0.47
1:D:418:LEU:HD13	2:D:872:HOH:O	2.14	0.47
1:C:136:LYS:HB2	2:C:729:HOH:O	2.14	0.47
1:C:375:ASP:OD1	1:D:192:SER:HB3	2.15	0.47
1:C:390:PHE:HA	1:C:397:GLY:HA3	1.97	0.47
1:D:46:ARG:NH2	1:D:295:HIS:CD2	2.83	0.47
1:D:119:PRO:HB2	1:D:122:GLN:HG3	1.96	0.47
1:D:230:LYS:NZ	1:D:230:LYS:HB3	2.30	0.47
1:D:414:ASN:O	1:D:418:LEU:HB2	2.14	0.47
1:A:45:PHE:CE1	1:A:49:MSE:HE1	2.50	0.47
1:A:607:SER:HB2	1:A:617:VAL:HG21	1.96	0.47
1:C:427:GLY:HA2	1:C:453:VAL:O	2.15	0.47
1:D:230:LYS:O	1:D:234:LEU:HG	2.15	0.47
1:D:336:PRO:HD3	2:D:766:HOH:O	2.14	0.47
1:A:314:GLU:HB2	2:A:1120:HOH:O	2.15	0.46
1:D:217:LEU:HB2	1:D:244:ILE:HG12	1.98	0.46
1:C:46:ARG:HD3	1:C:298:MSE:CE	2.44	0.46
2:C:901:HOH:O	1:D:480:MSE:SE	2.83	0.46
1:D:120:LEU:O	1:D:164:GLU:HG3	2.14	0.46
1:D:206:LEU:HD21	1:D:218:ARG:HG2	1.97	0.46
1:C:564:ARG:HB2	1:C:564:ARG:NH1	2.27	0.46
1:D:37:MSE:HE3	1:D:40:LEU:HD23	1.97	0.46
1:D:159:ASP:OD2	1:D:197:THR:HG21	2.15	0.46
1:D:289:PRO:HG2	1:D:292:VAL:HG21	1.97	0.46
1:B:215:GLN:HB3	2:B:1134:HOH:O	2.14	0.46
1:D:149:VAL:HG11	2:D:883:HOH:O	2.15	0.46
1:B:299:ARG:NH2	2:B:731:HOH:O	2.49	0.46
1:B:461:LEU:HD12	1:B:461:LEU:C	2.40	0.46
1:C:291:GLU:H	1:C:291:GLU:CD	2.23	0.46
1:D:240:ARG:NH2	1:D:392:ARG:HH12	2.13	0.46
1:D:295:HIS:HE1	2:D:879:HOH:O	1.98	0.46
1:D:389:ASP:OD1	1:D:401:HIS:HE1	1.99	0.46
1:D:419:HIS:ND1	2:D:866:HOH:O	2.36	0.46
1:D:610:TRP:C	1:D:612:ARG:N	2.73	0.46
1:D:627:ALA:HB3	1:D:632:VAL:HB	1.96	0.46
1:C:193:ILE:HD12	1:C:193:ILE:N	2.31	0.46
1:C:387:MSE:HE3	1:C:398:ARG:O	2.16	0.46
1:C:580:LEU:HD23	1:C:580:LEU:O	2.16	0.46
1:D:527:ARG:HE	1:D:530:LEU:HD12	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:GLN:HG3	1:D:561:ALA:N	2.30	0.46
1:C:234:LEU:HB3	2:C:916:HOH:O	2.15	0.46
1:D:30:HIS:CD2	1:D:70:HIS:HB2	2.51	0.46
1:D:76:TYR:HE2	1:D:94:PHE:HE1	1.64	0.46
1:D:541:GLU:HB2	2:D:724:HOH:O	2.14	0.46
1:C:530:LEU:O	1:C:580:LEU:HD21	2.15	0.46
1:D:413:LEU:HA	1:D:416:LEU:HD23	1.98	0.46
1:C:487:ARG:HG3	1:C:512:VAL:HB	1.97	0.46
1:D:16:ARG:HH12	1:D:223:ASN:ND2	2.14	0.46
1:D:71:GLY:C	2:D:892:HOH:O	2.59	0.46
1:D:134:GLU:HB2	1:D:151:HIS:CE1	2.51	0.46
1:D:180:SER:HB2	1:D:238:ASP:O	2.16	0.46
1:D:106:GLU:HA	1:D:116:THR:HG23	1.97	0.46
1:A:612:ARG:HA	1:B:611:GLU:HG2	1.97	0.45
1:D:7:LEU:HD23	1:D:7:LEU:N	2.31	0.45
1:D:297:ASP:OD1	1:D:299:ARG:HB2	2.16	0.45
1:D:364:PRO:HD3	2:D:886:HOH:O	2.16	0.45
1:D:557:LEU:HD23	1:D:572:VAL:HG11	1.99	0.45
1:B:369:LEU:CD1	1:B:425:TYR:HE2	2.30	0.45
1:D:335:LEU:H	1:D:335:LEU:CD2	2.22	0.45
1:D:543:GLN:HE21	1:D:569:ARG:HD3	1.81	0.45
1:C:158:SER:HB2	2:C:912:HOH:O	2.16	0.45
1:D:362:LEU:O	1:D:366:LEU:HG	2.16	0.45
1:B:215:GLN:HB2	2:B:1134:HOH:O	2.17	0.45
1:D:76:TYR:CE2	1:D:94:PHE:HE1	2.34	0.45
1:D:209:TYR:O	1:D:214:TRP:HB2	2.16	0.45
1:D:431:VAL:HG13	1:D:432:PHE:CD1	2.52	0.45
1:D:496:TYR:O	1:D:500:VAL:HG12	2.16	0.45
1:D:496:TYR:CB	1:D:529:LEU:HD12	2.47	0.45
1:D:539:VAL:O	1:D:542:PRO:HD3	2.16	0.45
1:A:214:TRP:CG	1:A:241:PRO:HG2	2.51	0.45
1:B:541:GLU:HB2	1:B:569:ARG:NH2	2.32	0.45
1:C:42:TYR:HE1	1:C:296:MSE:HE1	1.81	0.45
1:C:120:LEU:O	1:C:164:GLU:HG3	2.16	0.45
1:A:406:GLU:HG3	1:A:428:THR:HG21	1.98	0.45
1:C:430:LEU:HA	1:C:454:PHE:HB3	1.99	0.45
1:D:46:ARG:HH21	1:D:295:HIS:CD2	2.34	0.45
1:D:132:LEU:HD22	1:D:416:LEU:HD11	1.98	0.45
1:D:281:TRP:NE1	1:D:283:TYR:HB2	2.32	0.45
1:D:506:GLU:CD	1:D:506:GLU:N	2.75	0.45
1:A:594:PRO:HG2	1:A:597:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ARG:HD2	2:B:1095:HOH:O	2.16	0.45
1:B:566:LYS:NZ	1:B:566:LYS:HB3	2.31	0.45
1:C:62:ASP:CG	2:C:906:HOH:O	2.60	0.45
1:C:80:HIS:HB3	2:C:932:HOH:O	2.17	0.45
1:C:390:PHE:HB2	1:C:397:GLY:O	2.17	0.45
1:C:413:LEU:HD22	2:C:894:HOH:O	2.17	0.45
1:D:632:VAL:O	1:D:636:LEU:HB2	2.16	0.45
1:A:190:ARG:NH2	1:A:247:ARG:NH1	2.64	0.45
1:C:177:TRP:O	1:C:392:ARG:HG2	2.17	0.45
1:C:292:VAL:N	2:C:895:HOH:O	2.50	0.45
1:C:457:ASP:CB	1:C:512:VAL:HG12	2.47	0.45
1:A:418:LEU:HD11	1:A:446:MSE:SE	2.67	0.45
1:B:107:ARG:HD3	2:B:1069:HOH:O	2.17	0.45
1:D:191:ILE:HG23	2:D:887:HOH:O	2.16	0.45
1:D:241:PRO:HD3	2:D:846:HOH:O	2.16	0.45
1:D:252:PHE:CD2	1:D:257:GLN:NE2	2.85	0.45
1:D:436:MSE:O	1:D:440:ILE:HG13	2.17	0.45
1:B:475:MSE:HG3	1:B:608:LEU:O	2.17	0.45
1:B:595:PRO:HG2	2:B:1040:HOH:O	2.15	0.45
1:C:79:LEU:O	1:C:84:TYR:HB2	2.16	0.45
1:C:141:PHE:HB3	2:C:914:HOH:O	2.16	0.45
1:C:261:LYS:HB3	1:C:261:LYS:HZ2	1.80	0.45
1:C:349:ILE:CD1	1:C:520:LEU:HD11	2.47	0.45
1:C:469:GLN:HA	1:C:470:PRO:HD3	1.82	0.45
1:D:18:LEU:CD1	1:D:77:ALA:HB1	2.47	0.45
1:D:144:PRO:C	1:D:146:HIS:H	2.24	0.45
1:D:228:LEU:HD21	2:D:894:HOH:O	2.15	0.45
1:D:352:ARG:HG3	1:D:353:ALA:N	2.31	0.45
1:D:398:ARG:HG3	1:D:398:ARG:HH11	1.82	0.45
1:D:489:ALA:HB2	1:D:553:VAL:HG21	1.98	0.45
1:A:594:PRO:HA	1:A:595:PRO:HD2	1.88	0.44
1:A:609:GLY:HA2	1:B:609:GLY:HA2	1.99	0.44
1:B:45:PHE:CE1	1:B:49:MSE:HE1	2.53	0.44
1:B:100:LYS:NZ	2:B:930:HOH:O	2.50	0.44
1:C:95:ARG:HH11	1:D:463:GLU:HB3	1.81	0.44
1:C:352:ARG:HA	1:C:513:LEU:HD13	1.99	0.44
1:C:375:ASP:HA	1:D:194:ASP:OD1	2.17	0.44
1:C:429:PHE:HD2	1:C:432:PHE:CE2	2.35	0.44
1:D:17:PHE:O	1:D:18:LEU:C	2.59	0.44
1:D:88:LEU:HD11	1:D:286:PHE:HD1	1.82	0.44
1:D:190:ARG:C	1:D:197:THR:HG23	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:O	1:D:257:GLN:HA	2.16	0.44
1:D:524:GLU:HB3	2:D:890:HOH:O	2.16	0.44
1:B:584:GLN:HA	2:B:1120:HOH:O	2.17	0.44
1:C:571:ARG:NE	2:C:853:HOH:O	2.41	0.44
1:D:22:ALA:HB3	1:D:73:MSE:HE2	1.99	0.44
1:D:39:PRO:CG	1:D:222:VAL:HG22	2.45	0.44
1:D:65:VAL:HG12	2:D:837:HOH:O	2.17	0.44
1:D:77:ALA:HB2	2:D:907:HOH:O	2.17	0.44
1:A:68:ALA:HB1	1:A:70:HIS:CE1	2.53	0.44
1:C:42:TYR:O	1:C:46:ARG:HB2	2.18	0.44
1:D:61:ARG:CZ	1:D:63:ARG:NH2	2.80	0.44
1:D:205:VAL:CG2	1:D:206:LEU:N	2.80	0.44
1:D:282:PRO:HG2	2:D:880:HOH:O	2.17	0.44
1:D:644:ALA:O	1:D:648:LEU:HG	2.18	0.44
1:A:58:TRP:CD1	1:A:306:GLN:HG3	2.52	0.44
1:A:374:ALA:HB3	1:A:428:THR:CG2	2.43	0.44
1:B:527:ARG:NH1	1:B:527:ARG:HB2	2.33	0.44
1:B:594:PRO:CG	1:B:597:LEU:HD21	2.46	0.44
1:C:39:PRO:O	1:C:42:TYR:HB3	2.18	0.44
1:C:404:VAL:HG12	1:D:164:GLU:OE2	2.17	0.44
1:C:423:ARG:NH2	2:C:850:HOH:O	2.50	0.44
1:D:349:ILE:HG13	1:D:353:ALA:HB3	2.00	0.44
1:D:595:PRO:HB3	2:D:922:HOH:O	2.17	0.44
1:D:36:GLY:CA	2:D:848:HOH:O	2.65	0.44
1:D:59:PRO:HB2	1:D:309:TRP:CH2	2.52	0.44
1:D:63:ARG:HH21	1:D:63:ARG:CG	2.26	0.44
1:D:229:ARG:O	1:D:233:LYS:HG2	2.17	0.44
1:A:496:TYR:O	1:A:500:VAL:HG23	2.18	0.44
1:C:405:ARG:HH12	1:D:163:MSE:CE	2.13	0.44
1:D:269:PRO:HG2	1:D:270:GLU:H	1.81	0.44
1:D:336:PRO:HB2	1:D:337:PRO:HD2	1.99	0.44
1:D:492:TYR:CE1	1:D:523:PRO:HG3	2.53	0.44
1:A:247:ARG:HG3	2:A:1178:HOH:O	2.17	0.44
1:B:283:TYR:HA	1:B:284:PRO:HD3	1.79	0.44
1:B:342:PRO:HB3	1:B:495:PHE:CD2	2.53	0.44
1:C:80:HIS:CD2	2:C:932:HOH:O	2.71	0.44
1:D:148:VAL:HG12	2:D:899:HOH:O	2.17	0.44
1:A:545:VAL:HB	1:A:599:VAL:HG22	2.00	0.44
1:B:35:MSE:HE1	1:B:254:SER:HB3	1.99	0.44
1:B:540:GLU:HG2	2:B:1110:HOH:O	2.18	0.44
1:C:359:LEU:HB3	1:C:384:ALA:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD3	1:A:46:ARG:C	2.43	0.43
1:B:289:PRO:HG2	1:B:292:VAL:HG23	2.00	0.43
1:B:562:LEU:HD23	1:B:562:LEU:C	2.43	0.43
1:C:608:LEU:HD13	1:D:612:ARG:HH11	1.83	0.43
1:D:19:ALA:HA	1:D:73:MSE:HE2	2.00	0.43
1:D:124:ILE:CG2	1:D:125:SER:N	2.81	0.43
1:D:196:PRO:HD2	1:D:199:LEU:HD11	2.00	0.43
1:D:197:THR:C	1:D:199:LEU:H	2.26	0.43
1:D:295:HIS:CE1	2:D:879:HOH:O	2.71	0.43
1:D:352:ARG:HA	1:D:513:LEU:HD13	1.99	0.43
1:A:6:ASP:OD1	1:A:7:LEU:HD22	2.18	0.43
1:A:461:LEU:C	1:A:461:LEU:HD12	2.43	0.43
1:B:220:GLU:OE1	1:B:247:ARG:NH1	2.51	0.43
1:C:197:THR:C	1:C:199:LEU:H	2.26	0.43
1:D:133:ALA:HB2	2:D:849:HOH:O	2.17	0.43
1:D:256:LYS:O	1:D:262:ALA:HB2	2.18	0.43
1:D:288:VAL:O	1:D:293:TYR:HE2	2.01	0.43
1:C:188:ASP:OD1	1:C:190:ARG:CZ	2.67	0.43
1:D:93:SER:HA	2:D:906:HOH:O	2.17	0.43
1:D:416:LEU:HB2	1:D:424:ALA:HB3	2.00	0.43
1:B:527:ARG:HB2	1:B:527:ARG:HH11	1.83	0.43
1:B:629:TYR:CD1	1:B:630:PRO:HA	2.53	0.43
2:C:901:HOH:O	1:D:480:MSE:HE2	2.17	0.43
1:D:44:LEU:HA	1:D:48:VAL:HG13	1.96	0.43
1:D:116:THR:OG1	1:D:446:MSE:HG2	2.19	0.43
1:D:416:LEU:HD13	2:D:923:HOH:O	2.18	0.43
1:D:630:PRO:O	1:D:634:GLU:HG3	2.18	0.43
1:C:335:LEU:HD12	1:C:336:PRO:HD2	2.00	0.43
1:D:62:ASP:HA	2:D:852:HOH:O	2.18	0.43
1:D:141:PHE:O	1:D:142:ASN:C	2.60	0.43
1:D:349:ILE:HG13	1:D:350:ALA:N	2.34	0.43
1:C:230:LYS:HE2	1:C:230:LYS:HB3	1.89	0.43
1:C:407:HIS:HB3	2:C:904:HOH:O	2.18	0.43
1:C:418:LEU:HD11	1:C:446:MSE:SE	2.68	0.43
1:C:627:ALA:HB3	1:C:632:VAL:HB	2.00	0.43
1:D:191:ILE:HG13	2:D:937:HOH:O	2.18	0.43
1:C:429:PHE:HD1	1:C:455:THR:HG23	1.84	0.43
1:D:46:ARG:HA	1:D:298:MSE:SE	2.68	0.43
1:A:282:PRO:HA	2:A:990:HOH:O	2.19	0.43
1:A:404:VAL:HG12	1:B:164:GLU:OE2	2.19	0.43
1:A:405:ARG:HH12	1:B:163:MSE:HE2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:LEU:HD23	2:C:895:HOH:O	2.18	0.43
1:C:34:PRO:HA	1:C:74:LEU:HD13	2.00	0.43
1:C:136:LYS:HG3	1:C:422:TYR:CZ	2.54	0.43
1:D:133:ALA:HA	2:D:812:HOH:O	2.19	0.43
1:D:260:ALA:N	2:D:887:HOH:O	2.52	0.43
1:C:349:ILE:HD11	1:C:491:ALA:HB2	2.01	0.43
1:D:141:PHE:HA	2:D:908:HOH:O	2.19	0.43
1:D:252:PHE:CB	2:D:848:HOH:O	2.67	0.43
1:D:364:PRO:HD2	2:D:886:HOH:O	2.18	0.43
1:A:46:ARG:NH2	1:A:298:MSE:HE1	2.34	0.43
1:C:224:ASP:OD2	1:C:227:ALA:HB2	2.19	0.43
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.82	0.43
1:D:191:ILE:N	1:D:197:THR:HG23	2.33	0.43
1:D:380:ASN:HB3	1:D:382:THR:HG23	2.01	0.43
1:D:461:LEU:HD12	1:D:462:GLY:N	2.33	0.43
1:A:33:MSE:CE	1:A:71:GLY:HA3	2.49	0.42
1:A:540:GLU:HA	1:A:540:GLU:OE1	2.19	0.42
1:B:311:LYS:HD2	2:B:885:HOH:O	2.19	0.42
1:C:87:PRO:HG2	1:C:90:GLU:HG2	2.02	0.42
1:C:242:THR:CG2	2:C:939:HOH:O	2.64	0.42
1:C:400:LEU:HD12	1:C:400:LEU:N	2.34	0.42
1:C:629:TYR:CD1	1:C:630:PRO:HA	2.55	0.42
1:D:25:LYS:NZ	1:D:92:LYS:HB3	2.34	0.42
1:D:34:PRO:HA	2:D:829:HOH:O	2.19	0.42
1:D:111:PRO:HG3	2:D:792:HOH:O	2.18	0.42
1:C:392:ARG:NH1	2:C:884:HOH:O	2.50	0.42
1:C:635:ARG:HG2	1:C:635:ARG:HH11	1.84	0.42
1:D:120:LEU:H	1:D:120:LEU:CD2	2.32	0.42
1:D:148:VAL:HG23	1:D:313:LEU:HD22	2.01	0.42
1:D:240:ARG:HB3	1:D:241:PRO:HD2	2.00	0.42
1:A:296:MSE:O	1:A:298:MSE:HG2	2.18	0.42
1:A:437:ARG:HG2	2:A:1162:HOH:O	2.19	0.42
1:C:198:ASP:C	2:C:908:HOH:O	2.62	0.42
1:C:295:HIS:CD2	1:C:296:MSE:CE	3.02	0.42
1:C:329:ARG:NH2	1:C:334:GLU:O	2.52	0.42
1:C:404:VAL:HG21	1:D:160:GLY:CA	2.50	0.42
1:D:61:ARG:NH1	1:D:63:ARG:NH2	2.68	0.42
1:D:68:ALA:HB1	1:D:70:HIS:CD2	2.53	0.42
1:D:79:LEU:HD13	1:D:111:PRO:O	2.19	0.42
1:D:508:PRO:HD2	2:D:874:HOH:O	2.18	0.42
1:D:557:LEU:CD2	1:D:572:VAL:HG11	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:O	1:A:573:VAL:HG13	2.20	0.42
1:D:58:TRP:CH2	1:D:305:TRP:HB3	2.54	0.42
1:D:107:ARG:HD3	1:D:108:GLY:H	1.85	0.42
1:D:186:TRP:N	2:D:834:HOH:O	2.52	0.42
1:A:489:ALA:N	2:A:1175:HOH:O	2.52	0.42
1:B:630:PRO:O	1:B:634:GLU:HG3	2.19	0.42
1:C:647:PHE:CE2	1:C:651:VAL:HG22	2.55	0.42
1:D:394:ASN:C	1:D:394:ASN:HD22	2.27	0.42
1:D:498:TRP:O	1:D:502:LEU:HB2	2.19	0.42
1:D:636:LEU:HD12	1:D:636:LEU:HA	1.80	0.42
1:A:110:THR:HB	1:A:113:VAL:CG2	2.48	0.42
1:A:608:LEU:HD22	1:B:612:ARG:NH1	2.35	0.42
1:B:427:GLY:HA2	1:B:453:VAL:O	2.19	0.42
1:C:128:VAL:HG21	1:C:170:ALA:HB1	2.01	0.42
1:C:169:GLU:HB3	1:C:405:ARG:HD3	2.01	0.42
1:D:20:ILE:HD11	1:D:35:MSE:CG	2.44	0.42
1:D:314:GLU:O	1:D:317:ALA:HB3	2.19	0.42
1:D:327:LEU:O	1:D:331:LEU:CB	2.67	0.42
1:D:631:GLU:O	1:D:635:ARG:HG3	2.20	0.42
1:A:226:GLU:HG3	1:A:230:LYS:HE3	2.02	0.42
1:A:339:PRO:HB3	1:A:365:ARG:NH1	2.34	0.42
1:A:417:ASN:ND2	1:A:423:ARG:HA	2.34	0.42
1:B:332:ARG:HE	1:B:334:GLU:CD	2.27	0.42
1:C:218:ARG:HD3	1:C:245:ALA:HB3	2.01	0.42
1:D:72:SER:HB2	1:D:76:TYR:CE2	2.54	0.42
1:D:216:THR:HG22	1:D:243:LEU:HB3	2.01	0.42
1:D:301:LYS:HB2	2:D:807:HOH:O	2.19	0.42
1:D:354:ALA:CB	1:D:491:ALA:HA	2.50	0.42
1:A:329:ARG:NH1	1:A:336:PRO:HD3	2.34	0.42
1:C:31:PRO:O	1:C:34:PRO:HD2	2.20	0.42
1:C:230:LYS:O	1:C:234:LEU:HG	2.20	0.42
1:D:197:THR:C	1:D:199:LEU:N	2.78	0.42
1:D:266:PRO:C	2:D:858:HOH:O	2.60	0.42
1:D:484:PHE:HA	1:D:579:GLU:CG	2.47	0.42
1:A:636:LEU:HD23	1:A:636:LEU:HA	1.91	0.42
1:C:132:LEU:HD23	1:C:132:LEU:O	2.20	0.42
1:C:208:ARG:O	1:C:211:ALA:HB3	2.19	0.42
1:C:323:LEU:N	1:C:323:LEU:HD12	2.34	0.42
1:D:46:ARG:HG2	1:D:46:ARG:NH1	2.34	0.42
1:D:537:GLU:HG2	1:D:560:GLN:HE22	1.85	0.42
1:D:640:PRO:HG2	1:D:641:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HB2	1:B:76:TYR:CE2	2.55	0.42
1:B:289:PRO:HB2	1:B:291:GLU:CD	2.44	0.42
1:C:68:ALA:HB1	1:C:70:HIS:CE1	2.55	0.42
1:C:150:ASP:C	2:C:924:HOH:O	2.63	0.42
1:C:493:GLU:HG2	1:C:529:LEU:CD1	2.50	0.42
1:D:222:VAL:HG13	1:D:223:ASN:N	2.35	0.42
1:D:252:PHE:CA	1:D:257:GLN:HE21	2.33	0.42
1:D:286:PHE:HA	2:D:905:HOH:O	2.20	0.42
1:D:329:ARG:HG2	1:D:329:ARG:NH1	2.32	0.42
1:A:545:VAL:HG22	1:A:571:ARG:HG2	2.02	0.41
1:C:307:GLU:HG3	1:C:308:ALA:N	2.34	0.41
1:C:373:SER:CA	1:C:409:MSE:HE1	2.50	0.41
1:C:429:PHE:HD2	1:C:432:PHE:HE2	1.68	0.41
1:D:63:ARG:NH2	1:D:63:ARG:CG	2.83	0.41
1:D:561:ALA:O	1:D:564:ARG:HB3	2.20	0.41
1:A:587:ALA:O	1:A:591:GLU:HG3	2.20	0.41
1:B:285:PRO:O	1:B:286:PHE:HB2	2.19	0.41
1:C:457:ASP:HB3	1:C:512:VAL:HG12	2.03	0.41
1:D:461:LEU:CA	1:D:515:ARG:HD3	2.51	0.41
1:D:544:GLY:HA3	1:D:647:PHE:CE1	2.55	0.41
1:A:334:GLU:CD	2:A:1176:HOH:O	2.64	0.41
1:C:80:HIS:HD2	2:C:932:HOH:O	2.04	0.41
1:C:95:ARG:HH11	1:D:463:GLU:CB	2.34	0.41
1:D:100:LYS:HD2	2:D:882:HOH:O	2.20	0.41
1:D:132:LEU:HD23	1:D:132:LEU:C	2.44	0.41
1:D:324:HIS:C	1:D:326:GLU:N	2.69	0.41
1:D:326:GLU:OE2	1:D:329:ARG:NH2	2.54	0.41
1:D:338:LEU:HD21	1:D:503:ARG:NH1	2.35	0.41
1:D:347:LYS:HA	2:D:925:HOH:O	2.21	0.41
1:D:377:THR:N	1:D:378:PRO:HD2	2.35	0.41
1:B:59:PRO:CG	1:B:309:TRP:CH2	2.99	0.41
1:C:163:MSE:HE3	1:C:200:ALA:O	2.20	0.41
1:C:197:THR:HG22	1:C:201:PHE:HB3	2.01	0.41
1:D:143:ARG:HB3	1:D:144:PRO:HD2	2.03	0.41
1:A:43:LEU:HD23	1:A:47:GLU:HB2	2.02	0.41
1:A:434:ASP:OD1	1:B:437:ARG:HG2	2.20	0.41
1:B:190:ARG:N	1:B:190:ARG:CD	2.82	0.41
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.90	0.41
1:C:16:ARG:HG2	1:C:35:MSE:HA	2.03	0.41
1:D:206:LEU:HB3	1:D:210:ARG:HH22	1.86	0.41
1:D:394:ASN:ND2	1:D:394:ASN:C	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ALA:O	1:B:554:HIS:HE1	2.02	0.41
1:B:541:GLU:CB	1:B:569:ARG:NH2	2.83	0.41
1:D:25:LYS:HD2	2:D:919:HOH:O	2.20	0.41
1:D:61:ARG:HH21	1:D:61:ARG:HG2	1.85	0.41
1:D:292:VAL:O	1:D:296:MSE:HG2	2.20	0.41
1:D:527:ARG:NE	1:D:530:LEU:HD12	2.36	0.41
1:A:380:ASN:HA	1:A:455:THR:HG21	2.03	0.41
1:A:480:MSE:HA	1:A:481:PRO:HD3	1.93	0.41
1:B:163:MSE:HE3	1:B:201:PHE:CG	2.55	0.41
1:B:559:ALA:O	1:B:563:LEU:HD22	2.21	0.41
1:C:458:SER:HA	1:C:470:PRO:HD2	2.03	0.41
1:C:538:ASP:CG	2:C:853:HOH:O	2.63	0.41
1:C:571:ARG:CG	2:C:853:HOH:O	2.67	0.41
1:C:611:GLU:CD	1:D:612:ARG:HG3	2.45	0.41
1:D:62:ASP:OD1	1:D:152:TYR:HB2	2.21	0.41
1:D:94:PHE:HD2	2:D:891:HOH:O	2.03	0.41
1:D:120:LEU:HD22	1:D:120:LEU:N	2.34	0.41
1:D:522:SER:HB2	1:D:525:LYS:HB2	2.03	0.41
1:A:53:PRO:HB3	1:A:84:TYR:CD1	2.56	0.41
1:C:42:TYR:CE1	1:C:296:MSE:HE1	2.56	0.41
1:D:60:ASP:O	1:D:151:HIS:HB3	2.21	0.41
1:D:61:ARG:NH1	1:D:63:ARG:HH22	2.18	0.41
1:D:318:ARG:HG2	1:D:318:ARG:NH2	2.36	0.41
1:D:461:LEU:HD12	1:D:461:LEU:C	2.45	0.41
1:B:51:HIS:CE1	2:B:1087:HOH:O	2.74	0.41
1:C:52:ASN:HB2	2:C:929:HOH:O	2.21	0.41
1:C:169:GLU:CB	1:C:408:ALA:HB2	2.51	0.41
1:C:327:LEU:CA	2:C:870:HOH:O	2.69	0.41
1:D:35:MSE:SE	1:D:267:LEU:HD11	2.70	0.41
1:D:124:ILE:HG23	1:D:125:SER:N	2.35	0.41
1:D:317:ALA:O	1:D:320:TYR:O	2.39	0.41
1:D:372:GLY:N	2:D:861:HOH:O	2.52	0.41
1:C:65:VAL:HG13	1:C:115:VAL:HG12	2.02	0.41
1:C:547:VAL:O	1:C:601:ALA:HA	2.21	0.41
1:D:205:VAL:HG23	1:D:206:LEU:N	2.34	0.41
1:D:359:LEU:HD13	1:D:425:TYR:OH	2.21	0.41
1:D:408:ALA:O	1:D:412:ILE:HG13	2.21	0.41
1:A:54:LEU:HD21	1:A:299:ARG:CB	2.51	0.40
1:A:309:TRP:CH2	1:A:313:LEU:HD11	2.56	0.40
1:C:409:MSE:HE2	1:C:426:GLY:HA2	2.03	0.40
1:C:472:GLU:OE2	2:C:901:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:PHE:HA	1:D:20:ILE:CG1	2.50	0.40
1:D:351:THR:HA	1:D:354:ALA:HB3	2.03	0.40
1:D:415:GLY:O	1:D:416:LEU:C	2.64	0.40
1:D:432:PHE:C	1:D:434:ASP:N	2.77	0.40
1:D:632:VAL:HG13	1:D:633:TYR:N	2.37	0.40
1:A:430:LEU:HA	1:A:454:PHE:HB3	2.02	0.40
1:A:579:GLU:CD	1:A:579:GLU:N	2.75	0.40
1:B:268:GLY:O	1:B:272:VAL:HG23	2.21	0.40
1:B:561:ALA:O	1:B:564:ARG:HB3	2.21	0.40
1:C:214:TRP:CD2	1:C:241:PRO:HG2	2.56	0.40
1:C:558:ARG:NH1	2:C:814:HOH:O	2.54	0.40
1:D:20:ILE:CD1	1:D:35:MSE:SE	3.19	0.40
1:D:75:LEU:HD22	1:D:79:LEU:HG	2.02	0.40
1:A:594:PRO:HG2	1:A:597:LEU:CD2	2.51	0.40
1:B:555:LEU:HD21	1:B:639:THR:C	2.47	0.40
1:B:572:VAL:HG22	2:B:1114:HOH:O	2.20	0.40
1:C:168:GLY:N	2:C:787:HOH:O	2.54	0.40
1:C:370:LEU:C	2:C:879:HOH:O	2.64	0.40
1:C:371:GLY:HA3	1:C:387:MSE:HE1	2.04	0.40
1:C:377:THR:HB	1:C:378:PRO:CD	2.51	0.40
1:C:461:LEU:HG	1:C:469:GLN:HG2	2.02	0.40
1:C:641:GLU:O	1:C:645:GLU:HG3	2.21	0.40
1:D:146:HIS:HB3	1:D:316:TYR:CD1	2.56	0.40
1:D:161:ASP:HB3	2:D:844:HOH:O	2.21	0.40
1:D:233:LYS:O	1:D:237:LEU:HD13	2.21	0.40
1:D:555:LEU:HD23	1:D:555:LEU:O	2.21	0.40
1:A:135:ARG:HD3	1:A:135:ARG:C	2.47	0.40
1:A:469:GLN:OE1	1:A:624:GLY:HA3	2.21	0.40
1:A:604:ALA:HA	1:A:638:PHE:CZ	2.56	0.40
1:C:120:LEU:HD12	1:C:161:ASP:OD1	2.22	0.40
1:C:343:PRO:HG2	1:C:345:PHE:CZ	2.56	0.40
1:C:529:LEU:C	1:C:529:LEU:HD23	2.46	0.40
1:C:539:VAL:HG12	1:C:564:ARG:HH22	1.86	0.40
1:C:563:LEU:HD11	1:C:644:ALA:CA	2.50	0.40
1:D:469:GLN:OE1	1:D:624:GLY:HA3	2.21	0.40
1:D:486:ILE:HA	1:D:576:PRO:O	2.22	0.40
1:A:560:GLN:NE2	2:A:1170:HOH:O	2.54	0.40
1:B:220:GLU:OE2	1:B:247:ARG:NH1	2.55	0.40
1:B:442:LEU:CG	1:B:446:MSE:HE2	2.46	0.40
1:B:584:GLN:O	1:B:589:ARG:NH2	2.54	0.40
2:C:901:HOH:O	1:D:441:ARG:CG	2.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:THR:OG1	1:D:429:PHE:N	2.54	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	645/651 (99%)	632 (98%)	13 (2%)	0	100	100
1	B	645/651 (99%)	628 (97%)	17 (3%)	0	100	100
1	C	645/651 (99%)	619 (96%)	25 (4%)	1 (0%)	43	44
1	D	645/651 (99%)	584 (90%)	54 (8%)	7 (1%)	11	8
All	All	2580/2604 (99%)	2463 (96%)	109 (4%)	8 (0%)	36	36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	PRO
1	D	142	ASN
1	D	31	PRO
1	D	224	ASP
1	D	325	GLN
1	C	31	PRO
1	D	103	GLY
1	D	269	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/507 (102%)	502 (97%)	15 (3%)	37	42
1	B	517/507 (102%)	499 (96%)	18 (4%)	32	35
1	C	517/507 (102%)	499 (96%)	18 (4%)	32	35
1	D	517/507 (102%)	496 (96%)	21 (4%)	27	29
All	All	2068/2028 (102%)	1996 (96%)	72 (4%)	32	35

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	43	LEU
1	A	73	MSE
1	A	75	LEU
1	A	86	LEU
1	A	132	LEU
1	A	225	LEU
1	A	239	GLU
1	A	247	ARG
1	A	307	GLU
1	A	475	MSE
1	A	536	LEU
1	A	555	LEU
1	A	597	LEU
1	A	608	LEU
1	B	43	LEU
1	B	54	LEU
1	B	86	LEU
1	B	107	ARG
1	B	132	LEU
1	B	190	ARG
1	B	228	LEU
1	B	267	LEU
1	B	300	GLU
1	B	331	LEU
1	B	369	LEU
1	B	502	LEU
1	B	529	LEU
1	B	536	LEU
1	B	546	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	555	LEU
1	B	563	LEU
1	B	636	LEU
1	C	47	GLU
1	C	75	LEU
1	C	134	GLU
1	C	247	ARG
1	C	261	LYS
1	C	290	GLU
1	C	299	ARG
1	C	300	GLU
1	C	328	MSE
1	C	331	LEU
1	C	349	ILE
1	C	423	ARG
1	C	483	LEU
1	C	502	LEU
1	C	536	LEU
1	C	537	GLU
1	C	555	LEU
1	C	564	ARG
1	D	7	LEU
1	D	63	ARG
1	D	70	HIS
1	D	75	LEU
1	D	99	SER
1	D	107	ARG
1	D	124	ILE
1	D	134	GLU
1	D	205	VAL
1	D	215	GLN
1	D	220	GLU
1	D	236	LYS
1	D	239	GLU
1	D	277	ARG
1	D	314	GLU
1	D	338	LEU
1	D	368	GLU
1	D	529	LEU
1	D	555	LEU
1	D	579	GLU
1	D	580	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	215	GLN
1	A	380	ASN
1	A	394	ASN
1	A	417	ASN
1	A	554	HIS
1	A	560	GLN
1	A	584	GLN
1	B	109	HIS
1	B	215	GLN
1	B	278	ASN
1	B	324	HIS
1	B	380	ASN
1	B	394	ASN
1	B	417	ASN
1	B	482	ASN
1	B	554	HIS
1	C	70	HIS
1	C	96	GLN
1	C	122	GLN
1	C	146	HIS
1	C	215	GLN
1	C	263	HIS
1	C	381	ASN
1	C	394	ASN
1	C	482	ASN
1	C	543	GLN
1	D	30	HIS
1	D	122	GLN
1	D	215	GLN
1	D	257	GLN
1	D	295	HIS
1	D	394	ASN
1	D	401	HIS
1	D	482	ASN
1	D	543	GLN
1	D	560	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	632/651 (97%)	0.03	6 (0%) 81 83	14, 24, 38, 46	0
1	B	632/651 (97%)	0.01	6 (0%) 81 83	14, 25, 38, 54	0
1	C	632/651 (97%)	1.08	90 (14%) 6 6	27, 39, 52, 59	0
1	D	632/651 (97%)	1.75	233 (36%) 1 1	28, 47, 59, 64	0
All	All	2528/2604 (97%)	0.72	335 (13%) 7 7	14, 34, 55, 64	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	PHE	6.2
1	D	42	TYR	5.2
1	D	149	VAL	4.9
1	D	191	ILE	4.8
1	D	138	ALA	4.7
1	D	153	THR	4.4
1	D	217	LEU	4.4
1	D	309	TRP	4.4
1	D	18	LEU	4.4
1	B	651	VAL	4.3
1	D	38	ALA	4.3
1	C	147	VAL	4.3
1	D	137	LEU	4.3
1	D	252	PHE	4.3
1	D	205	VAL	4.2
1	D	154	TYR	4.0
1	D	209	TYR	4.0
1	D	41	ALA	4.0
1	C	148	VAL	4.0
1	D	10	LEU	4.0
1	D	222	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	395	PRO	3.9
1	D	13	ASN	3.9
1	D	246	VAL	3.8
1	D	17	PHE	3.8
1	D	287	VAL	3.8
1	D	32	GLY	3.8
1	D	40	LEU	3.8
1	D	228	LEU	3.8
1	D	58	TRP	3.7
1	D	152	TYR	3.7
1	D	75	LEU	3.7
1	D	20	ILE	3.7
1	D	250	ILE	3.7
1	D	64	PHE	3.7
1	D	331	LEU	3.7
1	D	141	PHE	3.7
1	D	232	ILE	3.7
1	D	241	PRO	3.6
1	D	305	TRP	3.6
1	C	141	PHE	3.6
1	D	15	ILE	3.6
1	D	26	ALA	3.6
1	C	199	LEU	3.6
1	D	321	PRO	3.6
1	D	371	GLY	3.6
1	D	70	HIS	3.6
1	D	240	ARG	3.6
1	D	211	ALA	3.6
1	D	301	LYS	3.6
1	D	12	VAL	3.6
1	D	39	PRO	3.5
1	D	74	LEU	3.5
1	D	16	ARG	3.5
1	D	227	ALA	3.5
1	D	78	VAL	3.5
1	D	179	LEU	3.4
1	C	177	TRP	3.4
1	D	62	ASP	3.4
1	D	323	LEU	3.4
1	D	56	PRO	3.4
1	D	198	ASP	3.4
1	D	86	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	312	ALA	3.4
1	D	317	ALA	3.4
1	D	225	LEU	3.4
1	D	185	PHE	3.4
1	D	186	TRP	3.3
1	D	324	HIS	3.3
1	D	48	VAL	3.3
1	D	19	ALA	3.3
1	C	205	VAL	3.3
1	D	316	TYR	3.3
1	D	243	LEU	3.3
1	D	536	LEU	3.3
1	C	322	ASP	3.3
1	C	386	GLY	3.3
1	D	112	GLY	3.3
1	C	260	ALA	3.3
1	D	157	ALA	3.3
1	D	130	LEU	3.3
1	D	267	LEU	3.3
1	C	214	TRP	3.2
1	C	211	ALA	3.2
1	D	271	ALA	3.2
1	D	302	GLY	3.2
1	D	313	LEU	3.2
1	D	370	LEU	3.2
1	D	190	ARG	3.2
1	D	59	PRO	3.2
1	D	155	VAL	3.2
1	D	315	ALA	3.2
1	D	34	PRO	3.2
1	D	292	VAL	3.1
1	D	54	LEU	3.1
1	D	418	LEU	3.1
1	D	242	THR	3.1
1	D	416	LEU	3.1
1	C	251	GLY	3.1
1	D	213	GLY	3.1
1	D	234	LEU	3.1
1	D	14	ALA	3.1
1	D	113	VAL	3.1
1	D	359	LEU	3.1
1	D	275	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	174	ALA	3.0
1	C	319	ALA	3.0
1	D	329	ARG	3.0
1	D	180	SER	3.0
1	D	218	ARG	3.0
1	D	253	GLY	3.0
1	D	111	PRO	3.0
1	C	209	TYR	3.0
1	D	148	VAL	3.0
1	D	320	TYR	3.0
1	D	21	ASP	2.9
1	C	364	PRO	2.9
1	D	284	PRO	2.9
1	D	68	ALA	2.9
1	C	175	GLY	2.9
1	D	76	TYR	2.9
1	C	309	TRP	2.9
1	D	279	LEU	2.9
1	D	327	LEU	2.9
1	D	238	ASP	2.9
1	C	130	LEU	2.8
1	D	44	LEU	2.8
1	D	162	LEU	2.8
1	C	522	SER	2.8
1	B	251	GLY	2.8
1	D	361	LEU	2.8
1	D	396	LEU	2.8
1	D	117	THR	2.8
1	D	288	VAL	2.8
1	D	187	ASP	2.8
1	C	131	ALA	2.8
1	D	237	LEU	2.8
1	C	304	ALA	2.8
1	D	139	ALA	2.8
1	D	283	TYR	2.8
1	D	29	GLY	2.7
1	D	447	GLY	2.7
1	D	260	ALA	2.7
1	C	338	LEU	2.7
1	C	115	VAL	2.7
1	D	223	ASN	2.7
1	D	308	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	323	LEU	2.7
1	D	63	ARG	2.7
1	D	303	ARG	2.7
1	D	272	VAL	2.7
1	D	183	ILE	2.7
1	D	83	GLY	2.7
1	C	218	ARG	2.7
1	D	207	ALA	2.7
1	D	255	PRO	2.7
1	D	269	PRO	2.7
1	D	249	HIS	2.7
1	D	399	TYR	2.7
1	C	108	GLY	2.7
1	D	397	GLY	2.7
1	D	214	TRP	2.7
1	C	353	ALA	2.6
1	D	88	LEU	2.6
1	D	216	THR	2.6
1	D	194	ASP	2.6
1	D	133	ALA	2.6
1	D	142	ASN	2.6
1	D	304	ALA	2.6
1	C	179	LEU	2.6
1	D	147	VAL	2.6
1	D	420	GLY	2.6
1	D	295	HIS	2.6
1	D	170	ALA	2.6
1	C	343	PRO	2.6
1	C	201	PHE	2.6
1	D	197	THR	2.6
1	D	202	THR	2.6
1	D	330	ARG	2.6
1	D	523	PRO	2.6
1	D	201	PHE	2.5
1	A	307	GLU	2.5
1	C	651	VAL	2.5
1	D	236	LYS	2.5
1	D	43	LEU	2.5
1	D	335	LEU	2.5
1	D	281	TRP	2.5
1	C	165	GLY	2.5
1	D	175	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	234	LEU	2.5
1	C	331	LEU	2.5
1	C	366	LEU	2.5
1	D	580	LEU	2.5
1	C	390	PHE	2.5
1	D	567	GLY	2.5
1	D	124	ILE	2.5
1	D	134	GLU	2.5
1	C	312	ALA	2.5
1	D	144	PRO	2.5
1	D	266	PRO	2.5
1	C	166	VAL	2.4
1	D	65	VAL	2.4
1	D	128	VAL	2.4
1	D	193	ILE	2.5
1	D	72	SER	2.4
1	C	233	LYS	2.4
1	D	81	LEU	2.4
1	C	405	ARG	2.4
1	D	109	HIS	2.4
1	D	135	ARG	2.4
1	A	6	ASP	2.4
1	D	258	ASP	2.4
1	C	42	TYR	2.4
1	D	212	TYR	2.4
1	C	231	ALA	2.4
1	D	131	ALA	2.4
1	D	262	ALA	2.4
1	A	54	LEU	2.4
1	D	206	LEU	2.4
1	D	263	HIS	2.4
1	D	495	PHE	2.4
1	D	150	ASP	2.4
1	D	244	ILE	2.4
1	D	422	TYR	2.4
1	D	189	ASN	2.4
1	C	232	ILE	2.4
1	D	184	VAL	2.4
1	D	31	PRO	2.4
1	D	177	TRP	2.4
1	D	285	PRO	2.4
1	D	84	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	226	GLU	2.3
1	D	415	GLY	2.3
1	D	390	PHE	2.3
1	D	542	PRO	2.3
1	C	217	LEU	2.3
1	D	502	LEU	2.3
1	D	393	ALA	2.3
1	C	5	ARG	2.3
1	D	66	LEU	2.3
1	D	123	GLY	2.3
1	C	349	ILE	2.3
1	B	570	VAL	2.3
1	D	52	ASN	2.3
1	B	564	ARG	2.3
1	C	135	ARG	2.3
1	C	204	ASP	2.3
1	D	60	ASP	2.3
1	C	465	GLY	2.3
1	C	206	LEU	2.3
1	C	327	LEU	2.3
1	D	132	LEU	2.3
1	D	192	SER	2.2
1	C	144	PRO	2.2
1	C	149	VAL	2.2
1	D	23	VAL	2.2
1	C	227	ALA	2.2
1	D	274	ALA	2.2
1	C	325	GLN	2.2
1	C	248	SER	2.2
1	C	216	THR	2.2
1	C	133	ALA	2.2
1	C	139	ALA	2.2
1	D	174	ALA	2.2
1	C	400	LEU	2.2
1	D	229	ARG	2.2
1	D	101	THR	2.2
1	D	282	PRO	2.2
1	D	219	VAL	2.2
1	D	251	GLY	2.2
1	C	308	ALA	2.2
1	D	22	ALA	2.2
1	D	325	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	520	LEU	2.2
1	D	521	LEU	2.2
1	D	597	LEU	2.2
1	D	6	ASP	2.2
1	D	85	ASP	2.2
1	D	368	GLU	2.1
1	C	426	GLY	2.1
1	D	268	GLY	2.1
1	B	597	LEU	2.1
1	C	120	LEU	2.1
1	C	370	LEU	2.1
1	C	259	SER	2.1
1	D	11	SER	2.1
1	C	428	THR	2.1
1	D	116	THR	2.1
1	C	252	PHE	2.1
1	A	651	VAL	2.1
1	C	184	VAL	2.1
1	C	222	VAL	2.1
1	D	264	GLY	2.1
1	C	245	ALA	2.1
1	D	319	ALA	2.1
1	D	67	SER	2.1
1	D	47	GLU	2.1
1	D	204	ASP	2.1
1	C	63	ARG	2.1
1	C	305	TRP	2.1
1	C	315	ALA	2.1
1	D	77	ALA	2.1
1	C	88	LEU	2.1
1	D	173	LEU	2.1
1	C	541	GLU	2.1
1	C	142	ASN	2.1
1	C	399	TYR	2.1
1	B	566	LYS	2.1
1	C	48	VAL	2.1
1	D	374	ALA	2.1
1	D	7	LEU	2.0
1	D	369	LEU	2.0
1	C	189	ASN	2.0
1	C	365	ARG	2.0
1	D	143	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	51	HIS	2.0
1	D	82	THR	2.0
1	D	367	PRO	2.0
1	D	165	GLY	2.0
1	D	372	GLY	2.0
1	C	246	VAL	2.0
1	C	431	VAL	2.0
1	A	312	ALA	2.0
1	C	200	ALA	2.0
1	C	510	ALA	2.0
1	C	580	LEU	2.0
1	D	257	GLN	2.0
1	D	562	LEU	2.0
1	A	303	ARG	2.0
1	C	423	ARG	2.0
1	C	249	HIS	2.0
1	C	230	LYS	2.0
1	D	87	PRO	2.0
1	D	110	THR	2.0
1	D	103	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.