



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 1ROV / pdb_00001rov
Title : Lipoygenase-3 Treated with Cumene Hydroperoxide
Authors : Vahedi-Faridi, A.; Brault, P.A.; Shah, P.; Kim, Y.W.; Dunham, W.R.; Funk, M.O.
Deposited on : 2003-12-02
Resolution : 2.00 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

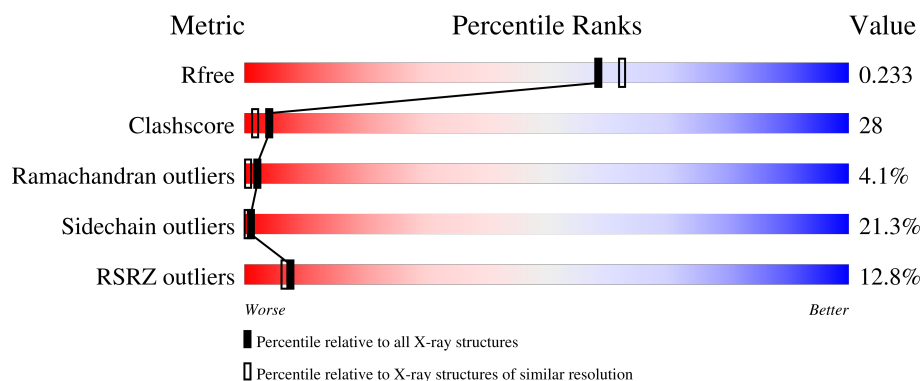
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	857	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	HTR	A	519	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7000 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 Seed lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6698	4278	1149	1253	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	HTR	TRP	modified residue	UNP P09186
A	565	HLU	LEU	modified residue	UNP P09186

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

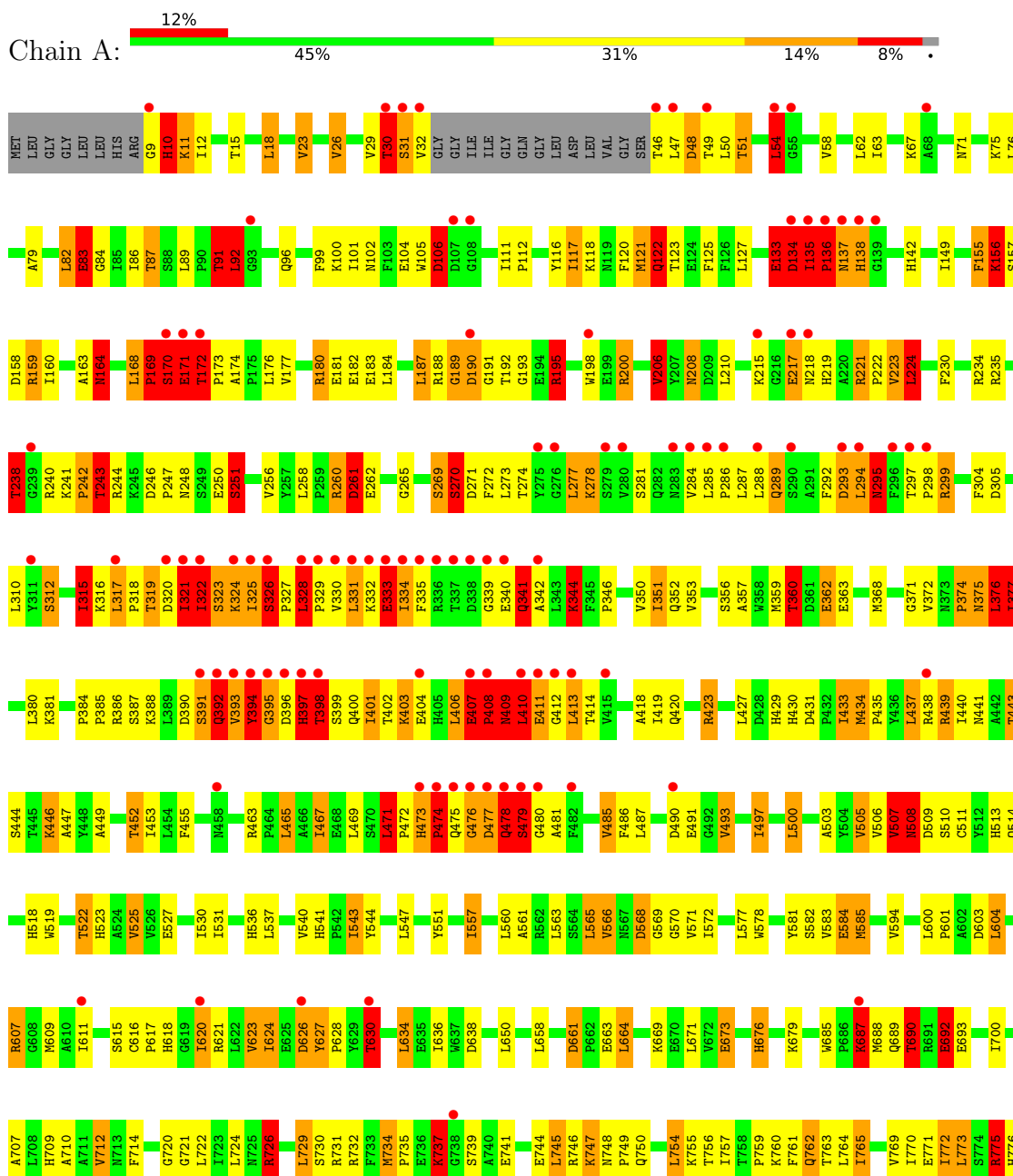
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	301	Total	O	0	0
			301	301		

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: Seed lipoxygenase-3





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.00Å 136.90Å 61.51Å 90.00° 96.24° 90.00°	Depositor
Resolution (Å)	43.37 – 2.00 43.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.0 (43.37-2.00) 78.1 (43.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.231 0.223 , 0.233	Depositor DCC
R_{free} test set	2419 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HTR, FE, HLU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.84	137/6841 (2.0%)	2.07	297/9286 (3.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	17

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	734	MET	SD-CE	-25.18	1.16	1.79
1	A	190	ASP	CA-C	19.03	1.78	1.52
1	A	585	MET	SD-CE	-16.02	1.39	1.79
1	A	676	HIS	ND1-CE1	12.70	1.45	1.32
1	A	190	ASP	C-O	11.73	1.38	1.24
1	A	171	GLU	N-CA	11.69	1.61	1.46
1	A	169	PRO	CA-C	-11.54	1.36	1.52
1	A	676	HIS	CE1-NE2	11.52	1.44	1.32
1	A	261	ASP	N-CA	11.22	1.60	1.46
1	A	473	HIS	CA-CB	10.68	1.61	1.52
1	A	117	ILE	CA-CB	10.43	1.69	1.54
1	A	789	PRO	CA-C	10.13	1.66	1.52
1	A	397	HIS	CA-C	9.95	1.66	1.52
1	A	676	HIS	CD2-NE2	-9.94	1.26	1.37
1	A	433	ILE	CA-CB	9.83	1.66	1.54
1	A	164	ASN	CB-CG	-9.74	1.27	1.52
1	A	407	GLU	CA-C	9.73	1.65	1.52
1	A	170	SER	CA-C	9.31	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	833	MET	SD-CE	-9.24	1.56	1.79
1	A	377	ILE	CA-CB	9.17	1.63	1.54
1	A	770	ILE	CA-CB	9.01	1.67	1.54
1	A	121	MET	CA-C	-8.94	1.40	1.52
1	A	790	ASN	CA-CB	-8.92	1.41	1.53
1	A	134	ASP	CA-C	-8.76	1.40	1.53
1	A	375	ASN	CB-CG	-8.75	1.30	1.52
1	A	261	ASP	CA-CB	8.68	1.68	1.53
1	A	49	THR	CA-CB	8.58	1.69	1.53
1	A	297	THR	CA-CB	8.56	1.68	1.54
1	A	398	THR	CA-CB	8.43	1.65	1.53
1	A	479	SER	N-CA	8.14	1.56	1.46
1	A	101	ILE	CA-CB	8.12	1.65	1.54
1	A	135	ILE	CA-CB	8.10	1.64	1.54
1	A	359	MET	SD-CE	-7.95	1.59	1.79
1	A	620	ILE	CA-CB	7.93	1.66	1.54
1	A	160	ILE	CA-CB	7.91	1.64	1.54
1	A	844	GLU	N-CA	7.86	1.56	1.46
1	A	206	VAL	CB-CG1	-7.71	1.27	1.52
1	A	785	GLU	C-O	-7.70	1.14	1.24
1	A	785	GLU	CA-C	-7.55	1.42	1.52
1	A	169	PRO	N-CA	-7.53	1.37	1.47
1	A	475	GLN	CA-C	7.52	1.61	1.52
1	A	787	ASP	CA-C	7.47	1.61	1.52
1	A	467	ILE	CA-CB	7.41	1.63	1.54
1	A	315	ILE	CA-CB	7.35	1.63	1.54
1	A	434	MET	SD-CE	-7.22	1.61	1.79
1	A	344	LYS	CA-C	7.21	1.62	1.52
1	A	700	ILE	CA-CB	7.18	1.62	1.54
1	A	120	PHE	CA-C	-7.03	1.42	1.52
1	A	177	VAL	CA-CB	6.97	1.62	1.54
1	A	172	THR	CB-CG2	-6.93	1.29	1.52
1	A	848	PHE	N-CA	6.92	1.55	1.46
1	A	174	ALA	CA-CB	6.88	1.61	1.53
1	A	407	GLU	N-CA	6.79	1.55	1.46
1	A	787	ASP	CB-CG	6.73	1.68	1.52
1	A	785	GLU	CB-CG	6.72	1.72	1.52
1	A	788	ASN	CB-CG	-6.67	1.35	1.52
1	A	224	LEU	CA-C	-6.67	1.44	1.52
1	A	531	ILE	CA-CB	6.64	1.62	1.54
1	A	737	LYS	CA-CB	6.59	1.64	1.53
1	A	843	LYS	C-O	-6.58	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	MET	SD-CE	-6.50	1.63	1.79
1	A	401	ILE	CA-C	6.48	1.60	1.52
1	A	322	ILE	CA-C	6.43	1.59	1.52
1	A	757	ILE	CA-CB	6.42	1.63	1.54
1	A	685	TRP	CA-C	-6.36	1.45	1.52
1	A	159	ARG	CD-NE	-6.32	1.37	1.46
1	A	785	GLU	CA-CB	6.28	1.64	1.53
1	A	414	THR	CA-CB	6.28	1.62	1.53
1	A	238	THR	CB-CG2	-6.23	1.31	1.52
1	A	661	ASP	C-O	-6.17	1.16	1.24
1	A	260	ARG	CA-C	-6.14	1.44	1.53
1	A	847	THR	CA-CB	-6.12	1.42	1.53
1	A	791	TRP	N-CA	-5.97	1.38	1.46
1	A	298	PRO	CA-C	5.92	1.59	1.52
1	A	137	ASN	CB-CG	5.92	1.66	1.52
1	A	171	GLU	C-O	5.90	1.31	1.24
1	A	505	VAL	CA-CB	-5.89	1.47	1.54
1	A	293	ASP	N-CA	5.89	1.53	1.46
1	A	360	THR	CB-CG2	-5.88	1.33	1.52
1	A	772	ILE	CA-C	5.85	1.59	1.52
1	A	471	LEU	C-O	5.84	1.28	1.24
1	A	123	THR	CA-C	5.84	1.60	1.52
1	A	687	LYS	N-CA	-5.83	1.38	1.46
1	A	294	LEU	N-CA	5.82	1.53	1.46
1	A	844	GLU	CA-C	-5.79	1.45	1.52
1	A	785	GLU	CD-OE1	5.79	1.36	1.25
1	A	293	ASP	CA-C	5.78	1.60	1.52
1	A	503	ALA	CA-CB	-5.74	1.44	1.53
1	A	775	ARG	CB-CG	-5.74	1.35	1.52
1	A	690	THR	CB-CG2	-5.73	1.33	1.52
1	A	99	PHE	CA-C	-5.61	1.45	1.52
1	A	295	ASN	CA-C	5.60	1.60	1.52
1	A	238	THR	C-O	-5.58	1.17	1.24
1	A	299	ARG	CA-C	5.57	1.60	1.52
1	A	841	SER	CA-C	-5.57	1.45	1.52
1	A	26	VAL	CA-CB	5.56	1.61	1.54
1	A	522	THR	CA-CB	-5.54	1.44	1.53
1	A	362	GLU	CG-CD	5.54	1.66	1.52
1	A	294	LEU	CA-C	5.53	1.60	1.52
1	A	398	THR	CA-C	5.51	1.59	1.52
1	A	83	GLU	N-CA	-5.50	1.39	1.46
1	A	737	LYS	CA-C	-5.50	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	855	ILE	CA-CB	5.47	1.59	1.53
1	A	392	GLN	CA-C	5.47	1.60	1.53
1	A	319	THR	CA-CB	5.46	1.61	1.53
1	A	609	MET	SD-CE	-5.45	1.66	1.79
1	A	317	LEU	CA-C	5.43	1.59	1.52
1	A	18	LEU	CA-C	-5.43	1.45	1.52
1	A	630	THR	CB-CG2	-5.43	1.34	1.52
1	A	172	THR	C-N	5.41	1.40	1.33
1	A	10	HIS	CA-C	5.39	1.59	1.52
1	A	630	THR	CA-CB	-5.38	1.44	1.53
1	A	134	ASP	CA-CB	5.38	1.62	1.53
1	A	419	ILE	CA-CB	5.38	1.60	1.54
1	A	333	GLU	CA-C	5.36	1.59	1.52
1	A	408	PRO	CA-C	5.36	1.60	1.52
1	A	710	ALA	CA-CB	5.33	1.61	1.53
1	A	10	HIS	N-CA	5.32	1.53	1.46
1	A	617	PRO	CA-C	5.29	1.59	1.52
1	A	624	ILE	CA-C	5.29	1.59	1.52
1	A	170	SER	C-O	5.22	1.30	1.24
1	A	570	GLY	C-O	-5.22	1.18	1.23
1	A	500	LEU	CG-CD1	-5.18	1.35	1.52
1	A	744	GLU	CA-C	5.18	1.59	1.52
1	A	394	TYR	N-CA	5.17	1.53	1.46
1	A	92	LEU	C-O	-5.15	1.17	1.24
1	A	262	GLU	CA-C	5.14	1.59	1.52
1	A	414	THR	CA-C	5.13	1.60	1.53
1	A	222	PRO	CA-C	-5.12	1.46	1.52
1	A	47	LEU	N-CA	5.10	1.52	1.46
1	A	790	ASN	CB-CG	-5.09	1.39	1.52
1	A	822	GLU	CA-C	5.08	1.59	1.52
1	A	452	THR	CB-CG2	-5.06	1.35	1.52
1	A	755	LYS	CA-C	-5.03	1.45	1.52
1	A	30	THR	CA-C	5.02	1.59	1.52
1	A	776	HIS	CA-CB	-5.02	1.46	1.53
1	A	270	SER	CA-C	-5.01	1.46	1.52

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	THR	N-CA-C	22.33	136.59	108.45
1	A	476	GLY	N-CA-C	22.10	132.01	111.67
1	A	473	HIS	CB-CA-C	18.21	124.13	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ASN	N-CA-C	-16.57	94.38	112.93
1	A	169	PRO	CA-C-O	-15.29	92.77	120.60
1	A	607	ARG	NE-CZ-NH2	-15.01	105.69	119.20
1	A	393	VAL	N-CA-C	14.35	125.78	112.29
1	A	847	THR	CA-C-N	-14.26	94.30	121.54
1	A	847	THR	C-N-CA	-14.26	94.30	121.54
1	A	159	ARG	NE-CZ-NH2	-14.19	106.43	119.20
1	A	189	GLY	CA-C-N	-12.45	97.77	121.54
1	A	189	GLY	C-N-CA	-12.45	97.77	121.54
1	A	159	ARG	CG-CD-NE	-12.30	84.95	112.00
1	A	747	LYS	N-CA-C	12.01	124.45	111.36
1	A	195	ARG	NE-CZ-NH1	-11.97	109.53	121.50
1	A	375	ASN	N-CA-C	11.80	127.86	113.23
1	A	240	ARG	NE-CZ-NH2	-11.70	108.67	119.20
1	A	726	ARG	NE-CZ-NH1	-11.36	110.14	121.50
1	A	847	THR	N-CA-CB	-10.62	94.00	111.20
1	A	493	VAL	CB-CA-C	-10.19	97.17	112.05
1	A	135	ILE	N-CA-CB	10.10	125.35	111.21
1	A	261	ASP	N-CA-CB	10.05	127.47	110.49
1	A	726	ARG	NE-CZ-NH2	10.01	128.21	119.20
1	A	221	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	A	786	ARG	CG-CD-NE	-9.91	90.21	112.00
1	A	164	ASN	CB-CG-ND2	-9.85	101.63	116.40
1	A	396	ASP	N-CA-C	-9.81	99.63	112.68
1	A	676	HIS	ND1-CE1-NE2	-9.79	98.61	108.40
1	A	712	VAL	N-CA-CB	-9.67	97.37	112.07
1	A	170	SER	CA-C-N	9.50	139.68	121.54
1	A	170	SER	C-N-CA	9.50	139.68	121.54
1	A	238	THR	O-C-N	-9.48	112.02	123.30
1	A	836	THR	N-CA-CB	-9.24	95.73	110.98
1	A	408	PRO	N-CA-C	9.21	131.45	112.47
1	A	785	GLU	CA-CB-CG	9.17	132.45	114.10
1	A	155	PHE	N-CA-C	9.10	128.21	110.56
1	A	164	ASN	CA-CB-CG	-9.08	103.52	112.60
1	A	607	ARG	NE-CZ-NH1	9.06	130.56	121.50
1	A	375	ASN	CB-CG-OD1	-9.04	102.72	120.80
1	A	342	ALA	N-CA-C	8.98	123.25	110.23
1	A	121	MET	CA-C-N	-8.87	104.60	121.54
1	A	121	MET	C-N-CA	-8.87	104.60	121.54
1	A	570	GLY	N-CA-C	8.84	126.39	111.98
1	A	54	LEU	N-CA-C	8.78	125.07	113.30
1	A	411	GLU	N-CA-C	8.77	129.48	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH1	8.44	129.94	121.50
1	A	847	THR	O-C-N	-8.35	111.92	123.11
1	A	394	TYR	CB-CA-C	-8.33	91.96	110.21
1	A	238	THR	CA-C-N	-8.32	105.11	121.41
1	A	238	THR	C-N-CA	-8.32	105.11	121.41
1	A	623	VAL	CB-CA-C	8.31	124.06	111.68
1	A	240	ARG	NE-CZ-NH1	8.25	129.75	121.50
1	A	200	ARG	NE-CZ-NH2	-8.24	111.78	119.20
1	A	133	GLU	CA-C-N	-8.15	106.50	123.20
1	A	133	GLU	C-N-CA	-8.15	106.50	123.20
1	A	775	ARG	CB-CA-C	-8.10	95.87	109.48
1	A	785	GLU	CG-CD-OE2	-8.10	99.77	118.40
1	A	843	LYS	CA-C-N	-8.10	106.07	121.54
1	A	843	LYS	C-N-CA	-8.10	106.07	121.54
1	A	731	ARG	CB-CA-C	-8.08	96.86	110.44
1	A	260	ARG	CA-C-N	-7.96	106.33	121.54
1	A	260	ARG	C-N-CA	-7.96	106.33	121.54
1	A	785	GLU	CA-C-O	-7.96	109.13	120.51
1	A	172	THR	CA-CB-OG1	7.91	121.46	109.60
1	A	452	THR	CA-CB-CG2	7.83	123.82	110.50
1	A	395	GLY	N-CA-C	7.75	131.55	113.18
1	A	260	ARG	N-CA-C	-7.74	100.31	110.53
1	A	48	ASP	N-CA-C	7.64	127.08	110.80
1	A	188	ARG	NE-CZ-NH2	-7.63	112.33	119.20
1	A	79	ALA	N-CA-C	-7.61	98.54	109.96
1	A	190	ASP	CA-C-O	7.61	131.38	120.51
1	A	825	ARG	NE-CZ-NH2	7.54	125.98	119.20
1	A	390	ASP	N-CA-C	7.53	126.83	110.80
1	A	480	GLY	N-CA-C	7.48	130.91	113.18
1	A	848	PHE	CB-CA-C	7.47	125.28	110.42
1	A	570	GLY	CA-C-O	-7.43	114.44	122.76
1	A	182	GLU	CA-CB-CG	7.43	128.96	114.10
1	A	288	LEU	N-CA-C	-7.42	104.83	114.04
1	A	376	LEU	N-CA-C	7.42	122.62	112.90
1	A	841	SER	CB-CA-C	-7.40	96.85	109.51
1	A	720	GLY	CA-C-O	7.39	125.77	119.04
1	A	785	GLU	CA-C-N	-7.39	112.21	122.93
1	A	785	GLU	C-N-CA	-7.39	112.21	122.93
1	A	134	ASP	CA-C-O	-7.36	111.67	121.46
1	A	623	VAL	N-CA-C	-7.30	97.58	109.12
1	A	522	THR	CA-CB-CG2	7.30	122.91	110.50
1	A	341	GLN	N-CA-C	7.28	126.30	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ILE	N-CA-C	7.27	120.81	113.47
1	A	473	HIS	N-CA-CB	-7.19	103.68	111.66
1	A	788	ASN	N-CA-C	7.17	125.65	109.81
1	A	789	PRO	CA-C-N	7.17	134.44	123.04
1	A	789	PRO	C-N-CA	7.17	134.44	123.04
1	A	362	GLU	CB-CG-CD	7.15	124.76	112.60
1	A	374	PRO	CA-C-N	7.14	134.22	121.66
1	A	374	PRO	C-N-CA	7.14	134.22	121.66
1	A	687	LYS	N-CA-C	-7.05	98.20	109.76
1	A	159	ARG	CD-NE-CZ	7.04	134.26	124.40
1	A	676	HIS	N-CA-C	-7.03	102.98	112.26
1	A	344	LYS	N-CA-C	7.02	119.89	110.35
1	A	785	GLU	N-CA-C	-7.01	95.86	110.80
1	A	238	THR	N-CA-CB	-7.00	98.92	110.68
1	A	164	ASN	N-CA-C	7.00	125.70	110.80
1	A	473	HIS	CA-CB-CG	6.98	120.78	113.80
1	A	607	ARG	CD-NE-CZ	6.93	134.11	124.40
1	A	407	GLU	CA-C-N	6.93	128.50	119.84
1	A	407	GLU	C-N-CA	6.93	128.50	119.84
1	A	375	ASN	CB-CG-ND2	6.86	126.69	116.40
1	A	269	SER	CA-C-N	-6.84	108.47	121.54
1	A	269	SER	C-N-CA	-6.84	108.47	121.54
1	A	795	THR	OG1-CB-CG2	6.84	122.97	109.30
1	A	536	HIS	N-CA-C	6.80	123.08	114.31
1	A	163	ALA	CA-C-N	6.78	134.49	121.54
1	A	163	ALA	C-N-CA	6.78	134.49	121.54
1	A	828	CYS	CA-CB-SG	-6.76	98.85	114.40
1	A	138	HIS	N-CA-CB	6.76	120.42	109.95
1	A	566	VAL	N-CA-CB	-6.75	100.02	111.50
1	A	92	LEU	O-C-N	-6.70	113.68	122.59
1	A	843	LYS	O-C-N	-6.67	113.25	122.46
1	A	360	THR	N-CA-CB	-6.66	100.16	110.29
1	A	394	TYR	O-C-N	6.66	131.28	122.43
1	A	413	LEU	N-CA-C	-6.64	100.69	110.52
1	A	260	ARG	O-C-N	-6.61	115.25	122.79
1	A	855	ILE	N-CA-C	-6.60	97.05	107.15
1	A	261	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	321	ILE	CB-CA-C	6.57	117.71	110.62
1	A	223	VAL	N-CA-CB	6.56	119.25	110.26
1	A	265	GLY	N-CA-C	-6.52	102.27	112.58
1	A	159	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	A	92	LEU	CA-C-N	-6.51	108.65	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	LEU	C-N-CA	-6.51	108.65	121.41
1	A	164	ASN	CB-CG-OD1	6.48	133.76	120.80
1	A	375	ASN	CA-CB-CG	-6.47	106.13	112.60
1	A	192	THR	N-CA-C	-6.46	99.48	109.24
1	A	737	LYS	CA-CB-CG	6.37	126.83	114.10
1	A	825	ARG	CB-CG-CD	6.36	125.94	111.30
1	A	439	ARG	N-CA-C	6.34	118.27	111.36
1	A	721	GLY	N-CA-C	-6.33	106.50	114.16
1	A	825	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	A	406	LEU	CA-C-N	6.32	137.22	121.80
1	A	406	LEU	C-N-CA	6.32	137.22	121.80
1	A	616	CYS	N-CA-C	6.29	118.57	110.39
1	A	157	SER	N-CA-C	-6.29	98.74	109.24
1	A	238	THR	N-CA-C	-6.27	98.69	108.90
1	A	394	TYR	N-CA-C	-6.23	105.40	112.87
1	A	473	HIS	CA-C-O	6.23	125.24	120.26
1	A	391	SER	N-CA-C	6.22	122.77	114.12
1	A	195	ARG	CG-CD-NE	6.21	125.66	112.00
1	A	771	GLU	CA-CB-CG	-6.21	101.69	114.10
1	A	329	PRO	N-CA-C	6.18	120.91	111.15
1	A	627	TYR	CB-CA-C	6.13	116.58	110.33
1	A	787	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	295	ASN	N-CA-C	6.10	123.80	110.80
1	A	171	GLU	CA-C-N	-6.09	106.93	121.80
1	A	171	GLU	C-N-CA	-6.09	106.93	121.80
1	A	270	SER	CA-CB-OG	6.08	123.27	111.10
1	A	269	SER	N-CA-C	-6.08	100.83	109.96
1	A	467	ILE	CA-CB-CG1	6.08	120.74	110.40
1	A	584	GLU	CB-CA-C	-6.08	100.70	110.79
1	A	714	PHE	N-CA-C	6.08	120.55	113.20
1	A	836	THR	OG1-CB-CG2	6.07	121.44	109.30
1	A	508	ASN	N-CA-C	-6.07	104.59	111.14
1	A	452	THR	CA-CB-OG1	6.06	118.69	109.60
1	A	467	ILE	CB-CG1-CD1	6.05	126.52	113.80
1	A	168	LEU	N-CA-CB	6.05	118.76	110.05
1	A	493	VAL	N-CA-CB	6.04	120.02	110.54
1	A	507	VAL	N-CA-CB	-6.03	99.86	110.77
1	A	479	SER	N-CA-CB	6.02	120.66	110.49
1	A	844	GLU	CB-CA-C	-6.01	98.45	110.42
1	A	790	ASN	N-CA-C	6.00	120.94	108.53
1	A	261	ASP	CB-CA-C	-5.97	98.53	110.42
1	A	431	ASP	N-CA-C	5.95	122.95	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	O-C-N	5.94	130.61	122.59
1	A	134	ASP	N-CA-C	5.92	119.32	109.96
1	A	188	ARG	CG-CD-NE	-5.92	98.97	112.00
1	A	712	VAL	CG1-CB-CG2	5.91	123.81	110.80
1	A	91	THR	N-CA-CB	-5.91	101.68	110.61
1	A	221	ARG	CG-CD-NE	-5.90	99.02	112.00
1	A	475	GLN	CB-CA-C	-5.86	98.83	109.38
1	A	568	ASP	CA-C-N	-5.85	105.50	122.46
1	A	568	ASP	C-N-CA	-5.85	105.50	122.46
1	A	410	LEU	N-CA-CB	5.83	119.67	110.39
1	A	346	PRO	CA-C-O	-5.82	116.14	120.73
1	A	508	ASN	CB-CA-C	-5.82	101.71	110.90
1	A	234	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	795	THR	N-CA-CB	-5.78	101.32	110.28
1	A	790	ASN	CA-CB-CG	-5.75	106.85	112.60
1	A	136	PRO	N-CA-C	5.74	124.30	112.47
1	A	563	LEU	N-CA-C	5.74	117.62	111.36
1	A	54	LEU	CA-C-N	-5.74	110.16	121.41
1	A	54	LEU	C-N-CA	-5.74	110.16	121.41
1	A	789	PRO	N-CA-C	5.73	124.27	112.47
1	A	401	ILE	N-CA-C	-5.72	102.20	109.58
1	A	692	GLU	CB-CA-C	-5.69	101.34	110.79
1	A	475	GLN	N-CA-C	-5.67	100.46	109.59
1	A	251	SER	CB-CA-C	-5.66	99.62	109.64
1	A	687	LYS	O-C-N	-5.65	116.58	123.19
1	A	775	ARG	CA-C-N	-5.65	114.93	122.72
1	A	775	ARG	C-N-CA	-5.65	114.93	122.72
1	A	827	ARG	CA-C-N	5.64	131.02	122.56
1	A	827	ARG	C-N-CA	5.64	131.02	122.56
1	A	840	PRO	N-CA-C	5.64	121.27	113.65
1	A	507	VAL	CB-CA-C	5.63	121.39	112.26
1	A	514	GLN	N-CA-C	5.62	117.21	111.14
1	A	585	MET	CG-SD-CE	5.62	113.26	100.90
1	A	221	ARG	CD-NE-CZ	5.61	132.25	124.40
1	A	321	ILE	N-CA-CB	-5.61	105.66	112.33
1	A	200	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	478	GLN	N-CA-C	-5.58	100.80	109.72
1	A	577	LEU	N-CA-C	5.58	117.80	111.11
1	A	122	GLN	CB-CG-CD	-5.54	103.19	112.60
1	A	663	GLU	N-CA-C	-5.52	104.90	111.69
1	A	106	ASP	N-CA-C	5.50	116.34	108.74
1	A	352	GLN	N-CA-C	5.49	118.02	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	ARG	CA-C-N	5.49	128.08	120.29
1	A	746	ARG	C-N-CA	5.49	128.08	120.29
1	A	673	GLU	N-CA-C	5.49	119.14	112.23
1	A	353	VAL	CB-CA-C	5.46	116.63	111.44
1	A	410	LEU	N-CA-C	5.46	118.32	109.86
1	A	851	ILE	CB-CG1-CD1	5.45	125.25	113.80
1	A	543	ILE	CB-CG1-CD1	5.45	125.25	113.80
1	A	687	LYS	CB-CA-C	5.45	118.63	109.48
1	A	23	VAL	N-CA-CB	-5.45	103.79	112.07
1	A	857	ILE	N-CA-C	-5.44	95.77	111.00
1	A	700	ILE	N-CA-CB	5.43	116.91	110.55
1	A	381	LYS	N-CA-C	-5.43	106.78	113.41
1	A	413	LEU	CB-CA-C	-5.43	100.32	109.83
1	A	748	ASN	N-CA-CB	-5.43	104.58	110.71
1	A	322	ILE	CB-CG1-CD1	5.40	125.14	113.80
1	A	371	GLY	CA-C-O	-5.40	116.39	121.90
1	A	485	VAL	N-CA-C	5.40	116.36	108.53
1	A	169	PRO	O-C-N	5.38	129.90	122.64
1	A	87	THR	N-CA-C	5.37	118.05	111.82
1	A	12	ILE	CB-CG1-CD1	5.37	125.07	113.80
1	A	764	LEU	N-CA-C	5.37	117.13	111.28
1	A	510	SER	CB-CA-C	-5.37	102.46	110.88
1	A	854	SER	N-CA-C	5.36	116.42	108.86
1	A	687	LYS	CA-C-N	-5.36	114.12	122.05
1	A	687	LYS	C-N-CA	-5.36	114.12	122.05
1	A	206	VAL	CG1-CB-CG2	-5.35	99.03	110.80
1	A	836	THR	CA-CB-CG2	5.35	119.59	110.50
1	A	172	THR	N-CA-C	5.34	121.61	109.81
1	A	238	THR	CB-CA-C	5.34	119.48	109.71
1	A	775	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	322	ILE	N-CA-C	-5.29	105.88	113.07
1	A	615	SER	CB-CA-C	-5.28	100.85	110.63
1	A	783	LEU	O-C-N	5.28	128.17	122.15
1	A	795	THR	CA-CB-CG2	5.28	119.47	110.50
1	A	843	LYS	CA-CB-CG	5.28	124.65	114.10
1	A	269	SER	CA-C-O	-5.27	114.75	120.81
1	A	91	THR	CB-CA-C	5.27	119.08	110.17
1	A	795	THR	CA-CB-OG1	5.27	117.50	109.60
1	A	180	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	478	GLN	CB-CA-C	5.26	119.69	109.33
1	A	193	GLY	CA-C-O	-5.25	117.79	121.88
1	A	47	LEU	CA-C-N	5.24	131.55	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	LEU	C-N-CA	5.24	131.55	121.54
1	A	71	ASN	N-CA-C	5.24	121.96	110.80
1	A	51	THR	N-CA-C	-5.22	105.67	111.36
1	A	449	ALA	N-CA-C	-5.22	100.73	109.24
1	A	474	PRO	CA-C-N	5.22	130.50	122.93
1	A	474	PRO	C-N-CA	5.22	130.50	122.93
1	A	679	LYS	CD-CE-NZ	5.22	128.59	111.90
1	A	195	ARG	NH1-CZ-NH2	-5.21	112.52	119.30
1	A	240	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	443	THR	N-CA-C	-5.19	101.81	109.86
1	A	840	PRO	CA-C-N	5.19	130.94	122.07
1	A	840	PRO	C-N-CA	5.19	130.94	122.07
1	A	339	GLY	N-CA-C	-5.18	100.90	113.18
1	A	217	GLU	CB-CA-C	5.18	119.95	110.11
1	A	628	PRO	N-CA-C	5.18	122.17	113.78
1	A	284	VAL	N-CA-C	5.17	117.55	111.09
1	A	707	ALA	N-CA-C	5.16	116.98	111.36
1	A	26	VAL	N-CA-C	5.15	116.49	110.62
1	A	636	ILE	CB-CG1-CD1	5.14	124.60	113.80
1	A	485	VAL	CB-CA-C	5.14	118.62	110.81
1	A	351	ILE	N-CA-C	5.12	117.82	112.90
1	A	844	GLU	N-CA-CB	5.12	119.14	110.49
1	A	775	ARG	N-CA-C	5.11	118.15	109.76
1	A	788	ASN	CA-C-N	5.11	126.23	119.84
1	A	788	ASN	C-N-CA	5.11	126.23	119.84
1	A	765	ILE	CB-CG1-CD1	5.11	124.52	113.80
1	A	169	PRO	N-CA-C	5.08	122.94	112.47
1	A	623	VAL	O-C-N	-5.07	116.27	122.61
1	A	584	GLU	N-CA-CB	5.07	117.57	110.12
1	A	791	TRP	N-CA-CB	-5.07	101.98	110.39
1	A	400	GLN	CB-CG-CD	5.06	121.20	112.60
1	A	506	VAL	N-CA-C	5.04	115.76	110.62
1	A	315	ILE	N-CA-CB	5.03	116.21	110.72
1	A	396	ASP	CB-CA-C	5.03	118.65	110.24
1	A	407	GLU	CA-CB-CG	5.03	124.17	114.10
1	A	582	SER	N-CA-C	5.03	117.16	111.02
1	A	183	GLU	N-CA-C	-5.02	105.88	111.36
1	A	234	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	328	LEU	CB-CA-C	5.02	116.36	108.63
1	A	763	THR	N-CA-C	-5.02	105.81	111.28
1	A	352	GLN	CA-C-N	-5.01	118.02	123.08
1	A	352	GLN	C-N-CA	-5.01	118.02	123.08

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	452	THR	CB
1	A	519	HTR	CB
1	A	522	THR	CB
1	A	795	THR	CB

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLN	Mainchain
1	A	133	GLU	Peptide
1	A	134	ASP	Mainchain
1	A	135	ILE	Mainchain
1	A	164	ASN	Mainchain
1	A	169	PRO	Peptide,Mainchain
1	A	171	GLU	Peptide,Mainchain
1	A	195	ARG	Sidechain
1	A	242	PRO	Mainchain
1	A	375	ASN	Sidechain,Mainchain
1	A	410	LEU	Peptide
1	A	478	GLN	Peptide
1	A	569	GLY	Peptide
1	A	726	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	6698	0	6614	368	1
2	A	1	0	0	0	0
3	A	301	0	0	78	1
All	All	7000	0	6614	368	2

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 (368) 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:190:ASP:C	1:A:190:ASP:CA	1.78	1.53
1:A:149:ILE:HG13	3:A:1034:HOH:O	1.16	1.28
1:A:121:MET:O	1:A:122:GLN:CB	1.79	1.25
1:A:734:MET:SD	1:A:734:MET:CE	1.16	1.25
1:A:851:ILE:HG12	3:A:951:HOH:O	1.06	1.22
1:A:269:SER:O	1:A:270:SER:CB	1.82	1.17
1:A:734:MET:SD	1:A:734:MET:HE3	1.74	1.14
1:A:857:ILE:HG13	3:A:935:HOH:O	1.44	1.13
1:A:734:MET:CE	1:A:734:MET:CG	2.28	1.11
1:A:734:MET:SD	1:A:734:MET:HE2	1.74	1.10
1:A:843:LYS:O	1:A:844:GLU:CB	1.91	1.09
1:A:789:PRO:C	3:A:1041:HOH:O	1.96	1.09
1:A:169:PRO:C	1:A:171:GLU:H	1.55	1.08
1:A:734:MET:SD	1:A:734:MET:HE1	1.74	1.06
1:A:572:ILE:HG12	3:A:1043:HOH:O	1.55	1.03
1:A:322:ILE:HG13	1:A:341:GLN:O	1.59	1.02
1:A:121:MET:O	1:A:122:GLN:HB2	1.21	1.00
1:A:269:SER:O	1:A:270:SER:HB3	1.18	1.00
1:A:171:GLU:HB3	1:A:180:ARG:HD3	1.44	0.99
1:A:287:LEU:HB3	1:A:321:ILE:HD11	1.44	0.98
1:A:806:ASN:HB2	3:A:924:HOH:O	1.63	0.98
1:A:127:LEU:CB	1:A:149:ILE:HD11	1.92	0.98
1:A:356:SER:HB3	3:A:1042:HOH:O	1.67	0.95
1:A:843:LYS:O	1:A:844:GLU:HB3	1.63	0.95
1:A:581:TYR:HB2	1:A:585:MET:HE2	1.49	0.94
1:A:127:LEU:HB2	1:A:149:ILE:HD11	1.48	0.94
1:A:578:TRP:HB3	1:A:585:MET:HE3	1.49	0.94
1:A:304:PHE:H	1:A:750:GLN:NE2	1.65	0.93
1:A:688:MET:N	3:A:957:HOH:O	2.02	0.92
1:A:473:HIS:HB2	1:A:476:GLY:C	1.94	0.91
1:A:783:LEU:O	1:A:785:GLU:N	2.02	0.91
1:A:518:HIS:O	1:A:522:THR:HG22	1.70	0.91
1:A:441:ASN:HD21	1:A:447:ALA:H	1.02	0.91
1:A:788:ASN:HB3	1:A:789:PRO:HD3	1.51	0.90
1:A:604:LEU:HD11	1:A:630:THR:OG1	1.71	0.90
1:A:785:GLU:HB2	1:A:805:GLY:HA3	1.53	0.89
1:A:412:GLY:HA2	3:A:945:HOH:O	1.73	0.89
1:A:788:ASN:CB	1:A:789:PRO:HD3	2.03	0.89
1:A:687:LYS:CA	3:A:957:HOH:O	2.20	0.89
1:A:376:LEU:HD22	3:A:1016:HOH:O	1.73	0.87
1:A:334:ILE:HB	3:A:1054:HOH:O	1.76	0.86
1:A:287:LEU:CB	1:A:321:ILE:HD11	2.04	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:HIS:O	1:A:474:PRO:C	2.20	0.85
1:A:190:ASP:OD1	1:A:191:GLY:N	2.09	0.85
1:A:687:LYS:C	3:A:957:HOH:O	2.20	0.85
1:A:441:ASN:ND2	1:A:447:ALA:H	1.75	0.84
1:A:170:SER:HB3	1:A:172:THR:OG1	1.76	0.84
1:A:190:ASP:CG	1:A:191:GLY:H	1.86	0.84
1:A:423:ARG:NH1	1:A:455:PHE:CZ	2.46	0.83
1:A:406:LEU:O	3:A:968:HOH:O	1.95	0.83
1:A:394:TYR:HB3	1:A:481:ALA:HB2	1.58	0.82
1:A:806:ASN:CB	3:A:924:HOH:O	2.21	0.82
1:A:819:ASN:ND2	1:A:827:ARG:HE	1.77	0.81
1:A:241:LYS:O	1:A:251:SER:OG	1.99	0.81
1:A:626:ASP:HB2	3:A:927:HOH:O	1.79	0.81
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.61	0.80
1:A:843:LYS:O	1:A:844:GLU:HB2	1.81	0.80
1:A:169:PRO:C	1:A:171:GLU:N	2.30	0.79
1:A:340:GLU:HG3	1:A:341:GLN:HE21	1.46	0.79
1:A:441:ASN:HD21	1:A:447:ALA:N	1.80	0.79
1:A:295:ASN:OD1	1:A:295:ASN:O	2.00	0.79
1:A:578:TRP:HB3	1:A:585:MET:CE	2.13	0.79
1:A:260:ARG:O	1:A:261:ASP:HB2	1.84	0.78
1:A:319:THR:N	1:A:341:GLN:OE1	2.17	0.78
1:A:409:ASN:HD22	1:A:409:ASN:C	1.92	0.78
1:A:83:GLU:C	1:A:83:GLU:OE2	2.27	0.77
1:A:190:ASP:CA	1:A:191:GLY:N	2.47	0.77
1:A:127:LEU:HB3	1:A:149:ILE:HD11	1.66	0.76
1:A:819:ASN:HD22	1:A:827:ARG:HE	1.32	0.75
1:A:393:VAL:C	1:A:395:GLY:H	1.93	0.75
1:A:304:PHE:H	1:A:750:GLN:HE21	1.31	0.74
1:A:206:VAL:HG12	1:A:224:LEU:O	1.87	0.74
1:A:190:ASP:C	1:A:190:ASP:HA	2.06	0.74
1:A:393:VAL:HG12	1:A:393:VAL:O	1.87	0.74
1:A:857:ILE:O	3:A:859:HOH:O	2.06	0.73
1:A:782:TYR:H	1:A:786:ARG:HD2	1.51	0.73
1:A:836:THR:HG21	3:A:1033:HOH:O	1.87	0.73
1:A:92:LEU:O	1:A:96:GLN:NE2	2.21	0.72
1:A:287:LEU:HB3	1:A:321:ILE:CD1	2.18	0.72
1:A:322:ILE:O	1:A:326:SER:HB2	1.89	0.72
1:A:581:TYR:CB	1:A:585:MET:HE2	2.18	0.72
1:A:326:SER:H	1:A:327:PRO:HD2	1.54	0.72
1:A:438:ARG:HB2	1:A:473:HIS:HE1	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:HB2	3:A:882:HOH:O	1.89	0.71
1:A:243:THR:HG22	1:A:246:ASP:H	1.53	0.71
1:A:789:PRO:HD2	3:A:1041:HOH:O	1.90	0.71
1:A:127:LEU:HB2	1:A:149:ILE:CD1	2.20	0.71
1:A:260:ARG:O	1:A:261:ASP:CB	2.36	0.71
1:A:319:THR:HA	1:A:341:GLN:HE22	1.54	0.70
1:A:376:LEU:HB2	3:A:1016:HOH:O	1.92	0.70
1:A:155:PHE:O	1:A:156:LYS:HB2	1.90	0.70
1:A:241:LYS:HE2	1:A:244:ARG:HH21	1.57	0.70
1:A:326:SER:H	1:A:327:PRO:CD	2.05	0.70
1:A:392:GLN:OE1	1:A:477:ASP:O	2.10	0.69
1:A:135:ILE:HG23	1:A:136:PRO:HD2	1.74	0.69
1:A:121:MET:O	1:A:122:GLN:CG	2.40	0.69
1:A:823:LYS:HE2	3:A:1047:HOH:O	1.91	0.69
1:A:238:THR:HG21	3:A:930:HOH:O	1.92	0.69
1:A:189:GLY:O	1:A:190:ASP:HB3	1.93	0.69
1:A:29:VAL:O	1:A:30:THR:C	2.36	0.68
1:A:318:PRO:C	1:A:341:GLN:OE1	2.36	0.68
1:A:376:LEU:CB	3:A:1016:HOH:O	2.41	0.68
1:A:626:ASP:CB	3:A:927:HOH:O	2.38	0.68
1:A:775:ARG:HH11	1:A:775:ARG:CG	2.04	0.68
1:A:658:LEU:HD11	1:A:664:LEU:HD12	1.75	0.68
1:A:785:GLU:HB2	1:A:805:GLY:CA	2.23	0.67
1:A:169:PRO:CA	1:A:171:GLU:H	2.06	0.67
1:A:292:PHE:O	1:A:294:LEU:N	2.28	0.67
1:A:775:ARG:CG	1:A:775:ARG:NH1	2.54	0.67
1:A:321:ILE:HD13	1:A:324:LYS:HB3	1.77	0.67
1:A:277:LEU:HD22	1:A:772:ILE:HG21	1.76	0.67
1:A:357:ALA:HB1	1:A:830:PRO:HB2	1.77	0.67
1:A:433:ILE:HG12	1:A:437:LEU:HD13	1.76	0.67
1:A:692:GLU:OE1	3:A:933:HOH:O	2.11	0.66
1:A:377:ILE:HB	3:A:1004:HOH:O	1.96	0.66
1:A:440:ILE:HD11	1:A:585:MET:HE1	1.78	0.65
1:A:189:GLY:O	1:A:190:ASP:CB	2.35	0.65
1:A:783:LEU:C	1:A:785:GLU:H	2.03	0.65
1:A:10:HIS:CD2	1:A:135:ILE:HB	2.31	0.65
1:A:412:GLY:CA	3:A:945:HOH:O	2.37	0.65
1:A:125:PHE:CE1	1:A:149:ILE:HD13	2.32	0.65
1:A:626:ASP:HB2	3:A:892:HOH:O	1.96	0.65
1:A:525:VAL:HG22	1:A:676:HIS:HE1	1.62	0.65
1:A:243:THR:CG2	1:A:246:ASP:H	2.09	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:SER:H	1:A:392:GLN:HE21	1.43	0.65
1:A:393:VAL:O	1:A:393:VAL:CG1	2.44	0.65
1:A:241:LYS:CE	1:A:244:ARG:HH21	2.09	0.64
1:A:838:LEU:HA	1:A:851:ILE:HD11	1.78	0.64
1:A:208:ASN:ND2	1:A:235:ARG:HH21	1.95	0.64
1:A:604:LEU:HD11	1:A:630:THR:HG1	1.62	0.64
1:A:522:THR:HG23	1:A:523:HIS:H	1.62	0.64
1:A:83:GLU:OE2	1:A:84:GLY:N	2.30	0.64
1:A:269:SER:O	1:A:270:SER:HB2	1.93	0.64
1:A:690:THR:HG22	1:A:693:GLU:H	1.61	0.63
1:A:618:HIS:HD2	1:A:638:ASP:OD2	1.82	0.63
1:A:318:PRO:HG2	1:A:321:ILE:HG22	1.80	0.63
1:A:149:ILE:N	1:A:149:ILE:HD12	2.13	0.62
1:A:368:MET:HB3	3:A:1004:HOH:O	1.99	0.62
1:A:621:ARG:HD2	3:A:944:HOH:O	1.98	0.62
1:A:83:GLU:OE2	1:A:83:GLU:CA	2.48	0.62
1:A:159:ARG:HD2	3:A:991:HOH:O	2.00	0.61
1:A:51:THR:O	1:A:54:LEU:HB2	2.00	0.61
1:A:171:GLU:CB	1:A:180:ARG:HD3	2.24	0.61
1:A:289:GLN:O	1:A:292:PHE:N	2.33	0.61
1:A:238:THR:CG2	1:A:250:GLU:OE2	2.49	0.60
1:A:687:LYS:O	1:A:693:GLU:OE1	2.20	0.60
1:A:136:PRO:C	1:A:138:HIS:H	2.07	0.59
1:A:315:ILE:HG13	1:A:317:LEU:CD2	2.31	0.59
1:A:584:GLU:HG3	3:A:894:HOH:O	2.01	0.59
1:A:438:ARG:CB	1:A:473:HIS:HE1	2.15	0.59
1:A:384:PRO:HG2	1:A:398:THR:OG1	2.03	0.59
1:A:15:THR:HG23	1:A:86:ILE:HD12	1.85	0.59
1:A:277:LEU:CD2	1:A:772:ILE:HG21	2.32	0.59
1:A:407:GLU:HB2	3:A:972:HOH:O	2.03	0.59
1:A:789:PRO:CD	3:A:1041:HOH:O	2.47	0.58
1:A:292:PHE:O	1:A:294:LEU:C	2.46	0.58
1:A:357:ALA:O	1:A:360:THR:HB	2.03	0.58
1:A:511:CYS:HG	1:A:578:TRP:CG	2.22	0.58
1:A:784:GLY:O	1:A:785:GLU:CB	2.52	0.58
1:A:784:GLY:O	1:A:785:GLU:HB3	2.03	0.58
1:A:687:LYS:HA	3:A:957:HOH:O	1.96	0.58
1:A:409:ASN:C	1:A:409:ASN:ND2	2.62	0.58
1:A:789:PRO:CA	3:A:1041:HOH:O	2.48	0.57
1:A:788:ASN:HB3	1:A:789:PRO:CD	2.28	0.57
1:A:376:LEU:CD2	3:A:1016:HOH:O	2.41	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:CG	3:A:1016:HOH:O	2.52	0.57
1:A:380:LEU:HD12	3:A:1018:HOH:O	2.03	0.57
1:A:561:ALA:HA	1:A:565:HLU:HB	1.87	0.57
1:A:581:TYR:HB2	1:A:585:MET:CE	2.30	0.57
1:A:857:ILE:HA	3:A:935:HOH:O	2.04	0.57
1:A:206:VAL:HG13	3:A:906:HOH:O	2.04	0.57
1:A:557:ILE:HD13	3:A:935:HOH:O	2.05	0.57
1:A:312:SER:O	1:A:344:LYS:HD3	2.05	0.56
1:A:423:ARG:NH1	1:A:455:PHE:CE1	2.74	0.56
1:A:473:HIS:HB2	1:A:477:ASP:N	2.21	0.56
1:A:775:ARG:HH11	1:A:775:ARG:HG3	1.70	0.56
1:A:817:GLU:HG3	3:A:950:HOH:O	2.03	0.56
1:A:469:LEU:HD12	1:A:486:PHE:CE1	2.39	0.56
1:A:603:ASP:OD1	1:A:607:ARG:CD	2.54	0.56
1:A:318:PRO:HA	1:A:341:GLN:OE1	2.06	0.56
1:A:407:GLU:CB	3:A:972:HOH:O	2.53	0.56
1:A:726:ARG:HD3	3:A:962:HOH:O	2.05	0.56
1:A:471:LEU:HB3	1:A:472:PRO:CD	2.36	0.56
1:A:430:HIS:HE1	1:A:434:MET:HE3	1.69	0.56
1:A:169:PRO:HA	1:A:171:GLU:H	1.69	0.56
1:A:669:LYS:HE2	1:A:673:GLU:OE1	2.06	0.55
1:A:360:THR:CG2	1:A:363:GLU:H	2.19	0.55
1:A:687:LYS:HB3	3:A:957:HOH:O	2.05	0.55
1:A:171:GLU:HB3	1:A:180:ARG:CD	2.28	0.55
1:A:318:PRO:CA	1:A:341:GLN:OE1	2.55	0.55
1:A:603:ASP:OD1	1:A:607:ARG:HD2	2.07	0.55
1:A:473:HIS:HB2	1:A:476:GLY:O	2.07	0.55
1:A:380:LEU:CD1	3:A:1018:HOH:O	2.55	0.54
1:A:618:HIS:HE1	3:A:884:HOH:O	1.90	0.54
1:A:393:VAL:C	1:A:395:GLY:N	2.59	0.54
1:A:83:GLU:OE2	1:A:83:GLU:HA	2.07	0.54
1:A:434:MET:HB3	1:A:435:PRO:HD3	1.90	0.54
1:A:438:ARG:HG2	3:A:865:HOH:O	2.07	0.54
1:A:315:ILE:HG13	1:A:317:LEU:HD23	1.88	0.54
1:A:350:VAL:O	1:A:831:VAL:HG23	2.07	0.54
1:A:497:ILE:HD13	1:A:734:MET:HE2	1.89	0.54
1:A:441:ASN:ND2	1:A:446:LYS:HA	2.23	0.54
1:A:455:PHE:HB2	1:A:465:LEU:HD22	1.89	0.54
1:A:135:ILE:HG23	1:A:136:PRO:CD	2.38	0.54
1:A:372:VAL:HG22	1:A:513:HIS:CE1	2.43	0.53
1:A:618:HIS:CD2	1:A:638:ASP:OD2	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HB3	1:A:169:PRO:CD	2.39	0.53
1:A:208:ASN:HD22	1:A:208:ASN:H	1.57	0.53
1:A:274:THR:HB	1:A:560:LEU:HD22	1.90	0.53
1:A:525:VAL:HG22	1:A:676:HIS:CE1	2.42	0.53
1:A:91:THR:HB	3:A:910:HOH:O	2.08	0.52
1:A:134:ASP:CG	1:A:135:ILE:H	2.17	0.52
1:A:238:THR:HG23	1:A:250:GLU:OE2	2.10	0.52
1:A:842:SER:OG	1:A:847:THR:HG21	2.09	0.52
1:A:243:THR:HG22	1:A:246:ASP:O	2.09	0.52
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.90	0.52
1:A:541:HIS:HE1	1:A:661:ASP:OD2	1.93	0.52
1:A:285:LEU:HB3	1:A:286:PRO:CD	2.40	0.52
1:A:294:LEU:O	1:A:295:ASN:HB2	2.09	0.52
1:A:709:HIS:CE1	1:A:857:ILE:OXT	2.62	0.52
1:A:248:ASN:OD1	1:A:248:ASN:N	2.43	0.51
1:A:26:VAL:HB	1:A:272:PHE:CE1	2.45	0.51
1:A:295:ASN:O	1:A:295:ASN:CG	2.54	0.51
1:A:630:THR:O	1:A:634:LEU:HD22	2.09	0.51
1:A:58:VAL:HB	1:A:82:LEU:HD22	1.93	0.51
1:A:411:GLU:HB3	3:A:911:HOH:O	2.10	0.51
1:A:471:LEU:HB3	1:A:472:PRO:HD2	1.91	0.51
1:A:170:SER:CB	1:A:172:THR:OG1	2.56	0.51
1:A:319:THR:CA	1:A:341:GLN:HE22	2.23	0.51
1:A:30:THR:O	1:A:31:SER:C	2.54	0.51
1:A:541:HIS:CD2	1:A:543:ILE:H	2.28	0.51
1:A:836:THR:HG22	1:A:848:PHE:CD2	2.46	0.51
1:A:142:HIS:ND1	3:A:869:HOH:O	2.34	0.50
1:A:734:MET:CE	1:A:734:MET:HG3	2.32	0.50
1:A:319:THR:OG1	1:A:341:GLN:NE2	2.43	0.50
1:A:626:ASP:CB	3:A:892:HOH:O	2.58	0.50
1:A:271:ASP:OD2	1:A:778:SER:OG	2.28	0.50
1:A:317:LEU:O	1:A:341:GLN:HB3	2.11	0.50
1:A:413:LEU:CD1	3:A:911:HOH:O	2.58	0.50
1:A:527:GLU:HA	1:A:530:ILE:HD12	1.93	0.50
1:A:788:ASN:CB	1:A:789:PRO:CD	2.84	0.50
1:A:155:PHE:O	1:A:156:LYS:CB	2.59	0.50
1:A:791:TRP:H	1:A:791:TRP:CD1	2.30	0.50
1:A:689:GLN:HG3	3:A:981:HOH:O	2.10	0.50
1:A:325:ILE:HA	1:A:328:LEU:HD11	1.94	0.49
1:A:117:ILE:HD13	1:A:127:LEU:HD22	1.94	0.49
1:A:135:ILE:CG1	1:A:136:PRO:N	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:LEU:C	1:A:729:LEU:CD2	2.86	0.49
1:A:831:VAL:HG22	1:A:831:VAL:O	2.11	0.49
1:A:135:ILE:HG13	1:A:136:PRO:N	2.27	0.49
1:A:837:LEU:O	1:A:851:ILE:HD11	2.13	0.49
1:A:118:LYS:HE2	1:A:158:ASP:OD1	2.12	0.49
1:A:63:ILE:HD11	1:A:116:TYR:CD2	2.48	0.49
1:A:505:VAL:O	1:A:508:ASN:HB2	2.13	0.49
1:A:136:PRO:C	1:A:138:HIS:N	2.70	0.49
1:A:410:LEU:HA	3:A:1002:HOH:O	2.13	0.49
1:A:412:GLY:N	3:A:945:HOH:O	2.45	0.49
1:A:401:ILE:HG21	1:A:453:ILE:HD12	1.94	0.48
1:A:30:THR:O	1:A:31:SER:O	2.31	0.48
1:A:190:ASP:CG	1:A:191:GLY:N	2.62	0.48
1:A:393:VAL:H	1:A:479:SER:HA	1.78	0.48
1:A:407:GLU:CA	3:A:972:HOH:O	2.62	0.48
1:A:600:LEU:HB3	1:A:601:PRO:HD3	1.96	0.48
1:A:530:ILE:HG12	1:A:551:TYR:CG	2.49	0.48
1:A:323:SER:O	1:A:327:PRO:CG	2.62	0.48
1:A:522:THR:HG23	1:A:523:HIS:N	2.27	0.48
1:A:430:HIS:HE1	1:A:434:MET:CE	2.26	0.48
1:A:413:LEU:HD23	1:A:418:ALA:HA	1.95	0.47
1:A:189:GLY:C	1:A:190:ASP:C	2.82	0.47
1:A:200:ARG:HD3	3:A:1067:HOH:O	2.14	0.47
1:A:287:LEU:HB2	1:A:321:ILE:HD11	1.93	0.47
1:A:305:ASP:CG	3:A:1031:HOH:O	2.57	0.47
1:A:440:ILE:O	1:A:443:THR:OG1	2.32	0.47
1:A:323:SER:O	1:A:327:PRO:HG3	2.14	0.47
1:A:218:ASN:HB3	1:A:219:HIS:CD2	2.49	0.47
1:A:295:ASN:HA	3:A:980:HOH:O	2.15	0.47
1:A:812:GLU:OE1	1:A:841:SER:HB2	2.15	0.47
1:A:391:SER:N	1:A:392:GLN:HE21	2.11	0.47
1:A:452:THR:HG23	3:A:977:HOH:O	2.14	0.47
1:A:278:LYS:NZ	3:A:1060:HOH:O	2.48	0.47
1:A:321:ILE:O	1:A:321:ILE:HD12	2.15	0.46
1:A:360:THR:HG22	1:A:363:GLU:H	1.80	0.46
1:A:408:PRO:CD	3:A:868:HOH:O	2.63	0.46
1:A:572:ILE:CG1	3:A:1043:HOH:O	2.33	0.46
1:A:292:PHE:C	1:A:294:LEU:N	2.73	0.46
1:A:10:HIS:NE2	1:A:135:ILE:HB	2.29	0.46
1:A:398:THR:OG1	1:A:399:SER:O	2.33	0.46
1:A:11:LYS:HG2	1:A:102:ASN:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD22	1:A:96:GLN:HB2	1.96	0.46
1:A:603:ASP:OD1	1:A:607:ARG:HD3	2.15	0.46
1:A:789:PRO:N	3:A:1041:HOH:O	2.49	0.46
1:A:658:LEU:CD1	1:A:664:LEU:HD12	2.43	0.46
1:A:750:GLN:O	1:A:754:LEU:HD22	2.16	0.46
1:A:790:ASN:HB2	3:A:1040:HOH:O	2.15	0.46
1:A:825:ARG:O	1:A:825:ARG:HD3	2.15	0.46
1:A:658:LEU:HD11	1:A:664:LEU:CD1	2.43	0.46
1:A:671:LEU:HD13	1:A:671:LEU:C	2.41	0.46
1:A:385:PRO:O	1:A:398:THR:HB	2.16	0.46
1:A:785:GLU:CB	1:A:805:GLY:HA3	2.37	0.46
1:A:600:LEU:HD23	1:A:634:LEU:HD13	1.97	0.45
1:A:312:SER:O	1:A:344:LYS:CD	2.65	0.45
1:A:218:ASN:HB3	1:A:219:HIS:HD2	1.82	0.45
1:A:230:PHE:CE1	1:A:584:GLU:HB3	2.51	0.45
1:A:430:HIS:CE1	1:A:434:MET:HE3	2.50	0.45
1:A:149:ILE:HD12	1:A:149:ILE:H	1.82	0.45
1:A:769:VAL:HG12	1:A:773:LEU:HD22	1.98	0.44
1:A:206:VAL:CG1	1:A:224:LEU:O	2.62	0.44
1:A:241:LYS:HB2	1:A:242:PRO:HD2	2.00	0.44
1:A:164:ASN:HD22	1:A:164:ASN:HA	0.78	0.44
1:A:331:LEU:HD23	1:A:334:ILE:HD11	1.99	0.44
1:A:806:ASN:O	1:A:810:GLN:HG3	2.18	0.44
1:A:438:ARG:CG	3:A:865:HOH:O	2.64	0.44
1:A:603:ASP:O	1:A:607:ARG:HD3	2.18	0.44
1:A:836:THR:HG23	1:A:849:ARG:HB3	1.98	0.43
1:A:172:THR:HG22	1:A:173:PRO:HD3	2.00	0.43
1:A:507:VAL:HG22	1:A:729:LEU:N	2.33	0.43
1:A:106:ASP:OD1	1:A:106:ASP:N	2.51	0.43
1:A:411:GLU:O	1:A:412:GLY:C	2.58	0.43
1:A:334:ILE:HG13	1:A:335:PHE:N	2.32	0.43
1:A:321:ILE:CD1	1:A:321:ILE:O	2.67	0.43
1:A:394:TYR:CB	1:A:481:ALA:HB2	2.38	0.43
1:A:159:ARG:HD2	1:A:159:ARG:HA	1.86	0.43
1:A:784:GLY:HA2	1:A:808:LEU:HD13	2.00	0.43
1:A:471:LEU:N	1:A:471:LEU:HD12	2.33	0.42
1:A:759:PRO:HG2	1:A:762:GLN:NE2	2.34	0.42
1:A:429:HIS:CE1	1:A:509:ASP:HA	2.54	0.42
1:A:837:LEU:HD13	1:A:848:PHE:CD1	2.53	0.42
1:A:208:ASN:ND2	1:A:235:ARG:NH2	2.63	0.42
1:A:287:LEU:HB3	1:A:321:ILE:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD23	1:A:295:ASN:N	2.34	0.42
1:A:409:ASN:ND2	1:A:409:ASN:O	2.53	0.42
1:A:760:LYS:O	1:A:761:PHE:C	2.60	0.42
1:A:788:ASN:HB2	1:A:789:PRO:HD3	1.97	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.20	0.42
1:A:745:LEU:O	1:A:749:PRO:HD3	2.20	0.42
1:A:323:SER:O	1:A:327:PRO:CD	2.67	0.42
1:A:273:LEU:HD13	1:A:857:ILE:HD12	2.02	0.42
1:A:407:GLU:HA	3:A:868:HOH:O	2.20	0.42
1:A:441:ASN:ND2	1:A:447:ALA:N	2.53	0.42
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.93	0.42
1:A:544:TYR:CD1	1:A:544:TYR:C	2.98	0.42
1:A:522:THR:CG2	1:A:523:HIS:H	2.32	0.42
1:A:181:GLU:HB3	3:A:958:HOH:O	2.19	0.41
1:A:402:THR:HG22	1:A:403:LYS:N	2.34	0.41
1:A:734:MET:HE3	1:A:735:PRO:HD2	2.02	0.41
1:A:9:GLY:N	3:A:1021:HOH:O	2.52	0.41
1:A:321:ILE:HD13	1:A:324:LYS:CB	2.48	0.41
1:A:376:LEU:HD11	3:A:1013:HOH:O	2.20	0.41
1:A:819:ASN:ND2	1:A:827:ARG:HH21	2.18	0.41
1:A:826:ASN:HB2	3:A:927:HOH:O	2.19	0.41
1:A:10:HIS:HB3	1:A:105:TRP:O	2.21	0.41
1:A:208:ASN:ND2	1:A:208:ASN:H	2.19	0.41
1:A:438:ARG:CD	3:A:865:HOH:O	2.69	0.41
1:A:581:TYR:OH	3:A:1023:HOH:O	2.20	0.41
1:A:839:LEU:O	1:A:851:ILE:HD13	2.21	0.41
1:A:159:ARG:NH1	3:A:1032:HOH:O	2.51	0.41
1:A:187:LEU:HD11	1:A:200:ARG:NH2	2.36	0.41
1:A:350:VAL:O	1:A:831:VAL:CG2	2.67	0.41
1:A:438:ARG:HG2	1:A:439:ARG:N	2.36	0.41
1:A:463:ARG:HG2	1:A:465:LEU:HD13	2.02	0.41
1:A:478:GLN:O	1:A:479:SER:C	2.63	0.41
1:A:795:THR:O	1:A:799:GLU:HG2	2.21	0.41
1:A:360:THR:HG22	1:A:363:GLU:CB	2.51	0.41
1:A:169:PRO:HD2	3:A:1081:HOH:O	2.22	0.40
1:A:75:LYS:HB3	1:A:75:LYS:HE3	1.90	0.40
1:A:189:GLY:O	1:A:190:ASP:C	2.65	0.40
1:A:518:HIS:O	1:A:522:THR:CG2	2.57	0.40
1:A:730:SER:HA	1:A:756:THR:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:946:HOH:O	3:A:946:HOH:O[2_655]	1.77	0.43
1:A:391:SER:O	1:A:802:LYS:NZ[1_556]	2.00	0.20

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
1	A	830/857 (97%)	748 (90%)	48 (6%)	34 (4%)	2 0

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	135	ILE
1	A	136	PRO
1	A	156	LYS
1	A	170	SER
1	A	293	ASP
1	A	295	ASN
1	A	326	SER
1	A	333	GLU
1	A	341	GLN
1	A	409	ASN
1	A	477	ASP
1	A	479	SER
1	A	737	LYS
1	A	739	SER
1	A	784	GLY
1	A	789	PRO
1	A	844	GLU
1	A	10	HIS
1	A	48	ASP
1	A	164	ASN
1	A	270	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	330	VAL
1	A	397	HIS
1	A	785	GLU
1	A	30	THR
1	A	31	SER
1	A	261	ASP
1	A	243	THR
1	A	407	GLU
1	A	624	ILE
1	A	788	ASN
1	A	408	PRO
1	A	474	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	733/747 (98%)	577 (79%)	156 (21%)	1 0

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	18	LEU
1	A	23	VAL
1	A	32	VAL
1	A	46	THR
1	A	50	LEU
1	A	54	LEU
1	A	62	LEU
1	A	67	LYS
1	A	76	LEU
1	A	82	LEU
1	A	83	GLU
1	A	87	THR
1	A	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	THR
1	A	92	LEU
1	A	100	LYS
1	A	104	GLU
1	A	106	ASP
1	A	133	GLU
1	A	134	ASP
1	A	135	ILE
1	A	137	ASN
1	A	156	LYS
1	A	164	ASN
1	A	171	GLU
1	A	172	THR
1	A	176	LEU
1	A	184	LEU
1	A	187	LEU
1	A	195	ARG
1	A	198	TRP
1	A	206	VAL
1	A	208	ASN
1	A	210	LEU
1	A	215	LYS
1	A	217	GLU
1	A	221	ARG
1	A	223	VAL
1	A	224	LEU
1	A	238	THR
1	A	243	THR
1	A	247	PRO
1	A	251	SER
1	A	256	VAL
1	A	258	LEU
1	A	277	LEU
1	A	278	LYS
1	A	281	SER
1	A	289	GLN
1	A	299	ARG
1	A	310	LEU
1	A	312	SER
1	A	315	ILE
1	A	316	LYS
1	A	320	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	321	ILE
1	A	322	ILE
1	A	323	SER
1	A	324	LYS
1	A	325	ILE
1	A	326	SER
1	A	328	LEU
1	A	331	LEU
1	A	334	ILE
1	A	344	LYS
1	A	351	ILE
1	A	360	THR
1	A	362	GLU
1	A	374	PRO
1	A	376	LEU
1	A	377	ILE
1	A	386	ARG
1	A	388	LYS
1	A	392	GLN
1	A	394	TYR
1	A	397	HIS
1	A	398	THR
1	A	403	LYS
1	A	404	GLU
1	A	409	ASN
1	A	410	LEU
1	A	420	GLN
1	A	423	ARG
1	A	427	LEU
1	A	437	LEU
1	A	444	SER
1	A	446	LYS
1	A	465	LEU
1	A	467	ILE
1	A	471	LEU
1	A	478	GLN
1	A	479	SER
1	A	485	VAL
1	A	487	LEU
1	A	490	ASP
1	A	491	GLU
1	A	493	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	497	ILE
1	A	500	LEU
1	A	507	VAL
1	A	508	ASN
1	A	525	VAL
1	A	537	LEU
1	A	540	VAL
1	A	547	LEU
1	A	557	ILE
1	A	566	VAL
1	A	568	ASP
1	A	571	VAL
1	A	583	VAL
1	A	594	VAL
1	A	604	LEU
1	A	611	ILE
1	A	620	ILE
1	A	623	VAL
1	A	626	ASP
1	A	627	TYR
1	A	630	THR
1	A	634	LEU
1	A	650	LEU
1	A	664	LEU
1	A	687	LYS
1	A	690	THR
1	A	692	GLU
1	A	712	VAL
1	A	722	LEU
1	A	724	LEU
1	A	729	LEU
1	A	732	ARG
1	A	737	LYS
1	A	741	GLU
1	A	745	LEU
1	A	747	LYS
1	A	754	LEU
1	A	762	GLN
1	A	765	ILE
1	A	773	LEU
1	A	775	ARG
1	A	785	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	787	ASP
1	A	796	ARG
1	A	798	LEU
1	A	814	LYS
1	A	815	LEU
1	A	823	LYS
1	A	825	ARG
1	A	836	THR
1	A	837	LEU
1	A	838	LEU
1	A	839	LEU
1	A	841	SER
1	A	843	LYS
1	A	847	THR
1	A	848	PHE
1	A	851	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	96	GLN
1	A	102	ASN
1	A	142	HIS
1	A	146	ASN
1	A	164	ASN
1	A	165	GLN
1	A	208	ASN
1	A	219	HIS
1	A	341	GLN
1	A	392	GLN
1	A	409	ASN
1	A	430	HIS
1	A	441	ASN
1	A	473	HIS
1	A	541	HIS
1	A	548	HIS
1	A	556	ASN
1	A	618	HIS
1	A	665	GLN
1	A	681	ASN
1	A	725	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	750	GLN
1	A	813	ASN
1	A	819	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	HLU	A	565	1	7,8,9	0.65	0	7,10,12	1.85	2 (28%)
1	HTR	A	519	1	13,16,17	1.32	2 (15%)	17,22,24	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HLU	A	565	1	-	6/9/10/12	-
1	HTR	A	519	1	1/1/2/3	3/9/10/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	HTR	CD1-CG	-2.71	1.33	1.36
1	A	519	HTR	CD2-CE2	-2.57	1.38	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	HLU	CD1-CG-CB	3.82	117.47	111.23
1	A	565	HLU	O-C-CA	-2.05	119.49	124.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	519	HTR	CB

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	565	HLU	C-CA-CB-OH
1	A	565	HLU	N-CA-CB-CG
1	A	565	HLU	C-CA-CB-CG
1	A	519	HTR	C-CA-CB-CG
1	A	565	HLU	N-CA-CB-OH
1	A	565	HLU	CA-CB-CG-CD1
1	A	519	HTR	C-CA-CB-OH
1	A	519	HTR	O-C-CA-CB
1	A	565	HLU	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	565	HLU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	834/857 (97%)	0.60	107 (12%) 7 6	13, 28, 65, 99	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	784	GLY	6.3
1	A	410	LEU	5.6
1	A	394	TYR	5.6
1	A	325	ILE	5.4
1	A	397	HIS	5.4
1	A	395	GLY	5.4
1	A	32	VAL	5.3
1	A	322	ILE	5.0
1	A	474	PRO	4.9
1	A	284	VAL	4.6
1	A	476	GLY	4.5
1	A	326	SER	4.5
1	A	393	VAL	4.5
1	A	9	GLY	4.5
1	A	47	LEU	4.4
1	A	137	ASN	4.3
1	A	806	ASN	4.3
1	A	398	THR	4.3
1	A	480	GLY	4.1
1	A	334	ILE	4.1
1	A	170	SER	4.1
1	A	473	HIS	4.0
1	A	391	SER	3.9
1	A	785	GLU	3.9
1	A	331	LEU	3.8
1	A	30	THR	3.8
1	A	392	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	3.7
1	A	190	ASP	3.6
1	A	294	LEU	3.6
1	A	275	TYR	3.6
1	A	479	SER	3.6
1	A	328	LEU	3.5
1	A	337	THR	3.5
1	A	288	LEU	3.4
1	A	396	ASP	3.4
1	A	46	THR	3.4
1	A	408	PRO	3.3
1	A	320	ASP	3.3
1	A	790	ASN	3.2
1	A	134	ASP	3.2
1	A	335	PHE	3.2
1	A	339	GLY	3.1
1	A	342	ALA	3.1
1	A	139	GLY	3.1
1	A	296	PHE	3.1
1	A	135	ILE	3.1
1	A	93	GLY	3.0
1	A	336	ARG	3.0
1	A	738	GLY	3.0
1	A	411	GLU	2.9
1	A	330	VAL	2.9
1	A	285	LEU	2.9
1	A	107	ASP	2.9
1	A	324	LYS	2.8
1	A	332	LYS	2.8
1	A	477	ASP	2.8
1	A	239	GLY	2.7
1	A	49	THR	2.7
1	A	329	PRO	2.7
1	A	283	ASN	2.7
1	A	279	SER	2.7
1	A	828	CYS	2.7
1	A	54	LEU	2.7
1	A	789	PRO	2.7
1	A	215	LYS	2.7
1	A	482	PHE	2.6
1	A	138	HIS	2.6
1	A	290	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	620	ILE	2.6
1	A	458	ASN	2.6
1	A	136	PRO	2.6
1	A	286	PRO	2.6
1	A	438	ARG	2.6
1	A	490	ASP	2.6
1	A	478	GLN	2.5
1	A	340	GLU	2.5
1	A	280	VAL	2.5
1	A	413	LEU	2.5
1	A	333	GLU	2.4
1	A	611	ILE	2.4
1	A	857	ILE	2.4
1	A	31	SER	2.3
1	A	404	GLU	2.3
1	A	218	ASN	2.3
1	A	475	GLN	2.3
1	A	108	GLY	2.3
1	A	687	LYS	2.3
1	A	311	TYR	2.2
1	A	172	THR	2.2
1	A	293	ASP	2.2
1	A	171	GLU	2.2
1	A	297	THR	2.2
1	A	298	PRO	2.2
1	A	415	VAL	2.2
1	A	317	LEU	2.2
1	A	626	ASP	2.2
1	A	68	ALA	2.1
1	A	217	GLU	2.1
1	A	338	ASP	2.1
1	A	276	GLY	2.1
1	A	630	THR	2.1
1	A	412	GLY	2.1
1	A	844	GLU	2.0
1	A	55	GLY	2.0
1	A	407	GLU	2.0
1	A	198	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HLU	A	565	9/10	0.82	0.14	26,29,33,36	0
1	HTR	A	519	15/16	0.93	0.08	17,19,21,30	0

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
2	FE	A	858	1/1	0.96	0.10	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.