Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:00 PM GMT

PDB ID	:	1ROV
Title	:	Lipoxygenase-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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		27
Ramachandran outliers		4.1%
Sidechain outliers		19.1%
RSRZ outliers		7.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
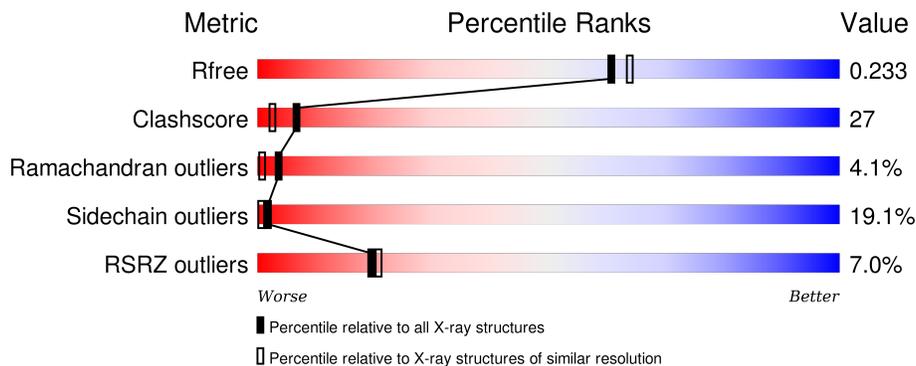
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 51% 27% 13% 6% •

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 (i)

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 6698	C 4278	N 1149	O 1253	S 18	0	0	0

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 (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
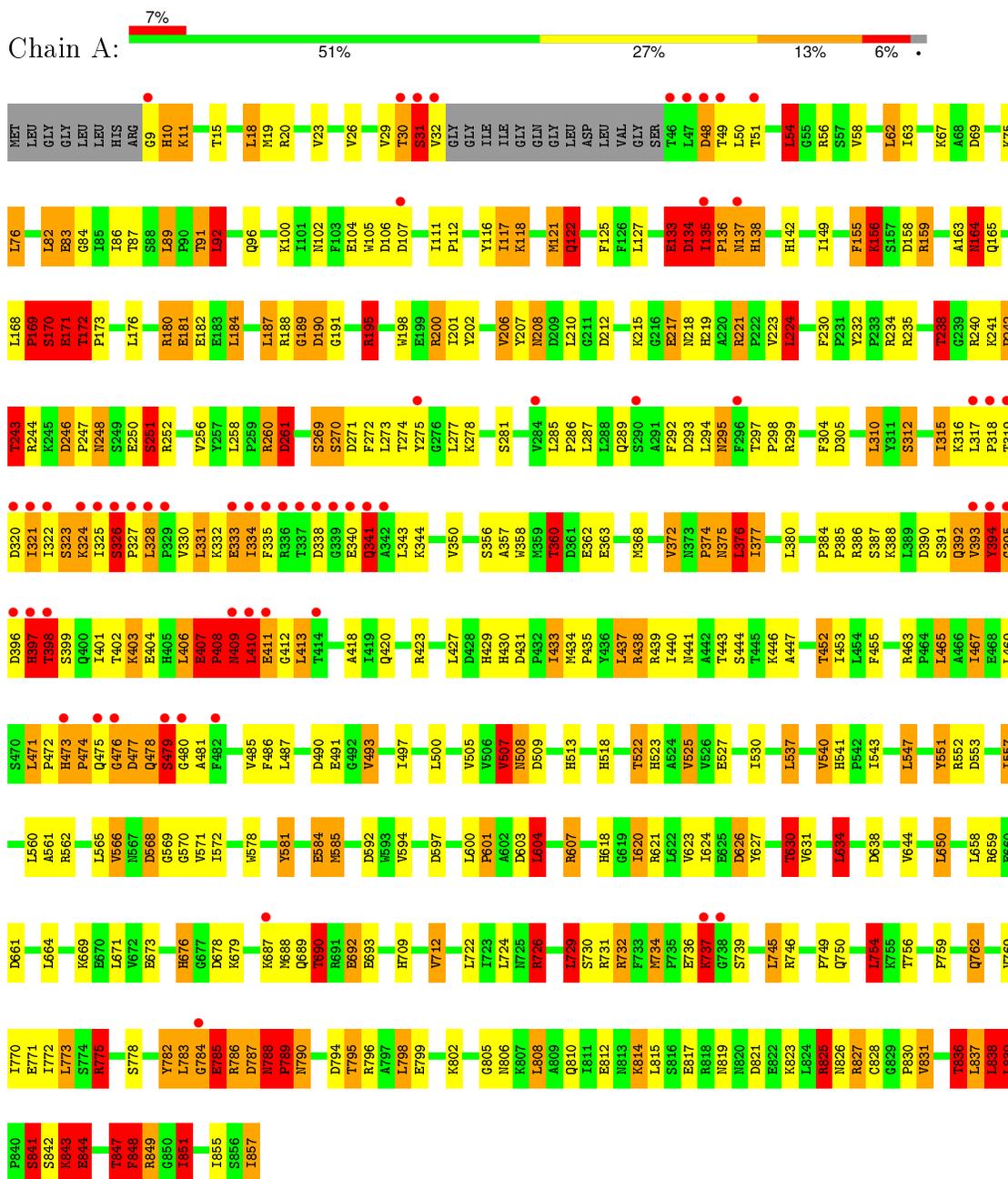
4 Data and refinement statistics (i)

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) 78.0 (43.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [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 (5.04%)	DCC
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 50653 reflections	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HLU, FE, HTR

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	1.45	64/6841 (0.9%)	1.87	205/9286 (2.2%)

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 (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	VAL	CB-CG1	-12.25	1.27	1.52
1	A	734	MET	SD-CE	-10.94	1.16	1.77
1	A	785	GLU	CB-CG	10.77	1.72	1.52
1	A	164	ASN	CB-CG	-10.15	1.27	1.51
1	A	190	ASP	CA-C	9.74	1.78	1.52
1	A	785	GLU	CD-OE1	9.72	1.36	1.25
1	A	362	GLU	CG-CD	9.31	1.66	1.51
1	A	375	ASN	CB-CG	-9.07	1.30	1.51
1	A	169	PRO	CA-C	-8.41	1.36	1.52
1	A	787	ASP	CB-CG	8.15	1.68	1.51
1	A	190	ASP	C-O	8.11	1.38	1.23
1	A	362	GLU	CB-CG	8.00	1.67	1.52
1	A	584	GLU	CB-CG	-7.51	1.37	1.52
1	A	171	GLU	N-CA	7.46	1.61	1.46
1	A	181	GLU	CG-CD	7.20	1.62	1.51
1	A	261	ASP	N-CA	7.16	1.60	1.46
1	A	394	TYR	CD2-CE2	-7.16	1.28	1.39
1	A	407	GLU	CB-CG	7.13	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	789	PRO	CA-C	6.97	1.66	1.52
1	A	137	ASN	CB-CG	6.87	1.66	1.51
1	A	172	THR	CB-CG2	-6.87	1.29	1.52
1	A	182	GLU	CG-CD	6.85	1.62	1.51
1	A	585	MET	SD-CE	-6.85	1.39	1.77
1	A	788	ASN	CB-CG	-6.82	1.35	1.51
1	A	644	VAL	CB-CG2	6.67	1.66	1.52
1	A	261	ASP	CA-CB	6.45	1.68	1.53
1	A	117	ILE	CA-CB	6.44	1.69	1.54
1	A	372	VAL	CB-CG2	-6.43	1.39	1.52
1	A	775	ARG	CB-CG	-6.42	1.35	1.52
1	A	394	TYR	CD1-CE1	-6.28	1.29	1.39
1	A	831	VAL	CB-CG2	-6.22	1.39	1.52
1	A	238	THR	CB-CG2	-6.17	1.31	1.52
1	A	49	THR	CA-CB	6.03	1.69	1.53
1	A	207	TYR	CD2-CE2	5.92	1.48	1.39
1	A	32	VAL	CA-CB	5.87	1.67	1.54
1	A	581	TYR	CD1-CE1	5.84	1.48	1.39
1	A	360	THR	CB-CG2	-5.82	1.33	1.52
1	A	690	THR	CB-CG2	-5.67	1.33	1.52
1	A	169	PRO	N-CA	-5.63	1.37	1.47
1	A	297	THR	CA-CB	5.61	1.68	1.53
1	A	171	GLU	CD-OE1	5.60	1.31	1.25
1	A	202	TYR	CD2-CE2	5.59	1.47	1.39
1	A	551	TYR	CD2-CE2	5.39	1.47	1.39
1	A	630	THR	CB-CG2	-5.37	1.34	1.52
1	A	358	TRP	CB-CG	-5.36	1.40	1.50
1	A	159	ARG	CD-NE	-5.32	1.37	1.46
1	A	736	GLU	CG-CD	5.30	1.59	1.51
1	A	770	ILE	CA-CB	5.27	1.67	1.54
1	A	433	ILE	CA-CB	5.20	1.66	1.54
1	A	407	GLU	CG-CD	5.18	1.59	1.51
1	A	479	SER	N-CA	5.17	1.56	1.46
1	A	135	ILE	C-N	5.17	1.44	1.34
1	A	551	TYR	CD1-CE1	5.13	1.47	1.39
1	A	771	GLU	CG-CD	-5.12	1.44	1.51
1	A	393	VAL	CB-CG1	5.11	1.63	1.52
1	A	790	ASN	CB-CG	-5.10	1.39	1.51
1	A	217	GLU	CG-CD	5.09	1.59	1.51
1	A	438	ARG	CG-CD	5.08	1.64	1.51
1	A	397	HIS	CA-C	5.06	1.66	1.52
1	A	217	GLU	CB-CG	5.04	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	782	TYR	CD1-CE1	5.02	1.46	1.39
1	A	620	ILE	CA-CB	5.02	1.66	1.54
1	A	676	HIS	CD2-NE2	-5.02	1.26	1.38
1	A	31	SER	CA-CB	5.00	1.60	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ARG	NE-CZ-NH2	-29.22	105.69	120.30
1	A	159	ARG	NE-CZ-NH2	-27.74	106.43	120.30
1	A	240	ARG	NE-CZ-NH2	-23.27	108.67	120.30
1	A	195	ARG	NE-CZ-NH1	-21.55	109.53	120.30
1	A	607	ARG	NE-CZ-NH1	20.51	130.56	120.30
1	A	726	ARG	NE-CZ-NH1	-20.32	110.14	120.30
1	A	221	ARG	NE-CZ-NH2	-20.12	110.24	120.30
1	A	221	ARG	NE-CZ-NH1	19.27	129.94	120.30
1	A	240	ARG	NE-CZ-NH1	18.90	129.75	120.30
1	A	200	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	A	188	ARG	NE-CZ-NH2	-15.94	112.33	120.30
1	A	726	ARG	NE-CZ-NH2	15.82	128.21	120.30
1	A	159	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	A	200	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	A	159	ARG	CG-CD-NE	-12.79	84.95	111.80
1	A	169	PRO	CA-C-O	-11.43	92.77	120.20
1	A	825	ARG	NE-CZ-NH2	11.37	125.98	120.30
1	A	847	THR	C-N-CA	-10.96	94.30	121.70
1	A	438	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	252	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	A	786	ARG	CG-CD-NE	-10.28	90.21	111.80
1	A	825	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	A	189	GLY	C-N-CA	-9.57	97.77	121.70
1	A	398	THR	N-CA-C	9.48	136.59	111.00
1	A	375	ASN	CB-CG-OD1	-9.44	102.72	121.60
1	A	261	ASP	N-CA-CB	9.37	127.47	110.60
1	A	188	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	A	785	GLU	CG-CD-OE2	-9.27	99.77	118.30
1	A	394	TYR	CB-CA-C	-9.22	91.96	110.40
1	A	212	ASP	CB-CG-OD1	8.78	126.20	118.30
1	A	786	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	785	GLU	CA-CB-CG	8.66	132.45	113.40
1	A	847	THR	N-CA-CB	-8.58	94.00	110.30
1	A	56	ARG	NE-CZ-NH2	-8.47	116.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	828	CYS	CA-CB-SG	-8.42	98.85	114.00
1	A	234	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	A	396	ASP	CB-CG-OD2	8.22	125.70	118.30
1	A	238	THR	C-N-CA	-8.19	105.11	122.30
1	A	585	MET	CG-SD-CE	8.16	113.26	100.20
1	A	452	THR	CA-CB-CG2	8.15	123.82	112.40
1	A	712	VAL	CG1-CB-CG2	8.07	123.81	110.90
1	A	568	ASP	C-N-CA	-8.00	105.50	122.30
1	A	224	LEU	CB-CG-CD1	7.94	124.50	111.00
1	A	89	LEU	CB-CG-CD1	7.86	124.36	111.00
1	A	597	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	18	LEU	CA-CB-CG	7.74	133.11	115.30
1	A	836	THR	N-CA-CB	-7.67	95.73	110.30
1	A	171	GLU	CA-C-N	-7.66	100.34	117.20
1	A	234	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	A	604	LEU	CB-CG-CD2	7.62	123.96	111.00
1	A	159	ARG	CD-NE-CZ	7.62	134.26	123.60
1	A	476	GLY	N-CA-C	7.56	132.01	113.10
1	A	607	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	522	THR	CA-CB-CG2	7.50	122.91	112.40
1	A	493	VAL	CB-CA-C	-7.49	97.17	111.40
1	A	408	PRO	N-CA-C	7.44	131.45	112.10
1	A	848	PHE	CB-CA-C	7.44	125.28	110.40
1	A	206	VAL	CG1-CB-CG2	-7.42	99.03	110.90
1	A	395	GLY	N-CA-C	7.38	131.55	113.10
1	A	678	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	69	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	679	LYS	CD-CE-NZ	7.34	128.59	111.70
1	A	19	MET	CG-SD-CE	7.28	111.85	100.20
1	A	180	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	775	ARG	CB-CA-C	-7.26	95.87	110.40
1	A	650	LEU	CA-CB-CG	7.22	131.90	115.30
1	A	170	SER	C-N-CA	7.19	139.68	121.70
1	A	480	GLY	N-CA-C	7.12	130.91	113.10
1	A	438	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	182	GLU	CA-CB-CG	7.07	128.96	113.40
1	A	56	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	252	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	547	LEU	CB-CG-CD1	7.04	122.97	111.00
1	A	20	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	841	SER	CB-CA-C	-6.97	96.85	110.10
1	A	390	ASP	CB-CG-OD2	6.97	124.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	732	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	473	HIS	CB-CA-C	6.87	124.13	110.40
1	A	411	GLU	N-CA-C	6.84	129.48	111.00
1	A	121	MET	C-N-CA	-6.84	104.60	121.70
1	A	592	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	838	LEU	CB-CG-CD1	6.80	122.57	111.00
1	A	89	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	479	SER	N-CA-CB	6.77	120.66	110.50
1	A	731	ARG	CB-CA-C	-6.77	96.86	110.40
1	A	847	THR	O-C-N	-6.74	111.92	122.70
1	A	557	ILE	CG1-CB-CG2	-6.68	96.69	111.40
1	A	507	VAL	CG1-CB-CG2	6.67	121.58	110.90
1	A	775	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	623	VAL	CB-CA-C	6.66	124.06	111.40
1	A	310	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	785	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	A	195	ARG	CG-CD-NE	6.60	125.66	111.80
1	A	238	THR	CA-C-N	6.60	129.39	116.20
1	A	238	THR	O-C-N	-6.57	112.02	123.20
1	A	92	LEU	C-N-CA	-6.50	108.65	122.30
1	A	184	LEU	CB-CG-CD1	6.47	122.01	111.00
1	A	712	VAL	N-CA-CB	-6.42	97.37	111.50
1	A	155	PHE	N-CA-C	6.38	128.21	111.00
1	A	659	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	634	LEU	CB-CG-CD1	6.36	121.81	111.00
1	A	135	ILE	N-CA-CB	6.33	125.35	110.80
1	A	164	ASN	CB-CG-ND2	-6.28	101.63	116.70
1	A	195	ARG	NH1-CZ-NH2	-6.25	112.52	119.40
1	A	843	LYS	C-N-CA	-6.25	106.07	121.70
1	A	568	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	375	ASN	N-CA-C	6.25	127.86	111.00
1	A	406	LEU	C-N-CA	6.21	137.22	121.70
1	A	221	ARG	CD-NE-CZ	6.18	132.25	123.60
1	A	847	THR	CA-C-N	6.18	130.79	117.20
1	A	137	ASN	N-CA-C	-6.16	94.38	111.00
1	A	172	THR	CA-CB-CG2	-6.16	103.78	112.40
1	A	260	ARG	C-N-CA	-6.15	106.33	121.70
1	A	107	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	746	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	188	ARG	CG-CD-NE	-6.11	98.97	111.80
1	A	737	LYS	CA-CB-CG	6.10	126.83	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	CG-CD-NE	-6.09	99.02	111.80
1	A	133	GLU	C-N-CA	-6.08	106.50	121.70
1	A	164	ASN	CB-CG-OD1	6.08	133.76	121.60
1	A	659	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	238	THR	N-CA-CB	-5.99	98.92	110.30
1	A	794	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	844	GLU	CB-CA-C	-5.97	98.45	110.40
1	A	48	ASP	N-CA-C	5.96	127.08	111.00
1	A	808	LEU	CB-CG-CD2	5.94	121.10	111.00
1	A	261	ASP	CB-CA-C	-5.93	98.53	110.40
1	A	172	THR	CA-CB-OG1	5.93	121.46	109.00
1	A	631	VAL	CG1-CB-CG2	-5.93	101.42	110.90
1	A	171	GLU	C-N-CA	-5.91	106.93	121.70
1	A	843	LYS	O-C-N	-5.91	113.25	122.70
1	A	783	LEU	CA-C-N	-5.88	104.44	116.20
1	A	190	ASP	CA-C-N	-5.87	104.46	116.20
1	A	390	ASP	N-CA-C	5.87	126.83	111.00
1	A	562	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	843	LYS	CA-C-N	5.81	129.97	117.20
1	A	475	GLN	CB-CA-C	-5.79	98.83	110.40
1	A	240	ARG	CD-NE-CZ	5.78	131.69	123.60
1	A	54	LEU	C-N-CA	-5.78	110.16	122.30
1	A	20	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	540	VAL	CG1-CB-CG2	5.72	120.05	110.90
1	A	851	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	A	341	GLN	N-CA-C	5.67	126.30	111.00
1	A	857	ILE	N-CA-C	-5.64	95.77	111.00
1	A	795	THR	OG1-CB-CG2	5.64	122.97	110.00
1	A	604	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	785	GLU	CA-C-N	5.61	129.55	117.20
1	A	785	GLU	N-CA-C	-5.61	95.86	111.00
1	A	92	LEU	O-C-N	-5.60	113.68	123.20
1	A	246	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	849	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	251	SER	CB-CA-C	-5.51	99.62	110.10
1	A	825	ARG	CB-CG-CD	5.51	125.94	111.60
1	A	790	ASN	CA-C-N	-5.51	105.08	117.20
1	A	118	LYS	CD-CE-NZ	-5.50	99.04	111.70
1	A	839	LEU	CB-CG-CD1	5.50	120.35	111.00
1	A	184	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	393	VAL	N-CA-C	5.47	125.78	111.00
1	A	814	LYS	CD-CE-NZ	5.47	124.28	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	HIS	N-CA-CB	5.46	120.42	110.60
1	A	181	GLU	CG-CD-OE2	5.45	129.21	118.30
1	A	821	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	164	ASN	N-CA-C	5.45	125.70	111.00
1	A	827	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	787	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	788	ASN	N-CA-C	5.43	125.65	111.00
1	A	376	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	76	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	552	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	754	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	190	ASP	CA-C-O	5.37	131.38	120.10
1	A	360	THR	N-CA-CB	-5.34	100.16	110.30
1	A	785	GLU	CG-CD-OE1	5.34	128.97	118.30
1	A	201	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	A	771	GLU	CA-CB-CG	-5.32	101.69	113.40
1	A	570	GLY	N-CA-C	5.32	126.39	113.10
1	A	362	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	269	SER	C-N-CA	-5.29	108.47	121.70
1	A	507	VAL	N-CA-CB	-5.29	99.86	111.50
1	A	537	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	507	VAL	CB-CA-C	5.25	121.39	111.40
1	A	787	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	A	785	GLU	CA-C-O	-5.22	109.13	120.10
1	A	566	VAL	N-CA-CB	-5.22	100.02	111.50
1	A	54	LEU	N-CA-C	5.21	125.07	111.00
1	A	413	LEU	CB-CA-C	-5.20	100.32	110.20
1	A	431	ASP	CB-CG-OD1	-5.19	113.62	118.30
1	A	798	LEU	CB-CG-CD2	5.18	119.80	111.00
1	A	431	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	855	ILE	N-CA-C	-5.17	97.05	111.00
1	A	836	THR	CA-CB-CG2	5.14	119.59	112.40
1	A	676	HIS	ND1-CE1-NE2	-5.13	98.61	109.90
1	A	467	ILE	CA-CB-CG1	5.12	120.74	111.00
1	A	48	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	163	ALA	C-N-CA	5.12	134.49	121.70
1	A	843	LYS	CA-CB-CG	5.12	124.65	113.40
1	A	343	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	789	PRO	C-N-CA	5.09	134.44	121.70
1	A	159	ARG	NH1-CZ-NH2	5.07	124.98	119.40
1	A	795	THR	CA-CB-CG2	5.05	119.47	112.40
1	A	62	LEU	CA-CB-CG	5.01	126.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	374	PRO	C-N-CA	5.01	134.22	121.70
1	A	729	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	732	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	Mainchain,Peptide
1	A	171	GLU	Mainchain,Peptide
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	361	1
2	A	1	0	0	0	0
3	A	301	0	0	78	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7000	0	6614	361	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 27.

All (361) 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:CA	1:A:190:ASP:C	1.78	1.50
1:A:149:ILE:HG13	3:A:1034:HOH:O	1.16	1.28
1:A:734:MET:SD	1:A:734:MET:CE	1.16	1.25
1:A:121:MET:O	1:A:122:GLN:CB	1.79	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:HE2	1:A:734:MET:SD	1.74	1.15
1:A:734:MET:HE1	1:A:734:MET:SD	1.74	1.13
1:A:857:ILE:HG13	3:A:935:HOH:O	1.44	1.13
1:A:734:MET:CG	1:A:734:MET:CE	2.28	1.11
1:A:734:MET:HE3	1:A:734:MET:SD	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	1.04
1:A:169:PRO:C	1:A:171:GLU:H	1.55	1.03
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:127:LEU:HB2	1:A:149:ILE:HD11	1.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:HIS:HB2	1:A:476:GLY:C	1.94	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
1:A:190:ASP:OD1	1:A:191:GLY:N	2.09	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: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:473:HIS:O	1:A:474:PRO:C	2.20	0.80
1:A:843:LYS:O	1:A:844:GLU:HB2	1.81	0.80
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.61	0.80
1:A:169:PRO:C	1:A:171:GLU:N	2.30	0.80
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:190:ASP:CG	1:A:191:GLY:H	1.86	0.79
1:A:578:TRP:HB3	1:A:585:MET:CE	2.13	0.79
1:A:295:ASN:OD1	1:A:295:ASN:O	2.00	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:190:ASP:CA	1:A:191:GLY:N	2.47	0.77
1:A:578:TRP:HB3	1:A:585:MET:HE1	1.65	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:581:TYR:HB2	1:A:585:MET:HE2	1.69	0.75
1:A:687:LYS:C	3:A:957:HOH:O	2.20	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: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:836:THR:HG21	3:A:1033:HOH:O	1.87	0.73
1:A:782:TYR:H	1:A:786:ARG:HD2	1.51	0.73
1:A:409:ASN:HD22	1:A:409:ASN:C	1.92	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:96:GLN:NE2	2.21	0.72
1:A:734:MET:CG	1:A:734:MET:HE2	2.05	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:83:GLU:C	1:A:83:GLU:OE2	2.27	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
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:393:VAL:C	1:A:395:GLY:H	1.93	0.70
1:A:155:PHE:O	1:A:156:LYS:HB2	1.90	0.70
1:A:190:ASP:HA	1:A:190:ASP:C	2.06	0.70
1:A:734:MET:HE2	1:A:734:MET:HG3	1.71	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: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:NH1	1:A:775:ARG:CG	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:433:ILE:HG12	1:A:437:LEU:HD13	1.76	0.67
1:A:357:ALA:HB1	1:A:830:PRO:HB2	1.77	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:189:GLY:O	1:A:190:ASP:CB	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLY:CA	3:A:945:HOH:O	2.37	0.65
1:A:10:HIS:CD2	1:A:135:ILE:HB	2.31	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:391:SER:H	1:A:392:GLN:HE21	1.43	0.65
1:A:393:VAL:CG1	1:A:393:VAL:O	2.44	0.65
1:A:243:THR:CG2	1:A:246:ASP:H	2.09	0.65
1:A:838:LEU:HA	1:A:851:ILE:HD11	1.78	0.64
1:A:241:LYS:CE	1:A:244:ARG:HH21	2.09	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:318:PRO:C	1:A:341:GLN:OE1	2.36	0.64
1:A:269:SER:O	1:A:270:SER:HB2	1.93	0.64
1:A:29:VAL:O	1:A:30:THR:C	2.36	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:HD12	1:A:149:ILE:N	2.13	0.62
1:A:581:TYR:HB2	1:A:585:MET:CE	2.30	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:CA	1:A:83:GLU:OE2	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:783:LEU:C	1:A:785:GLU:H	2.03	0.60
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: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:789:PRO:CA	3:A:1041:HOH:O	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ALA:O	1:A:360:THR:HB	2.03	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: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
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:857:ILE:HA	3:A:935:HOH:O	2.04	0.57
1:A:561:ALA:HA	1:A:565:HLU:HB	1.87	0.57
1:A:557:ILE:HD13	3:A:935:HOH:O	2.05	0.57
1:A:578:TRP:HB3	1:A:585:MET:HE3	1.87	0.57
1:A:206:VAL:HG13	3:A:906:HOH:O	2.04	0.57
1:A:312:SER:O	1:A:344:LYS:HD3	2.05	0.56
1:A:473:HIS:HB2	1:A:477:ASP:N	2.21	0.56
1:A:423:ARG:NH1	1:A:455:PHE:CE1	2.74	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:603:ASP:OD1	1:A:607:ARG:CD	2.54	0.56
1:A:469:LEU:HD12	1:A:486:PHE:CE1	2.39	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: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:578:TRP:CB	1:A:585:MET:HE1	2.35	0.55
1:A:136:PRO:C	1:A:138:HIS:H	2.07	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:618:HIS:HE1	3:A:884:HOH:O	1.90	0.54
1:A:380:LEU:CD1	3:A:1018:HOH:O	2.55	0.54
1:A:83:GLU:HA	1:A:83:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:292:PHE:O	1:A:294:LEU:C	2.46	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
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:525:VAL:HG22	1:A:676:HIS:CE1	2.42	0.53
1:A:274:THR:HB	1:A:560:LEU:HD22	1.90	0.53
1:A:91:THR:HB	3:A:910:HOH:O	2.08	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:541:HIS:HE1	1:A:661:ASP:OD2	1.93	0.52
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.90	0.52
1:A:294:LEU:O	1:A:295:ASN:HB2	2.09	0.52
1:A:285:LEU:HB3	1:A:286:PRO:CD	2.40	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:630:THR:O	1:A:634:LEU:HD22	2.09	0.51
1:A:411:GLU:HB3	3:A:911:HOH:O	2.10	0.51
1:A:58:VAL:HB	1:A:82:LEU:HD22	1.93	0.51
1:A:471:LEU:HB3	1:A:472:PRO:HD2	1.91	0.51
1:A:319:THR:CA	1:A:341:GLN:HE22	2.23	0.51
1:A:170:SER:CB	1:A:172:THR:OG1	2.56	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: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:788:ASN:CB	1:A:789:PRO:CD	2.84	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:409:ASN:ND2	1:A:409:ASN:C	2.62	0.50
1:A:527:GLU:HA	1:A:530:ILE:HD12	1.93	0.50
1:A:393:VAL:C	1:A:395:GLY:N	2.59	0.50
1:A:155:PHE:O	1:A:156:LYS:CB	2.59	0.50
1:A:135:ILE:HG13	1:A:136:PRO:N	2.27	0.50
1:A:689:GLN:HG3	3:A:981:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:831:VAL:HG22	1:A:831:VAL:O	2.11	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:412:GLY:N	3:A:945:HOH:O	2.45	0.49
1:A:410:LEU:HA	3:A:1002:HOH:O	2.13	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: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:430:HIS:HE1	1:A:434:MET:CE	2.26	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:134:ASP:CG	1:A:135:ILE:H	2.17	0.48
1:A:413:LEU:HD23	1:A:418:ALA:HA	1.95	0.47
1:A:287:LEU:HB2	1:A:321:ILE:HD11	1.93	0.47
1:A:200:ARG:HD3	3:A:1067:HOH:O	2.14	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:295:ASN:CG	1:A:295:ASN:O	2.54	0.47
1:A:278:LYS:NZ	3:A:1060:HOH:O	2.48	0.47
1:A:572:ILE:CG1	3:A:1043:HOH:O	2.33	0.46
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: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:30:THR:O	1:A:31:SER:C	2.54	0.46
1:A:789:PRO:N	3:A:1041:HOH:O	2.49	0.46
1:A:92:LEU:HD22	1:A:96:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ASP:OD1	1:A:607:ARG:HD3	2.15	0.46
1:A:11:LYS:HG2	1:A:102:ASN:HB3	1.97	0.46
1:A:750:GLN:O	1:A:754:LEU:HD22	2.16	0.46
1:A:658:LEU:CD1	1:A:664:LEU:HD12	2.43	0.46
1:A:825:ARG:O	1:A:825:ARG:HD3	2.15	0.46
1:A:790:ASN:HB2	3:A:1040:HOH:O	2.15	0.46
1:A:658:LEU:HD11	1:A:664:LEU:CD1	2.43	0.46
1:A:785:GLU:CB	1:A:805:GLY:HA3	2.37	0.46
1:A:385:PRO:O	1:A:398:THR:HB	2.16	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:430:HIS:HE1	1:A:434:MET:HE3	1.81	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:149:ILE:HD12	1:A:149:ILE:H	1.82	0.45
1:A:729:LEU:CD2	1:A:729:LEU:C	2.86	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:136:PRO:C	1:A:138:HIS:N	2.70	0.44
1:A:190:ASP:CG	1:A:191:GLY:N	2.62	0.44
1:A:331:LEU:HD23	1:A:334:ILE:HD11	1.99	0.44
1:A:164:ASN:HD22	1:A:164:ASN:HA	0.78	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:N	1:A:106:ASP:OD1	2.51	0.43
1:A:334:ILE:HG13	1:A:335:PHE:N	2.32	0.43
1:A:271:ASP:OD2	1:A:778:SER:OG	2.28	0.43
1:A:321:ILE:O	1:A:321:ILE:CD1	2.67	0.43
1:A:394:TYR:CB	1:A:481:ALA:HB2	2.38	0.43
1:A:784:GLY:HA2	1:A:808:LEU:HD13	2.00	0.43
1:A:159:ARG:HA	1:A:159:ARG:HD2	1.86	0.43
1:A:471:LEU:HD12	1:A:471:LEU:N	2.33	0.42
1:A:759:PRO:HG2	1:A:762:GLN:NE2	2.34	0.42
1:A:837:LEU:HD13	1:A:848:PHE:CD1	2.53	0.42
1:A:429:HIS:CE1	1:A:509:ASP:HA	2.54	0.42
1:A:208:ASN:ND2	1:A:235:ARG:NH2	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ASN:HB2	1:A:789:PRO:HD3	1.97	0.42
1:A:287:LEU:HB3	1:A:321:ILE:CG1	2.50	0.42
1:A:294:LEU:HD23	1:A:295:ASN:N	2.34	0.42
1:A:409:ASN:O	1:A:409:ASN:ND2	2.53	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:441:ASN:ND2	1:A:447:ALA:N	2.53	0.42
1:A:407:GLU:HA	3:A:868:HOH:O	2.20	0.42
1:A:305:ASP:CG	3:A:1031:HOH:O	2.57	0.42
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.93	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: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:411:GLU:O	1:A:412:GLY:C	2.58	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:438:ARG:CD	3:A:865:HOH:O	2.69	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:581:TYR:OH	3:A:1023:HOH:O	2.20	0.41
1:A:581:TYR:CB	1:A:585:MET:HE2	2.45	0.41
1:A:292:PHE:C	1:A:294:LEU:N	2.73	0.41
1:A:671:LEU:C	1:A:671:LEU:HD13	2.41	0.41
1:A:839:LEU:O	1:A:851:ILE:HD13	2.21	0.41
1:A:473:HIS:O	1:A:474:PRO:O	2.39	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:159:ARG:NH1	3:A:1032:HOH:O	2.51	0.41
1:A:350:VAL:O	1:A:831:VAL:CG2	2.67	0.41
1:A:187:LEU:HD11	1:A:200:ARG:NH2	2.36	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:518:HIS:O	1:A:522:THR:CG2	2.57	0.40
1:A:75:LYS:HE3	1:A:75:LYS:HB3	1.90	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 (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	830/857 (97%)	748 (90%)	48 (6%)	34 (4%)	3 1

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

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	164	ASN
1	A	270	SER
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 (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	733/747 (98%)	593 (81%)	140 (19%)	2	0

All (140) 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	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

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	THR
1	A	92	LEU
1	A	100	LYS
1	A	104	GLU
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	165	GLN
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	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	232	TYR
1	A	238	THR
1	A	243	THR
1	A	247	PRO
1	A	248	ASN
1	A	251	SER
1	A	256	VAL
1	A	258	LEU
1	A	275	TYR
1	A	281	SER
1	A	298	PRO
1	A	299	ARG
1	A	310	LEU
1	A	312	SER
1	A	315	ILE
1	A	316	LYS

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Mol	Chain	Res	Type
1	A	320	ASP
1	A	321	ILE
1	A	323	SER
1	A	324	LYS
1	A	326	SER
1	A	328	LEU
1	A	331	LEU
1	A	334	ILE
1	A	338	ASP
1	A	360	THR
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	427	LEU
1	A	437	LEU
1	A	444	SER
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
1	A	497	ILE
1	A	500	LEU
1	A	507	VAL
1	A	508	ASN
1	A	525	VAL

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Mol	Chain	Res	Type
1	A	537	LEU
1	A	540	VAL
1	A	547	LEU
1	A	553	ASP
1	A	566	VAL
1	A	568	ASP
1	A	571	VAL
1	A	594	VAL
1	A	601	PRO
1	A	604	LEU
1	A	620	ILE
1	A	626	ASP
1	A	627	TYR
1	A	630	THR
1	A	634	LEU
1	A	650	LEU
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	745	LEU
1	A	754	LEU
1	A	762	GLN
1	A	773	LEU
1	A	775	ARG
1	A	785	GLU
1	A	787	ASP
1	A	796	ARG
1	A	798	LEU
1	A	814	LYS
1	A	815	LEU
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

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Mol	Chain	Res	Type
1	A	847	THR
1	A	848	PHE
1	A	851	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	71	ASN
1	A	96	GLN
1	A	102	ASN
1	A	142	HIS
1	A	164	ASN
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	534	ASN
1	A	541	HIS
1	A	618	HIS
1	A	665	GLN
1	A	725	ASN
1	A	750	GLN
1	A	806	ASN
1	A	810	GLN
1	A	813	ASN
1	A	819	ASN

5.3.3　RNA (i)

There are no RNA molecules in this entry.

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

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

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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	HTR	A	519	1	15,16,17	1.75	3 (20%)	12,22,24	1.60	2 (16%)
1	HLU	A	565	1	7,8,9	0.60	0	8,10,12	2.36	3 (37%)

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	HTR	A	519	1	1/1/2/3	0/4/10/12	0/2/2/2
1	HLU	A	565	1	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	HTR	CA-CB	-4.00	1.47	1.54
1	A	519	HTR	CG-CB	-2.97	1.48	1.52
1	A	519	HTR	CD1-CG	-2.93	1.33	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	519	HTR	OH-CB-CG	-2.33	107.30	110.96
1	A	565	HLU	O-C-CA	-2.25	119.49	125.44
1	A	519	HTR	C-CA-N	2.91	115.91	109.83
1	A	565	HLU	CD1-CG-CB	3.71	117.47	111.26
1	A	565	HLU	C-CA-N	4.26	118.73	109.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	519	HTR	CB

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	834/857 (97%)	0.18	58 (6%)	19	21	13, 28, 65, 99	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	ILE	11.6
1	A	46	THR	9.2
1	A	47	LEU	8.3
1	A	397	HIS	8.3
1	A	410	LEU	7.6
1	A	321	ILE	7.2
1	A	395	GLY	6.8
1	A	339	GLY	6.5
1	A	31	SER	6.4
1	A	9	GLY	6.4
1	A	335	PHE	5.8
1	A	137	ASN	5.7
1	A	338	ASP	5.7
1	A	337	THR	5.6
1	A	107	ASP	5.3
1	A	340	GLU	5.1
1	A	396	ASP	4.7
1	A	30	THR	4.6
1	A	326	SER	4.5
1	A	48	ASP	4.2
1	A	333	GLU	4.2
1	A	476	GLY	4.2
1	A	784	GLY	4.1
1	A	32	VAL	3.9
1	A	296	PHE	3.8
1	A	317	LEU	3.7
1	A	322	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	3.7
1	A	341	GLN	3.6
1	A	394	TYR	3.5
1	A	49	THR	3.3
1	A	342	ALA	3.3
1	A	398	THR	3.3
1	A	409	ASN	3.3
1	A	336	ARG	3.2
1	A	479	SER	3.0
1	A	737	LYS	2.9
1	A	318	PRO	2.8
1	A	327	PRO	2.8
1	A	135	ILE	2.7
1	A	334	ILE	2.7
1	A	738	GLY	2.7
1	A	319	THR	2.7
1	A	275	TYR	2.7
1	A	290	SER	2.6
1	A	475	GLN	2.5
1	A	320	ASP	2.4
1	A	284	VAL	2.4
1	A	393	VAL	2.3
1	A	324	LYS	2.3
1	A	482	PHE	2.2
1	A	480	GLY	2.2
1	A	411	GLU	2.2
1	A	329	PRO	2.2
1	A	473	HIS	2.1
1	A	414	THR	2.0
1	A	51	THR	2.0
1	A	687	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	HTR	A	519	15/16	0.95	0.14	-	17,19,21,30	0
1	HLU	A	565	9/10	0.91	0.18	-	26,29,33,36	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE	A	858	1/1	0.98	0.06	-4.66	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.