



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 AM UTC

PDB ID : 2IUJ / pdb_00002iuj
Title : Crystal Structure of Soybean Lipxygenase-B
Authors : Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on : 2006-06-05
Resolution : 2.40 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

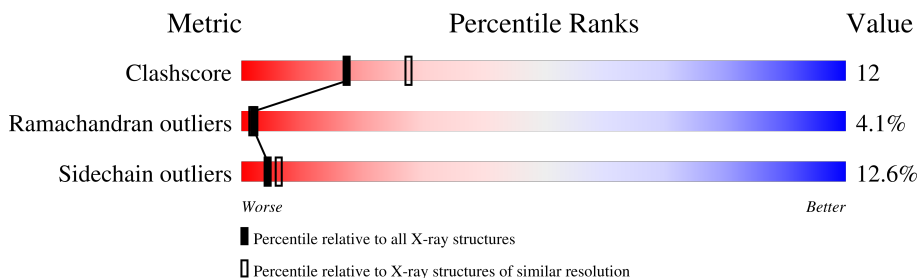
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	853	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6799 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 LIPOXYGENASE L-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6692	4307	1110	1262	13			

- 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.

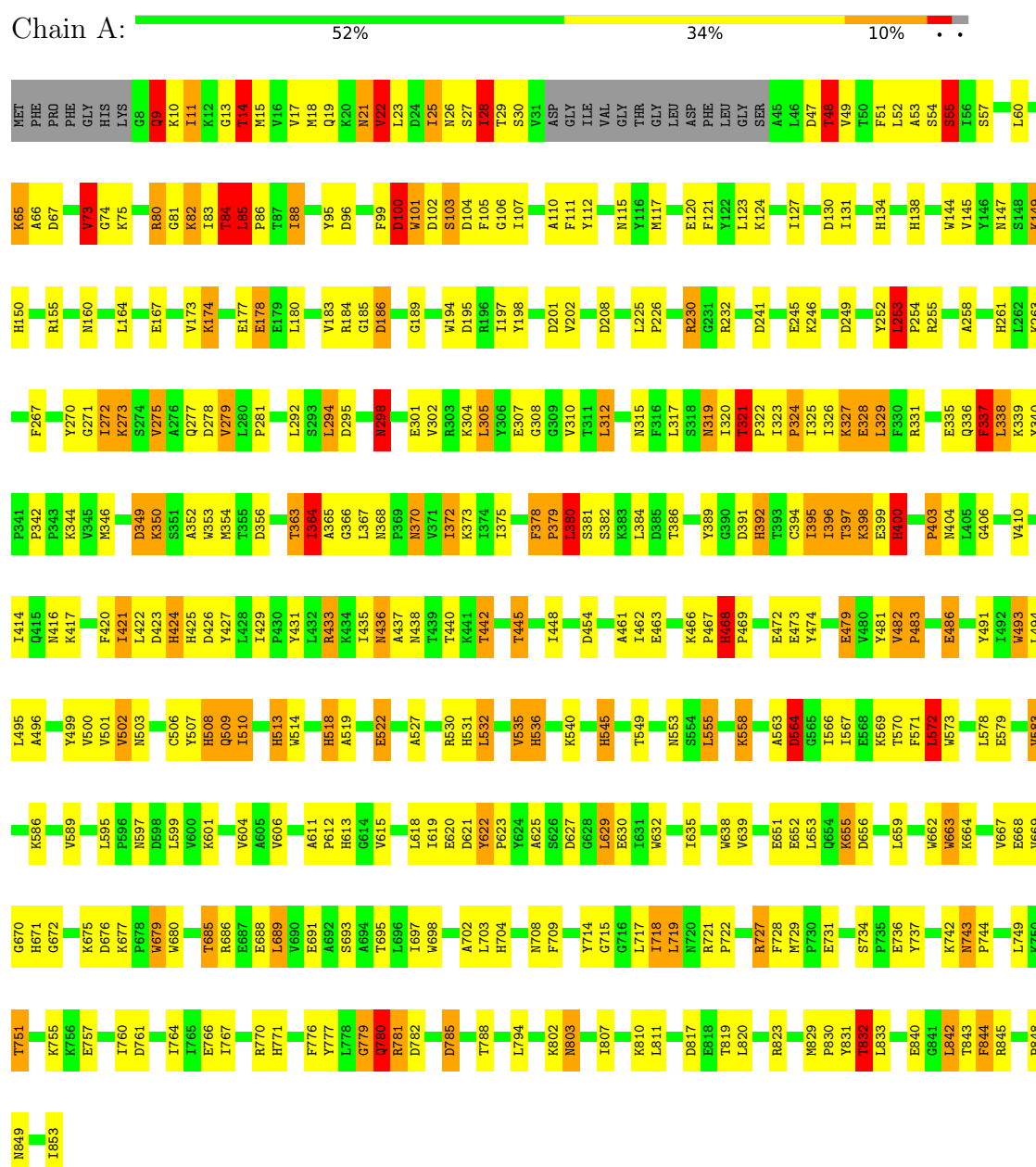
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: LIPOXYGENASE L-5



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.99Å 105.31Å 105.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	89.5 (15.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.050 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.03	30/6866 (0.4%)	1.95	218/9322 (2.3%)

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	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	ILE	CA-CB	7.58	1.57	1.54
1	A	771	HIS	CD2-NE2	-7.50	1.29	1.37
1	A	536	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	424	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	261	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	468	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	513	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	508	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	138	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	425	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	392	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	400	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	545	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	261	HIS	CG-ND1	-6.19	1.31	1.38
1	A	613	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	531	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	671	HIS	CD2-NE2	-6.01	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	518	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	73	VAL	CA-CB	5.62	1.62	1.54
1	A	14	THR	CA-CB	5.61	1.62	1.53
1	A	150	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	704	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	536	HIS	CG-ND1	-5.50	1.32	1.38
1	A	424	HIS	CG-ND1	-5.50	1.32	1.38
1	A	531	HIS	CG-ND1	-5.46	1.32	1.38
1	A	782	ASP	CA-CB	5.35	1.61	1.54
1	A	138	HIS	CG-ND1	-5.24	1.32	1.38
1	A	513	HIS	CG-ND1	-5.08	1.32	1.38
1	A	48	THR	CA-CB	5.05	1.62	1.53

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	ASP	CA-CB-CG	14.71	127.31	112.60
1	A	572	LEU	N-CA-C	10.88	124.49	111.33
1	A	186	ASP	N-CA-C	10.61	133.41	110.80
1	A	66	ALA	N-CA-C	10.08	124.96	110.14
1	A	329	LEU	N-CA-C	-9.98	96.28	111.56
1	A	275	VAL	N-CA-C	-9.53	102.62	111.67
1	A	337	PHE	N-CA-C	9.40	122.33	108.60
1	A	467	PRO	N-CA-C	9.28	127.27	113.81
1	A	100	ASP	CA-CB-CG	9.25	121.85	112.60
1	A	833	LEU	N-CA-C	9.21	121.39	111.36
1	A	709	PHE	CA-CB-CG	-9.20	104.61	113.80
1	A	328	GLU	N-CA-C	-8.47	101.19	112.72
1	A	395	ILE	N-CA-CB	-8.46	99.72	112.15
1	A	364	ILE	CB-CA-C	8.19	120.97	111.55
1	A	454	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	47	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	349	ASP	CA-CB-CG	7.72	120.32	112.60
1	A	423	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	49	VAL	N-CA-C	7.50	124.95	109.34
1	A	531	HIS	CA-CB-CG	-7.40	106.40	113.80
1	A	381	SER	N-CA-C	7.36	120.02	110.53
1	A	832	THR	N-CA-CB	-7.32	98.57	110.42
1	A	111	PHE	CA-CB-CG	7.31	121.11	113.80
1	A	743	ASN	CA-CB-CG	7.29	119.89	112.60
1	A	396	ILE	CB-CA-C	-7.28	102.01	111.25
1	A	364	ILE	N-CA-CB	-7.28	98.13	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	780	GLN	CA-C-N	7.28	132.30	122.84
1	A	780	GLN	C-N-CA	7.28	132.30	122.84
1	A	621	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	404	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	421	ILE	CB-CA-C	-7.24	100.84	111.19
1	A	298	ASN	CA-CB-CG	7.21	119.81	112.60
1	A	785	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	294	LEU	N-CA-C	7.16	121.11	112.38
1	A	337	PHE	CA-C-N	7.13	135.16	121.54
1	A	337	PHE	C-N-CA	7.13	135.16	121.54
1	A	844	PHE	N-CA-C	-7.08	104.57	112.57
1	A	426	ASP	N-CA-C	6.99	125.68	110.80
1	A	26	ASN	CA-CB-CG	6.98	119.58	112.60
1	A	391	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	466	LYS	CA-C-N	6.96	127.54	119.47
1	A	466	LYS	C-N-CA	6.96	127.54	119.47
1	A	429	ILE	CA-C-O	-6.94	113.44	118.71
1	A	370	ASN	N-CA-C	6.93	121.72	112.30
1	A	502	VAL	N-CA-CB	-6.92	102.83	110.51
1	A	638	TRP	CG-CD2-CE3	6.81	140.71	133.90
1	A	339	LYS	N-CA-C	6.76	120.65	108.48
1	A	519	ALA	N-CA-C	6.75	118.72	111.36
1	A	396	ILE	N-CA-C	-6.71	97.26	107.73
1	A	736	GLU	N-CA-C	-6.65	103.65	111.03
1	A	755	LYS	N-CA-C	6.58	119.01	111.11
1	A	780	GLN	N-CA-C	6.58	124.81	110.80
1	A	403	PRO	CA-C-N	6.56	129.40	120.54
1	A	403	PRO	C-N-CA	6.56	129.40	120.54
1	A	49	VAL	N-CA-CB	-6.54	100.44	111.23
1	A	9	GLN	N-CA-C	6.53	124.72	110.80
1	A	493	TRP	CG-CD2-CE3	6.53	140.43	133.90
1	A	392	HIS	CB-CG-CD2	-6.50	122.74	131.20
1	A	396	ILE	N-CA-CB	6.48	119.28	111.31
1	A	832	THR	CA-CB-CG2	6.48	121.52	110.50
1	A	771	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	819	THR	CA-CB-OG1	-6.42	99.96	109.60
1	A	144	TRP	CG-CD2-CE3	6.42	140.32	133.90
1	A	74	GLY	O-C-N	6.41	131.03	122.70
1	A	433	ARG	O-C-N	6.35	128.61	122.07
1	A	195	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	638	TRP	CB-CG-CD1	-6.30	117.45	126.90
1	A	319	ASN	CA-CB-CG	6.29	118.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	425	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	513	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	A	261	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	373	LYS	N-CA-C	6.21	118.39	109.14
1	A	844	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	189	GLY	O-C-N	6.16	128.19	122.47
1	A	832	THR	CA-CB-OG1	-6.14	100.38	109.60
1	A	535	VAL	N-CA-CB	-6.14	101.76	112.08
1	A	21	ASN	N-CA-C	6.11	120.20	112.87
1	A	788	THR	CA-C-N	6.11	128.38	120.44
1	A	788	THR	C-N-CA	6.11	128.38	120.44
1	A	514	TRP	CA-C-O	-6.10	114.59	121.00
1	A	755	LYS	CB-CG-CD	-6.08	97.31	111.30
1	A	420	PHE	N-CA-C	6.04	119.33	109.24
1	A	433	ARG	CA-C-N	6.02	128.35	120.28
1	A	433	ARG	C-N-CA	6.02	128.35	120.28
1	A	779	GLY	CA-C-N	6.02	133.04	121.54
1	A	779	GLY	C-N-CA	6.02	133.04	121.54
1	A	729	MET	CA-C-N	6.00	126.35	119.93
1	A	729	MET	C-N-CA	6.00	126.35	119.93
1	A	85	LEU	CA-C-N	5.97	127.08	120.45
1	A	85	LEU	C-N-CA	5.97	127.08	120.45
1	A	536	HIS	CA-C-N	5.97	127.30	119.84
1	A	536	HIS	C-N-CA	5.97	127.30	119.84
1	A	395	ILE	CB-CA-C	5.97	120.06	111.88
1	A	702	ALA	N-CA-C	5.96	119.02	111.69
1	A	445	THR	CA-C-N	5.94	131.73	121.64
1	A	445	THR	C-N-CA	5.94	131.73	121.64
1	A	473	GLU	N-CA-C	5.93	119.78	112.54
1	A	622	TYR	CA-C-N	5.92	126.33	119.47
1	A	622	TYR	C-N-CA	5.92	126.33	119.47
1	A	144	TRP	CE2-CD2-CG	-5.90	100.12	107.20
1	A	101	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	A	611	ALA	N-CA-C	5.89	118.25	110.36
1	A	173	VAL	CB-CA-C	-5.88	104.34	112.04
1	A	522	GLU	CA-C-N	5.86	125.54	119.56
1	A	522	GLU	C-N-CA	5.86	125.54	119.56
1	A	105	PHE	N-CA-C	-5.85	105.23	112.90
1	A	186	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	22	VAL	N-CA-CB	-5.84	99.33	111.24
1	A	368	ASN	CA-CB-CG	5.80	118.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	PHE	CA-C-N	5.78	128.30	120.38
1	A	571	PHE	C-N-CA	5.78	128.30	120.38
1	A	670	GLY	O-C-N	5.76	127.83	122.13
1	A	15	MET	CG-SD-CE	-5.75	88.25	100.90
1	A	619	ILE	N-CA-C	-5.74	98.36	107.15
1	A	448	ILE	CA-C-O	5.73	127.18	120.71
1	A	208	ASP	CA-C-N	5.71	125.33	119.56
1	A	208	ASP	C-N-CA	5.71	125.33	119.56
1	A	423	ASP	CA-C-O	5.71	127.05	120.60
1	A	379	PRO	CA-C-N	5.69	132.40	121.54
1	A	379	PRO	C-N-CA	5.69	132.40	121.54
1	A	445	THR	N-CA-C	5.69	118.20	110.35
1	A	22	VAL	CB-CA-C	5.63	119.59	111.65
1	A	632	TRP	CG-CD2-CE3	5.63	139.53	133.90
1	A	312	LEU	O-C-N	-5.63	116.31	122.06
1	A	669	VAL	N-CA-C	-5.63	107.18	111.62
1	A	178	GLU	CA-CB-CG	5.62	125.35	114.10
1	A	677	LYS	CA-C-N	5.62	125.32	119.64
1	A	677	LYS	C-N-CA	5.62	125.32	119.64
1	A	611	ALA	CA-C-N	5.58	125.42	119.28
1	A	611	ALA	C-N-CA	5.58	125.42	119.28
1	A	397	THR	CA-C-N	5.57	132.17	121.54
1	A	397	THR	C-N-CA	5.57	132.17	121.54
1	A	680	TRP	CG-CD2-CE3	5.57	139.47	133.90
1	A	253	LEU	CA-C-N	5.56	126.79	119.84
1	A	253	LEU	C-N-CA	5.56	126.79	119.84
1	A	372	ILE	N-CA-C	5.56	117.45	109.51
1	A	225	LEU	CA-C-N	5.54	125.86	119.93
1	A	225	LEU	C-N-CA	5.54	125.86	119.93
1	A	416	ASN	N-CA-C	5.52	119.72	113.15
1	A	429	ILE	CA-C-N	5.51	125.18	119.56
1	A	429	ILE	C-N-CA	5.51	125.18	119.56
1	A	101	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	A	255	ARG	N-CA-C	5.49	117.97	111.33
1	A	340	TYR	CA-C-N	5.48	126.03	120.38
1	A	340	TYR	C-N-CA	5.48	126.03	120.38
1	A	84	THR	N-CA-C	5.48	122.48	110.80
1	A	468	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	A	249	ASP	CA-CB-CG	5.47	118.08	112.60
1	A	83	ILE	N-CA-C	5.47	117.53	108.99
1	A	469	PRO	N-CA-C	5.47	120.95	113.84
1	A	144	TRP	CD1-CG-CD2	5.47	115.05	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	399	GLU	N-CA-C	5.46	116.92	110.97
1	A	55	SER	N-CA-C	-5.46	99.18	110.80
1	A	134	HIS	CB-CG-CD2	-5.46	124.11	131.20
1	A	493	TRP	CB-CG-CD1	-5.44	118.74	126.90
1	A	656	ASP	CA-C-N	5.41	124.93	119.19
1	A	656	ASP	C-N-CA	5.41	124.93	119.19
1	A	507	TYR	N-CA-C	-5.41	105.54	111.82
1	A	65	LYS	N-CA-C	5.41	117.77	109.07
1	A	241	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	536	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	514	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	A	273	LYS	N-CA-C	-5.39	105.48	111.36
1	A	679	TRP	CE2-CD2-CG	-5.39	100.74	107.20
1	A	632	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	A	680	TRP	CE2-CD2-CG	-5.38	100.75	107.20
1	A	261	HIS	N-CA-C	-5.36	99.58	108.75
1	A	620	GLU	N-CA-C	5.36	118.04	111.82
1	A	679	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	638	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	A	728	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	545	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	112	TYR	O-C-N	-5.30	116.99	123.19
1	A	656	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	436	ASN	N-CA-C	5.28	119.57	113.18
1	A	782	ASP	O-C-N	-5.26	116.10	122.68
1	A	731	GLU	CB-CG-CD	5.26	121.54	112.60
1	A	493	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	252	TYR	CA-C-O	5.25	126.96	120.92
1	A	386	THR	N-CA-C	5.24	117.08	111.36
1	A	782	ASP	N-CA-C	-5.24	101.43	108.19
1	A	635	ILE	N-CA-C	-5.21	105.52	110.42
1	A	246	LYS	CA-C-N	5.21	125.49	119.92
1	A	246	LYS	C-N-CA	5.21	125.49	119.92
1	A	363	THR	CA-C-N	5.18	128.46	122.35
1	A	363	THR	C-N-CA	5.18	128.46	122.35
1	A	803	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	510	ILE	N-CA-C	5.17	116.26	111.45
1	A	595	LEU	N-CA-C	5.16	120.49	113.16
1	A	708	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	438	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	527	ALA	N-CA-C	5.15	117.80	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	PHE	N-CA-C	5.15	119.43	113.20
1	A	663	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	315	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	612	PRO	N-CA-C	5.13	120.57	113.65
1	A	704	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	54	SER	CA-C-N	5.12	131.32	121.54
1	A	54	SER	C-N-CA	5.12	131.32	121.54
1	A	120	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	27	SER	CA-C-N	5.11	131.16	121.97
1	A	27	SER	C-N-CA	5.11	131.16	121.97
1	A	272	ILE	CA-CB-CG1	-5.09	101.74	110.40
1	A	397	THR	O-C-N	5.09	130.31	123.34
1	A	685	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	522	GLU	CA-C-O	-5.08	113.95	118.63
1	A	766	GLU	CA-CB-CG	-5.07	103.96	114.10
1	A	353	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	A	767	ILE	N-CA-C	-5.06	105.56	110.42
1	A	342	PRO	CA-C-N	5.06	124.99	119.78
1	A	342	PRO	C-N-CA	5.06	124.99	119.78
1	A	781	ARG	N-CA-C	5.04	116.82	108.20
1	A	396	ILE	CA-CB-CG2	-5.03	101.95	110.50
1	A	144	TRP	CB-CG-CD1	-5.02	119.38	126.90
1	A	549	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	398	LYS	N-CA-CB	-5.00	102.03	110.49

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	THR	Peptide
1	A	378	PHE	Peptide
1	A	85	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6692	0	6601	166	0
2	A	1	0	0	0	0
3	A	106	0	0	2	0
All	All	6799	0	6601	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (166) 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:718:ILE:HD13	1:A:718:ILE:H	1.31	0.92
1:A:253:LEU:HD21	1:A:258:ALA:HB2	1.53	0.90
1:A:82:LYS:HG3	1:A:95:TYR:HE2	1.37	0.87
1:A:653:LEU:HD13	1:A:686:ARG:HG3	1.66	0.78
1:A:653:LEU:HD11	1:A:689:LEU:HD12	1.67	0.77
1:A:328:GLU:HA	1:A:331:ARG:HA	1.65	0.77
1:A:394:CYS:SG	1:A:396:ILE:HG12	2.28	0.74
1:A:11:ILE:HG13	1:A:99:PHE:HB2	1.69	0.73
1:A:685:THR:HG22	1:A:688:GLU:H	1.55	0.71
1:A:510:ILE:HD11	1:A:567:ILE:HG21	1.72	0.71
1:A:718:ILE:H	1:A:718:ILE:CD1	2.05	0.70
1:A:518:HIS:HD1	1:A:553:ASN:ND2	1.91	0.69
1:A:442:THR:HG21	1:A:572:LEU:HD11	1.76	0.68
1:A:324:PRO:O	1:A:327:LYS:HB3	1.93	0.68
1:A:715:GLY:HA2	1:A:721:ARG:HB2	1.76	0.66
1:A:832:THR:HG23	1:A:845:ARG:HB3	1.76	0.65
1:A:202:VAL:O	1:A:230:ARG:HD2	1.97	0.65
1:A:51:PHE:H	1:A:82:LYS:HD2	1.62	0.65
1:A:82:LYS:HG3	1:A:95:TYR:CE2	2.28	0.64
1:A:21:ASN:HB2	1:A:28:ILE:HB	1.78	0.63
1:A:777:TYR:HA	1:A:848:PRO:HA	1.80	0.62
1:A:518:HIS:HD1	1:A:553:ASN:HD21	1.50	0.60
1:A:378:PHE:HZ	1:A:397:THR:HA	1.66	0.60
1:A:727:ARG:HB2	1:A:751:THR:HG23	1.83	0.60
1:A:509:GLN:NE2	1:A:509:GLN:HA	2.18	0.59
1:A:400:HIS:H	1:A:400:HIS:CD2	2.18	0.59
1:A:201:ASP:HB2	1:A:232:ARG:HG3	1.85	0.58
1:A:180:LEU:HB3	1:A:184:ARG:NH2	2.17	0.58
1:A:501:VAL:HG11	1:A:721:ARG:HA	1.84	0.58
1:A:28:ILE:HD13	1:A:29:THR:H	1.66	0.58
1:A:17:VAL:HG12	1:A:123:LEU:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:HD3	1:A:472:GLU:HG3	1.85	0.58
1:A:267:PHE:HB3	1:A:270:TYR:HB3	1.86	0.58
1:A:325:ILE:O	1:A:329:LEU:HB2	2.02	0.58
1:A:501:VAL:HG11	1:A:722:PRO:HD2	1.86	0.58
1:A:21:ASN:H	1:A:21:ASN:HD22	1.51	0.57
1:A:436:ASN:HA	1:A:440:THR:O	2.04	0.57
1:A:652:GLU:HA	1:A:655:LYS:HB2	1.86	0.57
1:A:302:VAL:O	1:A:305:LEU:HB2	2.04	0.57
1:A:583:VAL:HG12	1:A:586:LYS:HE2	1.86	0.57
1:A:145:VAL:HG22	1:A:155:ARG:HG3	1.86	0.57
1:A:102:ASP:CG	1:A:103:SER:H	2.13	0.56
1:A:506:CYS:HG	1:A:573:TRP:CG	2.23	0.56
1:A:9:GLN:NE2	1:A:10:LYS:H	2.04	0.56
1:A:479:GLU:HG3	1:A:481:TYR:HE1	1.70	0.56
1:A:651:GLU:O	1:A:655:LYS:HE3	2.05	0.56
1:A:532:LEU:HD13	1:A:662:TRP:HB2	1.88	0.56
1:A:298:ASN:HD22	1:A:301:GLU:H	1.53	0.56
1:A:365:ALA:HB2	1:A:623:PRO:HG2	1.89	0.55
1:A:509:GLN:HA	1:A:509:GLN:HE21	1.72	0.55
1:A:436:ASN:HD21	1:A:442:THR:N	2.04	0.55
1:A:734:SER:HB2	1:A:737:TYR:H	1.71	0.55
1:A:9:GLN:CD	1:A:10:LYS:H	2.14	0.55
1:A:337:PHE:HD1	1:A:338:LEU:H	1.55	0.54
1:A:823:ARG:O	1:A:830:PRO:HA	2.08	0.54
1:A:271:GLY:O	1:A:275:VAL:HG23	2.08	0.54
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.91	0.53
1:A:304:LYS:HA	1:A:307:GLU:HB2	1.89	0.53
1:A:570:THR:HG21	1:A:761:ASP:HB2	1.90	0.52
1:A:566:ILE:HG21	1:A:764:ILE:HG13	1.90	0.52
1:A:9:GLN:O	1:A:100:ASP:HA	2.08	0.52
1:A:327:LYS:C	1:A:329:LEU:H	2.17	0.52
1:A:384:LEU:HD13	1:A:389:TYR:HB2	1.92	0.52
1:A:445:THR:H	1:A:503:ASN:ND2	2.07	0.52
1:A:424:HIS:HB3	1:A:503:ASN:HD22	1.74	0.52
1:A:121:PHE:HE1	1:A:123:LEU:HB2	1.74	0.51
1:A:482:VAL:HG13	1:A:483:PRO:HD2	1.92	0.51
1:A:273:LYS:HB2	1:A:555:LEU:HD11	1.93	0.51
1:A:13:GLY:HA3	1:A:99:PHE:HE2	1.75	0.51
1:A:107:ILE:HD12	1:A:131:ILE:HD11	1.90	0.51
1:A:277:GLN:HE22	1:A:558:LYS:HE2	1.75	0.51
1:A:378:PHE:CZ	1:A:397:THR:HA	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:HIS:C	1:A:513:HIS:CD2	2.87	0.50
1:A:779:GLY:C	1:A:781:ARG:H	2.18	0.50
1:A:230:ARG:HA	1:A:522:GLU:HG2	1.94	0.50
1:A:164:LEU:HD23	3:A:2090:HOH:O	2.11	0.50
1:A:468:HIS:CD2	1:A:474:TYR:HB2	2.47	0.50
1:A:335:GLU:HG2	1:A:336:GLN:H	1.77	0.49
1:A:570:THR:CG2	1:A:761:ASP:HB2	2.42	0.49
1:A:275:VAL:HA	1:A:279:VAL:HB	1.94	0.49
1:A:832:THR:HG22	1:A:844:PHE:O	2.13	0.49
1:A:597:ASN:O	1:A:601:LYS:HG2	2.13	0.49
1:A:319:ASN:HB2	1:A:320:ILE:HD12	1.95	0.48
1:A:375:ILE:HG23	1:A:380:LEU:HD11	1.95	0.48
1:A:718:ILE:HD13	1:A:718:ILE:N	2.13	0.48
1:A:321:THR:HB	1:A:322:PRO:HG3	1.95	0.48
1:A:298:ASN:ND2	1:A:301:GLU:N	2.62	0.48
1:A:714:TYR:CE1	1:A:829:MET:SD	3.06	0.48
1:A:410:VAL:O	1:A:414:ILE:HG23	2.14	0.48
1:A:350:LYS:HD2	3:A:2062:HOH:O	2.14	0.47
1:A:198:TYR:HB2	1:A:530:ARG:HG3	1.97	0.47
1:A:445:THR:H	1:A:503:ASN:HD21	1.60	0.47
1:A:325:ILE:C	1:A:327:LYS:H	2.23	0.47
1:A:298:ASN:ND2	1:A:301:GLU:H	2.13	0.46
1:A:693:SER:O	1:A:697:ILE:HG13	2.15	0.46
1:A:310:VAL:HB	1:A:338:LEU:HB3	1.98	0.46
1:A:499:TYR:OH	1:A:751:THR:HG21	2.16	0.45
1:A:664:LYS:O	1:A:668:GLU:HB2	2.16	0.45
1:A:183:VAL:O	1:A:197:ILE:HA	2.16	0.45
1:A:436:ASN:HD21	1:A:442:THR:H	1.63	0.45
1:A:757:GLU:HA	1:A:760:ILE:HG12	1.97	0.45
1:A:253:LEU:HD21	1:A:258:ALA:CB	2.35	0.45
1:A:479:GLU:HG3	1:A:481:TYR:CE1	2.51	0.45
1:A:19:GLN:O	1:A:22:VAL:HB	2.17	0.45
1:A:115:ASN:HB2	1:A:145:VAL:HG12	1.98	0.45
1:A:672:GLY:HA2	1:A:675:LYS:HB3	1.99	0.45
1:A:389:TYR:HB3	1:A:392:HIS:CE1	2.52	0.44
1:A:14:THR:HG23	1:A:127:ILE:HG13	1.99	0.44
1:A:424:HIS:HA	1:A:427:TYR:CE2	2.52	0.44
1:A:417:LYS:HG2	1:A:618:LEU:HD13	1.99	0.44
1:A:278:ASP:HB3	1:A:323:ILE:HG12	1.99	0.44
1:A:400:HIS:CD2	1:A:400:HIS:N	2.85	0.44
1:A:344:LYS:C	1:A:346:MET:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:O	1:A:435:ILE:HG13	2.18	0.44
1:A:364:ILE:CD1	1:A:372:ILE:HG21	2.48	0.44
1:A:843:THR:HB	1:A:845:ARG:HG2	1.99	0.44
1:A:84:THR:HA	1:A:88:ILE:HD11	1.99	0.44
1:A:344:LYS:CB	1:A:829:MET:HE3	2.48	0.44
1:A:743:ASN:HA	1:A:744:PRO:HD3	1.75	0.44
1:A:85:LEU:N	1:A:86:PRO:HA	2.33	0.43
1:A:545:HIS:HE1	1:A:849:ASN:HD22	1.65	0.43
1:A:545:HIS:CE1	1:A:849:ASN:HD22	2.36	0.43
1:A:563:ALA:O	1:A:564:ASP:HB2	2.18	0.43
1:A:328:GLU:HA	1:A:331:ARG:CA	2.41	0.43
1:A:121:PHE:CE1	1:A:123:LEU:HB2	2.53	0.43
1:A:363:THR:HG21	1:A:372:ILE:HD12	2.01	0.43
1:A:653:LEU:CD1	1:A:689:LEU:HD12	2.43	0.43
1:A:382:SER:OG	1:A:384:LEU:HG	2.18	0.43
1:A:436:ASN:ND2	1:A:442:THR:H	2.17	0.43
1:A:10:LYS:HA	1:A:99:PHE:O	2.18	0.43
1:A:101:TRP:CZ3	1:A:106:GLY:O	2.72	0.43
1:A:807:ILE:O	1:A:811:LEU:HD13	2.19	0.43
1:A:18:MET:HE2	1:A:124:LYS:HD3	1.99	0.43
1:A:81:GLY:HA3	1:A:96:ASP:HB3	2.01	0.43
1:A:147:ASN:HD22	1:A:149:LYS:H	1.66	0.43
1:A:349:ASP:HB3	1:A:352:ALA:HB2	2.01	0.42
1:A:382:SER:HB2	1:A:392:HIS:O	2.19	0.42
1:A:536:HIS:O	1:A:540:LYS:HG3	2.19	0.42
1:A:776:PHE:HD1	1:A:781:ARG:HB3	1.85	0.42
1:A:65:LYS:NZ	1:A:104:ASP:HA	2.34	0.42
1:A:354:MET:HE3	1:A:494:LEU:HD11	2.00	0.42
1:A:717:LEU:HG	1:A:719:LEU:HB2	2.01	0.42
1:A:663:TRP:O	1:A:667:VAL:HG22	2.20	0.42
1:A:491:TYR:CD2	1:A:744:PRO:HB2	2.55	0.42
1:A:25:ILE:HD12	1:A:25:ILE:H	1.84	0.42
1:A:625:ALA:O	1:A:629:LEU:HD22	2.20	0.42
1:A:14:THR:HG23	1:A:127:ILE:CG1	2.50	0.41
1:A:21:ASN:H	1:A:21:ASN:ND2	2.17	0.41
1:A:817:ASP:OD1	1:A:820:LEU:HG	2.20	0.41
1:A:396:ILE:HD11	1:A:463:GLU:N	2.35	0.41
1:A:604:VAL:HG21	1:A:622:TYR:HE2	1.84	0.41
1:A:51:PHE:CZ	1:A:117:MET:SD	3.14	0.41
1:A:695:THR:O	1:A:698:TRP:HB3	2.21	0.41
1:A:174:LYS:O	1:A:178:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HD12	1:A:461:ALA:HB1	2.03	0.41
1:A:779:GLY:O	1:A:781:ARG:N	2.38	0.41
1:A:60:LEU:O	1:A:73:VAL:HA	2.21	0.41
1:A:734:SER:H	1:A:737:TYR:HB3	1.86	0.41
1:A:803:ASN:O	1:A:807:ILE:HG13	2.20	0.41
1:A:770:ARG:HG2	1:A:842:LEU:HB2	2.03	0.40
1:A:496:ALA:O	1:A:500:VAL:HG23	2.20	0.40
1:A:589:VAL:HG13	1:A:679:TRP:CD2	2.56	0.40
1:A:832:THR:HG22	1:A:844:PHE:C	2.46	0.40
1:A:366:GLY:HA2	1:A:714:TYR:CE2	2.56	0.40
1:A:462:ILE:HD12	1:A:493:TRP:CZ3	2.57	0.40
1:A:569:LYS:HA	1:A:569:LYS:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	829/853 (97%)	714 (86%)	81 (10%)	34 (4%)	 

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	48	THR
1	A	75	LYS
1	A	84	THR
1	A	186	ASP
1	A	380	LEU
1	A	398	LYS
1	A	780	GLN
1	A	55	SER

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	103	SER
1	A	130	ASP
1	A	185	GLY
1	A	53	ALA
1	A	80	ARG
1	A	110	ALA
1	A	327	LYS
1	A	403	PRO
1	A	564	ASP
1	A	831	TYR
1	A	167	GLU
1	A	308	GLY
1	A	437	ALA
1	A	468	HIS
1	A	486	GLU
1	A	508	HIS
1	A	30	SER
1	A	326	ILE
1	A	338	LEU
1	A	160	ASN
1	A	406	GLY
1	A	742	LYS
1	A	85	LEU
1	A	379	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	724/739 (98%)	633 (87%)	91 (13%)	4 6

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN

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Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	THR
1	A	22	VAL
1	A	23	LEU
1	A	25	ILE
1	A	28	ILE
1	A	48	THR
1	A	52	LEU
1	A	55	SER
1	A	57	SER
1	A	67	ASP
1	A	73	VAL
1	A	80	ARG
1	A	88	ILE
1	A	100	ASP
1	A	149	LYS
1	A	174	LYS
1	A	177	GLU
1	A	194	TRP
1	A	226	PRO
1	A	230	ARG
1	A	245	GLU
1	A	253	LEU
1	A	254	PRO
1	A	263	LYS
1	A	272	ILE
1	A	279	VAL
1	A	281	PRO
1	A	292	LEU
1	A	294	LEU
1	A	295	ASP
1	A	298	ASN
1	A	305	LEU
1	A	312	LEU
1	A	317	LEU
1	A	321	THR
1	A	324	PRO
1	A	337	PHE
1	A	350	LYS
1	A	364	ILE
1	A	367	LEU
1	A	370	ASN

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Mol	Chain	Res	Type
1	A	380	LEU
1	A	395	ILE
1	A	400	HIS
1	A	421	ILE
1	A	422	LEU
1	A	442	THR
1	A	479	GLU
1	A	482	VAL
1	A	483	PRO
1	A	486	GLU
1	A	495	LEU
1	A	502	VAL
1	A	509	GLN
1	A	532	LEU
1	A	535	VAL
1	A	555	LEU
1	A	558	LYS
1	A	564	ASP
1	A	572	LEU
1	A	578	LEU
1	A	579	GLU
1	A	583	VAL
1	A	599	LEU
1	A	606	VAL
1	A	615	VAL
1	A	629	LEU
1	A	630	GLU
1	A	639	VAL
1	A	655	LYS
1	A	659	LEU
1	A	676	ASP
1	A	689	LEU
1	A	691	GLU
1	A	703	LEU
1	A	718	ILE
1	A	719	LEU
1	A	727	ARG
1	A	749	LEU
1	A	751	THR
1	A	780	GLN
1	A	785	ASP
1	A	794	LEU

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Mol	Chain	Res	Type
1	A	802	LYS
1	A	810	LYS
1	A	832	THR
1	A	840	GLU
1	A	842	LEU
1	A	853	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	21	ASN
1	A	98	GLN
1	A	147	ASN
1	A	161	ASN
1	A	277	GLN
1	A	298	ASN
1	A	319	ASN
1	A	347	GLN
1	A	370	ASN
1	A	387	GLN
1	A	392	HIS
1	A	415	GLN
1	A	436	ASN
1	A	503	ASN
1	A	509	GLN
1	A	553	ASN
1	A	711	GLN
1	A	803	ASN
1	A	822	ASN
1	A	849	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.