



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:42 PM GMT

PDB ID : 1LNH
Title : LIPOXYGENASE-3(SOYBEAN) NON-HEME FE(II) METALLOPROTEIN
Authors : Skrzypczak-Jankun, E.
Deposited on : 1996-03-29
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

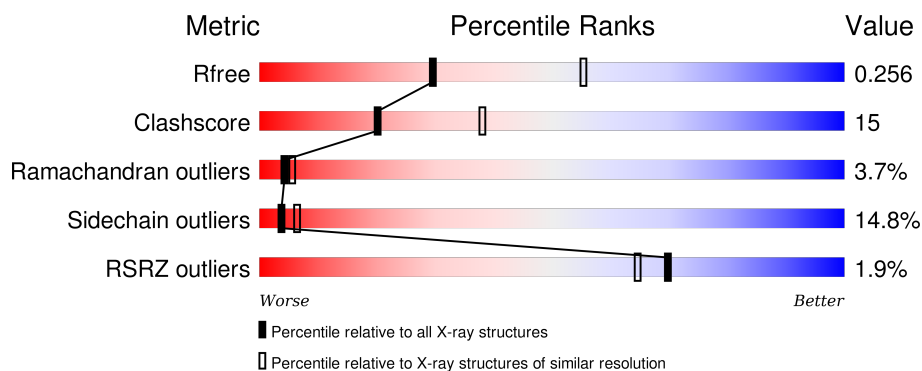
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

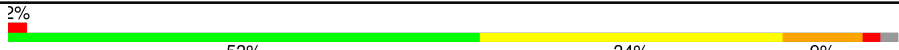
The reported resolution of this entry is 2.60 Å.

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 $\leq 5\%$. 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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6867 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6696	4278	1149	1251	18			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

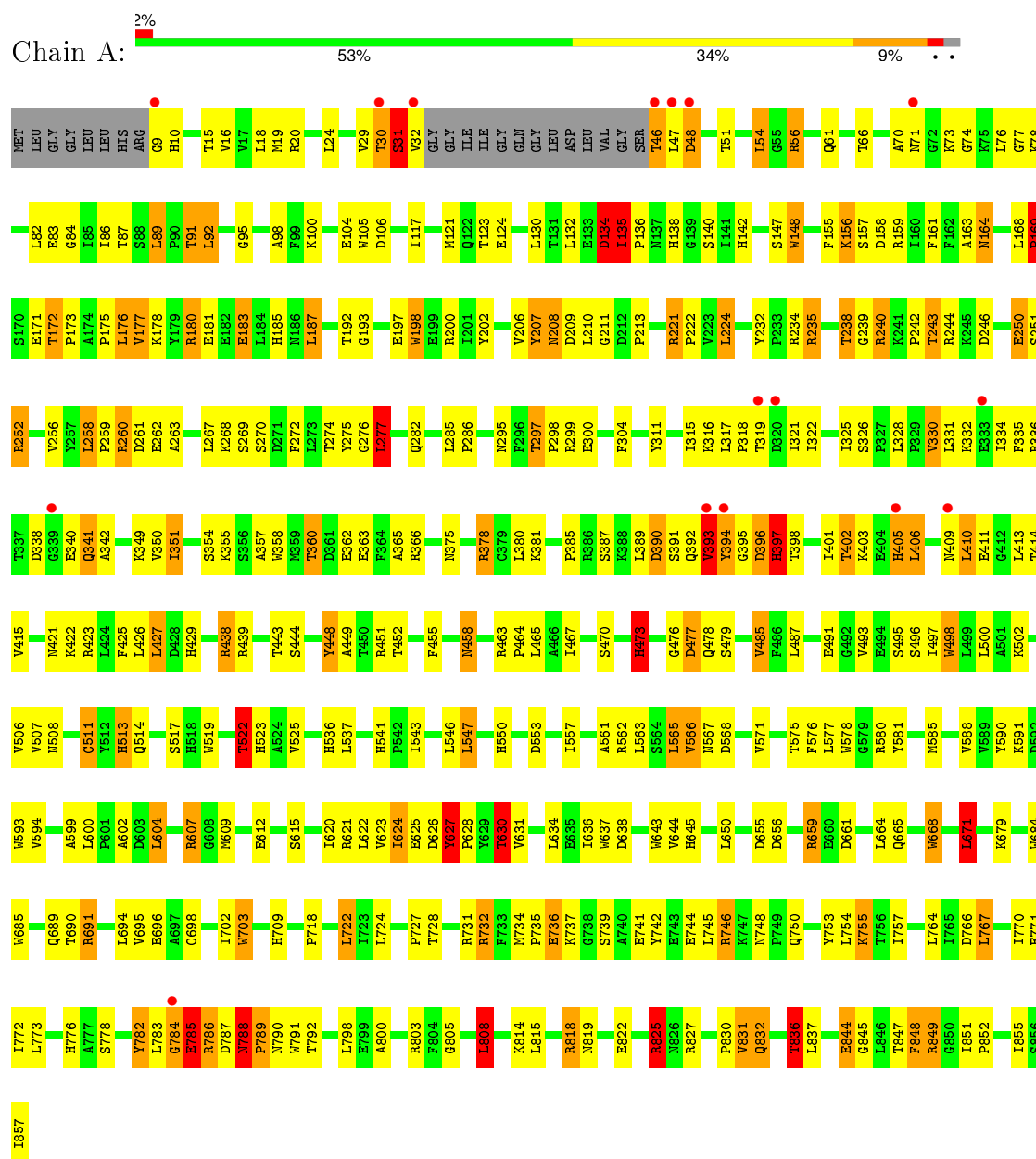
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		

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: 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	112.80 Å 137.40 Å 61.85 Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.1 (8.00-2.60) 80.9 (8.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.59 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.174 , 0.265 0.168 , 0.256	Depositor DCC
R_{free} test set	2236 reflections (9.96%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 87.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22440 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	3/6867 (0.0%)	1.76	171/9326 (1.8%)

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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	THR	C-N	17.20	1.73	1.34
1	A	31	SER	C-N	15.96	1.70	1.34
1	A	198	TRP	CG-CD2	-5.70	1.33	1.43

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	A	31	SER	O-C-N	-13.39	101.27	122.70
1	A	849	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	607	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	105	TRP	CD1-CG-CD2	9.49	113.90	106.30
1	A	684	TRP	CD1-CG-CD2	9.21	113.67	106.30
1	A	703	TRP	CD1-CG-CD2	9.17	113.63	106.30
1	A	791	TRP	CD1-CG-CD2	8.99	113.49	106.30
1	A	580	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	91	THR	N-CA-CB	-8.32	94.48	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	A	684	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	A	105	TRP	CE2-CD2-CG	-8.22	100.72	107.30
1	A	668	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	703	TRP	CE2-CD2-CG	-8.18	100.75	107.30
1	A	397	HIS	CA-CB-CG	8.17	127.48	113.60
1	A	637	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	659	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	358	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	643	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	498	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	643	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	A	849	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	A	511	CYS	CA-CB-SG	-7.85	99.86	114.00
1	A	637	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	A	198	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	358	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	685	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	498	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	691	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	439	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	148	TRP	CG-CD2-CE3	7.61	140.75	133.90
1	A	593	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	A	790	ASN	CA-C-N	-7.56	100.56	117.20
1	A	148	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	684	TRP	CB-CG-CD1	-7.51	117.24	127.00
1	A	685	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	671	LEU	CA-CB-CG	7.44	132.42	115.30
1	A	732	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	785	GLU	CA-CB-CG	7.40	129.68	113.40
1	A	637	TRP	CG-CD2-CE3	7.40	140.56	133.90
1	A	423	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	198	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	519	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	A	668	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	691	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	148	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	A	703	TRP	CB-CG-CD1	-7.29	117.52	127.00
1	A	134	ASP	N-CA-C	7.28	130.65	111.00
1	A	590	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	A	519	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	791	TRP	CE2-CD2-CG	-7.24	101.51	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	206	VAL	N-CA-CB	-7.22	95.62	111.50
1	A	836	THR	N-CA-CB	-7.03	96.94	110.30
1	A	240	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	18	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	48	ASP	CA-C-N	-6.95	101.90	117.20
1	A	463	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	703	TRP	CG-CD2-CE3	6.94	140.15	133.90
1	A	180	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	637	TRP	CB-CG-CD1	-6.91	118.02	127.00
1	A	831	VAL	CG1-CB-CG2	6.86	121.88	110.90
1	A	200	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	585	MET	CG-SD-CE	-6.83	89.27	100.20
1	A	627	TYR	CA-CB-CG	6.82	126.36	113.40
1	A	311	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	A	46	THR	O-C-N	-6.73	111.94	122.70
1	A	234	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	684	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	A	451	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	473	HIS	CA-CB-CG	6.64	124.89	113.60
1	A	56	ARG	CA-CB-CG	-6.62	98.84	113.40
1	A	172	THR	CA-C-N	6.61	135.61	117.10
1	A	578	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	358	TRP	CG-CD2-CE3	6.58	139.82	133.90
1	A	187	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	753	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	234	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	630	THR	CA-CB-OG1	-6.45	95.46	109.00
1	A	630	THR	N-CA-CB	-6.43	98.08	110.30
1	A	148	TRP	CB-CG-CD1	-6.42	118.65	127.00
1	A	522	THR	N-CA-CB	-6.42	98.10	110.30
1	A	20	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	746	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	625	GLU	CA-CB-CG	6.35	127.38	113.40
1	A	393	VAL	N-CA-C	6.30	128.01	111.00
1	A	685	TRP	CG-CD2-CE3	6.29	139.56	133.90
1	A	825	ARG	N-CA-C	6.29	127.98	111.00
1	A	782	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	221	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	498	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	358	TRP	CB-CG-CD1	-6.22	118.92	127.00
1	A	238	THR	CA-C-N	6.12	128.44	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	A	790	ASN	CA-CB-CG	-6.11	99.97	113.40
1	A	825	ARG	CB-CG-CD	6.10	127.46	111.60
1	A	845	GLY	CA-C-N	-6.10	103.79	117.20
1	A	105	TRP	CG-CD1-NE1	-6.08	104.02	110.10
1	A	375	ASN	N-CA-CB	-6.07	99.67	110.60
1	A	169	PRO	CA-CB-CG	-6.07	92.47	104.00
1	A	630	THR	CA-CB-CG2	6.02	120.83	112.40
1	A	643	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	A	156	LYS	CA-CB-CG	5.92	126.43	113.40
1	A	578	TRP	CD1-CG-CD2	5.88	111.00	106.30
1	A	438	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	746	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	172	THR	CA-C-O	-5.86	107.80	120.10
1	A	685	TRP	CB-CG-CD1	-5.85	119.39	127.00
1	A	578	TRP	CB-CG-CD1	-5.83	119.43	127.00
1	A	566	VAL	N-CA-CB	-5.82	98.69	111.50
1	A	791	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	A	637	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	A	848	PHE	N-CA-CB	-5.79	100.19	110.60
1	A	755	LYS	CA-CB-CG	5.76	126.08	113.40
1	A	163	ALA	CA-C-N	-5.76	104.53	117.20
1	A	473	HIS	N-CA-C	5.74	126.49	111.00
1	A	498	TRP	CG-CD2-CE3	5.72	139.04	133.90
1	A	448	TYR	CA-C-N	5.68	129.71	117.20
1	A	378	ARG	CG-CD-NE	-5.67	99.90	111.80
1	A	627	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	394	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	580	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	30	THR	N-CA-CB	-5.55	99.76	110.30
1	A	92	LEU	CA-C-N	5.50	127.20	116.20
1	A	593	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	A	498	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	478	GLN	N-CA-C	-5.49	96.19	111.00
1	A	679	LYS	CA-CB-CG	-5.47	101.36	113.40
1	A	684	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	410	LEU	N-CA-C	5.39	125.55	111.00
1	A	650	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	155	PHE	N-CA-C	5.35	125.45	111.00
1	A	221	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	685	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	163	ALA	O-C-N	5.32	131.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	668	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	A	105	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	A	336	ARG	CB-CG-CD	-5.31	97.81	111.60
1	A	643	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	123	THR	N-CA-C	-5.26	96.79	111.00
1	A	360	THR	N-CA-CB	-5.26	100.31	110.30
1	A	593	TRP	CG-CD1-NE1	-5.25	104.84	110.10
1	A	668	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	519	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	A	722	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	691	ARG	O-C-N	-5.24	114.32	122.70
1	A	238	THR	O-C-N	-5.21	114.34	123.20
1	A	825	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	847	THR	CA-CB-CG2	-5.18	105.15	112.40
1	A	82	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	238	THR	N-CA-C	-5.17	97.05	111.00
1	A	590	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	808	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	105	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	A	624	ILE	CA-C-N	-5.13	105.91	117.20
1	A	627	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	84	GLY	CA-C-N	-5.10	105.98	117.20
1	A	207	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	513	HIS	CA-C-N	5.08	128.38	117.20
1	A	121	MET	CG-SD-CE	-5.08	92.07	100.20
1	A	277	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	522	THR	O-C-N	-5.07	114.59	122.70
1	A	536	HIS	N-CA-C	5.07	124.67	111.00
1	A	358	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	792	THR	O-C-N	5.03	130.75	122.70
1	A	575	THR	OG1-CB-CG2	-5.03	98.43	110.00
1	A	209	ASP	N-CA-CB	-5.02	101.57	110.60
1	A	818	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	240	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	TYR	Sidechain
1	A	788	ASN	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	6696	0	6613	195	0
2	A	1	0	0	0	0
3	A	170	0	0	12	0
All	All	6867	0	6613	195	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 15.

All (195) 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:31:SER:C	1:A:32:VAL:N	1.70	1.40
1:A:46:THR:C	1:A:47:LEU:N	1.73	1.39
1:A:32:VAL:HG12	1:A:268:LYS:HA	1.43	0.99
1:A:138:HIS:HA	3:A:1143:HOH:O	1.78	0.83
1:A:394:TYR:HA	1:A:397:HIS:HB3	1.59	0.82
1:A:380:LEU:HD11	1:A:385:PRO:HG3	1.64	0.80
1:A:410:LEU:HD11	1:A:458:ASN:H	1.49	0.77
1:A:171:GLU:HB2	1:A:177:VAL:HG23	1.67	0.75
1:A:732:ARG:HH12	1:A:741:GLU:HB3	1.51	0.75
1:A:360:THR:HG21	1:A:830:PRO:HG3	1.69	0.74
1:A:612:GLU:HA	1:A:620:ILE:HG22	1.70	0.72
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.71	0.72
1:A:351:ILE:HB	1:A:355:LYS:HA	1.73	0.70
1:A:32:VAL:CG1	1:A:268:LYS:HG2	2.21	0.70
1:A:785:GLU:HB2	3:A:975:HOH:O	1.91	0.70
1:A:836:THR:HG22	1:A:848:PHE:O	1.92	0.69
1:A:318:PRO:HG2	1:A:321:ILE:HD13	1.75	0.69
1:A:825:ARG:HA	1:A:825:ARG:HE	1.58	0.67
1:A:360:THR:HG22	1:A:363:GLU:H	1.59	0.67
1:A:782:TYR:O	1:A:786:ARG:HB2	1.95	0.66
1:A:235:ARG:HH12	1:A:238:THR:HG22	1.61	0.66
1:A:185:HIS:HB2	3:A:1153:HOH:O	1.95	0.65
1:A:819:ASN:HD22	1:A:827:ARG:HE	1.43	0.65
1:A:402:THR:HA	3:A:1157:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PRO:HA	1:A:341:GLN:NE2	2.13	0.64
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.80	0.63
1:A:322:ILE:HG21	1:A:340:GLU:HA	1.81	0.63
1:A:467:ILE:HG12	1:A:498:TRP:CZ3	2.34	0.63
1:A:731:ARG:NH2	1:A:755:LYS:HA	2.14	0.63
1:A:318:PRO:HA	1:A:341:GLN:HE22	1.64	0.62
1:A:402:THR:HB	1:A:405:HIS:HB2	1.81	0.62
1:A:357:ALA:HB1	1:A:830:PRO:HB2	1.81	0.62
1:A:31:SER:O	1:A:32:VAL:N	2.30	0.61
1:A:24:LEU:HD23	1:A:148:TRP:CZ2	2.36	0.61
1:A:243:THR:HG22	1:A:246:ASP:H	1.65	0.61
1:A:242:PRO:HA	1:A:250:GLU:HA	1.83	0.60
1:A:319:THR:HA	1:A:322:ILE:HB	1.84	0.59
1:A:394:TYR:CA	1:A:397:HIS:HB3	2.32	0.59
1:A:46:THR:HG1	1:A:47:LEU:N	2.00	0.59
1:A:547:LEU:HD12	1:A:702:ILE:HD11	1.85	0.58
1:A:727:PRO:HB3	1:A:757:ILE:HB	1.85	0.58
1:A:321:ILE:HG22	1:A:325:ILE:HG12	1.84	0.58
1:A:9:GLY:HA2	1:A:106:ASP:HB3	1.85	0.58
1:A:836:THR:HG23	1:A:849:ARG:HB3	1.85	0.57
1:A:51:THR:HA	1:A:54:LEU:HD22	1.84	0.57
1:A:32:VAL:HG12	1:A:268:LYS:CA	2.26	0.57
1:A:350:VAL:O	1:A:831:VAL:HG21	2.04	0.57
1:A:644:VAL:HG12	1:A:695:VAL:HG13	1.87	0.57
1:A:766:ASP:O	1:A:770:ILE:HG12	2.05	0.57
1:A:815:LEU:HD12	1:A:818:ARG:HH12	1.69	0.56
1:A:698:CYS:O	1:A:702:ILE:HG12	2.04	0.56
1:A:316:LYS:HA	1:A:341:GLN:O	2.05	0.56
1:A:211:GLY:HA2	1:A:568:ASP:HB2	1.88	0.55
1:A:29:VAL:HG11	1:A:272:PHE:HE2	1.71	0.55
1:A:438:ARG:HD2	1:A:473:HIS:CE1	2.42	0.55
1:A:142:HIS:O	1:A:164:ASN:HB2	2.07	0.54
1:A:406:LEU:HG	1:A:465:LEU:HD23	1.89	0.54
1:A:783:LEU:O	1:A:785:GLU:N	2.41	0.54
1:A:427:LEU:HD13	1:A:429:HIS:CD2	2.43	0.54
1:A:562:ARG:O	1:A:567:ASN:HB3	2.07	0.53
1:A:438:ARG:HD2	1:A:473:HIS:HE1	1.72	0.53
1:A:32:VAL:HG11	1:A:267:LEU:O	2.07	0.53
1:A:588:VAL:O	1:A:591:LYS:HB2	2.07	0.53
1:A:664:LEU:HD21	1:A:694:LEU:HD13	1.90	0.53
1:A:496:SER:O	1:A:500:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ASN:ND2	1:A:827:ARG:HH21	2.07	0.52
1:A:168:LEU:HB3	1:A:169:PRO:HD2	1.91	0.52
1:A:171:GLU:HB3	1:A:180:ARG:HD3	1.91	0.52
1:A:270:SER:HA	1:A:330:VAL:HG13	1.91	0.52
1:A:171:GLU:HA	1:A:180:ARG:NH1	2.25	0.52
1:A:511:CYS:SG	1:A:576:PHE:HB3	2.49	0.52
1:A:304:PHE:H	1:A:750:GLN:NE2	2.08	0.52
1:A:736:GLU:O	1:A:742:TYR:HB2	2.10	0.52
1:A:202:TYR:HA	3:A:918:HOH:O	2.09	0.52
1:A:411:GLU:HB3	1:A:413:LEU:HD12	1.92	0.52
1:A:511:CYS:SG	1:A:577:LEU:HB3	2.50	0.51
1:A:169:PRO:HA	1:A:180:ARG:NH2	2.25	0.51
1:A:394:TYR:HA	1:A:397:HIS:CB	2.35	0.51
1:A:410:LEU:HD12	1:A:455:PHE:CE2	2.46	0.51
1:A:252:ARG:HH12	1:A:567:ASN:HD22	1.59	0.50
1:A:365:ALA:HB2	1:A:464:PRO:HD3	1.94	0.50
1:A:541:HIS:HD2	1:A:543:ILE:H	1.58	0.50
1:A:476:GLY:O	1:A:477:ASP:HB2	2.11	0.50
1:A:513:HIS:HA	1:A:517:SER:HB2	1.93	0.50
1:A:362:GLU:O	1:A:366:ARG:HB2	2.11	0.50
1:A:124:GLU:HG3	1:A:148:TRP:CE3	2.46	0.50
1:A:502:LYS:O	1:A:506:VAL:HG23	2.12	0.49
1:A:243:THR:HG22	1:A:246:ASP:O	2.12	0.49
1:A:773:LEU:HA	1:A:857:ILE:HG13	1.94	0.49
1:A:338:ASP:HB2	1:A:342:ALA:HB3	1.93	0.49
1:A:784:GLY:HA2	1:A:808:LEU:HD23	1.94	0.49
1:A:354:SER:H	1:A:831:VAL:HG23	1.77	0.49
1:A:132:LEU:O	1:A:140:SER:HA	2.12	0.49
1:A:522:THR:CG2	1:A:709:HIS:HD2	2.26	0.49
1:A:661:ASP:O	1:A:665:GLN:HG2	2.12	0.49
1:A:135:ILE:HG23	1:A:136:PRO:HD3	1.95	0.49
1:A:389:LEU:O	1:A:395:GLY:HA3	2.12	0.49
1:A:147:SER:OG	1:A:159:ARG:NH2	2.46	0.48
1:A:381:LYS:NZ	1:A:422:LYS:HE2	2.28	0.48
1:A:645:HIS:HE1	3:A:916:HOH:O	1.95	0.48
1:A:46:THR:O	1:A:47:LEU:C	2.52	0.48
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.95	0.48
1:A:315:ILE:HD13	1:A:764:LEU:HD11	1.95	0.48
1:A:709:HIS:CD2	1:A:855:ILE:HG23	2.49	0.48
1:A:626:ASP:HB3	3:A:1116:HOH:O	2.14	0.48
1:A:86:ILE:HD11	1:A:100:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:ND2	1:A:235:ARG:HH21	2.12	0.47
1:A:83:GLU:O	1:A:100:LYS:HG3	2.15	0.47
1:A:381:LYS:HZ2	1:A:422:LYS:HE2	1.79	0.47
1:A:546:LEU:HD21	1:A:644:VAL:HG22	1.97	0.47
1:A:522:THR:HG22	1:A:523:HIS:H	1.79	0.47
1:A:193:GLY:O	1:A:239:GLY:HA3	2.15	0.47
1:A:831:VAL:HG22	1:A:831:VAL:O	2.14	0.47
1:A:401:ILE:HA	1:A:485:VAL:HG11	1.97	0.47
1:A:497:ILE:HA	1:A:734:MET:HE1	1.97	0.47
1:A:815:LEU:HD12	1:A:818:ARG:NH1	2.29	0.47
1:A:668:TRP:CE3	1:A:671:LEU:HD11	2.50	0.47
1:A:357:ALA:O	1:A:360:THR:HB	2.15	0.46
1:A:690:THR:HG22	1:A:691:ARG:O	2.15	0.46
1:A:744:GLU:O	1:A:748:ASN:N	2.48	0.46
1:A:197:GLU:O	1:A:260:ARG:HG2	2.16	0.46
1:A:636:ILE:HD13	1:A:851:ILE:CD1	2.45	0.46
1:A:331:LEU:HD23	1:A:335:PHE:CE2	2.50	0.46
1:A:32:VAL:CG1	1:A:267:LEU:O	2.63	0.46
1:A:169:PRO:C	1:A:171:GLU:N	2.67	0.45
1:A:171:GLU:HA	1:A:180:ARG:HD3	1.98	0.45
1:A:183:GLU:HG2	3:A:1167:HOH:O	2.17	0.45
1:A:396:ASP:O	1:A:397:HIS:HB2	2.16	0.45
1:A:276:GLY:HA2	1:A:331:LEU:HD11	1.98	0.45
1:A:331:LEU:HD23	1:A:335:PHE:HE2	1.82	0.45
1:A:92:LEU:HD21	1:A:98:ALA:HB2	1.98	0.45
1:A:19:MET:HG2	1:A:95:GLY:O	2.16	0.45
1:A:785:GLU:HB2	1:A:805:GLY:HA3	1.98	0.45
1:A:836:THR:CG2	1:A:849:ARG:HB3	2.47	0.45
1:A:522:THR:HG21	1:A:709:HIS:HD2	1.81	0.45
1:A:825:ARG:HA	1:A:825:ARG:NE	2.24	0.44
1:A:222:PRO:O	1:A:224:LEU:HD13	2.16	0.44
1:A:252:ARG:NH1	1:A:567:ASN:HD22	2.15	0.44
1:A:277:LEU:HD13	1:A:772:ILE:HG21	1.99	0.44
1:A:256:VAL:HG13	1:A:563:LEU:HD13	1.98	0.44
1:A:117:ILE:HG21	1:A:161:PHE:HE2	1.83	0.44
1:A:403:LYS:HG3	1:A:415:VAL:HG21	1.99	0.44
1:A:51:THR:O	1:A:54:LEU:HB2	2.17	0.44
1:A:208:ASN:HD22	1:A:208:ASN:H	1.63	0.44
1:A:61:GLN:HG3	1:A:77:GLY:O	2.17	0.44
1:A:169:PRO:HG3	1:A:661:ASP:OD1	2.18	0.44
1:A:171:GLU:CB	1:A:180:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:HA2	1:A:331:LEU:CD1	2.48	0.43
1:A:317:LEU:O	1:A:341:GLN:HA	2.18	0.43
1:A:158:ASP:N	3:A:1130:HOH:O	2.51	0.43
1:A:240:ARG:HD2	1:A:251:SER:O	2.18	0.43
1:A:561:ALA:HA	1:A:565:LEU:HD22	2.01	0.43
1:A:819:ASN:HD22	1:A:827:ARG:NE	2.13	0.43
1:A:208:ASN:HA	3:A:931:HOH:O	2.19	0.43
1:A:157:SER:HB2	3:A:1130:HOH:O	2.18	0.43
1:A:178:LYS:HB2	3:A:933:HOH:O	2.18	0.43
1:A:207:TYR:HD2	1:A:210:LEU:HD11	1.83	0.43
1:A:776:HIS:O	1:A:844:GLU:O	2.37	0.43
1:A:259:PRO:O	1:A:262:GLU:HB2	2.19	0.43
1:A:565:LEU:HA	1:A:571:VAL:HG22	2.01	0.43
1:A:357:ALA:HB3	1:A:831:VAL:HB	2.00	0.42
1:A:550:HIS:CD2	1:A:702:ILE:HD12	2.54	0.42
1:A:299:ARG:HH11	1:A:299:ARG:HD3	1.74	0.42
1:A:607:ARG:NH2	1:A:609:MET:HG3	2.33	0.42
1:A:767:LEU:O	1:A:771:GLU:HB2	2.19	0.42
1:A:496:SER:HB3	1:A:745:LEU:HD22	2.02	0.42
1:A:814:LYS:HB2	1:A:814:LYS:HE3	1.78	0.42
1:A:173:PRO:HB2	1:A:176:LEU:HD22	2.01	0.42
1:A:297:THR:HA	1:A:298:PRO:HD2	1.79	0.42
1:A:655:ASP:O	1:A:659:ARG:HG3	2.19	0.42
1:A:627:TYR:HA	1:A:628:PRO:HD3	1.85	0.42
1:A:378:ARG:O	1:A:425:PHE:HA	2.20	0.42
1:A:169:PRO:HG3	1:A:661:ASP:CG	2.40	0.42
1:A:514:GLN:HG3	1:A:576:PHE:CZ	2.55	0.42
1:A:561:ALA:HA	1:A:565:LEU:HB2	2.02	0.42
1:A:74:GLY:HA2	1:A:175:PRO:HB3	2.00	0.42
1:A:208:ASN:ND2	1:A:235:ARG:NH2	2.68	0.41
1:A:16:VAL:CG2	1:A:130:LEU:HD13	2.50	0.41
1:A:385:PRO:HG2	1:A:426:LEU:HD13	2.02	0.41
1:A:800:ALA:HA	1:A:803:ARG:HH21	1.86	0.41
1:A:406:LEU:HD12	1:A:465:LEU:HB3	2.03	0.41
1:A:297:THR:HG21	1:A:315:ILE:HD11	2.01	0.41
1:A:61:GLN:NE2	1:A:76:LEU:HB3	2.36	0.41
1:A:178:LYS:HA	1:A:181:GLU:HG2	2.02	0.41
1:A:599:ALA:O	1:A:602:ALA:HB3	2.21	0.41
1:A:493:VAL:HG21	1:A:746:ARG:HH11	1.86	0.41
1:A:235:ARG:NH1	1:A:238:THR:HG22	2.33	0.41
1:A:507:VAL:HG23	1:A:728:THR:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD13	1:A:394:TYR:CE1	2.55	0.40
1:A:332:LYS:O	1:A:334:ILE:HD12	2.21	0.40
1:A:258:LEU:HD11	1:A:263:ALA:HB2	2.03	0.40
1:A:600:LEU:HD22	1:A:703:TRP:CH2	2.57	0.40
1:A:500:LEU:CD1	1:A:745:LEU:HD21	2.51	0.40
1:A:782:TYR:HA	1:A:852:PRO:HA	2.03	0.40
1:A:213:PRO:HG2	1:A:243:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	832/857 (97%)	725 (87%)	76 (9%)	31 (4%)	4 5

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ALA
1	A	73	LYS
1	A	78	LYS
1	A	164	ASN
1	A	172	THR
1	A	295	ASN
1	A	341	GLN
1	A	390	ASP
1	A	477	ASP
1	A	737	LYS
1	A	788	ASN
1	A	789	PRO
1	A	844	GLU
1	A	89	LEU

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Mol	Chain	Res	Type
1	A	134	ASP
1	A	156	LYS
1	A	326	SER
1	A	391	SER
1	A	397	HIS
1	A	402	THR
1	A	449	ALA
1	A	784	GLY
1	A	785	GLU
1	A	832	GLN
1	A	10	HIS
1	A	135	ILE
1	A	409	ASN
1	A	330	VAL
1	A	393	VAL
1	A	624	ILE
1	A	627	TYR

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	735/749 (98%)	626 (85%)	109 (15%)	4 6

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	30	THR
1	A	31	SER
1	A	48	ASP
1	A	54	LEU
1	A	56	ARG
1	A	66	THR
1	A	71	ASN
1	A	87	THR

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Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	THR
1	A	104	GLU
1	A	134	ASP
1	A	135	ILE
1	A	169	PRO
1	A	176	LEU
1	A	177	VAL
1	A	183	GLU
1	A	187	LEU
1	A	192	THR
1	A	198	TRP
1	A	208	ASN
1	A	221	ARG
1	A	224	LEU
1	A	232	TYR
1	A	235	ARG
1	A	243	THR
1	A	244	ARG
1	A	250	GLU
1	A	252	ARG
1	A	258	LEU
1	A	260	ARG
1	A	261	ASP
1	A	269	SER
1	A	274	THR
1	A	275	TYR
1	A	277	LEU
1	A	282	GLN
1	A	297	THR
1	A	300	GLU
1	A	328	LEU
1	A	349	LYS
1	A	351	ILE
1	A	390	ASP
1	A	392	GLN
1	A	393	VAL
1	A	396	ASP
1	A	398	THR
1	A	405	HIS
1	A	406	LEU
1	A	414	THR

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Mol	Chain	Res	Type
1	A	421	ASN
1	A	427	LEU
1	A	443	THR
1	A	444	SER
1	A	448	TYR
1	A	452	THR
1	A	458	ASN
1	A	470	SER
1	A	473	HIS
1	A	479	SER
1	A	485	VAL
1	A	487	LEU
1	A	491	GLU
1	A	495	SER
1	A	508	ASN
1	A	522	THR
1	A	525	VAL
1	A	537	LEU
1	A	547	LEU
1	A	553	ASP
1	A	557	ILE
1	A	565	LEU
1	A	566	VAL
1	A	594	VAL
1	A	604	LEU
1	A	615	SER
1	A	621	ARG
1	A	622	LEU
1	A	623	VAL
1	A	627	TYR
1	A	630	THR
1	A	634	LEU
1	A	638	ASP
1	A	656	ASP
1	A	671	LEU
1	A	689	GLN
1	A	696	GLU
1	A	718	PRO
1	A	722	LEU
1	A	724	LEU
1	A	735	PRO
1	A	736	GLU

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Mol	Chain	Res	Type
1	A	739	SER
1	A	754	LEU
1	A	767	LEU
1	A	778	SER
1	A	785	GLU
1	A	786	ARG
1	A	787	ASP
1	A	788	ASN
1	A	789	PRO
1	A	798	LEU
1	A	808	LEU
1	A	822	GLU
1	A	825	ARG
1	A	832	GLN
1	A	836	THR
1	A	837	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	219	HIS
1	A	352	GLN
1	A	392	GLN
1	A	421	ASN
1	A	441	ASN
1	A	458	ASN
1	A	473	HIS
1	A	521	ASN
1	A	534	ASN
1	A	541	HIS
1	A	665	GLN
1	A	750	GLN
1	A	788	ASN
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 [i](#)

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

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 ⓘ

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	836/857 (97%)	-0.72	16 (1%) 70 64	7, 28, 73, 93	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	VAL	4.7
1	A	9	GLY	3.0
1	A	32	VAL	3.0
1	A	409	ASN	2.7
1	A	30	THR	2.6
1	A	47	LEU	2.6
1	A	784	GLY	2.4
1	A	339	GLY	2.4
1	A	48	ASP	2.3
1	A	333	GLU	2.2
1	A	405	HIS	2.2
1	A	319	THR	2.1
1	A	71	ASN	2.1
1	A	320	ASP	2.1
1	A	394	TYR	2.1
1	A	46	THR	2.1

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

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

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
2	FE2	A	858	1/1	0.98	0.13	1.91	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.