



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:54 PM UTC

PDB ID : 6LST / pdb_00006lst
Title : Crystal structure of Uso1-1
Authors : Heo, Y.Y.; Lee, H.H.
Deposited on : 2020-01-20
Resolution : 2.94 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

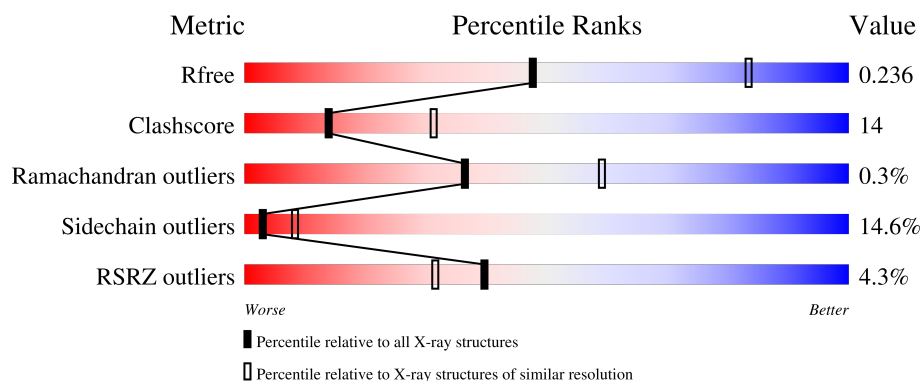
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	731	4% 55% 27% 6% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5333 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 Intracellular protein transport protein USO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	0	0
			5222	3368	858	979	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P25386
A	-3	ALA	-	expression tag	UNP P25386
A	-2	MET	-	expression tag	UNP P25386
A	-1	GLY	-	expression tag	UNP P25386
A	0	SER	-	expression tag	UNP P25386

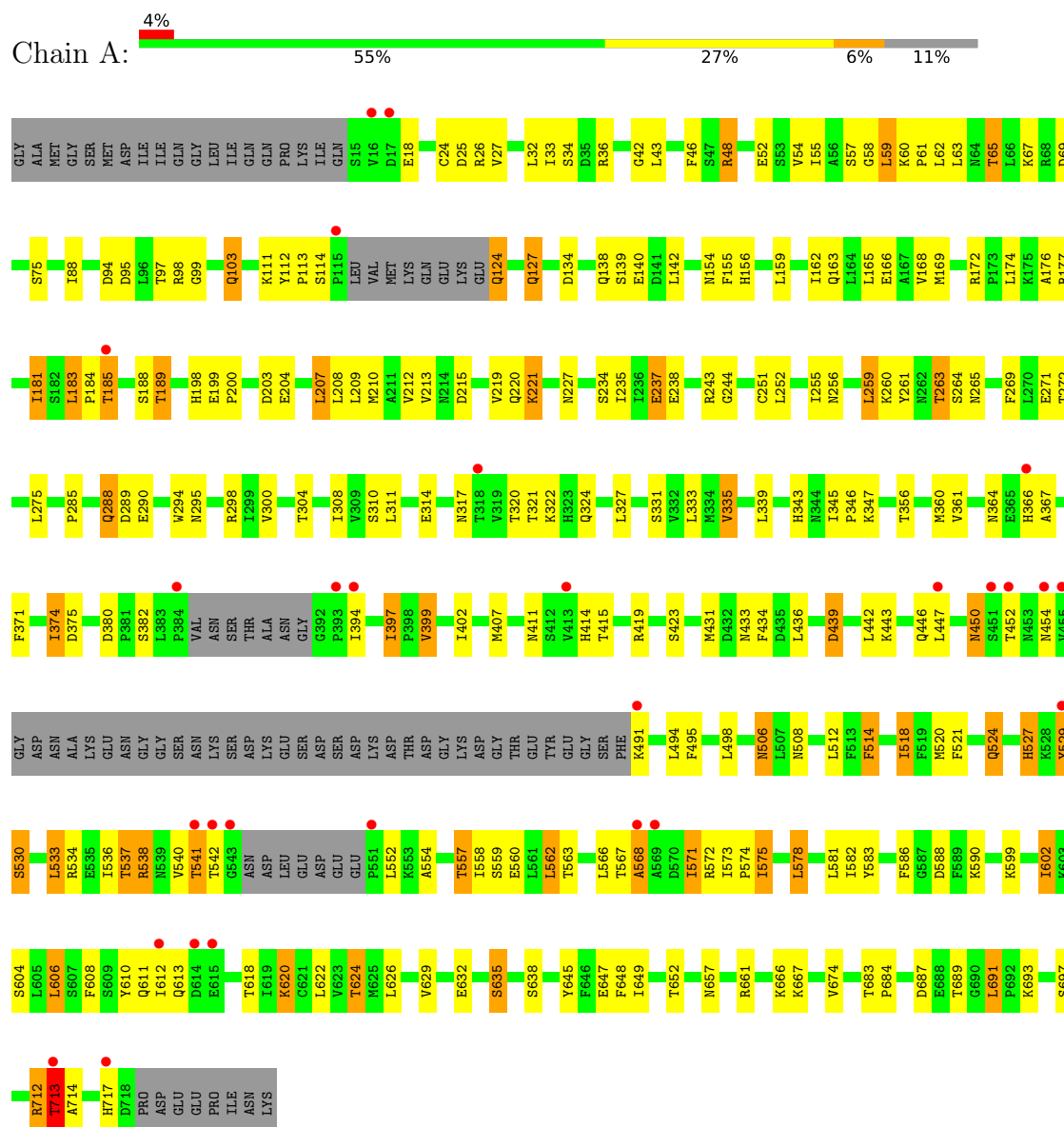
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Intracellular protein transport protein USO1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.37Å 114.37Å 193.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 2.94 49.22 – 2.94	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.22-2.94) 96.2 (49.22-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.27 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.252 (Not available) , 0.236	Depositor DCC
R_{free} test set	1550 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.19	6/5327 (0.1%)	1.64	41/7227 (0.6%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	HIS	CE1-NE2	9.01	1.41	1.32
1	A	717	HIS	CG-ND1	6.50	1.45	1.38
1	A	575	ILE	C-O	5.47	1.30	1.24
1	A	99	GLY	C-O	5.34	1.30	1.23
1	A	552	LEU	C-O	5.21	1.29	1.24
1	A	235	ILE	C-O	-5.18	1.18	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	THR	CA-CB-OG1	-8.41	96.99	109.60
1	A	185	THR	CA-CB-OG1	-8.03	97.55	109.60
1	A	215	ASP	CB-CA-C	-7.47	101.12	111.73
1	A	33	ILE	CA-C-N	7.41	130.54	120.54
1	A	33	ILE	C-N-CA	7.41	130.54	120.54
1	A	243	ARG	N-CA-C	-6.99	99.47	109.96
1	A	127	GLN	CB-CA-C	-6.51	99.99	110.79
1	A	237	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	566	LEU	CA-C-N	6.34	129.02	120.65
1	A	566	LEU	C-N-CA	6.34	129.02	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	PRO	CA-C-N	6.26	128.36	120.72
1	A	285	PRO	C-N-CA	6.26	128.36	120.72
1	A	154	ASN	CA-C-N	6.09	128.73	120.38
1	A	154	ASN	C-N-CA	6.09	128.73	120.38
1	A	454	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	356	THR	N-CA-C	-5.95	104.71	111.14
1	A	271	GLU	CA-C-N	5.86	130.79	121.18
1	A	271	GLU	C-N-CA	5.86	130.79	121.18
1	A	419	ARG	N-CA-C	-5.63	105.22	111.36
1	A	397	ILE	CB-CA-C	5.63	114.85	109.33
1	A	289	ASP	N-CA-C	-5.59	104.81	111.69
1	A	652	THR	CA-C-N	5.55	127.98	120.65
1	A	652	THR	C-N-CA	5.55	127.98	120.65
1	A	647	GLU	CA-C-N	5.45	127.90	120.54
1	A	647	GLU	C-N-CA	5.45	127.90	120.54
1	A	221	LYS	N-CA-C	-5.45	105.42	111.36
1	A	237	GLU	N-CA-C	-5.33	105.55	111.36
1	A	189	THR	N-CA-C	-5.31	105.57	111.36
1	A	610	TYR	CB-CA-C	-5.29	104.25	112.07
1	A	18	GLU	CA-C-N	5.28	127.81	120.63
1	A	18	GLU	C-N-CA	5.28	127.81	120.63
1	A	713	THR	CA-CB-CG2	5.27	119.45	110.50
1	A	512	LEU	N-CA-C	-5.22	105.26	111.69
1	A	203	ASP	CA-C-O	-5.11	115.44	120.70
1	A	343	HIS	CA-C-O	-5.10	115.64	121.00
1	A	52	GLU	CB-CA-C	5.09	120.45	110.67
1	A	310	SER	CA-C-O	-5.03	115.22	120.55
1	A	514	PHE	CA-C-N	5.02	126.97	120.44
1	A	514	PHE	C-N-CA	5.02	126.97	120.44
1	A	33	ILE	O-C-N	5.02	126.94	121.87
1	A	537	THR	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	GLY	Mainchain
1	A	540	VAL	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	5222	0	5256	151	0
2	A	111	0	0	6	0
All	All	5333	0	5256	151	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 14.

All (151) 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:124:GLN:HE21	1:A:124:GLN:HA	1.06	1.15
1:A:538:ARG:HG2	1:A:538:ARG:HH11	1.31	0.94
1:A:434:PHE:CE2	1:A:529:TYR:HB2	2.09	0.88
1:A:124:GLN:HA	1:A:124:GLN:NE2	1.86	0.85
1:A:27:VAL:O	1:A:36:ARG:HG2	1.78	0.83
1:A:32:LEU:HD23	1:A:32:LEU:H	1.42	0.82
1:A:434:PHE:HE2	1:A:529:TYR:HB2	1.48	0.77
1:A:407:MET:HE3	1:A:423:SER:HB2	1.68	0.76
1:A:48:ARG:HH11	1:A:48:ARG:HG2	1.50	0.75
1:A:506:ASN:HD22	1:A:506:ASN:H	1.32	0.74
1:A:156:HIS:ND1	2:A:802:HOH:O	2.20	0.74
1:A:407:MET:HE2	1:A:514:PHE:HB3	1.72	0.70
1:A:272:THR:O	1:A:272:THR:HG22	1.91	0.70
1:A:712:ARG:HD3	2:A:835:HOH:O	1.92	0.69
1:A:212:VAL:HG12	1:A:219:VAL:HG11	1.74	0.68
1:A:166:GLU:OE1	1:A:204:GLU:OE2	2.11	0.68
1:A:446:GLN:O	1:A:450:ASN:HB3	1.94	0.68
1:A:541:THR:HG22	1:A:541:THR:O	1.94	0.67
1:A:657:ASN:O	1:A:661:ARG:HG2	1.95	0.67
1:A:578:LEU:O	1:A:582:ILE:HG13	1.95	0.66
1:A:538:ARG:HG2	1:A:538:ARG:NH1	2.00	0.65
1:A:498:LEU:HG	1:A:558:ILE:HD11	1.80	0.64
1:A:645:TYR:CZ	1:A:649:ILE:HD11	2.33	0.64
1:A:364:ASN:HB3	1:A:367:ALA:HB3	1.80	0.63
1:A:713:THR:CG2	1:A:713:THR:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH1	1:A:95:ASP:OD2	2.32	0.62
1:A:620:LYS:O	1:A:624:THR:HG23	2.00	0.62
1:A:36:ARG:NH1	1:A:69:ASP:OD1	2.32	0.62
1:A:506:ASN:H	1:A:506:ASN:ND2	1.98	0.61
1:A:572:ARG:HH21	1:A:691:LEU:HD23	1.65	0.61
1:A:371:PHE:O	1:A:374:ILE:HG23	2.00	0.60
1:A:48:ARG:HH11	1:A:48:ARG:CG	2.13	0.60
1:A:414:HIS:HB2	2:A:841:HOH:O	2.01	0.60
1:A:314:GLU:O	1:A:320:THR:OG1	2.16	0.60
1:A:220:GLN:HB3	1:A:265:ASN:ND2	2.17	0.59
1:A:687:ASP:OD1	1:A:689:THR:N	2.34	0.58
1:A:433:ASN:C	1:A:433:ASN:HD22	2.11	0.58
1:A:55:ILE:O	1:A:59:LEU:HB2	2.04	0.58
1:A:394:ILE:O	1:A:394:ILE:HG23	2.04	0.58
1:A:571:ILE:HG13	1:A:571:ILE:O	2.02	0.58
1:A:572:ARG:NH2	1:A:691:LEU:HB3	2.18	0.58
1:A:433:ASN:OD1	1:A:436:LEU:HD12	2.04	0.58
1:A:558:ILE:HG22	1:A:581:LEU:HD11	1.86	0.57
1:A:263:THR:HG21	1:A:317:ASN:HD21	1.69	0.56
1:A:407:MET:HE3	1:A:423:SER:CB	2.36	0.56
1:A:606:LEU:HD23	1:A:648:PHE:CE2	2.41	0.56
1:A:165:LEU:O	1:A:169:MET:HB2	2.06	0.55
1:A:183:LEU:HD23	1:A:184:PRO:HD2	1.88	0.55
1:A:48:ARG:H	1:A:48:ARG:HD2	1.72	0.55
1:A:272:THR:O	1:A:272:THR:CG2	2.53	0.54
1:A:88:ILE:CG1	1:A:97:THR:HG21	2.38	0.54
1:A:320:THR:O	1:A:324:GLN:HG3	2.07	0.54
1:A:495:PHE:CE1	1:A:537:THR:HG23	2.44	0.53
1:A:169:MET:HE2	1:A:212:VAL:HA	1.90	0.53
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.23	0.53
1:A:183:LEU:HD23	1:A:184:PRO:CD	2.38	0.53
1:A:24:CYS:SG	1:A:57:SER:OG	2.58	0.53
1:A:124:GLN:HE21	1:A:124:GLN:CA	1.97	0.52
1:A:562:LEU:CD2	1:A:562:LEU:C	2.82	0.52
1:A:620:LYS:HB2	1:A:620:LYS:HZ3	1.74	0.52
1:A:524:GLN:O	1:A:530:SER:HB3	2.10	0.52
1:A:620:LYS:O	1:A:624:THR:CG2	2.57	0.52
1:A:140:GLU:HB2	2:A:812:HOH:O	2.09	0.52
1:A:124:GLN:N	2:A:816:HOH:O	2.43	0.51
1:A:602:ILE:HD13	1:A:602:ILE:N	2.24	0.51
1:A:518:ILE:O	1:A:521:PHE:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:PHE:HE2	1:A:529:TYR:O	1.94	0.51
1:A:27:VAL:O	1:A:65:THR:HG21	2.11	0.50
1:A:713:THR:O	1:A:713:THR:HG23	2.12	0.50
1:A:168:VAL:HG12	1:A:176:ALA:HB2	1.94	0.50
1:A:260:LYS:HE2	1:A:261:TYR:CE2	2.47	0.49
1:A:212:VAL:CG1	1:A:219:VAL:HG11	2.42	0.49
1:A:572:ARG:HH21	1:A:691:LEU:CD2	2.26	0.49
1:A:538:ARG:HH21	1:A:590:LYS:HD2	1.78	0.48
1:A:94:ASP:OD2	1:A:98:ARG:HB2	2.13	0.48
1:A:204:GLU:O	1:A:207:LEU:HB2	2.14	0.48
1:A:380:ASP:OD1	1:A:382:SER:OG	2.29	0.48
1:A:683:THR:N	1:A:684:PRO:HD3	2.28	0.48
1:A:288:GLN:HG3	1:A:290:GLU:O	2.14	0.48
1:A:495:PHE:HE1	1:A:537:THR:HG23	1.77	0.48
1:A:134:ASP:OD1	1:A:172:ARG:NH1	2.45	0.48
1:A:60:LYS:N	1:A:61:PRO:HD2	2.29	0.47
1:A:606:LEU:CD2	1:A:648:PHE:CE2	2.97	0.47
1:A:260:LYS:HA	1:A:311:LEU:HD22	1.96	0.47
1:A:611:GLN:HA	1:A:611:GLN:OE1	2.13	0.47
1:A:599:LYS:HA	1:A:602:ILE:HG12	1.97	0.47
1:A:541:THR:O	1:A:541:THR:CG2	2.58	0.47
1:A:524:GLN:O	1:A:527:HIS:HB2	2.15	0.47
1:A:554:ALA:HA	1:A:557:THR:HG23	1.97	0.46
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.84	0.46
1:A:567:THR:OG1	1:A:568:ALA:N	2.47	0.46
1:A:159:LEU:O	1:A:163:GLN:HG3	2.16	0.46
1:A:263:THR:CG2	1:A:317:ASN:HD21	2.29	0.46
1:A:687:ASP:OD1	1:A:689:THR:HB	2.17	0.45
1:A:54:VAL:O	1:A:58:GLY:N	2.47	0.45
1:A:199:GLU:N	1:A:200:PRO:CD	2.78	0.45
1:A:687:ASP:HA	1:A:693:LYS:HE2	1.98	0.45
1:A:32:LEU:HD23	1:A:32:LEU:N	2.21	0.45
1:A:42:GLY:O	1:A:46:PHE:HD1	2.00	0.45
1:A:562:LEU:HD11	1:A:578:LEU:HD13	1.99	0.45
1:A:295:ASN:OD1	1:A:298:ARG:HG3	2.16	0.45
1:A:559:SER:O	1:A:563:THR:HG23	2.16	0.44
1:A:32:LEU:H	1:A:32:LEU:CD2	2.22	0.44
1:A:333:LEU:CA	1:A:360:MET:HE1	2.48	0.44
1:A:439:ASP:O	1:A:443:LYS:HG2	2.18	0.44
1:A:162:ILE:HG21	1:A:204:GLU:HB3	1.99	0.44
1:A:199:GLU:N	1:A:200:PRO:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:O	1:A:210:MET:C	2.61	0.43
1:A:134:ASP:OD2	1:A:172:ARG:NH1	2.51	0.43
1:A:127:GLN:HE21	1:A:127:GLN:HB2	1.40	0.43
1:A:155:PHE:CE1	1:A:198:HIS:HB3	2.54	0.43
1:A:177:ARG:O	1:A:181:ILE:HG23	2.19	0.43
1:A:331:SER:O	1:A:335:VAL:HG12	2.19	0.43
1:A:533:LEU:HA	1:A:536:ILE:HD12	2.00	0.43
1:A:238:GLU:O	1:A:238:GLU:HG2	2.18	0.42
1:A:294:TRP:CD2	1:A:346:PRO:HG2	2.53	0.42
1:A:399:VAL:HA	1:A:402:ILE:HG22	2.01	0.42
1:A:112:TYR:HB2	1:A:300:VAL:HG13	2.00	0.42
1:A:446:GLN:O	1:A:450:ASN:N	2.52	0.42
1:A:434:PHE:CE2	1:A:529:TYR:HD2	2.37	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.96	0.42
1:A:602:ILE:HD13	1:A:602:ILE:H	1.83	0.42
1:A:520:MET:HG2	1:A:583:TYR:CD2	2.54	0.42
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.79	0.42
1:A:571:ILE:O	1:A:575:ILE:HG13	2.20	0.42
1:A:24:CYS:O	1:A:27:VAL:HB	2.20	0.42
1:A:27:VAL:HG12	1:A:65:THR:CG2	2.49	0.42
1:A:632:GLU:OE1	1:A:714:ALA:HA	2.19	0.42
1:A:288:GLN:HB2	1:A:290:GLU:O	2.20	0.41
1:A:411:ASN:ND2	1:A:508:ASN:HB2	2.36	0.41
1:A:259:LEU:HD11	1:A:269:PHE:HB2	2.03	0.41
1:A:645:TYR:CE1	1:A:649:ILE:HD11	2.55	0.41
1:A:204:GLU:HG2	2:A:819:HOH:O	2.21	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.87	0.41
1:A:60:LYS:N	1:A:61:PRO:CD	2.83	0.41
1:A:295:ASN:OD1	1:A:295:ASN:C	2.64	0.41
1:A:103:GLN:NE2	1:A:103:GLN:HA	2.35	0.41
1:A:112:TYR:N	1:A:113:PRO:HD3	2.35	0.41
1:A:111:LYS:HG3	1:A:304:THR:HG23	2.02	0.41
1:A:251:CYS:O	1:A:255:ILE:HG13	2.20	0.41
1:A:433:ASN:C	1:A:433:ASN:ND2	2.78	0.41
1:A:534:ARG:NH1	1:A:588:ASP:HB2	2.36	0.41
1:A:573:ILE:HB	1:A:574:PRO:HD3	2.02	0.41
1:A:608:PHE:CD1	1:A:608:PHE:C	2.99	0.41
1:A:494:LEU:HD13	1:A:518:ILE:HG21	2.03	0.40
1:A:586:PHE:C	1:A:586:PHE:CD1	2.99	0.40
1:A:626:LEU:O	1:A:626:LEU:HD12	2.21	0.40
1:A:213:VAL:O	1:A:213:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HG	1:A:622:LEU:HB3	2.04	0.40
1:A:60:LYS:HB3	1:A:61:PRO:HD3	2.02	0.40
1:A:333:LEU:N	1:A:360:MET:HE1	2.36	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	637/731 (87%)	598 (94%)	37 (6%)	2 (0%)	36 59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	ALA
1	A	635	SER

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	595/668 (89%)	508 (85%)	87 (15%)	3 8

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	26	ARG
1	A	34	SER
1	A	48	ARG
1	A	59	LEU
1	A	62	LEU
1	A	65	THR
1	A	67	LYS
1	A	75	SER
1	A	103	GLN
1	A	114	SER
1	A	124	GLN
1	A	138	GLN
1	A	139	SER
1	A	181	ILE
1	A	183	LEU
1	A	185	THR
1	A	188	SER
1	A	189	THR
1	A	207	LEU
1	A	208	LEU
1	A	221	LYS
1	A	227	ASN
1	A	234	SER
1	A	237	GLU
1	A	252	LEU
1	A	256	ASN
1	A	259	LEU
1	A	263	THR
1	A	264	SER
1	A	275	LEU
1	A	288	GLN
1	A	308	ILE
1	A	321	THR
1	A	322	LYS
1	A	327	LEU
1	A	335	VAL
1	A	339	LEU
1	A	345	ILE
1	A	347	LYS
1	A	361	VAL
1	A	366	HIS
1	A	374	ILE

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Mol	Chain	Res	Type
1	A	375	ASP
1	A	397	ILE
1	A	399	VAL
1	A	415	THR
1	A	431	MET
1	A	439	ASP
1	A	442	LEU
1	A	447	LEU
1	A	450	ASN
1	A	452	THR
1	A	491	LYS
1	A	506	ASN
1	A	518	ILE
1	A	524	GLN
1	A	527	HIS
1	A	529	TYR
1	A	530	SER
1	A	533	LEU
1	A	538	ARG
1	A	541	THR
1	A	542	THR
1	A	557	THR
1	A	560	GLU
1	A	562	LEU
1	A	571	ILE
1	A	578	LEU
1	A	602	ILE
1	A	604	SER
1	A	606	LEU
1	A	612	ILE
1	A	613	GLN
1	A	618	THR
1	A	620	LYS
1	A	624	THR
1	A	629	VAL
1	A	635	SER
1	A	638	SER
1	A	666	LYS
1	A	667	LYS
1	A	674	VAL
1	A	691	LEU
1	A	697	SER

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Mol	Chain	Res	Type
1	A	712	ARG
1	A	713	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	127	GLN
1	A	156	HIS
1	A	249	ASN
1	A	297	GLN
1	A	325	ASN
1	A	364	ASN
1	A	405	ASN
1	A	433	ASN
1	A	450	ASN
1	A	453	ASN
1	A	506	ASN
1	A	527	HIS
1	A	702	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	647/731 (88%)	-0.07	28 (4%) 40 31	46, 74, 121, 195	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	4.8
1	A	16	VAL	4.7
1	A	491	LYS	4.6
1	A	551	PRO	4.1
1	A	455	VAL	4.0
1	A	17	ASP	3.8
1	A	366	HIS	3.4
1	A	451	SER	3.4
1	A	394	ILE	3.2
1	A	543	GLY	3.2
1	A	615	GLU	3.0
1	A	529	TYR	2.9
1	A	393	PRO	2.9
1	A	454	ASN	2.9
1	A	717	HIS	2.8
1	A	713	THR	2.8
1	A	452	THR	2.7
1	A	614	ASP	2.7
1	A	568	ALA	2.6
1	A	541	THR	2.5
1	A	384	PRO	2.5
1	A	115	PRO	2.4
1	A	185	THR	2.2
1	A	542	THR	2.2
1	A	569	ALA	2.2
1	A	413	VAL	2.1
1	A	612	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	318	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.