



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:06 PM UTC

PDB ID : 6O0D / pdb_00006o0d
Title : Saxiphilin Apo structure
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Deposited on : 2019-02-16
Resolution : 2.50 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

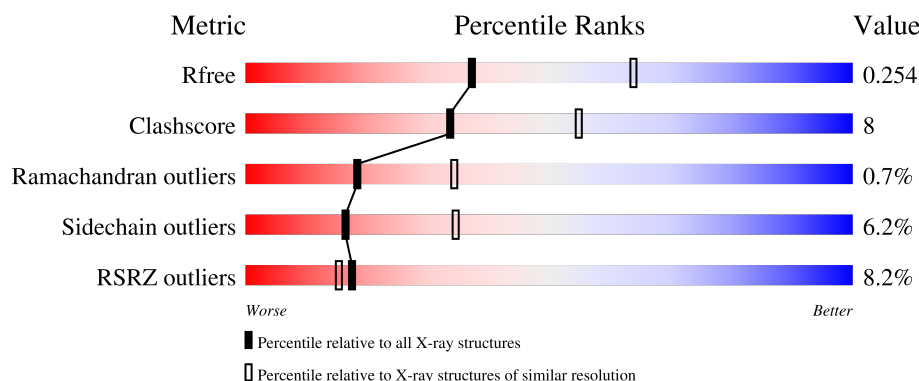
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	853	10% 75% 18% • 5%
1	B	853	6% 75% 19% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12705 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 Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	S	0	0	0
			6253	3912	1078	1204	59			
1	B	817	Total	C	N	O	S	0	0	0
			6306	3939	1088	1220	59			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	826	SER	-	expression tag	UNP P31226
A	827	ASN	-	expression tag	UNP P31226
A	828	SER	-	expression tag	UNP P31226
A	829	LEU	-	expression tag	UNP P31226
A	830	GLU	-	expression tag	UNP P31226
A	831	VAL	-	expression tag	UNP P31226
A	832	LEU	-	expression tag	UNP P31226
A	833	PHE	-	expression tag	UNP P31226
A	834	GLN	-	expression tag	UNP P31226
B	826	SER	-	expression tag	UNP P31226
B	827	ASN	-	expression tag	UNP P31226
B	828	SER	-	expression tag	UNP P31226
B	829	LEU	-	expression tag	UNP P31226
B	830	GLU	-	expression tag	UNP P31226
B	831	VAL	-	expression tag	UNP P31226
B	832	LEU	-	expression tag	UNP P31226
B	833	PHE	-	expression tag	UNP P31226
B	834	GLN	-	expression tag	UNP P31226

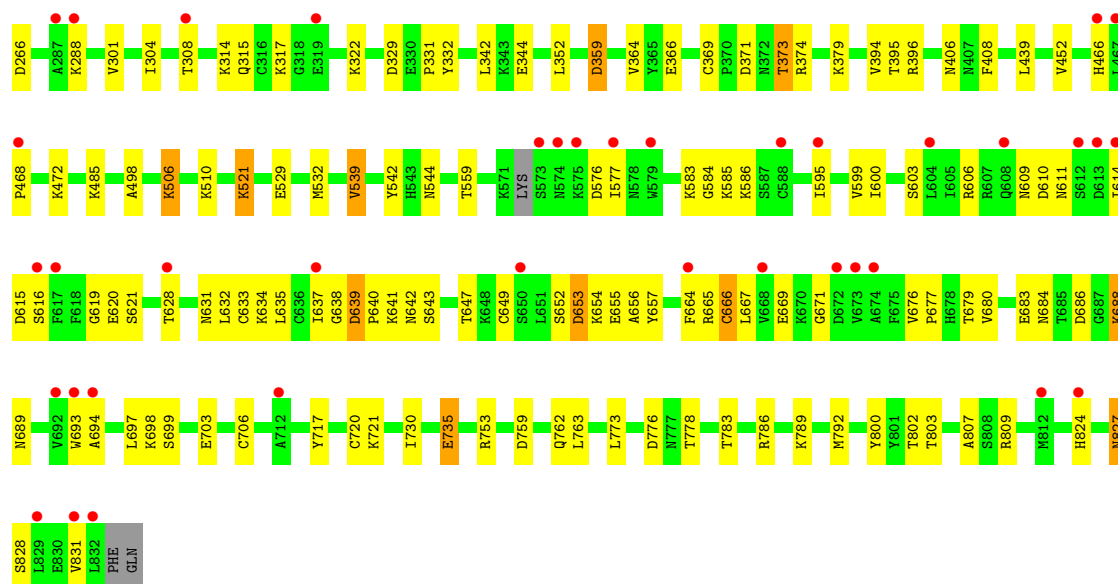
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	66	Total	O	0	0
			66	66		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.16Å 111.31Å 254.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.50 48.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.17-2.50) 99.8 (48.17-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.224 , 0.253 0.226 , 0.254	Depositor DCC
R_{free} test set	4737 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12705	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/6376	0.38	0/8602
1	B	0.13	0/6431	0.40	0/8679
All	All	0.13	0/12807	0.39	0/17281

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	ILE	Peptide

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	6253	0	6118	94	0
1	B	6306	0	6167	99	0
2	A	80	0	0	4	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	66	0	0	8	1
All	All	12705	0	12285	192	1

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 8.

All (192) 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:B:506:LYS:NZ	2:B:901:HOH:O	1.83	1.10
1:A:189:TYR:O	2:A:901:HOH:O	1.91	0.87
1:A:374:ARG:O	2:A:902:HOH:O	1.95	0.84
1:B:753:ARG:NH1	1:B:778:THR:O	2.11	0.83
1:B:242:LYS:NZ	1:B:342:LEU:O	2.11	0.83
1:A:614:ILE:O	1:A:616:SER:N	2.11	0.82
1:B:532:MET:HE1	1:B:809:ARG:HD3	1.67	0.76
1:B:606:ARG:HB2	1:B:611:ASN:HA	1.66	0.75
1:B:559:THR:OG1	2:B:902:HOH:O	2.04	0.74
1:A:86:ARG:NH1	1:A:228:HIS:O	2.19	0.74
1:A:164:GLU:HA	1:A:167:VAL:HG12	1.71	0.72
1:B:317:LYS:HB3	1:B:331:PRO:HG2	1.70	0.72
1:B:199:GLY:HA3	1:B:218:PRO:HB3	1.71	0.71
1:A:681:VAL:HG11	1:A:714:VAL:HG21	1.72	0.71
1:B:586:LYS:HB2	1:B:635:LEU:HD11	1.72	0.70
1:A:322:LYS:HD3	1:A:329:ASP:HB3	1.73	0.70
1:B:776:ASP:OD1	2:B:903:HOH:O	2.11	0.68
1:A:256:ARG:NH2	1:A:345:ASP:O	2.24	0.67
1:A:690:PRO:HA	1:A:695:LYS:HD2	1.76	0.67
1:B:43:GLU:HA	1:B:46:MET:HE2	1.76	0.67
1:A:269:LYS:NZ	1:A:458:MET:HE1	2.12	0.65
1:A:586:LYS:HD2	1:A:671:GLY:HA2	1.77	0.65
1:A:269:LYS:HZ2	1:A:458:MET:HE1	1.63	0.63
1:A:184:ASP:N	1:A:188:ASN:O	2.32	0.63
1:A:301:VAL:HG22	1:A:315:GLN:HG2	1.81	0.61
1:A:410:MET:HE1	1:A:438:ALA:HA	1.81	0.61
1:B:72:TYR:HB3	1:B:74:LEU:HD22	1.82	0.61
1:B:603:SER:OG	1:B:803:THR:O	2.20	0.60
1:A:43:GLU:HA	1:A:46:MET:HE2	1.83	0.60
1:A:662:GLY:C	1:A:664:PHE:H	2.10	0.59
1:A:587:SER:HA	1:A:673:VAL:HG13	1.83	0.59
1:A:242:LYS:NZ	1:A:345:ASP:OD1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLY:HA3	1:A:218:PRO:HG3	1.84	0.59
1:A:489:TRP:HE1	1:A:747:GLN:HG2	1.67	0.59
1:B:127:GLY:HA3	1:B:146:PRO:HG3	1.85	0.58
1:B:55:ASP:O	1:B:395:THR:HG23	2.04	0.58
1:A:63:GLU:HG2	1:A:263:SER:HB2	1.85	0.58
1:B:206:ALA:HB3	1:B:824:HIS:NE2	2.19	0.58
1:A:600:ILE:HG13	1:A:601:PRO:HD3	1.85	0.58
1:B:639:ASP:HB2	1:B:656:ALA:N	2.18	0.57
1:B:301:VAL:HG22	1:B:315:GLN:HG2	1.86	0.57
1:B:138:LYS:NZ	2:B:913:HOH:O	2.38	0.56
1:B:472:LYS:HE3	1:B:498:ALA:HB2	1.87	0.56
1:B:395:THR:HG22	1:B:396:ARG:H	1.70	0.56
1:B:639:ASP:HB3	1:B:654:LYS:O	2.06	0.56
1:A:262:VAL:HG23	1:A:305:PRO:O	2.06	0.56
1:B:532:MET:HA	1:B:532:MET:HE3	1.88	0.56
1:B:165:ARG:HG3	1:B:183:CYS:SG	2.46	0.55
1:A:336:TYR:CZ	1:A:426:LYS:HD3	2.42	0.55
1:A:570:VAL:HG13	1:A:705:LEU:HD21	1.88	0.55
1:A:668:VAL:HG21	1:A:693:TRP:CE3	2.41	0.55
1:A:155:ARG:HE	1:A:157:GLU:CD	2.15	0.54
1:A:570:VAL:HG11	1:A:577:ILE:HG21	1.90	0.54
1:A:668:VAL:HG23	1:A:669:GLU:HG3	1.89	0.54
1:A:689:ASN:O	1:A:694:ALA:HB3	2.07	0.54
1:A:138:LYS:HZ2	1:A:138:LYS:HB3	1.73	0.54
1:B:679:THR:O	1:B:683:GLU:HG3	2.08	0.53
1:B:369:CYS:HB2	1:B:371:ASP:OD1	2.08	0.53
1:B:619:GLY:O	1:B:631:ASN:HB3	2.08	0.53
1:B:676:VAL:HB	1:B:680:VAL:HG11	1.91	0.53
1:B:786:ARG:NH2	1:B:789:LYS:O	2.42	0.53
1:A:704:LEU:HD22	1:A:714:VAL:HA	1.90	0.53
1:B:359:ASP:OD1	1:B:359:ASP:N	2.37	0.53
1:B:245:SER:HB2	1:B:374:ARG:HH22	1.73	0.52
1:A:706:CYS:N	1:A:720:CYS:SG	2.82	0.52
1:A:483:LYS:HE3	1:A:487:ASP:OD2	2.09	0.52
1:A:537:PRO:HB3	1:A:729:ALA:HB1	1.90	0.52
1:B:74:LEU:O	2:B:904:HOH:O	2.19	0.52
1:B:151:ALA:N	2:B:912:HOH:O	2.37	0.52
1:B:631:ASN:HA	1:B:634:LYS:HD2	1.92	0.52
1:A:262:VAL:HG22	1:A:304:ILE:HG22	1.92	0.51
1:B:827:ASN:O	1:B:827:ASN:ND2	2.37	0.51
1:B:641:LYS:C	1:B:643:SER:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LYS:O	1:B:643:SER:N	2.43	0.51
1:A:366:GLU:OE2	1:A:374:ARG:HD3	2.13	0.49
1:B:184:ASP:N	1:B:188:ASN:O	2.44	0.49
1:B:205:ASN:HB2	1:B:209:GLU:HB2	1.94	0.49
1:A:266:ASP:OD1	1:A:266:ASP:N	2.25	0.49
1:A:703:GLU:OE2	1:A:713:PRO:HA	2.13	0.49
1:A:489:TRP:HE1	1:A:747:GLN:CG	2.26	0.49
1:A:615:ASP:HB3	1:A:631:ASN:HB2	1.94	0.48
1:B:655:GLU:OE2	1:B:657:TYR:N	2.43	0.48
1:B:759:ASP:OD1	1:B:759:ASP:N	2.46	0.48
1:B:156:HIS:HB2	2:B:946:HOH:O	2.13	0.48
1:A:615:ASP:CB	1:A:631:ASN:HB2	2.44	0.47
1:B:243:LYS:HG2	1:B:366:GLU:HB2	1.95	0.47
1:B:686:ASP:OD1	1:B:699:SER:N	2.43	0.47
1:A:268:TRP:O	1:A:270:ALA:N	2.44	0.47
1:A:206:ALA:HB2	1:A:228:HIS:HB3	1.96	0.47
1:A:589:HIS:ND1	1:A:597:GLY:O	2.30	0.47
1:B:653:ASP:OD1	1:B:653:ASP:N	2.41	0.47
1:B:802:THR:HG22	1:B:807:ALA:HB2	1.96	0.47
1:B:90:LYS:NZ	1:B:135:MET:O	2.48	0.47
1:B:595:ILE:HA	1:B:599:VAL:HB	1.96	0.47
1:B:664:PHE:HD2	1:B:693:TRP:HZ3	1.64	0.47
1:B:108:ILE:O	1:B:110:GLN:NE2	2.48	0.46
1:A:98:ALA:O	1:A:106:HIS:NE2	2.43	0.46
1:B:652:SER:OG	1:B:654:LYS:HG2	2.15	0.46
1:B:706:CYS:N	1:B:720:CYS:SG	2.88	0.46
1:A:587:SER:CA	1:A:673:VAL:HG13	2.44	0.46
1:B:205:ASN:N	1:B:209:GLU:O	2.49	0.46
1:B:694:ALA:HA	1:B:697:LEU:HB2	1.96	0.46
1:A:539:VAL:HG12	1:A:783:THR:HA	1.98	0.46
1:B:717:TYR:O	1:B:721:LYS:HB3	2.16	0.46
1:A:598:TRP:C	1:A:601:PRO:HD2	2.41	0.46
1:B:665:ARG:HE	1:B:669:GLU:CD	2.23	0.45
1:B:198:THR:HG22	1:B:199:GLY:H	1.81	0.45
1:B:332:TYR:OH	1:B:344:GLU:OE1	2.30	0.45
1:A:647:THR:HG22	1:A:648:LYS:HG3	1.99	0.45
1:B:539:VAL:HG12	1:B:730:ILE:HD13	1.97	0.45
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.17	0.45
1:A:202:TRP:HB3	1:A:215:LYS:HG2	1.99	0.45
1:A:682:PHE:HA	1:A:685:THR:HG22	1.99	0.45
1:A:69:LYS:HB3	1:A:69:LYS:HE2	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD11	1:A:826:SER:HB2	1.98	0.45
1:B:677:PRO:O	1:B:680:VAL:HG12	2.17	0.45
1:A:623:ALA:HB3	1:A:632:LEU:HD22	1.99	0.45
1:B:639:ASP:HB3	1:B:640:PRO:HD3	1.99	0.45
1:A:590:THR:HG22	1:A:597:GLY:HA3	1.99	0.44
1:A:752:GLY:HA2	1:A:763:LEU:H	1.81	0.44
1:A:450:LEU:HD22	1:A:454:LEU:HD13	2.00	0.44
1:B:59:LEU:HD12	1:B:394:VAL:HG11	2.00	0.44
1:B:189:TYR:HB3	1:B:204:VAL:HG11	2.00	0.44
1:A:460:ALA:HA	1:A:465:ALA:HB2	1.99	0.44
1:A:756:PHE:C	1:A:757:GLU:OE2	2.60	0.44
1:B:583:LYS:H	1:B:583:LYS:HG3	1.60	0.44
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.98	0.44
1:B:220:LYS:N	1:B:220:LYS:HD2	2.33	0.44
1:A:621:SER:HA	1:A:635:LEU:HD12	2.00	0.44
1:A:615:ASP:C	1:A:617:PHE:H	2.26	0.43
1:A:759:ASP:OD1	1:A:759:ASP:N	2.42	0.43
1:A:245:SER:HG	1:A:374:ARG:HH22	1.63	0.43
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.99	0.43
1:B:600:ILE:HD11	1:B:800:TYR:CE2	2.52	0.43
1:A:473:VAL:HG23	1:A:743:ILE:HD12	1.99	0.43
1:B:466:HIS:O	1:B:468:PRO:HD3	2.18	0.43
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.99	0.43
1:B:586:LYS:HA	1:B:620:GLU:O	2.18	0.43
1:A:293:ARG:NE	1:B:308:THR:OG1	2.52	0.43
1:B:621:SER:HA	1:B:635:LEU:HD12	1.99	0.43
1:A:662:GLY:O	1:A:664:PHE:N	2.51	0.43
1:B:162:LEU:HD23	1:B:165:ARG:HB2	2.00	0.43
1:A:693:TRP:CD1	1:A:693:TRP:H	2.35	0.43
1:B:69:LYS:HB3	1:B:69:LYS:HE2	1.85	0.43
1:A:259:HIS:HB2	1:A:304:ILE:HG23	2.00	0.43
1:A:610:ASP:OD1	1:A:610:ASP:N	2.52	0.43
1:B:506:LYS:HD2	1:B:510:LYS:HE3	2.01	0.42
1:A:563:THR:HG22	1:A:725:ILE:O	2.19	0.42
1:B:161:CYS:HB3	1:B:187:GLY:O	2.20	0.42
1:B:521:LYS:HG2	1:B:773:LEU:O	2.19	0.42
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.54	0.42
1:A:182:GLN:HE22	1:A:194:PHE:HB3	1.83	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.91	0.42
1:A:43:GLU:OE2	1:A:326:ASN:ND2	2.34	0.42
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLY:C	1:B:585:LYS:HD2	2.45	0.42
1:B:371:ASP:OD1	1:B:373:THR:HG22	2.20	0.42
1:B:684:ASN:HA	1:B:689:ASN:HB2	2.02	0.42
1:A:717:TYR:O	1:A:721:LYS:HB3	2.20	0.42
1:A:32:ILE:HG21	1:A:408:PHE:HB2	2.02	0.41
1:A:618:PHE:HB3	1:A:619:GLY:H	1.66	0.41
1:B:735:GLU:H	1:B:735:GLU:HG3	1.40	0.41
1:B:789:LYS:HE3	1:B:789:LYS:HB2	1.89	0.41
1:A:86:ARG:NH2	2:A:901:HOH:O	2.51	0.41
1:B:521:LYS:O	1:B:521:LYS:HG3	2.21	0.41
1:B:686:ASP:HB2	1:B:688:LYS:NZ	2.36	0.41
1:A:19:LYS:HD2	1:A:422:SER:HB2	2.03	0.41
1:A:232:THR:O	2:A:903:HOH:O	2.21	0.41
1:A:574:ASN:O	1:A:574:ASN:ND2	2.53	0.41
1:A:621:SER:N	1:A:635:LEU:HD12	2.35	0.41
1:A:667:LEU:HD22	1:A:672:ASP:HA	2.01	0.41
1:B:577:ILE:HD12	1:B:585:LYS:HG2	2.03	0.41
1:A:166:GLN:C	1:A:168:ALA:H	2.28	0.41
1:B:641:LYS:HD3	1:B:641:LYS:HA	1.72	0.41
1:A:697:LEU:H	1:A:697:LEU:HD22	1.86	0.41
1:A:8:ARG:HG2	1:A:35:VAL:HB	2.03	0.41
1:A:256:ARG:NH1	1:A:348:ASP:OD1	2.53	0.41
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.56	0.41
1:B:379:LYS:HA	1:B:379:LYS:HD3	1.89	0.41
1:B:485:LYS:NZ	1:B:763:LEU:O	2.37	0.41
1:A:603:SER:HB3	1:A:803:THR:O	2.21	0.41
1:A:243:LYS:NZ	1:A:363:GLU:O	2.54	0.40
1:A:268:TRP:HD1	1:A:269:LYS:HG2	1.86	0.40
1:A:158:LEU:HD12	1:A:159:PRO:HD2	2.02	0.40
1:B:165:ARG:HE	1:B:165:ARG:HB3	1.51	0.40
1:B:637:ILE:HG22	1:B:638:GLY:H	1.86	0.40
1:B:529:GLU:HG3	2:B:911:HOH:O	2.21	0.40
1:B:641:LYS:C	1:B:643:SER:N	2.79	0.40
1:B:666:CYS:SG	1:B:667:LEU:N	2.94	0.40
1:A:689:ASN:O	1:A:690:PRO:C	2.64	0.40
1:B:631:ASN:C	1:B:633:CYS:H	2.29	0.40
1:B:647:THR:HG21	1:B:654:LYS:HB3	2.02	0.40

All (1) 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)
2:A:956:HOH:O	2:B:959:HOH:O[4_455]	1.86	0.34

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	798/853 (94%)	764 (96%)	28 (4%)	6 (1%)	16	31
1	B	811/853 (95%)	768 (95%)	37 (5%)	6 (1%)	18	34
All	All	1609/1706 (94%)	1532 (95%)	65 (4%)	12 (1%)	18	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	615	ASP
1	A	690	PRO
1	B	206	ALA
1	B	610	ASP
1	A	2	PRO
1	B	615	ASP
1	A	633	CYS
1	B	632	LEU
1	B	642	ASN
1	B	671	GLY
1	A	167	VAL
1	A	772	LEU

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	696/731 (95%)	650 (93%)	46 (7%)	15	32
1	B	703/731 (96%)	662 (94%)	41 (6%)	18	38
All	All	1399/1462 (96%)	1312 (94%)	87 (6%)	16	34

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

Mol	Chain	Res	Type
1	A	43	GLU
1	A	85	ASN
1	A	88	LEU
1	A	92	LEU
1	A	104	ILE
1	A	132	VAL
1	A	138	LYS
1	A	156	HIS
1	A	157	GLU
1	A	164	GLU
1	A	209	GLU
1	A	220	LYS
1	A	266	ASP
1	A	284	ASP
1	A	352	LEU
1	A	371	ASP
1	A	409	LEU
1	A	419	LEU
1	A	454	LEU
1	A	563	THR
1	A	574	ASN
1	A	575	LYS
1	A	577	ILE
1	A	582	ILE
1	A	586	LYS
1	A	590	THR
1	A	604	LEU
1	A	607	ARG
1	A	609	ASN
1	A	610	ASP
1	A	651	LEU
1	A	654	LYS
1	A	661	GLN
1	A	666	CYS

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Mol	Chain	Res	Type
1	A	673	VAL
1	A	676	VAL
1	A	684	ASN
1	A	697	LEU
1	A	705	LEU
1	A	722	LEU
1	A	741	VAL
1	A	757	GLU
1	A	773	LEU
1	A	824	HIS
1	A	827	ASN
1	A	831	VAL
1	B	74	LEU
1	B	132	VAL
1	B	157	GLU
1	B	158	LEU
1	B	163	LYS
1	B	165	ARG
1	B	182	GLN
1	B	184	ASP
1	B	198	THR
1	B	204	VAL
1	B	224	THR
1	B	266	ASP
1	B	288	LYS
1	B	314	LYS
1	B	352	LEU
1	B	359	ASP
1	B	364	VAL
1	B	373	THR
1	B	452	VAL
1	B	506	LYS
1	B	521	LYS
1	B	539	VAL
1	B	576	ASP
1	B	609	ASN
1	B	614	ILE
1	B	616	SER
1	B	628	THR
1	B	639	ASP
1	B	649	CYS
1	B	653	ASP

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Mol	Chain	Res	Type
1	B	666	CYS
1	B	688	LYS
1	B	698	LYS
1	B	703	GLU
1	B	735	GLU
1	B	762	GLN
1	B	783	THR
1	B	792	MET
1	B	827	ASN
1	B	828	SER
1	B	831	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	118	GLN
1	A	128	HIS
1	A	143	ASN
1	A	205	ASN
1	A	248	GLN
1	A	323	ASN
1	A	574	ASN
1	A	747	GLN
1	A	762	GLN
1	B	118	GLN
1	B	195	HIS
1	B	248	GLN
1	B	315	GLN
1	B	323	ASN
1	B	660	ASN
1	B	684	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](#)

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	810/853 (94%)	0.59	84 (10%) 11 10	42, 73, 150, 178	0
1	B	817/853 (95%)	0.58	50 (6%) 27 23	41, 74, 129, 169	0
All	All	1627/1706 (95%)	0.59	134 (8%) 17 15	41, 74, 144, 178	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	TRP	6.1
1	B	831	VAL	6.0
1	B	832	LEU	5.7
1	A	1	ALA	5.2
1	A	287	ALA	4.7
1	B	88	LEU	4.7
1	B	829	LEU	4.7
1	B	614	ILE	4.5
1	B	579	TRP	4.3
1	B	85	ASN	4.2
1	B	574	ASN	4.0
1	A	647	THR	3.9
1	A	2	PRO	3.9
1	B	5	LYS	3.7
1	B	168	ALA	3.7
1	B	179	PHE	3.7
1	A	619	GLY	3.6
1	B	577	ILE	3.6
1	B	824	HIS	3.5
1	A	258	CYS	3.4
1	A	635	LEU	3.4
1	A	614	ILE	3.3
1	B	163	LYS	3.2
1	A	711	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	636	CYS	3.2
1	B	668	VAL	3.1
1	B	258	CYS	3.1
1	A	582	ILE	3.1
1	A	717	TYR	3.0
1	A	156	HIS	3.0
1	A	804	VAL	3.0
1	B	466	HIS	3.0
1	A	180	VAL	3.0
1	B	167	VAL	3.0
1	A	833	PHE	3.0
1	A	692	VAL	2.9
1	B	613	ASP	2.9
1	B	674	ALA	2.9
1	A	726	PRO	2.9
1	A	575	LYS	2.8
1	A	163	LYS	2.8
1	A	606	ARG	2.8
1	A	288	LYS	2.8
1	A	579	TRP	2.7
1	B	612	SER	2.7
1	A	672	ASP	2.7
1	A	577	ILE	2.7
1	A	202	TRP	2.7
1	B	617	PHE	2.7
1	A	569	LEU	2.6
1	A	632	LEU	2.6
1	A	626	SER	2.6
1	B	287	ALA	2.6
1	A	194	PHE	2.6
1	A	574	ASN	2.6
1	A	468	PRO	2.5
1	B	637	ILE	2.5
1	B	319	GLU	2.5
1	A	170	GLY	2.5
1	A	729	ALA	2.5
1	A	621	SER	2.5
1	A	808	SER	2.5
1	A	707	LEU	2.5
1	A	205	ASN	2.5
1	B	694	ALA	2.5
1	B	573	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	604	LEU	2.5
1	A	722	LEU	2.5
1	A	567	VAL	2.5
1	B	588	CYS	2.4
1	A	564	LEU	2.4
1	A	689	ASN	2.4
1	B	288	LYS	2.4
1	B	575	LYS	2.4
1	B	628	THR	2.4
1	A	664	PHE	2.4
1	B	468	PRO	2.4
1	A	725	ILE	2.4
1	B	467	LEU	2.4
1	A	670	LYS	2.4
1	A	562	GLY	2.3
1	B	812	MET	2.3
1	A	675	PHE	2.3
1	A	85	ASN	2.3
1	A	590	THR	2.3
1	A	693	TRP	2.3
1	B	693	TRP	2.3
1	A	157	GLU	2.3
1	A	682	PHE	2.3
1	A	554	PRO	2.3
1	B	224	THR	2.2
1	B	616	SER	2.2
1	B	650	SER	2.2
1	B	204	VAL	2.2
1	B	712	ALA	2.2
1	B	213	GLY	2.2
1	A	467	LEU	2.2
1	A	796	PHE	2.2
1	A	566	ALA	2.2
1	A	724	GLY	2.2
1	A	653	ASP	2.2
1	A	293	ARG	2.2
1	A	82	TYR	2.2
1	A	805	TYR	2.2
1	A	179	PHE	2.2
1	A	648	LYS	2.2
1	A	673	VAL	2.1
1	A	595	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	692	VAL	2.1
1	A	226	GLN	2.1
1	A	609	ASN	2.1
1	B	664	PHE	2.1
1	A	525	GLN	2.1
1	A	599	VAL	2.1
1	B	673	VAL	2.1
1	A	605	ILE	2.1
1	B	595	ILE	2.1
1	A	546	ASP	2.1
1	A	613	ASP	2.1
1	A	630	SER	2.1
1	A	690	PRO	2.1
1	A	772	LEU	2.1
1	A	563	THR	2.1
1	A	782	ILE	2.1
1	B	672	ASP	2.1
1	A	710	SER	2.1
1	B	604	LEU	2.0
1	A	801	TYR	2.0
1	B	608	GLN	2.0
1	A	568	ALA	2.0
1	A	705	LEU	2.0
1	B	205	ASN	2.0
1	B	308	THR	2.0
1	A	286	PRO	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.