Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:48 AM EDT

PDB ID	:	6O0D
Title	:	Saxiphilin Apo structure
Authors	:	Yen, T.J.; Lolicato, M.; Minor, D.L.
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:

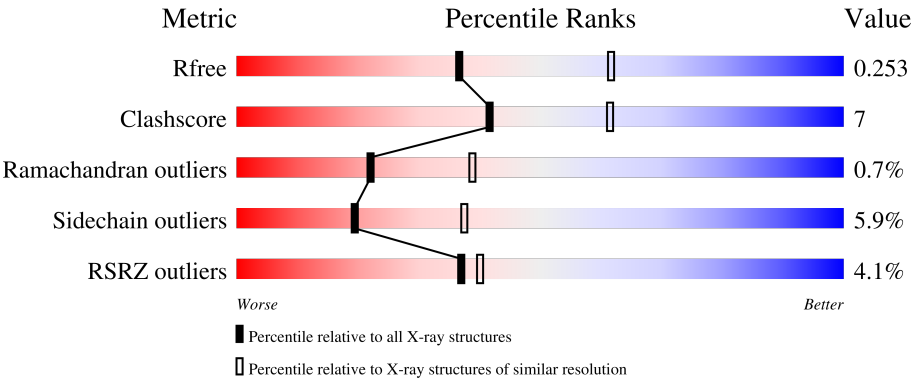
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	5% 75% 18% · 5%
1	B	853	3% 77% 17% · ·

2 Entry composition (i)

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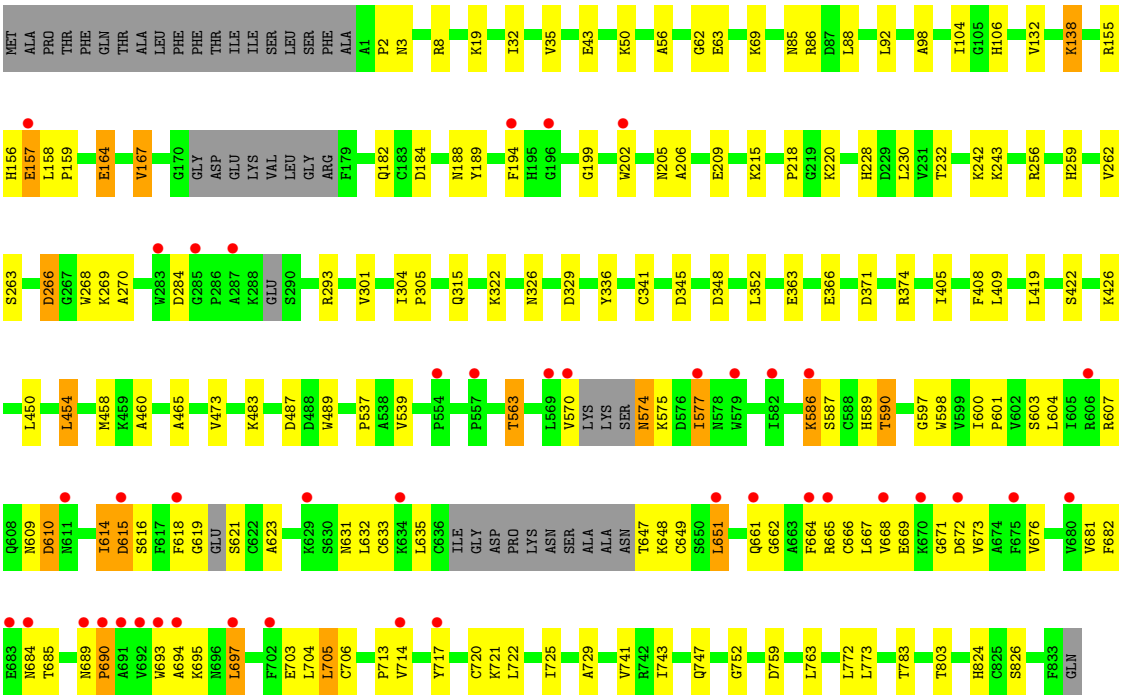
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	66	Total	O	0	0
			66	66		

3 Residue-property plots (i)

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.

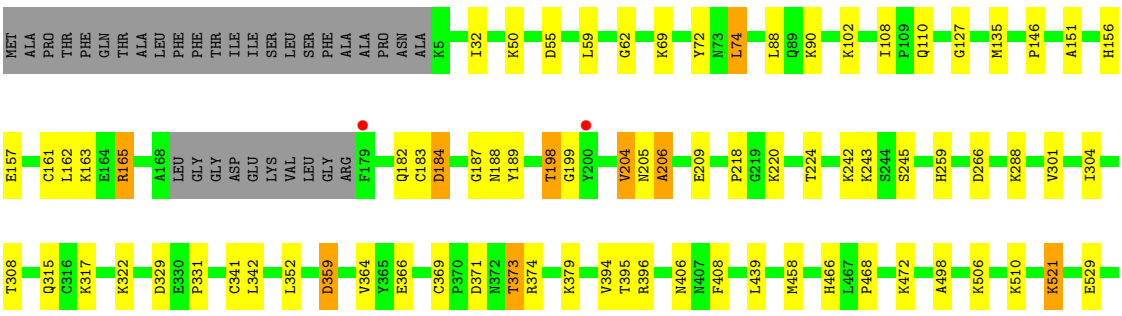
• Molecule 1: Saxiphilin

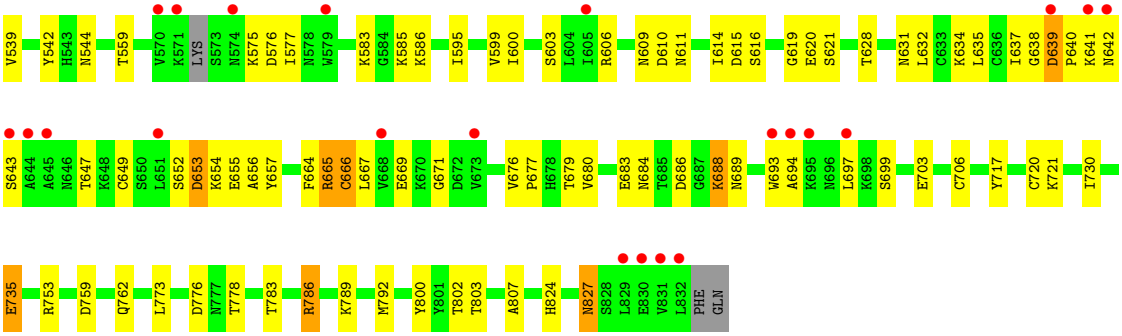
Chain A:



• Molecule 1: Saxiphilin

Chain B:




V539 Y542 H543 N544 T559 V570 K571 LYS S573 N574 K575 D576 I577 N578 W579 K583 G584 K585 K586 I595 V599 I600 S603 L604 I605 R606 N609 D610 N611 I614 D615 S616 G619 E620 S621 T628 N631 L632 C633 K634 L635 C636 I637 G638 D639 P640 K641 N642
S643 A644 A645 N646 T647 K648 C649 S650 L651 S652 D653 K654 E655 A656 Y657 F664 R665 C666 L667 V668 E669 K670 G671 D672 V673 V676 P677 H678 T679 V680 E683 N684 T685 D686 G687 K688 N689 W693 A694 K695 N696 L697 K698 S699 E703 C706 Y717 C720 K721 I730
E735 R753 D759 Q762 L773 D776 N777 T778 T783 R786 K789 M792 Y800 Y801 T802 T803 A807 H824 N827 S828 L829 E830 V831 L832 PHE GLN

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.64 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.224 , 0.253 0.224 , 0.253	Depositor DCC
R_{free} test set	4737 reflections (4.98%)	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 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/6376	0.48	0/8602
1	B	0.26	0/6431	0.47	0/8679
All	All	0.26	0/12807	0.47	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

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	85	0
1	B	6306	0	6167	91	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	7	1
All	All	12705	0	12285	175	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 7.

All (175) 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: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:A:586:LYS:HD2	1:A:671:GLY:HA2	1.77	0.65
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:662:GLY:C	1:A:664:PHE:H	2.10	0.55
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:O	1:B:643:SER:N	2.43	0.51
1:B:62:GLY:O	1:B:458:MET:HE1	2.12	0.50
1:A:155:ARG:HE	1:A:157:GLU:CD	2.15	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:641:LYS:C	1:B:643:SER:H	2.18	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:B:198:THR:HG22	1:B:199:GLY:H	1.81	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
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:62:GLY:O	1:A:458:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ALA:HA	1:A:465:ALA:HB2	1.99	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:759:ASP:OD1	1:A:759:ASP:N	2.42	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:641:LYS:HD3	1:B:641:LYS:HA	1.72	0.41
1:A:598:TRP:C	1:A:601:PRO:HD2	2.41	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:665:ARG:HE	1:B:669:GLU:CD	2.23	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:666:CYS:SG	1:B:667:LEU:N	2.94	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%)	19 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	811/853 (95%)	768 (95%)	37 (5%)	6 (1%)	22 39
All	All	1609/1706 (94%)	1532 (95%)	65 (4%)	12 (1%)	22 39

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%)	651 (94%)	45 (6%)	17 33
1	B	703/731 (96%)	665 (95%)	38 (5%)	22 42
All	All	1399/1462 (96%)	1316 (94%)	83 (6%)	19 37

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	50	LYS
1	A	85	ASN
1	A	88	LEU

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Mol	Chain	Res	Type
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	205	ASN
1	A	209	GLU
1	A	220	LYS
1	A	266	ASP
1	A	284	ASP
1	A	341	CYS
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	586	LYS
1	A	590	THR
1	A	604	LEU
1	A	607	ARG
1	A	609	ASN
1	A	610	ASP
1	A	649	CYS
1	A	651	LEU
1	A	661	GLN
1	A	665	ARG
1	A	666	CYS
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	773	LEU
1	A	824	HIS
1	B	50	LYS

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Mol	Chain	Res	Type
1	B	74	LEU
1	B	102	LYS
1	B	157	GLU
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	341	CYS
1	B	352	LEU
1	B	359	ASP
1	B	364	VAL
1	B	373	THR
1	B	521	LYS
1	B	575	LYS
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
1	B	665	ARG
1	B	666	CYS
1	B	688	LYS
1	B	703	GLU
1	B	735	GLU
1	B	762	GLN
1	B	783	THR
1	B	786	ARG
1	B	792	MET
1	B	827	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.29	42 (5%)	27	29	42, 73, 150, 178	0
1	B	817/853 (95%)	0.24	24 (2%)	51	55	41, 74, 129, 169	0
All	All	1627/1706 (95%)	0.27	66 (4%)	37	40	41, 74, 144, 178	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	VAL	7.2
1	B	644	ALA	6.3
1	A	690	PRO	6.2
1	A	691	ALA	5.1
1	A	697	LEU	4.7
1	A	582	ILE	4.6
1	A	689	ASN	4.5
1	B	639	ASP	4.5
1	A	717	TYR	4.5
1	A	579	TRP	4.4
1	B	694	ALA	4.4
1	A	283	TRP	4.3
1	A	670	LYS	4.2
1	A	693	TRP	4.2
1	A	714	VAL	4.2
1	A	615	ASP	4.2
1	A	569	LEU	4.1
1	B	693	TRP	4.0
1	B	574	ASN	4.0
1	A	554	PRO	3.7
1	B	642	ASN	3.7
1	A	702	PHE	3.6
1	A	694	ALA	3.5
1	A	692	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	570	VAL	3.5
1	A	668	VAL	3.5
1	B	643	SER	3.4
1	B	645	ALA	3.4
1	A	664	PHE	3.4
1	B	831	VAL	3.4
1	B	179	PHE	3.3
1	B	673	VAL	3.3
1	A	287	ALA	3.3
1	A	683	GLU	3.2
1	A	196	GLY	3.2
1	A	202	TRP	3.2
1	A	606	ARG	3.0
1	B	829	LEU	2.9
1	A	675	PHE	2.9
1	A	680	VAL	2.9
1	A	684	ASN	2.9
1	A	618	PHE	2.9
1	A	661	GLN	2.8
1	A	672	ASP	2.8
1	A	629	LYS	2.7
1	A	611	ASN	2.7
1	B	200	TYR	2.6
1	B	695	LYS	2.6
1	A	665	ARG	2.6
1	A	577	ILE	2.5
1	A	285	GLY	2.5
1	B	651	LEU	2.4
1	B	579	TRP	2.4
1	B	571	LYS	2.4
1	A	651	LEU	2.4
1	B	641	LYS	2.4
1	B	830	GLU	2.4
1	B	570	VAL	2.3
1	A	194	PHE	2.3
1	A	586	LYS	2.3
1	A	557	PRO	2.2
1	B	832	LEU	2.2
1	A	634	LYS	2.1
1	B	697	LEU	2.1
1	A	157	GLU	2.0
1	B	605	ILE	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 monosaccharides 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.