



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:36 PM UTC

PDB ID : 5GKO / pdb_00005gko
Title : Crystal structure of tripartite-type ABC transporter, MacB from *Acinetobacter baumannii*
Authors : Murakami, S.; Okada, U.; Yamashita, E.
Deposited on : 2016-07-04
Resolution : 3.39 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

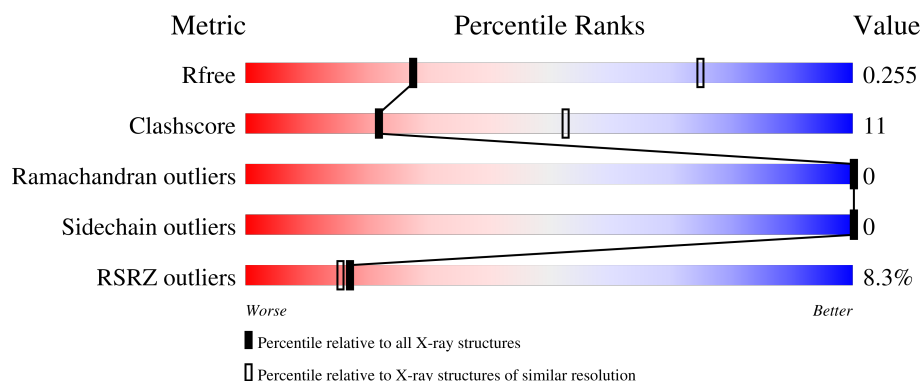
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	671	8% 71% 26% .
1	B	671	8% 73% 24% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9770 atoms, of which 0 are hydrogens and 0 are deuteriums.

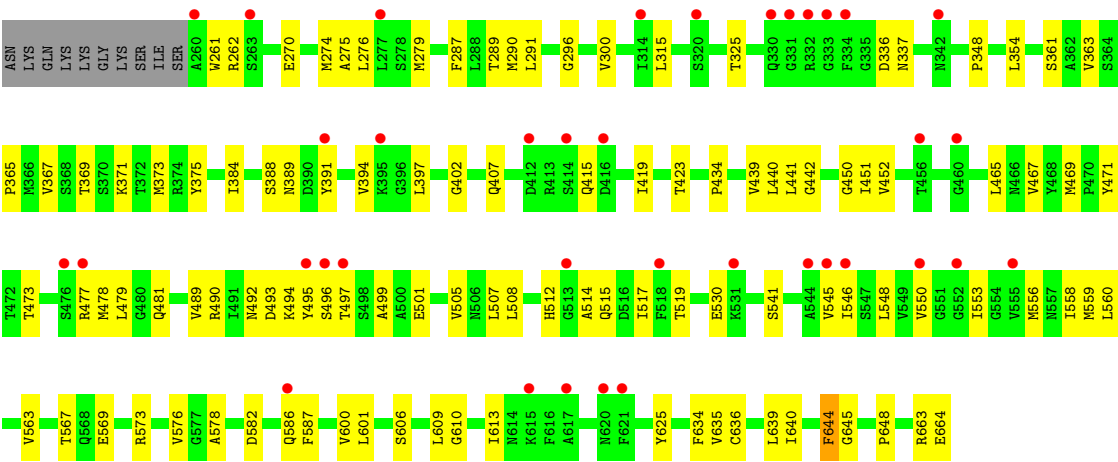
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Macrolide export ATP-binding/permease protein MacB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	Se	0	0	0
			4885	3056	854	952	3	20			
1	B	650	Total	C	N	O	S	Se	0	0	0
			4885	3056	854	952	3	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MSE	-	expression tag	UNP A0A0D8G707
A	-5	HIS	-	expression tag	UNP A0A0D8G707
A	-4	HIS	-	expression tag	UNP A0A0D8G707
A	-3	HIS	-	expression tag	UNP A0A0D8G707
A	-2	HIS	-	expression tag	UNP A0A0D8G707
A	-1	HIS	-	expression tag	UNP A0A0D8G707
A	0	HIS	-	expression tag	UNP A0A0D8G707
B	-6	MSE	-	expression tag	UNP A0A0D8G707
B	-5	HIS	-	expression tag	UNP A0A0D8G707
B	-4	HIS	-	expression tag	UNP A0A0D8G707
B	-3	HIS	-	expression tag	UNP A0A0D8G707
B	-2	HIS	-	expression tag	UNP A0A0D8G707
B	-1	HIS	-	expression tag	UNP A0A0D8G707
B	0	HIS	-	expression tag	UNP A0A0D8G707



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	229.15Å 229.15Å 155.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.96 – 3.39 43.96 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.96-3.39) 99.1 (43.96-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.223 , 0.255 0.227 , 0.255	Depositor DCC
R_{free} test set	2909 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 138.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9770	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9358e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.19	0/4925	0.50	0/6643
1	B	0.19	0/4925	0.53	1/6643 (0.0%)
All	All	0.19	0/9850	0.51	1/13286 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	644	PHE	N-CA-C	10.94	123.20	111.28

There are no chirality outliers.

There are no planarity outliers.

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	4885	0	4973	111	0
1	B	4885	0	4973	105	0
All	All	9770	0	9946	210	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 11.

All (210) 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:546:ILE:O	1:B:550:VAL:HB	1.57	1.05
1:A:547:SER:HB3	1:B:548:LEU:HD12	1.60	0.83
1:A:109:VAL:HG12	1:A:162:MSE:HE2	1.62	0.79
1:A:394:VAL:HG23	1:A:490:ARG:HB2	1.65	0.78
1:B:109:VAL:HG12	1:B:162:MSE:HE2	1.63	0.78
1:A:330:GLN:HE22	1:A:345:THR:H	1.32	0.77
1:A:419:ILE:HG23	1:A:423:THR:HB	1.68	0.76
1:B:53:MSE:HE1	1:B:171:ASP:HB2	1.71	0.73
1:A:13:VAL:HB	1:A:64:SER:HB3	1.69	0.73
1:B:394:VAL:HG23	1:B:490:ARG:HB2	1.71	0.71
1:B:296:GLY:HA2	1:B:548:LEU:HD13	1.75	0.67
1:B:289:THR:HG21	1:B:558:ILE:HG21	1.75	0.66
1:A:87:ARG:HG3	1:A:577:GLY:HA3	1.78	0.65
1:A:225:SER:OG	1:A:227:ARG:NH1	2.32	0.63
1:A:120:PRO:HA	1:A:123:ARG:HG2	1.79	0.62
1:B:115:TYR:OH	1:B:573:ARG:HD2	1.98	0.62
1:B:373:MSE:HE3	1:B:439:VAL:HG21	1.82	0.62
1:A:144:PRO:O	1:A:152:GLN:NE2	2.33	0.61
1:B:144:PRO:O	1:B:152:GLN:NE2	2.33	0.61
1:A:139:LYS:HD2	1:A:142:ASN:ND2	2.15	0.61
1:A:363:VAL:HG12	1:A:489:VAL:HG22	1.81	0.61
1:B:369:THR:HB	1:B:479:LEU:HD21	1.83	0.61
1:B:139:LYS:HD2	1:B:142:ASN:ND2	2.15	0.61
1:B:402:GLY:HA3	1:B:450:GLY:HA2	1.83	0.60
1:A:95:GLN:HA	1:A:172:GLU:O	2.02	0.60
1:A:373:MSE:HE3	1:A:439:VAL:HG21	1.84	0.60
1:A:505:VAL:HG13	1:A:515:GLN:HE22	1.67	0.59
1:A:11:ASN:N	1:A:30:ASP:OD1	2.30	0.59
1:A:598:GLY:HA2	1:A:601:LEU:HB2	1.86	0.58
1:A:369:THR:HB	1:A:479:LEU:HD21	1.86	0.58
1:B:9:VAL:HG13	1:B:12:LEU:HG	1.85	0.58
1:B:325:THR:HA	1:B:489:VAL:O	2.04	0.58
1:A:546:ILE:O	1:A:550:VAL:HB	2.04	0.57
1:B:300:VAL:HG13	1:B:545:VAL:HG22	1.85	0.57
1:A:217:GLU:HB3	1:A:225:SER:HB3	1.86	0.57
1:A:100:LEU:HD22	1:A:569:GLU:HG3	1.86	0.57
1:A:267:ARG:HH21	1:A:579:ARG:NH1	2.02	0.57
1:B:287:PHE:O	1:B:291:LEU:HB2	2.03	0.57
1:B:91:GLY:C	1:B:92:PHE:HD1	2.13	0.57
1:B:169:LEU:HD23	1:B:200:ILE:HB	1.87	0.56
1:B:174:THR:HG23	1:B:186:MSE:HE3	1.87	0.56
1:B:434:PRO:HG2	1:B:451:ILE:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:MSE:HB2	1:B:644:PHE:HB3	1.85	0.56
1:A:91:GLY:C	1:A:92:PHE:HD1	2.14	0.56
1:A:330:GLN:NE2	1:A:344:LYS:HA	2.19	0.56
1:B:100:LEU:HD22	1:B:569:GLU:HG3	1.87	0.56
1:B:501:GLU:HG3	1:B:519:THR:OG1	2.06	0.56
1:A:350:ASP:OD1	1:A:511:ARG:NH1	2.29	0.55
1:A:533:THR:HA	1:A:536:MSE:HE2	1.89	0.55
1:A:606:SER:O	1:A:625:TYR:OH	2.25	0.55
1:A:415:GLN:NE2	1:A:445:PRO:O	2.39	0.55
1:B:663:ARG:O	1:B:664:GLU:HG3	2.07	0.55
1:B:300:VAL:HG22	1:B:545:VAL:HG22	1.89	0.55
1:A:115:TYR:CD2	1:A:578:ALA:HA	2.42	0.54
1:A:456:THR:OG1	1:A:458:GLY:O	2.25	0.54
1:A:332:ARG:HB3	1:B:515:GLN:HE22	1.73	0.54
1:B:11:ASN:N	1:B:30:ASP:OD1	2.36	0.54
1:A:402:GLY:HA3	1:A:450:GLY:HA2	1.89	0.53
1:B:89:TYR:O	1:B:166:ASP:HB2	2.08	0.53
1:A:574:MSE:HA	1:A:578:ALA:HB3	1.90	0.53
1:B:93:ILE:HG23	1:B:153:GLN:NE2	2.24	0.53
1:A:169:LEU:HD23	1:A:200:ILE:HB	1.91	0.53
1:A:112:PRO:HG3	1:A:576:VAL:HB	1.90	0.52
1:A:306:LEU:HA	1:A:623:VAL:HG12	1.91	0.52
1:B:517:ILE:O	1:B:517:ILE:HD12	2.09	0.52
1:A:139:LYS:HD2	1:A:142:ASN:HD21	1.74	0.52
1:A:636:CYS:O	1:A:640:ILE:HG12	2.08	0.52
1:B:276:LEU:HA	1:B:279:MSE:HE2	1.91	0.52
1:B:17:PRO:HA	1:B:22:THR:HA	1.92	0.52
1:A:508:LEU:HB2	1:A:517:ILE:HD13	1.92	0.51
1:B:560:LEU:HD23	1:B:648:PRO:HB3	1.92	0.51
1:A:311:GLN:HB2	1:A:533:THR:HG21	1.90	0.51
1:B:569:GLU:OE2	1:B:573:ARG:NH2	2.43	0.51
1:A:328:VAL:HG22	1:A:519:THR:HG22	1.93	0.51
1:B:606:SER:O	1:B:625:TYR:OH	2.24	0.51
1:A:110:GLU:HA	1:A:162:MSE:HE3	1.92	0.51
1:A:272:PHE:CE1	1:A:593:LEU:HD21	2.46	0.51
1:B:423:THR:HA	1:B:465:LEU:HD22	1.93	0.51
1:B:636:CYS:O	1:B:640:ILE:HG12	2.09	0.51
1:A:329:PHE:CE1	1:A:520:MSE:HE2	2.46	0.51
1:A:375:TYR:HB2	1:A:439:VAL:HG12	1.93	0.51
1:A:384:ILE:HD11	1:A:441:LEU:HB3	1.94	0.50
1:B:70:ASN:HB2	1:B:89:TYR:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HA	1:A:606:SER:HB2	1.93	0.50
1:A:550:VAL:O	1:A:553:ILE:HG23	2.11	0.50
1:A:197:HIS:CE1	1:A:246:PRO:HA	2.46	0.50
1:A:389:ASN:HD21	1:A:407:GLN:HG3	1.76	0.50
1:B:550:VAL:O	1:B:553:ILE:HG23	2.12	0.49
1:B:139:LYS:HD2	1:B:142:ASN:HD21	1.76	0.49
1:A:267:ARG:HH21	1:A:579:ARG:HH12	1.60	0.49
1:A:505:VAL:O	1:A:509:THR:OG1	2.27	0.49
1:A:360:VAL:HG11	1:A:363:VAL:HG13	1.93	0.49
1:B:541:SER:O	1:B:545:VAL:HG23	2.11	0.49
1:B:508:LEU:O	1:B:512:HIS:HD2	1.96	0.48
1:A:114:VAL:HG22	1:A:123:ARG:NH1	2.27	0.48
1:B:164:GLY:HA2	1:B:247:ALA:HB3	1.94	0.48
1:A:61:ARG:HD2	1:A:75:GLY:O	2.13	0.48
1:B:644:PHE:N	1:B:645:GLY:HA3	2.29	0.48
1:B:115:TYR:CE2	1:B:578:ALA:HB2	2.47	0.48
1:B:270:GLU:O	1:B:274:MSE:HG2	2.13	0.48
1:B:315:LEU:HD11	1:B:530:GLU:HG2	1.95	0.48
1:B:389:ASN:HD21	1:B:407:GLN:HG3	1.79	0.48
1:A:7:LEU:HB2	1:A:33:ILE:HB	1.95	0.47
1:A:134:LEU:HD12	1:A:158:ALA:HB2	1.96	0.47
1:B:363:VAL:HG23	1:B:489:VAL:HG12	1.96	0.47
1:A:359:TYR:O	1:A:492:ASN:N	2.39	0.47
1:A:42:VAL:HA	1:A:203:THR:O	2.14	0.47
1:B:197:HIS:CE1	1:B:246:PRO:HA	2.50	0.47
1:A:315:LEU:HD22	1:A:526:ARG:HG3	1.95	0.47
1:A:327:THR:HG22	1:A:488:VAL:HG12	1.96	0.47
1:B:361:SER:HB3	1:B:492:ASN:HB2	1.96	0.47
1:A:354:LEU:HD23	1:A:507:LEU:HD23	1.96	0.47
1:B:365:PRO:HD2	1:B:388:SER:HB2	1.97	0.47
1:B:496:SER:HB2	1:B:499:ALA:HB3	1.97	0.47
1:B:600:VAL:HG22	1:B:634:PHE:CE1	2.49	0.47
1:A:332:ARG:CD	1:B:505:VAL:HG21	2.45	0.47
1:B:118:VAL:HG11	1:B:123:ARG:HD3	1.96	0.47
1:B:473:THR:O	1:B:477:ARG:HB2	2.14	0.47
1:B:275:ALA:O	1:B:279:MSE:HG3	2.15	0.47
1:A:9:VAL:HG13	1:A:12:LEU:HD23	1.96	0.47
1:A:366:MSE:HB3	1:A:486:ASN:OD1	2.15	0.47
1:B:375:TYR:HB2	1:B:439:VAL:HG12	1.96	0.47
1:B:217:GLU:HB3	1:B:225:SER:HB3	1.97	0.47
1:B:300:VAL:HG22	1:B:545:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:HG3	1:B:478:MSE:CE	2.45	0.46
1:A:609:LEU:O	1:A:613:ILE:HG12	2.15	0.46
1:B:59:LEU:HD11	1:B:92:PHE:HE2	1.80	0.46
1:B:609:LEU:O	1:B:613:ILE:HG12	2.16	0.46
1:A:440:LEU:HD13	1:A:442:GLY:O	2.16	0.46
1:B:134:LEU:HD12	1:B:158:ALA:HB2	1.98	0.46
1:A:343:PHE:HD2	1:B:514:ALA:HA	1.80	0.45
1:A:456:THR:HB	1:A:462:ASP:HB3	1.98	0.45
1:B:61:ARG:HD2	1:B:75:GLY:O	2.15	0.45
1:B:348:PRO:HB3	1:B:471:TYR:HE2	1.81	0.45
1:A:384:ILE:CD1	1:A:441:LEU:HB3	2.46	0.45
1:A:423:THR:HA	1:A:465:LEU:HD22	1.99	0.45
1:B:38:LEU:HB2	1:B:193:ASN:ND2	2.30	0.45
1:A:307:GLY:HA3	1:A:537:THR:HG21	1.98	0.45
1:B:384:ILE:CD1	1:B:441:LEU:HB3	2.47	0.45
1:A:345:THR:OG1	1:A:516:ASP:OD2	2.25	0.45
1:A:556:MSE:HE3	1:A:644:PHE:HA	1.98	0.45
1:A:210:LYS:HA	1:A:215:ILE:HD11	1.98	0.45
1:B:546:ILE:O	1:B:550:VAL:CB	2.47	0.45
1:B:610:GLY:HA3	1:B:625:TYR:OH	2.17	0.45
1:A:397:LEU:HD13	1:A:452:VAL:HG11	1.99	0.45
1:B:419:ILE:HG22	1:B:467:VAL:HG22	1.99	0.45
1:A:395:LYS:HE3	1:A:488:VAL:HG11	1.98	0.45
1:B:112:PRO:HB3	1:B:576:VAL:HG13	1.99	0.45
1:B:384:ILE:HD11	1:B:441:LEU:HB3	1.99	0.45
1:A:5:ALA:HB1	1:A:34:TYR:HA	1.99	0.44
1:A:361:SER:N	1:A:492:ASN:HB2	2.32	0.44
1:B:494:LYS:HG3	1:B:497:THR:HB	1.99	0.44
1:A:184:GLU:O	1:A:187:ARG:HG2	2.18	0.44
1:A:592:ILE:HD11	1:A:642:VAL:HG22	2.00	0.44
1:B:261:TRP:CD1	1:B:262:ARG:HB2	2.52	0.44
1:B:394:VAL:HA	1:B:490:ARG:HD2	1.99	0.44
1:B:563:VAL:HG22	1:B:587:PHE:CE2	2.53	0.44
1:B:391:TYR:HA	1:B:394:VAL:HG12	1.98	0.43
1:A:15:GLU:HG2	1:A:24:GLN:HG2	1.99	0.43
1:A:428:PHE:CE2	1:A:434:PRO:HA	2.52	0.43
1:B:354:LEU:HD23	1:B:507:LEU:HD23	2.00	0.43
1:A:7:LEU:HD22	1:A:67:TYR:OH	2.18	0.43
1:A:111:VAL:HB	1:A:112:PRO:HD3	1.99	0.43
1:A:120:PRO:O	1:A:124:LYS:HG3	2.18	0.43
1:B:118:VAL:HG13	1:B:123:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:CG1	1:A:363:VAL:HG13	2.49	0.43
1:B:397:LEU:HD13	1:B:452:VAL:HG11	2.00	0.43
1:B:493:ASP:HB3	1:B:495:TYR:HB2	2.01	0.43
1:A:62:PRO:O	1:A:63:THR:OG1	2.33	0.43
1:A:548:LEU:HA	1:A:548:LEU:HD23	1.79	0.43
1:A:38:LEU:HG	1:A:212:ALA:HA	2.01	0.42
1:A:326:ILE:HD12	1:A:501:GLU:HG3	2.00	0.42
1:A:547:SER:HB3	1:B:548:LEU:CD1	2.41	0.42
1:B:42:VAL:HA	1:B:203:THR:O	2.19	0.42
1:B:348:PRO:HB3	1:B:471:TYR:CE2	2.54	0.42
1:A:337:ASN:O	1:A:341:ALA:HB3	2.19	0.42
1:B:567:THR:HG21	1:B:663:ARG:NH1	2.35	0.42
1:B:440:LEU:HD13	1:B:442:GLY:O	2.20	0.42
1:B:582:ASP:O	1:B:586:GLN:HG3	2.19	0.42
1:A:473:THR:O	1:A:477:ARG:HB2	2.19	0.42
1:B:40:ALA:HA	1:B:201:LEU:O	2.20	0.42
1:B:110:GLU:HA	1:B:162:MSE:HE3	2.02	0.42
1:A:89:TYR:O	1:A:166:ASP:HB2	2.20	0.42
1:B:508:LEU:O	1:B:512:HIS:CD2	2.73	0.42
1:A:59:LEU:HD11	1:A:92:PHE:HE2	1.84	0.42
1:A:105:ALA:O	1:A:109:VAL:HG23	2.20	0.42
1:A:596:LEU:HB2	1:A:638:THR:HG22	2.02	0.42
1:A:14:ARG:HB3	1:A:26:LEU:HB2	2.01	0.41
1:B:336:ASP:OD1	1:B:337:ASN:N	2.51	0.41
1:A:38:LEU:HB2	1:A:193:ASN:ND2	2.35	0.41
1:A:297:ILE:HA	1:A:300:VAL:HG12	2.02	0.41
1:A:350:ASP:HA	1:A:511:ARG:NH1	2.35	0.41
1:A:406:ASP:OD1	1:A:407:GLN:N	2.53	0.41
1:A:332:ARG:HD3	1:B:505:VAL:HG21	2.01	0.41
1:A:559:MSE:O	1:A:563:VAL:HG23	2.21	0.41
1:B:41:ILE:O	1:B:202:VAL:HA	2.20	0.41
1:A:521:ASN:HB3	1:A:524:SER:OG	2.21	0.41
1:B:290:MSE:HE2	1:B:601:LEU:HD12	2.02	0.41
1:B:553:ILE:O	1:B:556:MSE:N	2.53	0.41
1:A:391:TYR:HA	1:A:394:VAL:HG12	2.02	0.41
1:B:367:VAL:HG21	1:B:481:GLN:NE2	2.36	0.41
1:B:415:GLN:HA	1:B:469:MSE:HE3	2.02	0.41
1:B:559:MSE:O	1:B:563:VAL:HG23	2.22	0.41
1:B:635:VAL:O	1:B:639:LEU:HG	2.21	0.40
1:A:543:ILE:O	1:A:547:SER:HB2	2.21	0.40
1:A:419:ILE:O	1:A:451:ILE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:GLU:O	1:B:573:ARG:HG2	2.20	0.40
1:B:600:VAL:HG22	1:B:634:PHE:HE1	1.86	0.40
1:A:505:VAL:CG1	1:A:515:GLN:HE22	2.34	0.40
1:A:647:LEU:HB3	1:A:648:PRO:HD3	2.03	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	646/671 (96%)	618 (96%)	28 (4%)	0	100	100
1	B	646/671 (96%)	613 (95%)	33 (5%)	0	100	100
All	All	1292/1342 (96%)	1231 (95%)	61 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	538/536 (100%)	538 (100%)	0	100	100
1	B	538/536 (100%)	538 (100%)	0	100	100
All	All	1076/1072 (100%)	1076 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	337	ASN
1	A	481	GLN
1	A	515	GLN
1	B	98	HIS
1	B	153	GLN
1	B	211	ASN
1	B	233	GLN
1	B	378	ASN
1	B	424	GLN
1	B	426	GLN
1	B	481	GLN

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 oligosaccharides 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, 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	630/671 (93%)	0.39	53 (8%) 17 15	98, 144, 239, 333	0
1	B	630/671 (93%)	0.42	51 (8%) 18 16	109, 156, 255, 334	0
All	All	1260/1342 (93%)	0.41	104 (8%) 17 15	98, 150, 249, 334	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	546	ILE	6.1
1	A	546	ILE	5.9
1	A	45	SER	5.6
1	B	412	ASP	5.0
1	B	617	ALA	4.9
1	B	477	ARG	4.8
1	A	518	PHE	4.7
1	A	238	VAL	4.6
1	B	460	GLY	4.2
1	B	476	SER	4.1
1	A	550	VAL	4.0
1	B	333	GLY	3.8
1	B	331	GLY	3.7
1	B	117	GLY	3.7
1	A	22	THR	3.7
1	B	334	PHE	3.6
1	A	141	GLN	3.5
1	B	34	TYR	3.5
1	A	333	GLY	3.5
1	B	518	PHE	3.4
1	A	531	LYS	3.4
1	B	332	ARG	3.3
1	B	141	GLN	3.3
1	A	334	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	496	SER	3.2
1	A	544	ALA	3.2
1	B	263	SER	3.1
1	A	493	ASP	3.0
1	B	243	ASP	3.0
1	B	207	GLN	3.0
1	B	260	ALA	2.9
1	A	285	ARG	2.9
1	A	628	THR	2.9
1	A	261	TRP	2.9
1	A	44	GLN	2.9
1	B	235	LEU	2.9
1	B	314	ILE	2.9
1	B	50	SER	2.8
1	B	238	VAL	2.8
1	B	277	LEU	2.8
1	B	550	VAL	2.7
1	A	235	LEU	2.7
1	A	23	ILE	2.7
1	B	497	THR	2.7
1	A	232	ASP	2.6
1	A	242	PRO	2.6
1	A	246	PRO	2.6
1	A	243	ASP	2.6
1	A	337	ASN	2.6
1	A	595	CYS	2.5
1	B	234	SER	2.5
1	B	620	ASN	2.5
1	A	494	LYS	2.5
1	A	321	LEU	2.5
1	B	395	LYS	2.4
1	B	320	SER	2.4
1	B	456	THR	2.4
1	A	97	TYR	2.3
1	A	376	GLN	2.3
1	A	616	PHE	2.3
1	B	586	GLN	2.3
1	A	119	THR	2.3
1	A	282	HIS	2.3
1	A	34	TYR	2.3
1	A	102	ASP	2.3
1	A	412	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	THR	2.3
1	B	391	TYR	2.3
1	A	11	ASN	2.3
1	B	555	VAL	2.3
1	A	244	ALA	2.3
1	B	552	GLY	2.3
1	B	16	PHE	2.3
1	B	621	PHE	2.3
1	A	207	GLN	2.3
1	B	414	SER	2.2
1	A	663	ARG	2.2
1	B	531	LYS	2.2
1	B	495	TYR	2.2
1	B	342	ASN	2.2
1	A	529	ILE	2.2
1	A	597	ILE	2.2
1	B	244	ALA	2.2
1	A	549	VAL	2.2
1	A	443	SER	2.2
1	A	482	ALA	2.2
1	B	545	VAL	2.1
1	B	246	PRO	2.1
1	B	513	GLY	2.1
1	A	634	PHE	2.1
1	A	277	LEU	2.1
1	A	513	GLY	2.1
1	A	664	GLU	2.1
1	B	615	LYS	2.1
1	B	544	ALA	2.1
1	A	535	THR	2.1
1	B	22	THR	2.1
1	A	46	GLY	2.1
1	B	44	GLN	2.1
1	B	330	GLN	2.1
1	A	436	GLY	2.0
1	A	342	ASN	2.0
1	B	416	ASP	2.0
1	A	555	VAL	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 [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.