Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 03:42 am BST

PDB ID	:	5GKO
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 following versions of software and data (see references ⓘ) were used in the production of this report:

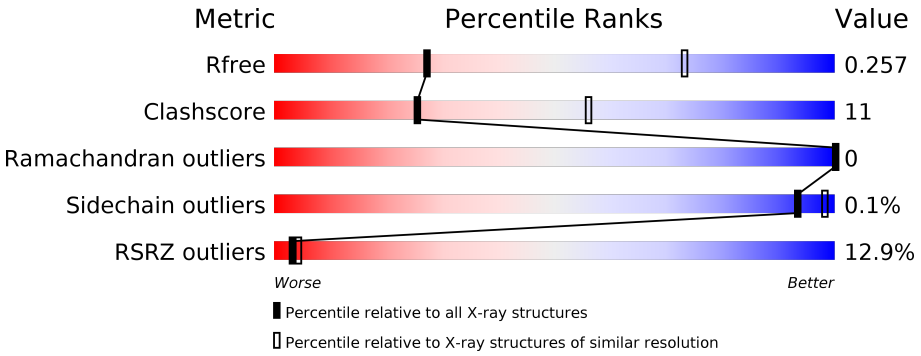
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	671	11% 71% 25%
1	B	671	13% 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:

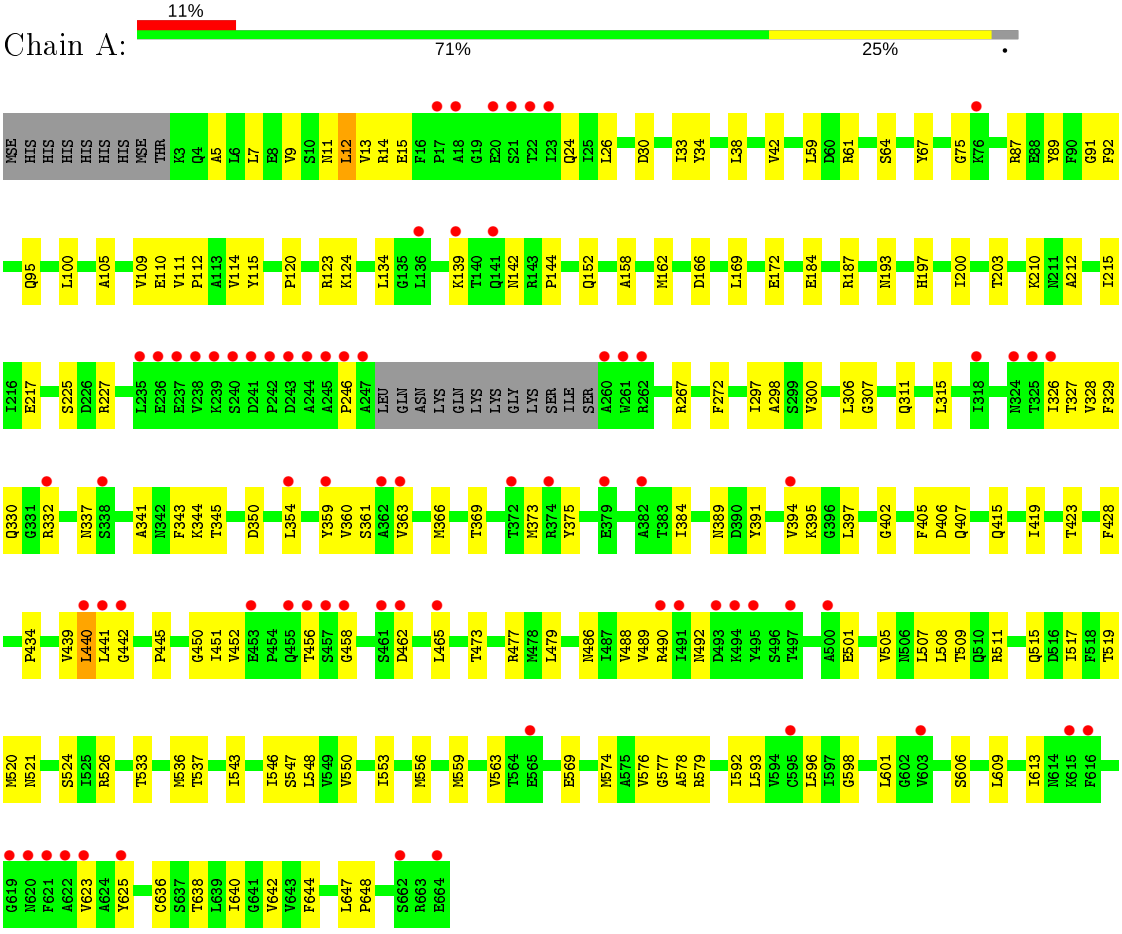
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MSE	-	expression tag	UNP A0A0D8G707
A	-5	HIS	-	expression tag	UNP A0A0D8G707
A	-4	HIS	-	expression tag	UNP A0A0D8G707
A	-3	HIS	-	expression tag	UNP A0A0D8G707
A	-2	HIS	-	expression tag	UNP A0A0D8G707
A	-1	HIS	-	expression tag	UNP A0A0D8G707
A	0	HIS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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

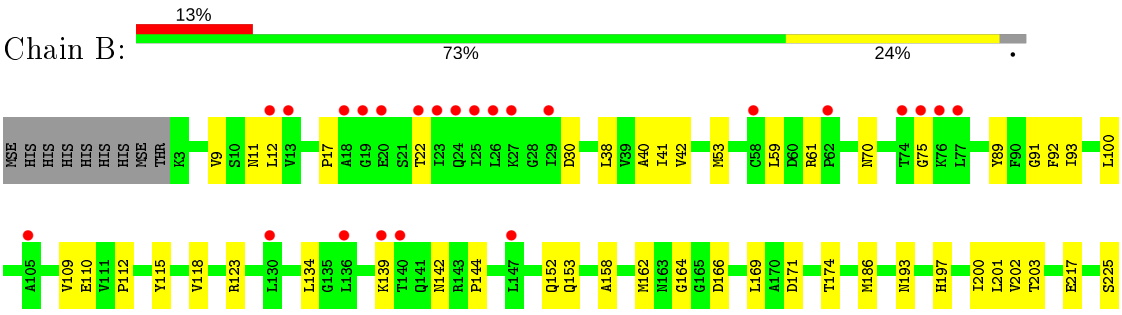
- Molecule 1: Macrolide export ATP-binding/permease protein MacB

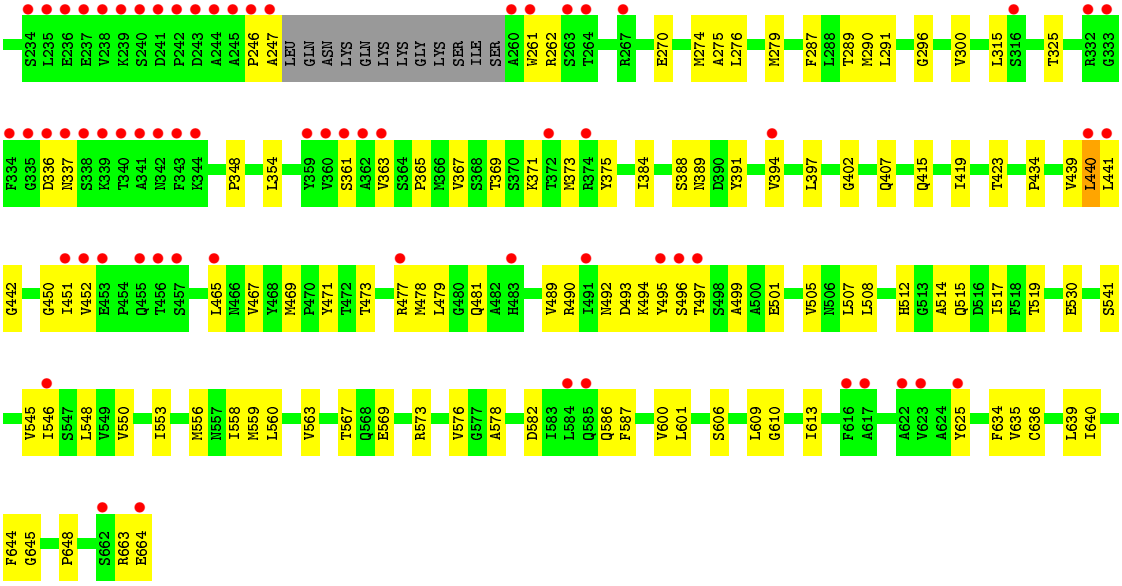
Chain A:



- Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain B:




S234 L235 E236 E237 V238 K239 S240 D241 P242 D243 A244 A245 P246 A247 LEU GLN ASN LYS GLN LYS LYS GLY LYS SER ILE SER A260 W261 R262 S263 T264 R267 E270 M274 A275 L276 M279 F287 L288 T289 M290 L291 G296 V300 L315 S316 T325 R332 G333
F334 G335 D336 N337 S338 K339 T340 A341 N342 F343 K344 P348 L354 Y359 V360 S361 A362 V363 S364 P365 M366 V367 S368 T369 S370 K371 T372 M373 R374 Y375 I384 S388 N389 D390 Y391 V394 L397 G402 Q407 Q415 I419 T423 P434 V439 L440 L441
G442 G450 I451 V452 E453 P454 Q455 T456 S457 L465 N466 V467 Y468 M469 P470 Y471 T472 T473 R477 M478 L479 G480 Q481 A482 H483 V489 R490 I491 N492 D493 K494 Y495 S496 T497 S498 A499 A500 E501 V505 N506 L507 L508 B512 G513 A514 Q515 D516 I517 F518 T519 E530 S541
V545 I546 S547 L548 V549 V550 I553 M556 N557 I558 M559 L560 V563 T567 Q568 E569 R573 V576 G577 A578 D582 I583 L584 Q585 Q586 F587 V600 L601 S606 L609 G610 I613 F616 A617 A622 V623 A624 Y625 F634 V635 C636 L639 I640
F644 G645 P648 S662 R663 E664

4 Data and refinement statistics (i)

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 45.23 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.96-3.39) 99.2 (45.23-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.223 , 0.255 0.224 , 0.257	Depositor DCC
R_{free} test set	2909 reflections (5.07%)	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)	0.31 , 123.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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	0.28	0/4925	0.54	2/6643 (0.0%)
1	B	0.28	0/4925	0.54	1/6643 (0.0%)
All	All	0.28	0/9850	0.54	3/13286 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	440	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	440	LEU	CA-CB-CG	5.91	128.89	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4885	0	4973	109	0
1	B	4885	0	4973	105	0
All	All	9770	0	9946	208	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 (208) 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: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
1:B:556:MSE:HB2	1:B:644:PHE:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	1:B:517:ILE:O	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:91:GLY:C	1:B:92:PHE:HD1	2.13	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:A:91:GLY:C	1:A:92:PHE:HD1	2.14	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:A:606:SER:O	1:A:625:TYR:OH	2.25	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:505:VAL:O	1:A:509:THR:OG1	2.27	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: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:134:LEU:HD12	1:A:158:ALA:HB2	1.96	0.47
1:A:7:LEU:HB2	1:A:33:ILE:HB	1.95	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:B:473:THR:O	1:B:477:ARG:HB2	2.14	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:275:ALA:O	1:B:279:MSE:HG3	2.15	0.47
1:A:366:MSE:HB3	1:A:486:ASN:OD1	2.15	0.47
1:A:9:VAL:HG13	1:A:12:LEU:HD23	1.96	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:348:PRO:HB3	1:B:471:TYR:HE2	1.81	0.45
1:B:61:ARG:HD2	1:B:75:GLY:O	2.15	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: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:384:ILE:HD11	1:B:441:LEU:HB3	1.99	0.45
1:B:112:PRO:HB3	1:B:576:VAL:HG13	1.99	0.45
1:A:361:SER:N	1:A:492:ASN:HB2	2.32	0.44
1:A:5:ALA:HB1	1:A:34:TYR:HA	1.99	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: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:A:7:LEU:HD22	1:A:67:TYR:OH	2.18	0.43
1:B:118:VAL:HG13	1:B:123:ARG:HH11	1.84	0.43
1:A:360:VAL:CG1	1:A:363:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:110:GLU:HA	1:B:162:MSE:HE3	2.02	0.42
1:B:40:ALA:HA	1:B:201:LEU:O	2.20	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:297:ILE:HA	1:A:300:VAL:HG12	2.02	0.41
1:A:38:LEU:HB2	1:A:193:ASN:ND2	2.35	0.41
1:A:406:ASP:OD1	1:A:407:GLN:N	2.53	0.41
1:A:350:ASP:HA	1:A:511:ARG:NH1	2.35	0.41
1:A:559:MSE:O	1:A:563:VAL:HG23	2.21	0.41
1:A:332:ARG:HD3	1:B:505:VAL:HG21	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	537 (100%)	1 (0%)	93	98
1	B	538/536 (100%)	538 (100%)	0	100	100
All	All	1076/1072 (100%)	1075 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	193	ASN
1	A	330	GLN
1	B	153	GLN
1	B	193	ASN
1	B	512	HIS

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 carbohydrates 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	630/671 (93%)	0.70	72 (11%)	5 6	98, 144, 239, 333	0
1	B	630/671 (93%)	0.83	90 (14%)	2 3	109, 156, 255, 334	0
All	All	1260/1342 (93%)	0.77	162 (12%)	3 4	98, 150, 249, 334	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	12.2
1	A	261	TRP	10.2
1	A	243	ASP	10.2
1	A	244	ALA	8.5
1	A	239	LYS	8.5
1	B	242	PRO	7.7
1	B	235	LEU	7.4
1	B	247	ALA	7.2
1	B	261	TRP	7.2
1	A	664	GLU	7.2
1	B	457	SER	7.0
1	B	244	ALA	7.0
1	B	456	THR	6.9
1	B	260	ALA	6.8
1	A	240	SER	6.8
1	A	247	ALA	6.7
1	B	333	GLY	6.6
1	B	239	LYS	6.3
1	A	260	ALA	6.1
1	A	457	SER	5.9
1	B	455	GLN	5.5
1	A	622	ALA	5.3
1	B	237	GLU	5.2
1	A	621	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	5.0
1	B	62	PRO	5.0
1	B	341	ALA	4.9
1	A	324	ASN	4.9
1	B	246	PRO	4.8
1	B	240	SER	4.8
1	B	241	ASP	4.6
1	B	332	ARG	4.5
1	B	625	TYR	4.5
1	B	25	ILE	4.4
1	A	458	GLY	4.4
1	A	491	ILE	4.4
1	A	242	PRO	4.3
1	B	245	ALA	4.2
1	B	359	TYR	4.2
1	A	237	GLU	4.1
1	B	23	ILE	4.1
1	A	620	ASN	4.1
1	B	27	LYS	4.0
1	A	20	GLU	4.0
1	B	360	VAL	4.0
1	B	20	GLU	4.0
1	A	625	TYR	4.0
1	B	617	ALA	4.0
1	B	24	GLN	4.0
1	B	264	THR	3.8
1	B	26	LEU	3.8
1	A	246	PRO	3.8
1	A	623	VAL	3.8
1	B	496	SER	3.8
1	B	267	ARG	3.7
1	B	477	ARG	3.7
1	B	338	SER	3.7
1	B	18	ALA	3.7
1	B	363	VAL	3.7
1	A	456	THR	3.6
1	B	238	VAL	3.6
1	B	334	PHE	3.5
1	B	336	ASP	3.5
1	A	465	LEU	3.4
1	B	19	GLY	3.4
1	A	238	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	22	THR	3.4
1	A	374	ARG	3.4
1	A	616	PHE	3.4
1	B	236	GLU	3.4
1	A	441	LEU	3.4
1	A	235	LEU	3.3
1	A	326	ILE	3.3
1	A	461	SER	3.3
1	B	491	ILE	3.3
1	B	362	ALA	3.3
1	B	263	SER	3.3
1	B	340	THR	3.2
1	B	495	TYR	3.2
1	B	337	ASN	3.2
1	B	76	LYS	3.1
1	A	22	THR	3.1
1	B	136	LEU	3.1
1	A	18	ALA	3.0
1	B	623	VAL	3.0
1	B	483	HIS	3.0
1	B	342	ASN	3.0
1	B	234	SER	2.9
1	A	359	TYR	2.9
1	A	379	GLU	2.9
1	B	139	LYS	2.9
1	A	236	GLU	2.8
1	A	442	GLY	2.8
1	A	462	ASP	2.8
1	A	241	ASP	2.8
1	B	335	GLY	2.8
1	B	664	GLU	2.8
1	A	23	ILE	2.7
1	B	497	THR	2.7
1	B	440	LEU	2.7
1	A	76	LYS	2.7
1	A	603	VAL	2.7
1	A	453	GLU	2.7
1	B	394	VAL	2.7
1	A	619	GLY	2.6
1	A	136	LEU	2.6
1	B	585	GLN	2.6
1	B	12	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	455	GLN	2.6
1	A	497	THR	2.6
1	A	500	ALA	2.5
1	B	77	LEU	2.5
1	A	354	LEU	2.5
1	A	490	ARG	2.5
1	B	622	ALA	2.5
1	B	74	THR	2.5
1	A	382	ALA	2.5
1	B	58	CYS	2.5
1	A	662	SER	2.4
1	B	316	SER	2.4
1	A	262	ARG	2.4
1	A	494	LYS	2.4
1	B	584	LEU	2.4
1	A	493	ASP	2.4
1	B	452	VAL	2.4
1	A	325	THR	2.4
1	A	372	THR	2.4
1	B	339	LYS	2.4
1	A	595	CYS	2.4
1	A	338	SER	2.4
1	A	565	GLU	2.4
1	B	662	SER	2.3
1	B	29	ILE	2.3
1	A	394	VAL	2.3
1	B	453	GLU	2.3
1	B	372	THR	2.3
1	B	374	ARG	2.3
1	A	139	LYS	2.3
1	B	130	LEU	2.3
1	A	332	ARG	2.3
1	B	546	ILE	2.3
1	A	363	VAL	2.2
1	A	495	TYR	2.2
1	B	140	THR	2.2
1	B	344	LYS	2.2
1	B	13	VAL	2.2
1	B	616	PHE	2.2
1	A	362	ALA	2.2
1	A	17	PRO	2.1
1	B	343	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	615	LYS	2.1
1	B	441	LEU	2.1
1	A	21	SER	2.1
1	B	75	GLY	2.1
1	B	147	LEU	2.1
1	A	318	ILE	2.1
1	B	361	SER	2.1
1	B	465	LEU	2.0
1	A	141	GLN	2.0
1	B	105	ALA	2.0
1	B	451	ILE	2.0
1	A	440	LEU	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 carbohydrates 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.