



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:02 AM UTC

PDB ID : 5MKK / pdb_00005mkk
Title : Crystal structure of the heterodimeric ABC transporter TmrAB, a homolog of the antigen translocation complex TAP
Authors : Noell, A.; Thomas, C.; Tomasiak, T.M.; Olieric, V.; Wang, M.; Diederichs, K.; Stroud, R.M.; Pos, K.M.; Tampe, R.
Deposited on : 2016-12-05
Resolution : 2.70 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

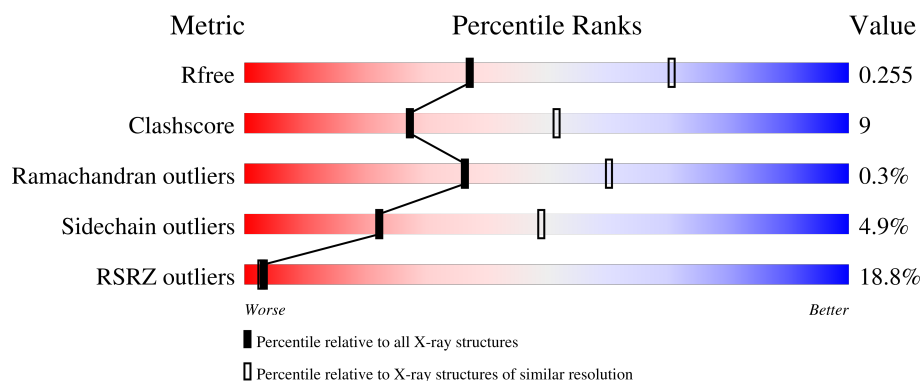
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	611	19% 72% 24% ..
2	B	577	18% 76% 23% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9311 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 Multidrug resistance ABC transporter ATP-binding and per-mease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4739	3085	824	822	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	601	LYS	-	expression tag	UNP Q72J05
A	602	LEU	-	expression tag	UNP Q72J05
A	603	GLY	-	expression tag	UNP Q72J05
A	604	GLY	-	expression tag	UNP Q72J05
A	605	GLY	-	expression tag	UNP Q72J05
A	606	GLY	-	expression tag	UNP Q72J05
A	607	GLU	-	expression tag	UNP Q72J05
A	608	ASN	-	expression tag	UNP Q72J05
A	609	LEU	-	expression tag	UNP Q72J05
A	610	TYR	-	expression tag	UNP Q72J05
A	611	PHE	-	expression tag	UNP Q72J05
A	612	GLN	-	expression tag	UNP Q72J05

- Molecule 2 is a protein called Multidrug resistance ABC transporter ATP-binding and per-mease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	577	Total	C	N	O	S	0	0	0
			4552	2939	815	786	12			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

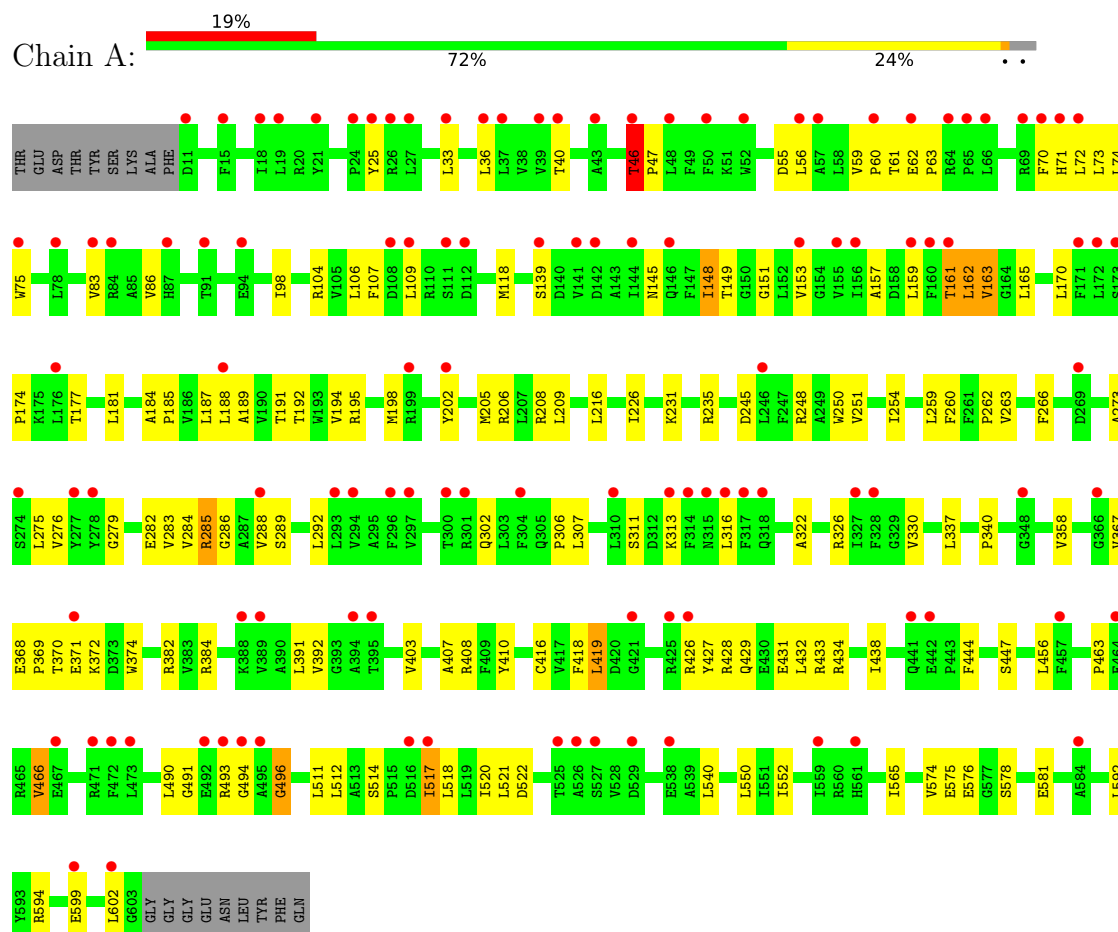
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	6	Total	O	0	0
			6	6		

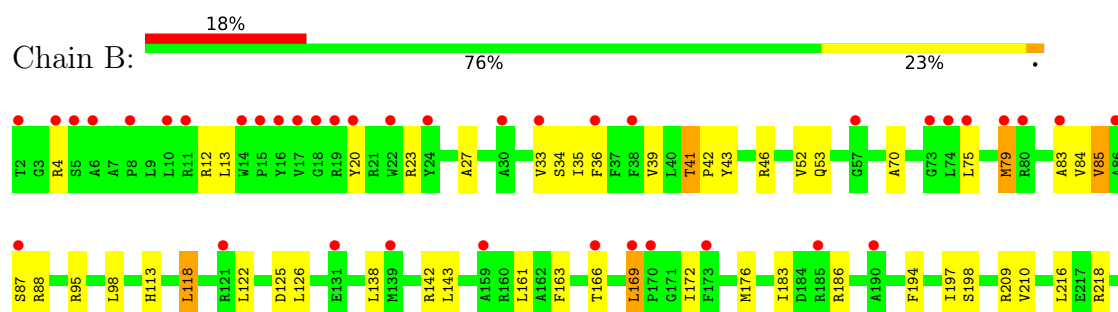
3 Residue-property plots

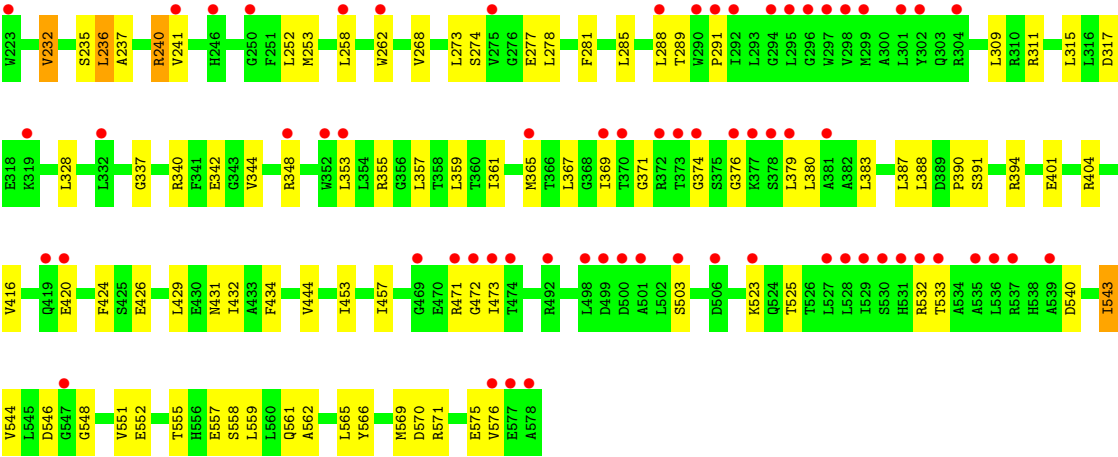
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein



- Molecule 2: Multidrug resistance ABC transporter ATP-binding and permease protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.37Å 93.37Å 1043.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.90 – 2.70 48.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.90-2.70) 100.0 (48.90-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.272 (Not available) , 0.255	Depositor DCC
R_{free} test set	4814 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9311	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.52	0/4843	0.88	8/6568 (0.1%)
2	B	0.51	0/4641	0.88	8/6282 (0.1%)
All	All	0.52	0/9484	0.88	16/12850 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LYS	N-CA-C	-7.59	104.92	114.56
2	B	420	GLU	CA-C-N	7.07	127.05	119.76
2	B	420	GLU	C-N-CA	7.07	127.05	119.76
1	A	496	GLY	N-CA-C	-5.97	107.59	114.69
2	B	41	THR	CA-C-N	-5.81	113.69	119.56
2	B	41	THR	C-N-CA	-5.81	113.69	119.56
1	A	46	THR	CA-C-N	-5.63	113.96	120.04
1	A	46	THR	C-N-CA	-5.63	113.96	120.04
2	B	355	ARG	N-CA-C	5.46	117.39	108.76
1	A	368	GLU	CA-C-N	5.37	125.29	119.76
1	A	368	GLU	C-N-CA	5.37	125.29	119.76
1	A	184	ALA	CA-C-N	-5.30	114.21	119.56
1	A	184	ALA	C-N-CA	-5.30	114.21	119.56
2	B	416	VAL	N-CA-C	5.23	115.49	108.17
2	B	387	LEU	N-CA-C	-5.13	105.86	111.82
2	B	548	GLY	N-CA-C	-5.10	108.29	114.92

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	4739	0	4868	92	0
2	B	4552	0	4716	95	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	4	0	0	0	0
4	B	6	0	0	0	0
All	All	9311	0	9584	171	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 9.

All (171) 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)
2:B:46:ARG:HD2	2:B:277:GLU:HG2	1.60	0.83
2:B:361:ILE:HG23	2:B:365:MET:HE2	1.63	0.81
1:A:514:SER:HB3	1:A:517:ILE:HG23	1.62	0.81
2:B:340:ARG:NH1	2:B:342:GLU:OE1	2.14	0.79
2:B:533:THR:HG21	2:B:570:ASP:HB2	1.62	0.79
1:A:208:ARG:HD3	1:A:245:ASP:HB3	1.65	0.79
2:B:143:LEU:HB3	2:B:291:PRO:HB3	1.66	0.77
1:A:371:GLU:HA	1:A:374:TRP:CD1	2.23	0.73
1:A:195:ARG:HH22	1:A:311:SER:HA	1.54	0.72
1:A:574:VAL:HG12	1:A:575:GLU:HG3	1.73	0.71
1:A:594:ARG:HG3	2:B:571:ARG:HH12	1.56	0.70
2:B:344:VAL:HG13	2:B:390:PRO:HB3	1.76	0.68
2:B:371:GLY:HA2	2:B:569:MET:HE1	1.75	0.68
2:B:13:LEU:HB2	2:B:309:LEU:HD21	1.77	0.66
2:B:186:ARG:HE	2:B:237:ALA:HB1	1.61	0.66
1:A:578:SER:HB3	1:A:581:GLU:HG3	1.79	0.65
2:B:41:THR:HG23	2:B:42:PRO:HD3	1.79	0.65
1:A:98:ILE:HD13	1:A:153:VAL:HG11	1.77	0.65
1:A:599:GLU:HG3	2:B:565:LEU:HD11	1.78	0.65
1:A:151:GLY:HA2	1:A:313:LYS:HD2	1.80	0.64
1:A:282:GLU:OE2	1:A:285:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:O	1:A:191:THR:HG23	1.98	0.62
1:A:118:MET:HA	1:A:118:MET:HE2	1.81	0.62
2:B:374:GLY:N	3:B:601:SO4:O4	2.31	0.62
1:A:410:TYR:OH	2:B:209:ARG:NH2	2.34	0.61
1:A:106:LEU:HD13	1:A:145:ASN:HB2	1.83	0.60
1:A:148:ILE:HG13	1:A:149:THR:HG23	1.82	0.60
1:A:40:THR:HG22	1:A:161:THR:HG22	1.83	0.60
1:A:521:LEU:HD13	1:A:540:LEU:HD13	1.84	0.60
1:A:434:ARG:HH22	2:B:218:ARG:HH22	1.49	0.60
2:B:533:THR:HG23	2:B:566:TYR:CZ	2.36	0.59
1:A:70:PHE:O	1:A:74:LEU:HB3	2.04	0.58
2:B:84:VAL:O	2:B:87:SER:OG	2.22	0.58
1:A:170:LEU:HG	1:A:177:THR:HG21	1.86	0.58
2:B:285:LEU:O	2:B:289:THR:HG23	2.03	0.58
2:B:359:LEU:HD22	2:B:543:ILE:HD12	1.85	0.58
1:A:391:LEU:HD11	1:A:550:LEU:HD23	1.86	0.57
2:B:348:ARG:HH21	2:B:388:LEU:HD22	1.70	0.57
1:A:25:TYR:CZ	1:A:104:ARG:HB3	2.41	0.56
1:A:273:ALA:HA	1:A:276:VAL:HG12	1.88	0.55
1:A:283:VAL:HG11	2:B:52:VAL:HG13	1.87	0.55
1:A:447:SER:HA	1:A:490:LEU:O	2.07	0.55
1:A:284:VAL:C	1:A:286:GLY:H	2.15	0.55
2:B:172:ILE:HD13	2:B:253:MET:SD	2.45	0.55
2:B:471:ARG:O	2:B:473:ILE:N	2.34	0.55
2:B:183:ILE:HG22	2:B:241:VAL:HG12	1.88	0.55
2:B:43:TYR:HE1	2:B:46:ARG:HH11	1.55	0.55
1:A:407:ALA:O	1:A:433:ARG:HD3	2.06	0.54
2:B:503:SER:O	2:B:532:ARG:NH2	2.41	0.54
2:B:169:LEU:HD21	2:B:288:LEU:HD21	1.89	0.54
1:A:55:ASP:O	1:A:56:LEU:HD23	2.07	0.54
1:A:107:PHE:HB2	2:B:232:VAL:HG21	1.88	0.54
1:A:198:MET:HE3	1:A:202:TYR:HE2	1.72	0.53
1:A:194:VAL:HG21	1:A:260:PHE:HD1	1.73	0.53
2:B:365:MET:HE3	2:B:367:LEU:HB2	1.90	0.53
1:A:463:PRO:HA	1:A:466:VAL:HG13	1.90	0.53
2:B:83:ALA:HB3	2:B:138:LEU:HD11	1.91	0.53
2:B:337:GLY:O	2:B:525:THR:OG1	2.21	0.53
1:A:181:LEU:O	1:A:185:PRO:HD3	2.09	0.52
2:B:328:LEU:HD21	2:B:404:ARG:NH2	2.24	0.52
1:A:61:THR:C	1:A:63:PRO:HD3	2.34	0.52
1:A:511:LEU:HD23	1:A:517:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ARG:HB2	2:B:126:LEU:HD21	1.91	0.52
2:B:118:LEU:O	2:B:122:LEU:HB2	2.09	0.52
2:B:394:ARG:NH1	2:B:401:GLU:HG2	2.25	0.52
2:B:394:ARG:HH11	2:B:401:GLU:HG2	1.75	0.52
2:B:544:VAL:HB	2:B:552:GLU:HB3	1.91	0.52
2:B:376:GLY:HA2	2:B:379:LEU:HD23	1.92	0.51
1:A:428:ARG:NH1	1:A:431:GLU:OE1	2.39	0.51
1:A:494:GLY:O	1:A:496:GLY:N	2.37	0.51
2:B:348:ARG:HB2	2:B:353:LEU:HD11	1.92	0.51
1:A:382:ARG:HH22	1:A:384:ARG:HG2	1.76	0.50
1:A:56:LEU:HD13	1:A:72:LEU:HD13	1.93	0.50
2:B:253:MET:HE2	2:B:289:THR:HG22	1.92	0.50
1:A:408:ARG:O	1:A:433:ARG:NH1	2.45	0.50
1:A:36:LEU:HD21	1:A:157:ALA:HA	1.94	0.50
1:A:444:PHE:HB3	2:B:210:VAL:HG21	1.94	0.50
2:B:27:ALA:HB1	2:B:83:ALA:HB2	1.93	0.49
1:A:61:THR:HG22	1:A:62:GLU:N	2.27	0.49
1:A:522:ASP:OD2	1:A:552:ILE:HD12	2.13	0.49
2:B:533:THR:HG21	2:B:570:ASP:CB	2.38	0.49
2:B:544:VAL:HG21	2:B:566:TYR:HB2	1.95	0.48
2:B:163:PHE:HA	2:B:166:THR:HG22	1.93	0.48
1:A:419:LEU:HD22	1:A:432:LEU:HD11	1.94	0.48
2:B:161:LEU:HD23	2:B:281:PHE:CE2	2.48	0.48
1:A:162:LEU:HD11	1:A:307:LEU:HD12	1.94	0.48
1:A:205:MET:HE1	1:A:209:LEU:HD22	1.95	0.48
1:A:174:PRO:HA	1:A:177:THR:HG22	1.95	0.48
1:A:226:ILE:HD13	1:A:235:ARG:HG3	1.95	0.48
1:A:245:ASP:OD1	1:A:248:ARG:NH1	2.46	0.47
1:A:205:MET:HE2	1:A:209:LEU:HB2	1.96	0.47
2:B:571:ARG:O	2:B:575:GLU:HB2	2.13	0.47
1:A:205:MET:HE3	1:A:250:TRP:CZ2	2.49	0.47
1:A:466:VAL:HB	1:A:512:LEU:HD11	1.97	0.47
1:A:250:TRP:HB3	2:B:88:ARG:HG3	1.97	0.47
2:B:559:LEU:HB3	2:B:566:TYR:CD2	2.48	0.47
2:B:559:LEU:HD23	2:B:559:LEU:HA	1.80	0.47
1:A:514:SER:O	1:A:517:ILE:HG12	2.15	0.47
2:B:429:LEU:HD12	2:B:444:VAL:HG11	1.97	0.47
1:A:340:PRO:HG3	1:A:426:ARG:HA	1.97	0.46
1:A:46:THR:HG22	1:A:47:PRO:HD3	1.96	0.46
1:A:266:PHE:HE1	2:B:70:ALA:HB2	1.81	0.46
2:B:33:VAL:HG12	2:B:75:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:MET:HG3	2:B:289:THR:CG2	2.45	0.46
2:B:39:VAL:O	2:B:42:PRO:HD2	2.15	0.46
2:B:253:MET:HG3	2:B:289:THR:HG22	1.97	0.46
1:A:288:VAL:HB	1:A:292:LEU:HD22	1.98	0.46
1:A:594:ARG:HG3	2:B:571:ARG:NH1	2.28	0.46
2:B:431:ASN:O	2:B:434:PHE:HB2	2.15	0.46
1:A:61:THR:O	1:A:63:PRO:HD3	2.16	0.45
1:A:74:LEU:HD13	2:B:262:TRP:CZ2	2.51	0.45
2:B:79:MET:HE1	2:B:142:ARG:HD2	1.98	0.45
1:A:159:LEU:O	1:A:163:VAL:HG13	2.16	0.45
2:B:176:MET:HA	2:B:176:MET:HE2	1.97	0.45
2:B:41:THR:CG2	2:B:42:PRO:HD3	2.47	0.45
2:B:98:LEU:HD13	2:B:122:LEU:HD11	1.98	0.45
2:B:125:ASP:OD1	2:B:311:ARG:NH2	2.47	0.45
1:A:157:ALA:O	1:A:161:THR:HG23	2.17	0.45
1:A:74:LEU:HG	1:A:75:TRP:HD1	1.82	0.44
1:A:216:LEU:HD21	2:B:122:LEU:HD23	1.98	0.44
2:B:113:HIS:HB3	2:B:118:LEU:HD22	2.00	0.44
2:B:453:ILE:HG13	2:B:457:ILE:HG13	2.00	0.44
1:A:367:VAL:O	1:A:369:PRO:HD3	2.18	0.44
2:B:546:ASP:HB2	2:B:551:VAL:HG11	1.99	0.44
1:A:456:LEU:HD22	2:B:216:LEU:HD11	1.99	0.44
2:B:432:ILE:HG21	2:B:444:VAL:HG13	2.00	0.44
2:B:12:ARG:HH22	2:B:317:ASP:CG	2.26	0.44
1:A:189:ALA:O	1:A:192:THR:HG22	2.17	0.44
2:B:424:PHE:O	2:B:426:GLU:N	2.47	0.43
2:B:561:GLN:O	2:B:562:ALA:HB3	2.18	0.43
1:A:565:ILE:O	1:A:576:GLU:HA	2.18	0.43
1:A:494:GLY:C	1:A:496:GLY:H	2.25	0.43
2:B:236:LEU:O	2:B:240:ARG:HD3	2.18	0.43
1:A:403:VAL:HG13	1:A:520:ILE:HG21	2.00	0.43
2:B:555:THR:HG23	2:B:558:SER:H	1.84	0.43
2:B:23:ARG:NH1	2:B:85:VAL:HG12	2.33	0.42
2:B:172:ILE:HG12	2:B:252:LEU:HB3	2.00	0.42
2:B:194:PHE:O	2:B:197:ILE:HG22	2.20	0.42
1:A:231:LYS:HG2	2:B:434:PHE:CZ	2.54	0.42
2:B:557:GLU:C	2:B:559:LEU:H	2.27	0.42
1:A:61:THR:HG22	1:A:62:GLU:H	1.85	0.42
1:A:251:VAL:HG22	2:B:85:VAL:HG22	2.02	0.42
1:A:322:ALA:HB1	1:A:326:ARG:HH12	1.84	0.42
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:HD3	2:B:88:ARG:HA	1.86	0.41
1:A:370:THR:O	1:A:371:GLU:HB2	2.20	0.41
2:B:344:VAL:HG11	2:B:383:LEU:HD13	2.02	0.41
1:A:275:LEU:O	1:A:279:GLY:HA3	2.20	0.41
1:A:602:LEU:O	2:B:551:VAL:HG21	2.21	0.41
1:A:427:TYR:CD2	1:A:432:LEU:HD13	2.56	0.41
2:B:23:ARG:HH11	2:B:85:VAL:HG12	1.86	0.41
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.88	0.41
1:A:429:GLN:OE1	1:A:433:ARG:NH2	2.52	0.41
2:B:35:ILE:HD13	2:B:35:ILE:HA	1.76	0.41
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.84	0.41
1:A:151:GLY:HA3	1:A:316:LEU:HD23	2.02	0.41
1:A:491:GLY:C	1:A:493:ARG:H	2.29	0.41
2:B:33:VAL:O	2:B:36:PHE:HB3	2.21	0.41
2:B:274:SER:OG	2:B:277:GLU:HG3	2.21	0.41
2:B:361:ILE:HG12	2:B:367:LEU:HD22	2.03	0.41
2:B:533:THR:HG23	2:B:566:TYR:OH	2.20	0.41
2:B:348:ARG:HD3	2:B:348:ARG:HA	1.79	0.40
1:A:162:LEU:HD12	1:A:306:PRO:HB2	2.03	0.40
2:B:98:LEU:HD22	2:B:315:LEU:HD23	2.02	0.40
1:A:165:LEU:HD21	1:A:302:GLN:OE1	2.21	0.40
1:A:416:CYS:HB2	1:A:418:PHE:CE1	2.56	0.40
2:B:20:TYR:HB3	2:B:23:ARG:HH21	1.85	0.40
2:B:268:VAL:HA	2:B:273:LEU:O	2.22	0.40
2:B:383:LEU:HD22	2:B:390:PRO:HD3	2.03	0.40
1:A:259:LEU:C	1:A:262:PRO:HD2	2.46	0.40
1:A:382:ARG:NH2	1:A:384:ARG:HG2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	591/611 (97%)	559 (95%)	30 (5%)	2 (0%)	36 60
2	B	575/577 (100%)	534 (93%)	39 (7%)	2 (0%)	36 60
All	All	1166/1188 (98%)	1093 (94%)	69 (6%)	4 (0%)	36 60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ARG
2	B	576	VAL
2	B	472	GLY
1	A	60	PRO

5.3.2 Protein sidechains ⓘ

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	495/510 (97%)	469 (95%)	26 (5%)	20 46
2	B	463/463 (100%)	442 (96%)	21 (4%)	24 52
All	All	958/973 (98%)	911 (95%)	47 (5%)	22 49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	46	THR
1	A	59	VAL
1	A	71	HIS
1	A	83	VAL
1	A	86	VAL
1	A	109	LEU
1	A	139	SER
1	A	148	ILE
1	A	161	THR
1	A	162	LEU
1	A	163	VAL

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	206	ARG
1	A	263	VAL
1	A	289	SER
1	A	330	VAL
1	A	337	LEU
1	A	358	VAL
1	A	392	VAL
1	A	419	LEU
1	A	438	ILE
1	A	466	VAL
1	A	517	ILE
1	A	518	LEU
1	A	592	LEU
2	B	4	ARG
2	B	34	SER
2	B	53	GLN
2	B	79	MET
2	B	85	VAL
2	B	118	LEU
2	B	169	LEU
2	B	198	SER
2	B	232	VAL
2	B	235	SER
2	B	236	LEU
2	B	240	ARG
2	B	258	LEU
2	B	278	LEU
2	B	357	LEU
2	B	369	ILE
2	B	380	LEU
2	B	391	SER
2	B	523	LYS
2	B	540	ASP
2	B	543	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN
2	B	303	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	701	-	4,4,4	0.30	0	6,6,6	0.34	0
3	SO4	B	601	-	4,4,4	0.29	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	SO4	1	0

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	593/611 (97%)	0.99	115 (19%) 3 2	63, 103, 161, 227	0
2	B	577/577 (100%)	0.91	105 (18%) 3 3	63, 102, 149, 210	0
All	All	1170/1188 (98%)	0.95	220 (18%) 3 3	63, 102, 154, 227	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	499	ASP	9.4
2	B	297	TRP	9.0
2	B	378	SER	7.6
2	B	578	ALA	7.2
2	B	577	GLU	6.6
1	A	57	ALA	6.6
1	A	172	LEU	6.1
2	B	2	THR	6.1
2	B	419	GLN	5.9
2	B	536	LEU	5.6
1	A	310	LEU	5.6
1	A	442	GLU	5.4
1	A	142	ASP	5.4
2	B	529	ILE	5.4
1	A	171	PHE	5.4
2	B	420	GLU	5.2
2	B	528	LEU	5.2
1	A	421	GLY	5.0
2	B	294	GLY	5.0
2	B	14	TRP	5.0
1	A	25	TYR	4.9
2	B	83	ALA	4.9
2	B	381	ALA	4.9
2	B	469	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	173	PHE	4.9
2	B	473	ILE	4.8
1	A	495	ALA	4.7
1	A	274	SER	4.7
1	A	146	GLN	4.7
2	B	576	VAL	4.7
1	A	471	ARG	4.6
1	A	559	ILE	4.5
1	A	278	TYR	4.5
1	A	153	VAL	4.4
1	A	313	LYS	4.4
1	A	69	ARG	4.3
1	A	21	TYR	4.3
1	A	64	ARG	4.2
1	A	24	PRO	4.2
1	A	75	TRP	4.2
1	A	314	PHE	4.2
1	A	304	PHE	4.1
1	A	141	VAL	4.1
1	A	538	GLU	4.0
2	B	527	LEU	4.0
2	B	500	ASP	4.0
1	A	70	PHE	4.0
1	A	84	ARG	4.0
2	B	33	VAL	4.0
2	B	295	LEU	3.9
1	A	315	ASN	3.9
1	A	111	SER	3.9
1	A	441	GLN	3.9
2	B	74	LEU	3.9
2	B	376	GLY	3.9
1	A	301	ARG	3.8
2	B	372	ARG	3.7
1	A	66	LEU	3.7
2	B	10	LEU	3.7
2	B	353	LEU	3.7
2	B	262	TRP	3.7
1	A	317	PHE	3.7
1	A	395	THR	3.6
1	A	108	ASP	3.5
1	A	160	PHE	3.5
1	A	472	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	3.5
2	B	373	THR	3.5
2	B	474	THR	3.4
1	A	39	VAL	3.4
1	A	83	VAL	3.4
1	A	18	ILE	3.3
2	B	75	LEU	3.3
1	A	602	LEU	3.3
2	B	241	VAL	3.3
1	A	71	HIS	3.3
2	B	530	SER	3.3
2	B	57	GLY	3.3
1	A	328	PHE	3.3
1	A	56	LEU	3.2
1	A	72	LEU	3.2
1	A	493	ARG	3.2
2	B	258	LEU	3.2
2	B	503	SER	3.2
2	B	6	ALA	3.2
2	B	535	ALA	3.2
1	A	112	ASP	3.2
2	B	139	MET	3.2
1	A	526	ALA	3.2
1	A	371	GLU	3.2
1	A	46	THR	3.2
2	B	319	LYS	3.1
2	B	80	ARG	3.1
1	A	516	ASP	3.1
1	A	78	LEU	3.1
1	A	155	VAL	3.1
2	B	472	GLY	3.1
2	B	170	PRO	3.0
2	B	370	THR	3.0
2	B	159	ALA	3.0
2	B	532	ARG	3.0
2	B	301	LEU	3.0
1	A	91	THR	3.0
2	B	290	TRP	3.0
2	B	79	MET	3.0
1	A	87	HIS	3.0
2	B	298	VAL	3.0
2	B	537	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	65	PRO	2.9
1	A	199	ARG	2.9
2	B	250	GLY	2.9
1	A	300	THR	2.9
2	B	30	ALA	2.9
2	B	377	LYS	2.9
2	B	374	GLY	2.9
2	B	121	ARG	2.8
1	A	156	ILE	2.8
1	A	36	LEU	2.8
2	B	166	THR	2.8
1	A	388	LYS	2.8
2	B	190	ALA	2.8
2	B	5	SER	2.7
2	B	22	TRP	2.7
2	B	539	ALA	2.7
1	A	188	LEU	2.7
2	B	291	PRO	2.7
2	B	292	ILE	2.7
1	A	426	ARG	2.7
2	B	547	GLY	2.7
1	A	173	SER	2.7
1	A	297	VAL	2.7
1	A	40	THR	2.7
1	A	139	SER	2.6
1	A	464	GLU	2.6
2	B	533	THR	2.6
1	A	109	LEU	2.6
2	B	131	GLU	2.6
2	B	17	VAL	2.6
2	B	288	LEU	2.5
1	A	60	PRO	2.5
2	B	36	PHE	2.5
2	B	185	ARG	2.5
2	B	379	LEU	2.5
2	B	18	GLY	2.5
2	B	352	TRP	2.5
2	B	506	ASP	2.5
1	A	527	SER	2.5
2	B	492	ARG	2.5
1	A	529	ASP	2.5
1	A	176	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	467	GLU	2.4
1	A	202	TYR	2.4
1	A	37	LEU	2.4
2	B	246	HIS	2.4
1	A	15	PHE	2.4
2	B	299	MET	2.4
1	A	366	GLY	2.4
2	B	275	VAL	2.4
1	A	277	TYR	2.4
2	B	348	ARG	2.4
1	A	269	ASP	2.4
1	A	318	GLN	2.4
2	B	304	ARG	2.4
1	A	457	PHE	2.4
1	A	327	ILE	2.3
2	B	223	TRP	2.3
2	B	11	ARG	2.3
2	B	24	TYR	2.3
1	A	561	HIS	2.3
1	A	296	PHE	2.3
1	A	525	THR	2.3
2	B	15	PRO	2.3
2	B	19	ARG	2.3
1	A	494	GLY	2.3
1	A	19	LEU	2.3
1	A	394	ALA	2.3
2	B	531	HIS	2.3
1	A	492	GLU	2.3
2	B	4	ARG	2.3
2	B	87	SER	2.3
1	A	159	LEU	2.3
1	A	517	ILE	2.2
1	A	246	LEU	2.2
2	B	498	LEU	2.2
1	A	599	GLU	2.2
2	B	302	TYR	2.2
2	B	471	ARG	2.2
1	A	11	ASP	2.2
1	A	62	GLU	2.2
2	B	8	PRO	2.2
1	A	48	LEU	2.2
2	B	523	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	33	LEU	2.2
1	A	473	LEU	2.2
1	A	288	VAL	2.2
1	A	50	PHE	2.2
2	B	38	PHE	2.2
2	B	20	TYR	2.1
1	A	293	LEU	2.1
1	A	144	ILE	2.1
2	B	369	ILE	2.1
1	A	584	ALA	2.1
2	B	86	ALA	2.1
1	A	348	GLY	2.1
2	B	16	TYR	2.1
1	A	425	ARG	2.1
2	B	169	LEU	2.1
2	B	332	LEU	2.1
2	B	73	GLY	2.1
1	A	389	VAL	2.1
1	A	94	GLU	2.0
2	B	501	ALA	2.0
1	A	52	TRP	2.0
1	A	161	THR	2.0
1	A	27	LEU	2.0
1	A	294	VAL	2.0
1	A	26	ARG	2.0
1	A	43	ALA	2.0
2	B	365	MET	2.0
2	B	296	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	601	5/5	0.86	0.31	96,100,109,114	0
3	SO4	A	701	5/5	0.92	0.11	72,78,85,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.