



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 02:10 PM JST

PDB ID : 8Z1U / pdb_00008z1u
Title : Crystal structure of aminoglycoside efflux transporter MexY from *Pseudomonas aeruginosa*
Authors : Murakami, S.; Yamashita, E.; Okada, U.; Aoki, M.
Deposited on : 2024-04-12
Resolution : 2.89 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

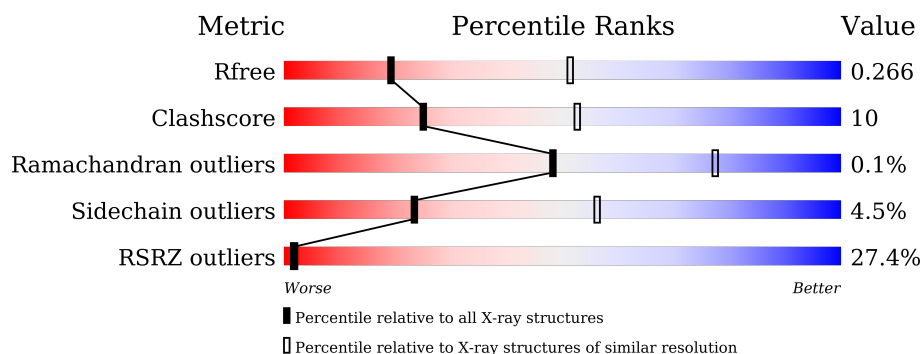
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	1054	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7938 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.

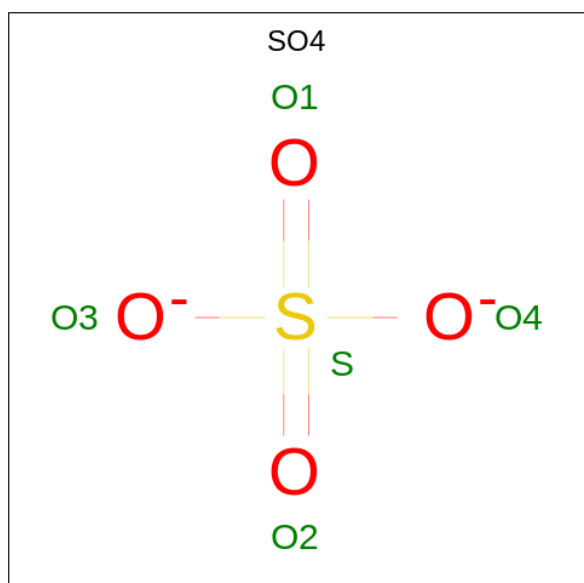
- Molecule 1 is a protein called Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1027	7798	5008	1335	1420	35	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1046	HIS	-	expression tag	UNP Q9RG59
A	1047	HIS	-	expression tag	UNP Q9RG59
A	1048	HIS	-	expression tag	UNP Q9RG59
A	1049	HIS	-	expression tag	UNP Q9RG59
A	1050	HIS	-	expression tag	UNP Q9RG59
A	1051	HIS	-	expression tag	UNP Q9RG59
A	1052	HIS	-	expression tag	UNP Q9RG59
A	1053	HIS	-	expression tag	UNP Q9RG59
A	1054	HIS	-	expression tag	UNP Q9RG59

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

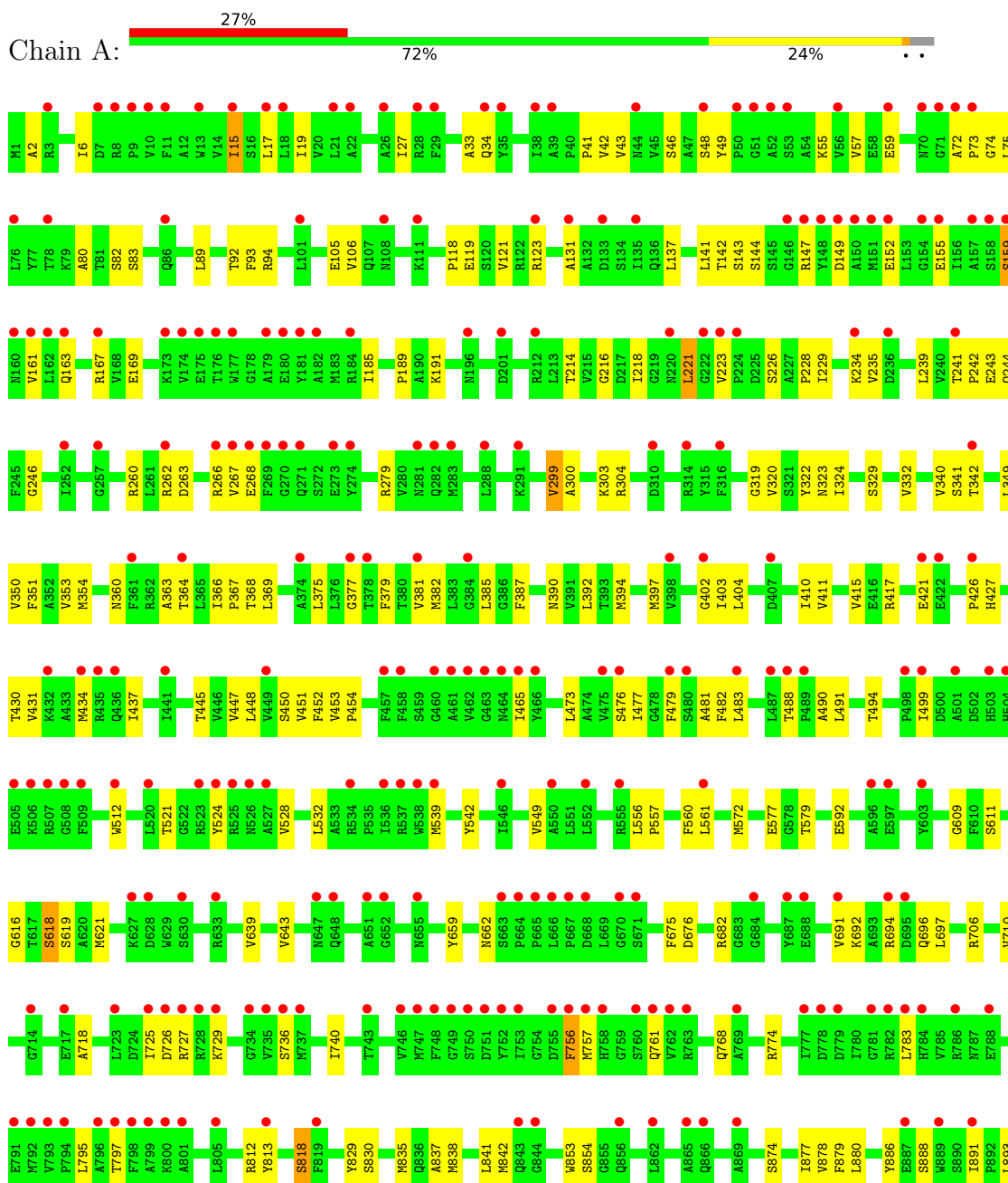
- Molecule 3 is water.

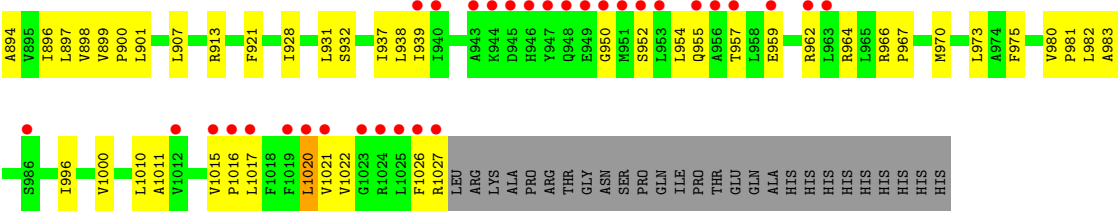
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		

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: Efflux pump membrane transporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.43Å 186.43Å 374.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	161.45 – 2.89 161.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.2 (161.45-2.89) 94.6 (161.45-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.253 , 0.270 0.244 , 0.266	Depositor DCC
R_{free} test set	4061 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7938	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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	0.17	0/7949	0.36	0/10807

There are no bond length outliers.

There are no bond angle outliers.

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	7798	0	7972	152	0
2	A	55	0	0	2	0
3	A	85	0	0	2	0
All	All	7938	0	7972	152	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 10.

All (152) 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:A:959:GLU:HG2	1:A:962:ARG:HH21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:THR:HG21	1:A:1020:LEU:HD21	1.72	0.71
1:A:72:ALA:HB3	1:A:75:LEU:HB2	1.71	0.71
1:A:141:LEU:HD11	1:A:161:VAL:HG21	1.77	0.67
1:A:415:VAL:HG22	1:A:430:THR:HA	1.75	0.66
1:A:697:LEU:HD21	1:A:838:MET:HE1	1.77	0.66
1:A:42:VAL:HB	1:A:131:ALA:HB3	1.78	0.66
1:A:80:ALA:HB3	1:A:812:ARG:HB2	1.77	0.66
1:A:579:THR:HB	1:A:618:SER:HB3	1.78	0.66
1:A:43:VAL:HG11	1:A:106:VAL:HG21	1.78	0.66
1:A:375:LEU:HD13	1:A:397:MET:HE3	1.78	0.64
1:A:239:LEU:HD22	1:A:244:GLN:HB3	1.79	0.63
1:A:74:GLY:O	1:A:94:ARG:N	2.26	0.62
1:A:144:SER:HB3	1:A:319:GLY:HA2	1.82	0.62
1:A:34:GLN:HB2	1:A:332:VAL:HG22	1.82	0.62
1:A:366:ILE:HD12	1:A:491:LEU:HB3	1.82	0.61
1:A:886:TYR:HD1	1:A:891:ILE:HG21	1.65	0.61
1:A:725:ILE:O	1:A:761:GLN:HA	2.01	0.60
1:A:279:ARG:NH1	1:A:592:GLU:OE2	2.34	0.60
1:A:410:ILE:HG22	1:A:437:ILE:HD12	1.83	0.59
1:A:757:MET:HG3	1:A:761:GLN:O	2.03	0.59
1:A:351:PHE:HD1	1:A:368:THR:HG21	1.67	0.59
1:A:445:THR:HG21	1:A:481:ALA:HB2	1.83	0.59
1:A:404:LEU:HD21	1:A:476:SER:HB2	1.85	0.59
1:A:379:PHE:HA	1:A:382:MET:HE2	1.85	0.58
1:A:727:ARG:O	1:A:729:LYS:N	2.36	0.58
1:A:879:PHE:HD2	1:A:896:ILE:HG13	1.68	0.58
1:A:74:GLY:HA2	1:A:94:ARG:CZ	2.34	0.58
1:A:149:ASP:HB2	1:A:152:GLU:HB3	1.84	0.58
1:A:385:LEU:HB3	1:A:387:PHE:HE2	1.69	0.58
1:A:385:LEU:HB3	1:A:387:PHE:CE2	2.39	0.58
1:A:966:ARG:O	1:A:970:MET:HG2	2.03	0.58
1:A:692:LYS:NZ	3:A:1201:HOH:O	2.36	0.57
1:A:322:TYR:C	1:A:323:ASN:HD22	2.12	0.57
1:A:379:PHE:HZ	1:A:394:MET:HE1	1.70	0.57
1:A:266:ARG:NE	1:A:268:GLU:OE2	2.38	0.56
1:A:403:ILE:HG12	1:A:931:LEU:HD21	1.86	0.56
1:A:528:VAL:HG22	1:A:532:LEU:HD11	1.88	0.56
1:A:879:PHE:CD2	1:A:896:ILE:HG13	2.40	0.56
1:A:451:VAL:HA	1:A:877:ILE:HD11	1.87	0.55
1:A:675:PHE:HZ	1:A:710:VAL:HG22	1.71	0.55
1:A:59:GLU:HG3	1:A:756:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:O	1:A:532:LEU:HD12	2.07	0.54
1:A:73:PRO:HD3	1:A:105:GLU:HG2	1.88	0.54
1:A:490:ALA:O	1:A:494:THR:HG22	2.08	0.53
1:A:894:ALA:HB2	1:A:1022:VAL:HG21	1.90	0.53
1:A:901:LEU:HD12	1:A:1010:LEU:HD23	1.90	0.53
1:A:342:THR:HG23	1:A:981:PRO:HB2	1.90	0.53
1:A:366:ILE:HG22	1:A:488:THR:HG22	1.90	0.52
1:A:234:LYS:NZ	2:A:1110:SO4:O2	2.43	0.52
1:A:41:PRO:HG2	1:A:93:PHE:HB2	1.92	0.51
1:A:143:SER:HB2	1:A:147:ARG:HB3	1.92	0.51
1:A:893:LEU:O	1:A:897:LEU:HD23	2.10	0.51
1:A:2:ALA:O	1:A:6:ILE:HG13	2.11	0.50
1:A:59:GLU:HG3	1:A:756:PHE:CZ	2.46	0.50
1:A:119:GLU:O	1:A:123:ARG:HG3	2.11	0.50
1:A:542:TYR:CE2	1:A:897:LEU:HD12	2.47	0.50
1:A:169:GLU:O	1:A:304:ARG:NH1	2.43	0.50
1:A:260:ARG:NH1	2:A:1106:SO4:O1	2.45	0.50
1:A:898:VAL:HG13	1:A:932:SER:HB3	1.94	0.50
1:A:1022:VAL:O	1:A:1026:PHE:HB2	2.11	0.50
1:A:1011:ALA:O	1:A:1015:VAL:HG22	2.12	0.49
1:A:556:LEU:HD12	1:A:557:PRO:HD2	1.95	0.49
1:A:185:ILE:HB	1:A:229:ILE:HB	1.94	0.49
1:A:966:ARG:HB3	1:A:967:PRO:HD3	1.95	0.49
1:A:218:ILE:HG22	1:A:774:ARG:HA	1.95	0.48
1:A:682:ARG:NH2	3:A:1203:HOH:O	2.45	0.48
1:A:950:GLY:HA3	1:A:1027:ARG:HD2	1.94	0.48
1:A:448:LEU:HB3	1:A:477:ILE:HD13	1.96	0.48
1:A:572:MET:HB2	1:A:659:TYR:HB3	1.95	0.48
1:A:223:VAL:HG12	1:A:223:VAL:O	2.13	0.48
1:A:426:PRO:O	1:A:430:THR:HG23	2.12	0.48
1:A:609:GLY:HA2	1:A:616:GLY:O	2.12	0.48
1:A:842:MET:HB3	1:A:842:MET:HE3	1.72	0.48
1:A:1015:VAL:N	1:A:1016:PRO:HD2	2.29	0.48
1:A:216:GLY:O	1:A:228:PRO:HA	2.13	0.48
1:A:560:PHE:O	1:A:561:LEU:HD23	2.14	0.48
1:A:430:THR:O	1:A:434:MET:HG2	2.14	0.47
1:A:447:VAL:HG12	1:A:878:VAL:HG13	1.96	0.47
1:A:33:ALA:O	1:A:390:ASN:HA	2.14	0.47
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.74	0.47
1:A:73:PRO:HD2	1:A:93:PHE:HE2	1.80	0.47
1:A:353:VAL:HG11	1:A:973:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:VAL:HG13	1:A:694:ARG:NH2	2.30	0.47
1:A:736:SER:O	1:A:740:ILE:HG13	2.15	0.47
1:A:300:ALA:O	1:A:304:ARG:HG3	2.14	0.46
1:A:450:SER:O	1:A:453:VAL:HG22	2.15	0.46
1:A:49:TYR:HB3	1:A:57:VAL:HG22	1.98	0.46
1:A:706:ARG:HG2	1:A:829:TYR:CE1	2.51	0.46
1:A:377:GLY:O	1:A:381:VAL:HG23	2.16	0.46
1:A:360:ASN:OD1	1:A:363:ALA:HB3	2.16	0.46
1:A:835:MET:HE3	1:A:853:TRP:CE2	2.50	0.45
1:A:155:GLU:O	1:A:159:SER:HB2	2.15	0.45
1:A:1017:LEU:O	1:A:1021:VAL:HG23	2.16	0.45
1:A:189:PRO:HG3	1:A:221:LEU:HB2	1.99	0.45
1:A:939:ILE:HG22	1:A:964:ARG:HB2	1.99	0.45
1:A:427:HIS:O	1:A:431:VAL:HG23	2.16	0.45
1:A:15:ILE:O	1:A:19:ILE:HG12	2.17	0.45
1:A:448:LEU:HD21	1:A:931:LEU:HD23	1.99	0.44
1:A:639:VAL:O	1:A:643:VAL:HG13	2.17	0.44
1:A:147:ARG:HG2	1:A:320:VAL:HG23	1.99	0.44
1:A:964:ARG:C	1:A:967:PRO:HD2	2.42	0.44
1:A:402:GLY:HA3	1:A:975:PHE:HA	1.99	0.44
1:A:907:LEU:HD23	1:A:921:PHE:HZ	1.82	0.44
1:A:411:VAL:HG12	1:A:437:ILE:HD11	1.99	0.44
1:A:512:TRP:CD1	1:A:512:TRP:C	2.96	0.44
1:A:452:PHE:CE2	1:A:473:LEU:HD23	2.52	0.43
1:A:42:VAL:HG22	1:A:92:THR:HG23	1.99	0.43
1:A:137:LEU:HD21	1:A:324:ILE:HD13	2.01	0.43
1:A:246:GLY:O	1:A:262:ARG:HG2	2.17	0.43
1:A:524:TYR:O	1:A:528:VAL:HG12	2.18	0.43
1:A:959:GLU:HG2	1:A:962:ARG:NH2	2.29	0.43
1:A:144:SER:N	1:A:319:GLY:O	2.28	0.43
1:A:783:LEU:HB3	1:A:795:LEU:HD12	2.01	0.43
1:A:621:MET:HE3	1:A:621:MET:HB3	1.82	0.43
1:A:639:VAL:HG11	1:A:662:ASN:OD1	2.18	0.43
1:A:913:ARG:NH1	1:A:983:ALA:O	2.37	0.43
1:A:982:LEU:HD13	1:A:996:ILE:HG23	2.00	0.43
1:A:49:TYR:CE2	1:A:118:PRO:HG2	2.53	0.43
1:A:417:ARG:O	1:A:421:GLU:HB2	2.18	0.43
1:A:350:VAL:O	1:A:354:MET:HG3	2.19	0.43
1:A:577:GLU:HG3	1:A:718:ALA:HB2	2.00	0.43
1:A:74:GLY:HA2	1:A:94:ARG:NE	2.33	0.42
1:A:539:MET:HE2	1:A:1021:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:TYR:N	1:A:818:SER:OG	2.52	0.42
1:A:118:PRO:HB2	1:A:121:VAL:HG23	2.01	0.42
1:A:364:THR:O	1:A:367:PRO:HD2	2.19	0.42
1:A:382:MET:HE2	1:A:382:MET:HB2	1.93	0.42
1:A:768:GLN:NE2	1:A:774:ARG:HH21	2.18	0.42
1:A:837:ALA:O	1:A:841:LEU:HG	2.19	0.42
1:A:191:LYS:HE2	1:A:263:ASP:O	2.19	0.42
1:A:417:ARG:HE	1:A:417:ARG:HB3	1.61	0.42
1:A:479:PHE:O	1:A:482:PHE:N	2.53	0.41
1:A:676:ASP:HB3	1:A:854:SER:O	2.20	0.41
1:A:299:VAL:O	1:A:303:LYS:HG3	2.20	0.41
1:A:241:THR:OG1	1:A:243:GLU:OE1	2.39	0.41
1:A:454:PRO:HG3	1:A:877:ILE:HG12	2.03	0.41
1:A:899:VAL:CG2	1:A:900:PRO:HD3	2.51	0.41
1:A:899:VAL:HG23	1:A:900:PRO:HD3	2.03	0.41
1:A:954:LEU:O	1:A:955:GLN:C	2.64	0.41
1:A:392:LEU:HD11	1:A:465:ILE:HG12	2.02	0.41
1:A:369:LEU:HD23	1:A:369:LEU:HA	1.92	0.41
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.88	0.41
1:A:479:PHE:C	1:A:483:LEU:HD12	2.46	0.41
1:A:454:PRO:HG2	1:A:874:SER:HA	2.03	0.40
1:A:928:ILE:HD13	1:A:928:ILE:HA	1.84	0.40
1:A:27:ILE:HD11	1:A:379:PHE:CE2	2.56	0.40
1:A:163:GLN:O	1:A:167:ARG:HG3	2.22	0.40
1:A:973:LEU:HD23	1:A:973:LEU:HA	1.82	0.40
1:A:242:PRO:HB3	1:A:267:VAL:HG12	2.02	0.40
1:A:379:PHE:CZ	1:A:394:MET:HE1	2.53	0.40
1:A:452:PHE:CE2	1:A:473:LEU:HB3	2.57	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	1025/1054 (97%)	987 (96%)	37 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	952	SER

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	817/841 (97%)	780 (96%)	37 (4%)	23 56

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	17	LEU
1	A	46	SER
1	A	48	SER
1	A	55	LYS
1	A	82	SER
1	A	83	SER
1	A	89	LEU
1	A	142	THR
1	A	159	SER
1	A	214	THR
1	A	221	LEU
1	A	226	SER
1	A	235	VAL
1	A	299	VAL
1	A	329	SER
1	A	340	VAL
1	A	341	SER
1	A	349	LEU
1	A	499	ILE

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Mol	Chain	Res	Type
1	A	521	THR
1	A	549	VAL
1	A	611	SER
1	A	618	SER
1	A	619	SER
1	A	696	GLN
1	A	726	ASP
1	A	756	PHE
1	A	797	THR
1	A	818	SER
1	A	830	SER
1	A	880	LEU
1	A	888	SER
1	A	937	ILE
1	A	980	VAL
1	A	1000	VAL
1	A	1020	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	323	ASN
1	A	436	GLN
1	A	566	GLN
1	A	741	ASN
1	A	824	GLN
1	A	856	GLN
1	A	946	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
2	SO4	A	1103	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	1108	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	1101	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	A	1111	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	A	1105	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	A	1109	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	1102	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	1107	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	1106	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	1110	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	A	1104	-	4,4,4	0.16	0	6,6,6	0.08	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1106	SO4	1	0
2	A	1110	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	1027/1054 (97%)	1.39	281 (27%) 2 2	51, 88, 143, 237	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	SER	12.0
1	A	152	GLU	11.3
1	A	160	ASN	10.3
1	A	163	GLN	10.0
1	A	503	HIS	9.3
1	A	151	MET	8.8
1	A	756	PHE	8.5
1	A	148	TYR	8.3
1	A	155	GLU	8.3
1	A	798	PHE	7.8
1	A	778	ASP	7.6
1	A	158	SER	7.4
1	A	762	VAL	7.1
1	A	269	PHE	7.0
1	A	507	ARG	6.8
1	A	181	TYR	6.7
1	A	782	ARG	6.4
1	A	793	VAL	6.4
1	A	236	ASP	6.4
1	A	750	SER	6.3
1	A	461	ALA	6.2
1	A	123	ARG	6.2
1	A	1019	PHE	6.1
1	A	951	MET	6.1
1	A	21	LEU	6.0
1	A	947	TYR	6.0
1	A	499	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	133	ASP	5.9
1	A	268	GLU	5.9
1	A	52	ALA	5.7
1	A	512	TRP	5.7
1	A	666	LEU	5.7
1	A	149	ASP	5.6
1	A	38	ILE	5.4
1	A	108	ASN	5.4
1	A	843	GLN	5.3
1	A	688	GLU	5.3
1	A	479	PHE	5.2
1	A	488	THR	5.2
1	A	963	LEU	5.2
1	A	714	GLY	5.1
1	A	755	ASP	5.0
1	A	154	GLY	5.0
1	A	945	ASP	5.0
1	A	157	ALA	5.0
1	A	266	ARG	4.9
1	A	797	THR	4.9
1	A	957	THR	4.9
1	A	555	ARG	4.8
1	A	757	MET	4.8
1	A	1016	PRO	4.8
1	A	691	VAL	4.7
1	A	180	GLU	4.7
1	A	952	SER	4.7
1	A	73	PRO	4.6
1	A	752	TYR	4.6
1	A	146	GLY	4.6
1	A	799	ALA	4.6
1	A	889	TRP	4.6
1	A	506	LYS	4.5
1	A	464	ASN	4.5
1	A	162	LEU	4.5
1	A	792	MET	4.4
1	A	728	ARG	4.4
1	A	668	ASP	4.4
1	A	695	ASP	4.4
1	A	224	PRO	4.4
1	A	667	PRO	4.4
1	A	135	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	783	LEU	4.3
1	A	664	PRO	4.2
1	A	779	ASP	4.2
1	A	760	SER	4.2
1	A	794	PRO	4.1
1	A	51	GLY	4.1
1	A	270	GLY	4.1
1	A	1020	LEU	4.1
1	A	487	LEU	4.1
1	A	378	THR	4.1
1	A	729	LYS	4.1
1	A	537	ARG	4.0
1	A	761	GLN	4.0
1	A	949	GLU	4.0
1	A	39	ALA	4.0
1	A	475	VAL	4.0
1	A	179	ALA	4.0
1	A	483	LEU	4.0
1	A	727	ARG	3.9
1	A	17	LEU	3.9
1	A	940	ILE	3.9
1	A	865	ALA	3.9
1	A	1017	LEU	3.8
1	A	725	ILE	3.8
1	A	11	PHE	3.8
1	A	175	GLU	3.8
1	A	788	GLU	3.8
1	A	520	LEU	3.8
1	A	50	PRO	3.7
1	A	953	LEU	3.7
1	A	504	HIS	3.7
1	A	651	ALA	3.6
1	A	384	GLY	3.6
1	A	174	VAL	3.6
1	A	460	GLY	3.6
1	A	862	LEU	3.6
1	A	597	GLU	3.5
1	A	3	ARG	3.5
1	A	603	TYR	3.5
1	A	956	ALA	3.5
1	A	252	ILE	3.5
1	A	784	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	3.4
1	A	212	ARG	3.4
1	A	1024	ARG	3.4
1	A	726	ASP	3.4
1	A	435	ARG	3.4
1	A	944	LYS	3.3
1	A	223	VAL	3.3
1	A	525	ARG	3.3
1	A	271	GLN	3.2
1	A	1025	LEU	3.2
1	A	866	GLN	3.2
1	A	35	TYR	3.2
1	A	781	GLY	3.2
1	A	763	ARG	3.1
1	A	421	GLU	3.1
1	A	655	ASN	3.1
1	A	758	HIS	3.1
1	A	694	ARG	3.1
1	A	56	VAL	3.1
1	A	449	VAL	3.1
1	A	196	ASN	3.1
1	A	939	ILE	3.1
1	A	71	GLY	3.0
1	A	684	GLY	3.0
1	A	476	SER	3.0
1	A	596	ALA	3.0
1	A	462	VAL	3.0
1	A	786	ARG	3.0
1	A	176	THR	3.0
1	A	550	ALA	3.0
1	A	962	ARG	3.0
1	A	509	PHE	3.0
1	A	527	ALA	3.0
1	A	167	ARG	3.0
1	A	955	GLN	3.0
1	A	274	TYR	3.0
1	A	663	SER	3.0
1	A	34	GLN	2.9
1	A	281	ASN	2.9
1	A	182	ALA	2.9
1	A	314	ARG	2.9
1	A	950	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	131	ALA	2.9
1	A	526	ASN	2.9
1	A	536	ILE	2.8
1	A	7	ASP	2.8
1	A	633	ARG	2.8
1	A	546	ILE	2.8
1	A	891	ILE	2.8
1	A	959	GLU	2.8
1	A	101	LEU	2.8
1	A	267	VAL	2.8
1	A	801	ALA	2.8
1	A	687	TYR	2.8
1	A	800	LYS	2.8
1	A	458	PHE	2.8
1	A	508	GLY	2.8
1	A	647	ASN	2.7
1	A	887	GLU	2.7
1	A	377	GLY	2.7
1	A	735	VAL	2.7
1	A	805	LEU	2.7
1	A	813	TYR	2.7
1	A	943	ALA	2.7
1	A	628	ASP	2.7
1	A	364	THR	2.7
1	A	9	PRO	2.7
1	A	737	MET	2.7
1	A	1026	PHE	2.7
1	A	734	GLY	2.7
1	A	538	TRP	2.6
1	A	15	ILE	2.6
1	A	407	ASP	2.6
1	A	173	LYS	2.6
1	A	282	GLN	2.6
1	A	222	GLY	2.6
1	A	523	ARG	2.6
1	A	670	GLY	2.6
1	A	342	THR	2.6
1	A	29	PHE	2.5
1	A	316	PHE	2.5
1	A	465	ILE	2.5
1	A	748	PHE	2.5
1	A	147	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	946	HIS	2.5
1	A	78	THR	2.5
1	A	150	ALA	2.5
1	A	177	TRP	2.5
1	A	717	GLU	2.5
1	A	283	MET	2.5
1	A	539	MET	2.5
1	A	753	ILE	2.5
1	A	749	GLY	2.5
1	A	10	VAL	2.5
1	A	288	LEU	2.5
1	A	398	VAL	2.5
1	A	819	PHE	2.5
1	A	498	PRO	2.5
1	A	234	LYS	2.4
1	A	561	LEU	2.4
1	A	161	VAL	2.4
1	A	70	ASN	2.4
1	A	374	ALA	2.4
1	A	844	GLY	2.4
1	A	59	GLU	2.4
1	A	466	TYR	2.4
1	A	1027	ARG	2.4
1	A	665	PRO	2.4
1	A	630	SER	2.4
1	A	777	ILE	2.4
1	A	22	ALA	2.4
1	A	1023	GLY	2.4
1	A	856	GLN	2.3
1	A	432	LYS	2.3
1	A	262	ARG	2.3
1	A	652	GLY	2.3
1	A	53	SER	2.3
1	A	948	GLN	2.3
1	A	1021	VAL	2.3
1	A	361	PHE	2.3
1	A	426	PRO	2.3
1	A	220	ASN	2.3
1	A	402	GLY	2.3
1	A	310	ASP	2.3
1	A	273	GLU	2.2
1	A	747	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	18	LEU	2.2
1	A	552	LEU	2.2
1	A	111	LYS	2.2
1	A	1015	VAL	2.2
1	A	28	ARG	2.2
1	A	26	ALA	2.2
1	A	769	ALA	2.2
1	A	791	GLU	2.2
1	A	13	TRP	2.2
1	A	434	MET	2.2
1	A	480	SER	2.2
1	A	241	THR	2.2
1	A	441	ILE	2.2
1	A	257	GLY	2.2
1	A	436	GLN	2.2
1	A	8	ARG	2.2
1	A	501	ALA	2.2
1	A	723	LEU	2.2
1	A	291	LYS	2.1
1	A	489	PRO	2.1
1	A	72	ALA	2.1
1	A	201	ASP	2.1
1	A	534	ARG	2.1
1	A	457	PHE	2.1
1	A	627	LYS	2.1
1	A	648	GLN	2.1
1	A	505	GLU	2.1
1	A	184	ARG	2.1
1	A	743	THR	2.1
1	A	86	GLN	2.1
1	A	524	TYR	2.1
1	A	1012	VAL	2.1
1	A	671	SER	2.0
1	A	736	SER	2.0
1	A	422	GLU	2.0
1	A	746	VAL	2.0
1	A	463	GLY	2.0
1	A	76	LEU	2.0
1	A	751	ASP	2.0
1	A	796	ALA	2.0
1	A	869	ALA	2.0
1	A	48	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	986	SER	2.0
1	A	44	ASN	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(\AA^2)	Q<0.9
2	SO4	A	1111	5/5	0.55	0.15	127,144,169,184	0
2	SO4	A	1107	5/5	0.59	0.14	101,110,142,144	0
2	SO4	A	1108	5/5	0.60	0.17	153,155,161,169	0
2	SO4	A	1105	5/5	0.70	0.12	120,131,164,166	0
2	SO4	A	1110	5/5	0.72	0.10	110,122,135,144	0
2	SO4	A	1104	5/5	0.75	0.14	88,112,138,139	0
2	SO4	A	1106	5/5	0.80	0.11	114,129,141,154	0
2	SO4	A	1109	5/5	0.84	0.09	90,106,129,145	0
2	SO4	A	1102	5/5	0.88	0.21	55,90,109,112	0
2	SO4	A	1103	5/5	0.93	0.08	95,114,122,127	0
2	SO4	A	1101	5/5	0.94	0.11	52,53,79,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.