



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 5XU1 / pdb_00005xu1
Title : Structure of a non-canonical ABC transporter from *Streptococcus pneumoniae* R6
Authors : Yang, H.B.; Jiang, Y.L.; Hou, W.T.; Chen, M.T.; Chen, Y.; Zhou, C.Z.
Deposited on : 2017-06-22
Resolution : 3.30 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
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

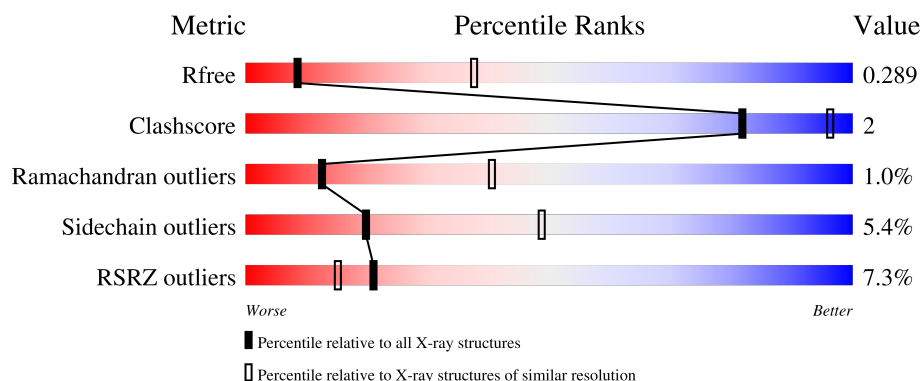
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	245	4% 85% 5% 10%
1	B	245	6% 80% 12% 8%
2	M	419	8% 80% 12% 7%
2	S	419	7% 79% 10% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9287 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 ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1712	1080	296	331	5			
1	B	226	Total	C	N	O	S	0	0	0
			1752	1101	306	340	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q8DQF8
A	-10	GLY	-	expression tag	UNP Q8DQF8
A	-9	GLY	-	expression tag	UNP Q8DQF8
A	-8	SER	-	expression tag	UNP Q8DQF8
A	-7	HIS	-	expression tag	UNP Q8DQF8
A	-6	HIS	-	expression tag	UNP Q8DQF8
A	-5	HIS	-	expression tag	UNP Q8DQF8
A	-4	HIS	-	expression tag	UNP Q8DQF8
A	-3	HIS	-	expression tag	UNP Q8DQF8
A	-2	HIS	-	expression tag	UNP Q8DQF8
A	-1	GLY	-	expression tag	UNP Q8DQF8
A	0	THR	-	expression tag	UNP Q8DQF8
B	-11	MET	-	expression tag	UNP Q8DQF8
B	-10	GLY	-	expression tag	UNP Q8DQF8
B	-9	GLY	-	expression tag	UNP Q8DQF8
B	-8	SER	-	expression tag	UNP Q8DQF8
B	-7	HIS	-	expression tag	UNP Q8DQF8
B	-6	HIS	-	expression tag	UNP Q8DQF8
B	-5	HIS	-	expression tag	UNP Q8DQF8
B	-4	HIS	-	expression tag	UNP Q8DQF8
B	-3	HIS	-	expression tag	UNP Q8DQF8
B	-2	HIS	-	expression tag	UNP Q8DQF8
B	-1	GLY	-	expression tag	UNP Q8DQF8
B	0	THR	-	expression tag	UNP Q8DQF8

- Molecule 2 is a protein called ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	390	Total	C	N	O	S	0	0	0
			2950	1890	486	562	12			
2	S	378	Total	C	N	O	S	0	0	0
			2855	1830	469	543	13			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

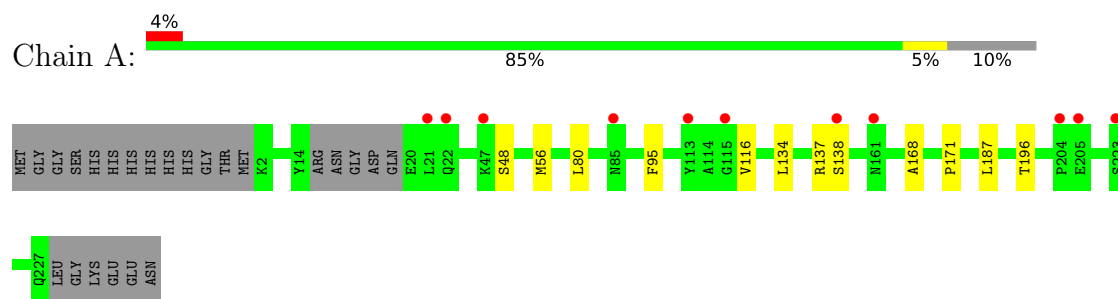
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	5	Total	O	0	0
			5	5		
4	M	2	Total	O	0	0
			2	2		
4	S	7	Total	O	0	0
			7	7		

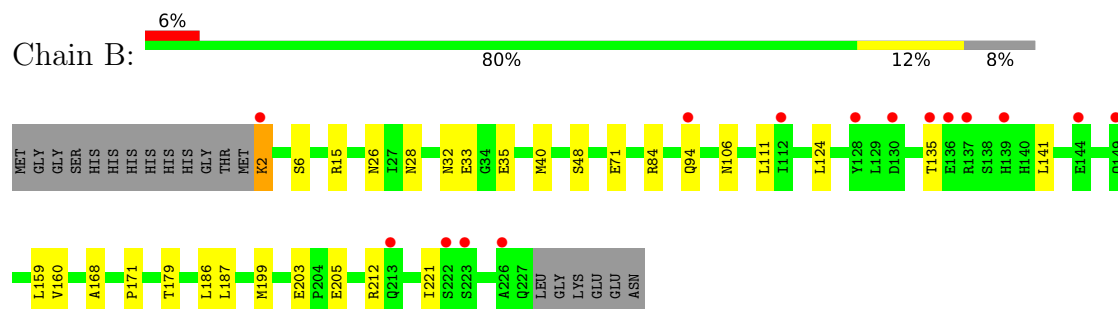
3 Residue-property plots [i](#)

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

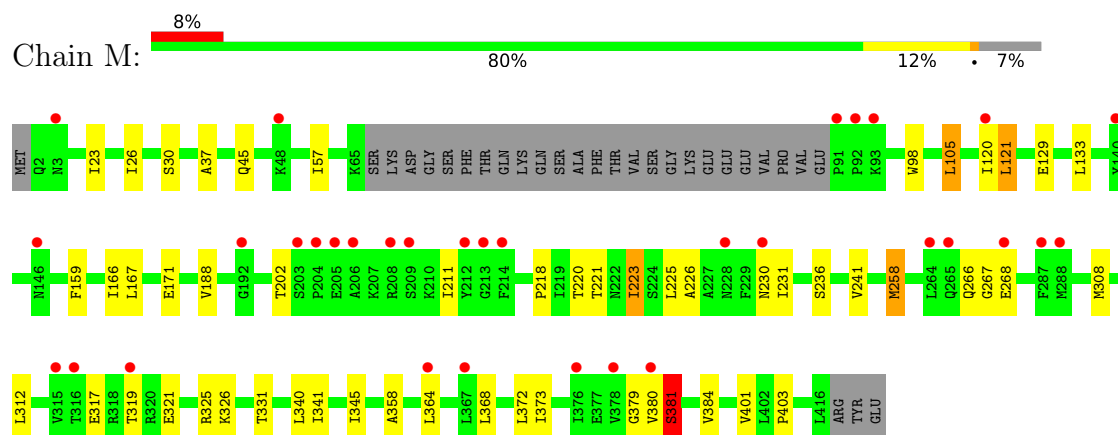
- Molecule 1: ABC transporter ATP-binding protein



- Molecule 1: ABC transporter ATP-binding protein



- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease

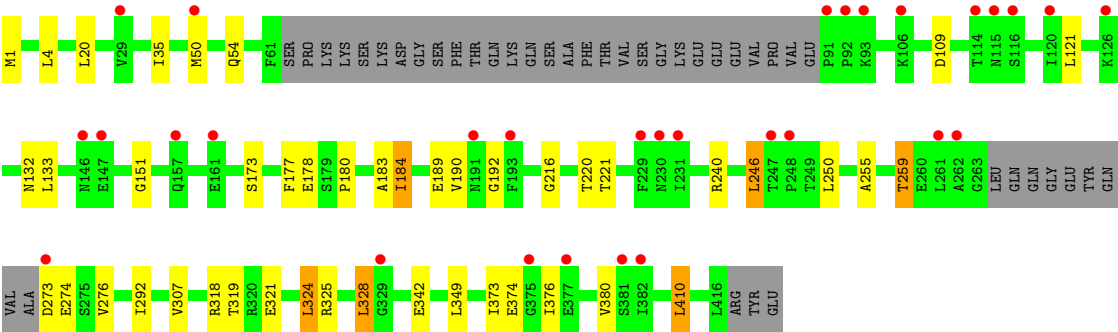
Chain S:

7%

79%

10%

10%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.05Å 154.99Å 205.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.30) 99.5 (50.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.234 , 0.289 0.234 , 0.289	Depositor DCC
R_{free} test set	1729 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9287	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	0/1732	0.85	0/2333
1	B	0.60	0/1773	0.87	2/2389 (0.1%)
2	M	0.62	0/2989	0.91	1/4040 (0.0%)
2	S	0.64	0/2891	0.93	1/3906 (0.0%)
All	All	0.62	0/9385	0.90	4/12668 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLN	N-CA-C	-7.07	100.01	110.48
2	M	121	LEU	N-CA-C	6.45	120.14	111.24
2	S	274	GLU	N-CA-C	6.20	118.33	110.33
1	B	160	VAL	N-CA-C	5.13	118.25	111.17

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	1712	0	1761	2	0
1	B	1752	0	1796	7	0
2	M	2950	0	3072	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	2855	0	2978	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
4	M	2	0	0	0	0
4	S	7	0	0	1	0
All	All	9287	0	9607	47	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 2.

All (47) 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:M:45:GLN:HE22	2:M:373:ILE:HG23	1.58	0.68
1:B:26:ASN:OD1	1:B:28:ASN:ND2	2.27	0.68
2:S:151:GLY:HA3	2:S:184:ILE:HD11	1.78	0.65
2:M:340:LEU:HD11	2:M:401:VAL:HG12	1.87	0.57
2:S:324:LEU:O	2:S:328:LEU:HD22	2.06	0.56
2:S:373:ILE:HG22	2:S:376:ILE:HD11	1.86	0.56
2:M:166:ILE:HD11	2:M:218:PRO:HB2	1.88	0.55
2:M:258:MET:HE3	2:M:258:MET:HA	1.90	0.53
2:M:159:PHE:HA	2:M:223:ILE:HD11	1.91	0.53
2:M:98:TRP:HB3	2:M:258:MET:HE2	1.90	0.51
1:B:84:ARG:NH1	2:M:326:LYS:O	2.45	0.50
2:S:319:THR:HG22	2:S:410:LEU:HD11	1.93	0.50
2:M:133:LEU:CD2	2:M:225:LEU:HD11	2.43	0.48
2:S:35:ILE:HD13	2:S:292:ILE:HG22	1.94	0.48
2:M:230:ASN:CG	2:S:192:GLY:HA3	2.40	0.46
2:M:321:GLU:OE2	2:M:325:ARG:NH2	2.49	0.46
1:A:168:ALA:HB1	1:A:171:PRO:HG3	1.98	0.45
1:B:35:GLU:OE2	1:B:212:ARG:NH1	2.47	0.45
2:M:120:ILE:HA	2:M:129:GLU:HA	1.99	0.45
1:B:168:ALA:HB1	1:B:171:PRO:HG3	1.99	0.45
2:M:341:ILE:O	2:M:345:ILE:HG12	2.17	0.45
2:S:133:LEU:HD22	2:S:190:VAL:HG11	1.98	0.45
2:M:211:ILE:HG23	2:M:373:ILE:HD11	1.98	0.45
2:M:308:MET:HE2	2:S:20:LEU:HD21	1.98	0.45
2:M:37:ALA:HB1	2:M:379:GLY:HA3	1.99	0.44
2:S:121:LEU:HG	2:S:190:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:380:VAL:O	2:M:381:SER:C	2.61	0.44
2:S:50:MET:HE3	2:S:54:GLN:NE2	2.32	0.44
2:M:220:THR:HG23	2:M:225:LEU:HD13	2.00	0.44
1:B:2:LYS:O	1:B:33:GLU:N	2.46	0.43
2:S:318:ARG:NH2	2:S:342:GLU:OE1	2.51	0.43
2:S:177:PHE:HB2	2:S:183:ALA:HB2	2.00	0.43
2:M:226:ALA:HA	2:M:231:ILE:O	2.18	0.43
2:M:312:LEU:HG	2:M:403:PRO:HG3	2.01	0.43
2:S:255:ALA:O	2:S:259:THR:OG1	2.35	0.43
1:B:168:ALA:O	1:B:199:MET:HA	2.18	0.42
2:M:23:ILE:HA	2:M:26:ILE:HG12	2.01	0.42
2:S:321:GLU:OE2	2:S:325:ARG:NH2	2.53	0.42
2:S:132:ASN:N	2:S:216:GLY:O	2.46	0.42
2:S:220:THR:OG1	2:S:221:THR:N	2.53	0.42
2:M:57:ILE:HD12	2:M:241:VAL:HG21	2.02	0.41
2:M:220:THR:OG1	2:M:221:THR:N	2.53	0.41
2:S:246:LEU:HD22	2:S:250:LEU:HD12	2.01	0.41
1:A:56:MET:HB3	1:A:80:LEU:HG	2.01	0.41
2:S:240:ARG:HD2	4:S:503:HOH:O	2.21	0.41
2:M:30:SER:HA	2:M:358:ALA:HB2	2.03	0.40
1:B:32:ASN:O	1:B:35:GLU:HB2	2.22	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	217/245 (89%)	209 (96%)	7 (3%)	1 (0%)	24	55
1	B	224/245 (91%)	206 (92%)	16 (7%)	2 (1%)	14	43
2	M	386/419 (92%)	354 (92%)	26 (7%)	6 (2%)	7	31
2	S	372/419 (89%)	343 (92%)	26 (7%)	3 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1199/1328 (90%)	1112 (93%)	75 (6%)	12 (1%)	12	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	372	LEU
2	M	368	LEU
2	S	276	VAL
1	B	15	ARG
2	M	267	GLY
2	M	381	SER
1	A	95	PHE
2	M	105	LEU
2	M	268	GLU
2	S	374	GLU
2	S	180	PRO
1	B	221	ILE

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	189/208 (91%)	182 (96%)	7 (4%)	30	58
1	B	193/208 (93%)	177 (92%)	16 (8%)	10	34
2	M	327/353 (93%)	311 (95%)	16 (5%)	22	51
2	S	317/353 (90%)	301 (95%)	16 (5%)	22	50
All	All	1026/1122 (91%)	971 (95%)	55 (5%)	20	49

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	116	VAL
1	A	134	LEU

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Mol	Chain	Res	Type
1	A	137	ARG
1	A	138	SER
1	A	187	LEU
1	A	196	THR
1	B	2	LYS
1	B	6	SER
1	B	40	MET
1	B	48	SER
1	B	71	GLU
1	B	106	ASN
1	B	111	LEU
1	B	124	LEU
1	B	135	THR
1	B	141	LEU
1	B	159	LEU
1	B	179	THR
1	B	186	LEU
1	B	187	LEU
1	B	203	GLU
1	B	205	GLU
2	M	105	LEU
2	M	121	LEU
2	M	167	LEU
2	M	171	GLU
2	M	188	VAL
2	M	202	THR
2	M	223	ILE
2	M	236	SER
2	M	258	MET
2	M	266	GLN
2	M	317	GLU
2	M	319	THR
2	M	331	THR
2	M	364	LEU
2	M	381	SER
2	M	384	VAL
2	S	1	MET
2	S	4	LEU
2	S	109	ASP
2	S	173	SER
2	S	178	GLU
2	S	184	ILE

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Mol	Chain	Res	Type
2	S	189	GLU
2	S	246	LEU
2	S	259	THR
2	S	273	ASP
2	S	307	VAL
2	S	324	LEU
2	S	328	LEU
2	S	349	LEU
2	S	380	VAL
2	S	410	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	94	GLN
1	A	162	ASN
1	B	139	HIS
1	B	182	GLN
1	B	213	GLN
2	M	3	ASN
2	M	14	HIS
2	M	45	GLN
2	M	118	ASN
2	M	185	ASN
2	M	228	ASN
2	S	54	GLN
2	S	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	221/245 (90%)	0.31	11 (4%) 34 23	53, 76, 102, 125	0
1	B	226/245 (92%)	0.42	15 (6%) 24 16	58, 78, 114, 140	0
2	M	390/419 (93%)	0.43	33 (8%) 16 13	54, 78, 120, 148	0
2	S	378/419 (90%)	0.63	30 (7%) 18 14	50, 88, 132, 149	0
All	All	1215/1328 (91%)	0.47	89 (7%) 21 15	50, 80, 125, 149	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	230	ASN	6.1
2	M	378	VAL	5.9
2	S	377	GLU	4.8
1	B	135	THR	4.7
2	S	106	LYS	4.6
2	S	116	SER	4.6
2	S	229	PHE	4.5
2	M	205	GLU	4.3
2	M	212	TYR	4.2
1	B	136	GLU	4.1
2	M	208	ARG	3.9
2	S	262	ALA	3.8
2	M	91	PRO	3.7
2	M	93	LYS	3.7
1	B	2	LYS	3.6
1	A	113	TYR	3.5
2	S	120	ILE	3.5
2	M	213	GLY	3.3
2	M	268	GLU	3.3
1	A	85	ASN	3.3
1	B	226	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	S	147	GLU	3.2
2	S	329	GLY	3.2
2	S	230	ASN	3.2
2	M	214	PHE	3.2
2	M	288	MET	3.1
1	A	205	GLU	3.1
1	A	115	GLY	3.0
2	S	381	SER	3.0
1	B	128	TYR	3.0
2	M	228	ASN	2.9
2	S	92	PRO	2.9
1	A	138	SER	2.8
2	M	319	THR	2.8
2	M	380	VAL	2.8
1	A	223	SER	2.8
2	S	382	ILE	2.8
2	S	91	PRO	2.8
1	A	204	PRO	2.7
2	S	126	LYS	2.6
2	M	192	GLY	2.6
2	S	115	ASN	2.6
2	M	204	PRO	2.5
2	M	209	SER	2.5
2	M	367	LEU	2.5
2	M	316	THR	2.5
2	S	114	THR	2.5
2	S	261	LEU	2.5
2	M	3	ASN	2.5
2	M	287	PHE	2.5
2	M	146	ASN	2.5
1	B	94	GLN	2.5
1	B	213	GLN	2.5
2	M	92	PRO	2.4
2	S	248	PRO	2.4
1	B	149	GLN	2.4
2	S	191	ASN	2.4
1	A	22	GLN	2.3
1	B	144	GLU	2.3
2	M	206	ALA	2.3
2	S	157	GLN	2.3
2	S	161	GLU	2.3
2	S	50	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	161	ASN	2.3
2	S	93	LYS	2.3
2	M	264	LEU	2.2
2	S	193	PHE	2.2
2	M	376	ILE	2.2
1	B	139	HIS	2.2
2	S	29	VAL	2.2
2	M	364	LEU	2.2
1	B	130	ASP	2.2
2	S	273	ASP	2.2
2	M	315	VAL	2.2
1	B	222	SER	2.2
1	B	223	SER	2.2
1	A	47	LYS	2.2
2	M	265	GLN	2.1
2	M	48	LYS	2.1
1	A	21	LEU	2.1
2	S	247	THR	2.1
2	M	120	ILE	2.1
2	S	231	ILE	2.1
1	B	137	ARG	2.1
2	M	203	SER	2.1
2	S	146	ASN	2.1
2	M	140	TYR	2.1
1	B	112	ILE	2.0
2	S	375	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($\text{\AA}^2$)	Q<0.9
3	MG	B	301	1/1	0.93	0.11	49,49,49,49	0
3	MG	A	301	1/1	0.94	0.20	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.