



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 2F1M / pdb_00002f1m
Title : Conformational flexibility in the multidrug efflux system protein AcrA
Authors : Mikolosko, J.; Bobyk, K.; Zgurskaya, H.I.; Ghosh, P.
Deposited on : 2005-11-14
Resolution : 2.71 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

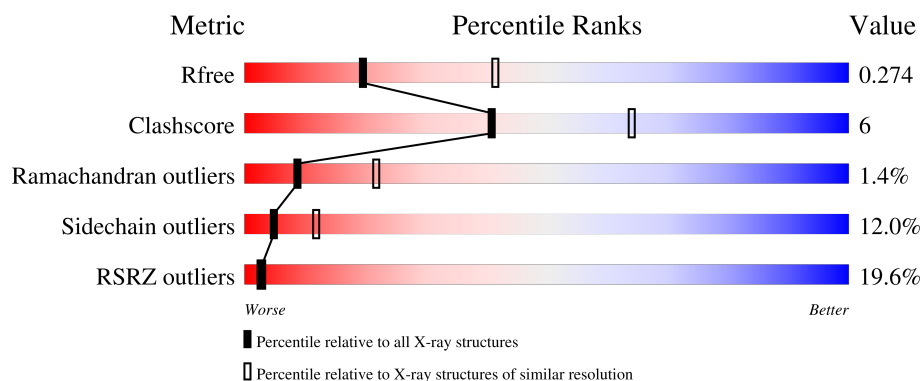
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	277	16% 68% 13% • 17%
1	B	277	11% 62% 15% • 19%
1	C	277	13% 70% 14% • • 11%
1	D	277	25% 65% 13% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7000 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 Acriflavine resistance protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	Se	20	0	0
			1728	1076	300	348	4			
1	B	223	Total	C	N	O	Se	25	0	0
			1680	1049	292	336	3			
1	C	247	Total	C	N	O	Se	0	0	0
			1870	1161	327	377	5			
1	D	224	Total	C	N	O	Se	21	0	0
			1686	1053	294	336	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MSE	-	initiating methionine	UNP P0AE06
A	223	MSE	PHE	engineered mutation	UNP P0AE06
A	224	MSE	LEU	engineered mutation	UNP P0AE06
A	287	MSE	LEU	engineered mutation	UNP P0AE06
A	288	MSE	LEU	engineered mutation	UNP P0AE06
A	291	MSE	MET	modified residue	UNP P0AE06
A	313	LEU	-	cloning artifact	UNP P0AE06
A	314	GLU	-	cloning artifact	UNP P0AE06
A	315	HIS	-	cloning artifact	UNP P0AE06
A	316	HIS	-	cloning artifact	UNP P0AE06
A	317	HIS	-	cloning artifact	UNP P0AE06
A	318	HIS	-	cloning artifact	UNP P0AE06
A	319	HIS	-	cloning artifact	UNP P0AE06
A	320	HIS	-	cloning artifact	UNP P0AE06
B	44	MSE	-	initiating methionine	UNP P0AE06
B	223	MSE	PHE	engineered mutation	UNP P0AE06
B	224	MSE	LEU	engineered mutation	UNP P0AE06
B	287	MSE	LEU	engineered mutation	UNP P0AE06
B	288	MSE	LEU	engineered mutation	UNP P0AE06
B	291	MSE	MET	modified residue	UNP P0AE06
B	313	LEU	-	cloning artifact	UNP P0AE06

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Chain	Residue	Modelled	Actual	Comment	Reference
B	314	GLU	-	cloning artifact	UNP P0AE06
B	315	HIS	-	cloning artifact	UNP P0AE06
B	316	HIS	-	cloning artifact	UNP P0AE06
B	317	HIS	-	cloning artifact	UNP P0AE06
B	318	HIS	-	cloning artifact	UNP P0AE06
B	319	HIS	-	cloning artifact	UNP P0AE06
B	320	HIS	-	cloning artifact	UNP P0AE06
C	44	MSE	-	initiating methionine	UNP P0AE06
C	223	MSE	PHE	engineered mutation	UNP P0AE06
C	224	MSE	LEU	engineered mutation	UNP P0AE06
C	287	MSE	LEU	engineered mutation	UNP P0AE06
C	288	MSE	LEU	engineered mutation	UNP P0AE06
C	291	MSE	MET	modified residue	UNP P0AE06
C	313	LEU	-	cloning artifact	UNP P0AE06
C	314	GLU	-	cloning artifact	UNP P0AE06
C	315	HIS	-	cloning artifact	UNP P0AE06
C	316	HIS	-	cloning artifact	UNP P0AE06
C	317	HIS	-	cloning artifact	UNP P0AE06
C	318	HIS	-	cloning artifact	UNP P0AE06
C	319	HIS	-	cloning artifact	UNP P0AE06
C	320	HIS	-	cloning artifact	UNP P0AE06
D	44	MSE	-	initiating methionine	UNP P0AE06
D	223	MSE	PHE	engineered mutation	UNP P0AE06
D	224	MSE	LEU	engineered mutation	UNP P0AE06
D	287	MSE	LEU	engineered mutation	UNP P0AE06
D	288	MSE	LEU	engineered mutation	UNP P0AE06
D	291	MSE	MET	modified residue	UNP P0AE06
D	313	LEU	-	cloning artifact	UNP P0AE06
D	314	GLU	-	cloning artifact	UNP P0AE06
D	315	HIS	-	cloning artifact	UNP P0AE06
D	316	HIS	-	cloning artifact	UNP P0AE06
D	317	HIS	-	cloning artifact	UNP P0AE06
D	318	HIS	-	cloning artifact	UNP P0AE06
D	319	HIS	-	cloning artifact	UNP P0AE06
D	320	HIS	-	cloning artifact	UNP P0AE06

- Molecule 2 is water.

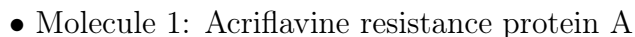
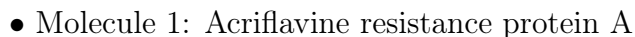
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	10	Total O 10 10	0	0

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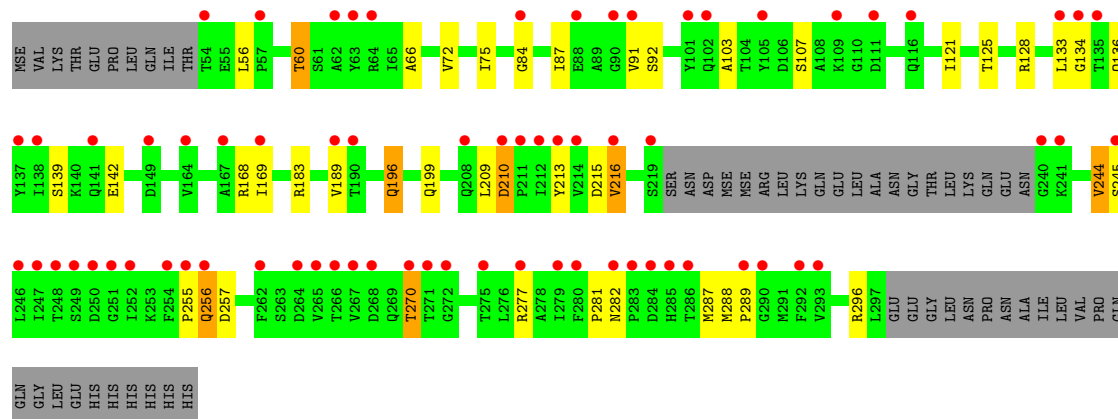
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	8	Total	O	0	0
			8	8		
2	D	4	Total	O	0	0
			4	4		

- Molecule 1: Acriflavine resistance protein A



- Molecule 1: Acriflavine resistance protein A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.79Å 100.03Å 332.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.71 50.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.71) 96.6 (50.00-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.275 0.233 , 0.274	Depositor DCC
R_{free} test set	1972 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.9	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	0.89	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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](#)

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	0.60	0/1746	1.03	0/2364
1	B	0.59	0/1699	1.08	5/2304 (0.2%)
1	C	0.57	0/1888	1.12	3/2552 (0.1%)
1	D	0.54	0/1705	1.02	3/2310 (0.1%)
All	All	0.58	0/7038	1.06	11/9530 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	210	ASP	CA-C-N	-12.72	104.48	120.51
1	C	210	ASP	C-N-CA	-12.72	104.48	120.51
1	B	210	ASP	CA-C-N	-8.19	109.60	119.84
1	B	210	ASP	C-N-CA	-8.19	109.60	119.84
1	D	210	ASP	CA-C-N	-7.99	109.47	120.25
1	D	210	ASP	C-N-CA	-7.99	109.47	120.25
1	D	270	THR	N-CA-C	-5.76	102.67	110.68
1	C	220	SER	N-CA-C	5.62	118.26	111.40
1	B	254	PHE	CA-C-N	5.54	125.38	119.28
1	B	254	PHE	C-N-CA	5.54	125.38	119.28
1	B	269	GLN	CB-CA-C	-5.16	100.77	110.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ASP	Peptide

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	1728	0	1735	18	0
1	B	1680	0	1692	24	0
1	C	1870	0	1881	31	0
1	D	1686	0	1701	20	0
2	A	14	0	0	1	0
2	B	10	0	0	0	0
2	C	8	0	0	0	0
2	D	4	0	0	0	0
All	All	7000	0	7009	89	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 6.

All (89) 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:91:VAL:HG22	1:D:91:VAL:HG22	1.49	0.95
1:B:277:ARG:HH11	1:B:277:ARG:HG3	1.32	0.92
1:C:236:LYS:HD2	1:C:237:GLN:H	1.37	0.88
1:C:191:GLU:O	1:D:66:ALA:HA	1.79	0.83
1:D:60:THR:HG22	1:D:289:PRO:HA	1.60	0.83
1:C:56:LEU:HB3	1:C:218:GLN:HE21	1.47	0.80
1:D:215:ASP:OD1	1:D:277:ARG:HD3	1.81	0.79
1:D:196:GLN:H	1:D:199:GLN:HE21	1.31	0.78
1:B:87:ILE:HG13	1:B:93:LEU:HD21	1.73	0.71
1:D:196:GLN:H	1:D:199:GLN:NE2	1.90	0.70
1:C:139:SER:HB2	1:C:141:GLN:HE21	1.57	0.70
1:B:139:SER:OG	1:B:142:GLU:HB2	1.92	0.69
1:B:248:THR:HG22	1:B:287:MSE:HE1	1.76	0.68
1:A:191:GLU:O	1:B:66:ALA:HA	1.94	0.68
1:C:236:LYS:CD	1:C:237:GLN:H	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:THR:HG21	1:C:288:MSE:O	2.00	0.62
1:A:63:TYR:HB2	1:A:211:PRO:O	2.02	0.60
1:C:135:THR:HG23	1:C:137:TYR:H	1.68	0.58
1:A:209:LEU:C	1:A:210:ASP:O	2.46	0.58
1:A:210:ASP:HB3	1:A:211:PRO:CD	2.35	0.57
1:A:210:ASP:O	1:A:211:PRO:C	2.48	0.56
1:B:246:LEU:HG	1:B:280:PHE:CE2	2.40	0.56
1:D:213:TYR:CG	1:D:277:ARG:HD2	2.41	0.56
1:A:210:ASP:HB3	1:A:211:PRO:HD2	1.87	0.55
1:D:209:LEU:HD13	1:D:288:MSE:HE1	1.89	0.55
1:D:256:GLN:HB2	1:D:281:PRO:HG2	1.88	0.55
1:B:55:GLU:HG3	1:B:294:ARG:HE	1.72	0.54
1:B:246:LEU:HD22	1:B:293:VAL:CG1	2.37	0.53
1:B:87:ILE:HG13	1:B:93:LEU:CD2	2.37	0.53
1:C:244:VAL:HG12	1:C:280:PHE:HZ	1.74	0.53
1:A:246:LEU:HD22	1:A:293:VAL:CG1	2.39	0.53
1:D:245:SER:OG	1:D:296:ARG:HG3	2.08	0.53
1:C:60:THR:HG23	1:C:289:PRO:HA	1.92	0.52
1:B:210:ASP:O	1:B:282:ASN:N	2.43	0.51
1:C:132:LEU:O	1:C:135:THR:HG22	2.11	0.51
1:C:237:GLN:O	1:C:238:GLU:HB2	2.11	0.51
1:D:103:ALA:O	1:D:107:SER:HB2	2.11	0.50
1:C:265:VAL:HG12	1:C:276:LEU:CD2	2.41	0.50
1:C:265:VAL:HG12	1:C:276:LEU:HD23	1.93	0.50
1:B:283:PRO:HB2	1:D:168:ARG:CZ	2.42	0.50
1:A:201:THR:HG23	2:A:29:HOH:O	2.11	0.50
1:D:56:LEU:HB3	1:D:216:VAL:HG11	1.93	0.50
1:D:244:VAL:O	1:D:257:ASP:HB2	2.11	0.50
1:A:165:GLU:OE1	1:A:168:ARG:NH1	2.44	0.50
1:A:56:LEU:HD23	1:A:217:THR:O	2.12	0.49
1:C:60:THR:CG2	1:C:288:MSE:O	2.60	0.49
1:C:135:THR:CG2	1:C:137:TYR:H	2.26	0.49
1:D:84:GLY:O	1:D:183:ARG:HD2	2.13	0.48
1:C:244:VAL:CG1	1:C:295:ALA:HB1	2.44	0.48
1:D:139:SER:HB3	1:D:142:GLU:HB2	1.94	0.48
1:C:135:THR:HG23	1:C:137:TYR:N	2.29	0.48
1:D:121:ILE:O	1:D:125:THR:HG23	2.14	0.47
1:A:56:LEU:HD22	1:A:216:VAL:HG13	1.96	0.47
1:A:243:LYS:HB2	1:A:298:GLU:HB2	1.97	0.47
1:C:265:VAL:CG1	1:C:276:LEU:CD2	2.93	0.46
1:D:210:ASP:O	1:D:282:ASN:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLN:C	1:B:271:THR:H	2.24	0.45
1:C:135:THR:HG23	1:C:137:TYR:HD2	1.82	0.45
1:C:244:VAL:HG12	1:C:280:PHE:CZ	2.52	0.45
1:C:117:ALA:O	1:C:121:ILE:HG12	2.16	0.45
1:A:71:GLN:O	1:A:197:ASN:ND2	2.50	0.45
1:B:76:ILE:HD11	1:B:195:VAL:HG11	1.97	0.45
1:B:264:ASP:N	1:B:264:ASP:OD1	2.50	0.44
1:D:287:MSE:O	1:D:288:MSE:HE2	2.17	0.44
1:D:56:LEU:CB	1:D:216:VAL:HG11	2.48	0.44
1:B:212:ILE:HG21	1:B:287:MSE:HG2	1.99	0.43
1:B:287:MSE:HE2	1:B:291:MSE:SE	2.68	0.43
1:C:210:ASP:O	1:C:282:ASN:N	2.51	0.43
1:C:234:THR:H	1:C:235:LEU:HD23	1.83	0.43
1:B:246:LEU:HD22	1:B:293:VAL:HG11	2.01	0.43
1:C:82:LYS:HD3	1:C:82:LYS:HA	1.87	0.43
1:A:105:TYR:CZ	1:A:168:ARG:HG3	2.54	0.43
1:A:210:ASP:O	1:A:211:PRO:O	2.37	0.42
1:B:215:ASP:OD1	1:B:277:ARG:NH1	2.53	0.42
1:C:265:VAL:CG1	1:C:276:LEU:HD21	2.49	0.42
1:A:72:VAL:HG13	1:A:101:TYR:CZ	2.54	0.42
1:C:236:LYS:C	1:C:237:GLN:HE21	2.28	0.42
1:B:60:THR:HG22	1:B:214:VAL:HG22	2.01	0.41
1:B:254:PHE:HA	1:B:255:PRO:HD3	1.82	0.41
1:C:236:LYS:CG	1:C:237:GLN:H	2.33	0.41
1:B:269:GLN:C	1:B:271:THR:N	2.79	0.41
1:C:241:LYS:HD3	1:C:261:GLU:HB3	2.03	0.41
1:C:87:ILE:HD12	1:C:87:ILE:HA	1.78	0.41
1:C:244:VAL:HG13	1:C:295:ALA:HB1	2.03	0.41
1:C:60:THR:HG22	1:C:291:MSE:H	1.85	0.41
1:A:105:TYR:CZ	1:A:109:LYS:HD2	2.55	0.41
1:B:244:VAL:O	1:B:257:ASP:HB2	2.22	0.40
1:B:59:ARG:HH11	1:B:59:ARG:HB2	1.86	0.40
1:A:135:THR:C	1:A:137:TYR:H	2.29	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	225/277 (81%)	213 (95%)	8 (4%)	4 (2%)	6	16
1	B	219/277 (79%)	209 (95%)	7 (3%)	3 (1%)	9	22
1	C	245/277 (88%)	236 (96%)	6 (2%)	3 (1%)	10	25
1	D	220/277 (79%)	208 (94%)	9 (4%)	3 (1%)	9	22
All	All	909/1108 (82%)	866 (95%)	30 (3%)	13 (1%)	9	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	C	236	LYS
1	C	238	GLU
1	D	136	GLN
1	A	136	GLN
1	B	263	SER
1	B	268	ASP
1	A	211	PRO
1	A	263	SER
1	C	235	LEU
1	D	255	PRO
1	B	270	THR
1	D	134	GLY

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	184/220 (84%)	163 (89%)	21 (11%)	5	13
1	B	178/220 (81%)	155 (87%)	23 (13%)	4	10
1	C	199/220 (90%)	168 (84%)	31 (16%)	2	6
1	D	178/220 (81%)	164 (92%)	14 (8%)	11	27
All	All	739/880 (84%)	650 (88%)	89 (12%)	5	12

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	72	VAL
1	A	75	ILE
1	A	87	ILE
1	A	116	GLN
1	A	121	ILE
1	A	147	LEU
1	A	158	THR
1	A	166	THR
1	A	169	ILE
1	A	183	ARG
1	A	189	VAL
1	A	201	THR
1	A	206	VAL
1	A	216	VAL
1	A	220	SER
1	A	244	VAL
1	A	253	LYS
1	A	264	ASP
1	A	270	THR
1	A	293	VAL
1	B	56	LEU
1	B	59	ARG
1	B	72	VAL
1	B	87	ILE
1	B	120	ASN
1	B	121	ILE
1	B	142	GLU
1	B	147	LEU
1	B	169	ILE
1	B	183	ARG
1	B	189	VAL
1	B	194	LEU

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Mol	Chain	Res	Type
1	B	206	VAL
1	B	216	VAL
1	B	243	LYS
1	B	252	ILE
1	B	256	GLN
1	B	262	PHE
1	B	270	THR
1	B	275	THR
1	B	277	ARG
1	B	287	MSE
1	B	293	VAL
1	C	56	LEU
1	C	60	THR
1	C	72	VAL
1	C	87	ILE
1	C	116	GLN
1	C	135	THR
1	C	138	ILE
1	C	145	GLN
1	C	157	VAL
1	C	169	ILE
1	C	189	VAL
1	C	196	GLN
1	C	201	THR
1	C	206	VAL
1	C	216	VAL
1	C	220	SER
1	C	223	MSE
1	C	226	LEU
1	C	229	GLU
1	C	235	LEU
1	C	237	GLN
1	C	238	GLU
1	C	244	VAL
1	C	246	LEU
1	C	247	ILE
1	C	253	LYS
1	C	257	ASP
1	C	265	VAL
1	C	274	ILE
1	C	277	ARG
1	C	299	GLU

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Mol	Chain	Res	Type
1	D	60	THR
1	D	72	VAL
1	D	75	ILE
1	D	87	ILE
1	D	92	SER
1	D	128	ARG
1	D	133	LEU
1	D	169	ILE
1	D	189	VAL
1	D	196	GLN
1	D	216	VAL
1	D	244	VAL
1	D	256	GLN
1	D	270	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	207	GLN
1	A	269	GLN
1	B	116	GLN
1	B	151	GLN
1	B	207	GLN
1	B	218	GLN
1	C	71	GLN
1	C	80	ASN
1	C	120	ASN
1	C	141	GLN
1	C	154	ASN
1	C	218	GLN
1	C	221	ASN
1	C	237	GLN
1	D	71	GLN
1	D	80	ASN
1	D	95	GLN
1	D	197	ASN
1	D	199	GLN
1	D	208	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](#)

There are no ligands in this entry.

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	225/277 (81%)	1.16	43 (19%)	3 3	33, 62, 67, 72	5 (2%)
1	B	220/277 (79%)	1.11	30 (13%)	7 6	28, 60, 68, 74	6 (2%)
1	C	242/277 (87%)	0.85	35 (14%)	6 5	52, 61, 66, 70	0
1	D	221/277 (79%)	1.60	70 (31%)	1 1	34, 62, 69, 71	5 (2%)
All	All	908/1108 (81%)	1.17	178 (19%)	3 3	28, 61, 68, 74	16 (1%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	285	HIS	7.5
1	B	211	PRO	6.5
1	D	282	ASN	6.3
1	A	211	PRO	6.0
1	A	212	ILE	5.6
1	A	292	PHE	5.6
1	B	210	ASP	5.3
1	D	293	VAL	5.2
1	D	292	PHE	5.2
1	D	283	PRO	5.1
1	D	286	THR	5.0
1	B	134	GLY	4.9
1	D	211	PRO	4.7
1	A	290	GLY	4.6
1	D	248	THR	4.6
1	B	289	PRO	4.6
1	D	289	PRO	4.6
1	D	210	ASP	4.5
1	C	249	SER	4.5
1	C	219	SER	4.4
1	D	137	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	212	ILE	4.3
1	B	282	ASN	4.3
1	D	256	GLN	4.3
1	D	264	ASP	4.1
1	B	283	PRO	4.0
1	B	290	GLY	4.0
1	D	247	ILE	4.0
1	D	167	ALA	4.0
1	A	289	PRO	3.9
1	B	285	HIS	3.9
1	D	266	THR	3.9
1	C	276	LEU	3.9
1	A	210	ASP	3.9
1	A	241	LYS	3.9
1	D	134	GLY	3.8
1	A	172	ALA	3.7
1	D	251	GLY	3.7
1	B	248	THR	3.7
1	C	210	ASP	3.7
1	A	286	THR	3.7
1	B	247	ILE	3.7
1	A	148	ALA	3.6
1	D	105	TYR	3.6
1	B	167	ALA	3.6
1	D	272	GLY	3.5
1	D	267	VAL	3.5
1	B	212	ILE	3.5
1	D	271	THR	3.5
1	D	268	ASP	3.5
1	B	267	VAL	3.5
1	D	284	ASP	3.5
1	D	169	ILE	3.4
1	D	101	TYR	3.4
1	B	262	PHE	3.4
1	D	290	GLY	3.3
1	D	240	GLY	3.3
1	B	286	THR	3.3
1	C	275	THR	3.3
1	C	292	PHE	3.3
1	C	274	ILE	3.3
1	A	275	THR	3.2
1	D	255	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	135	THR	3.2
1	B	120	ASN	3.2
1	A	209	LEU	3.2
1	B	135	THR	3.2
1	A	252	ILE	3.1
1	A	266	THR	3.1
1	B	252	ILE	3.1
1	C	213	TYR	3.1
1	D	90	GLY	3.1
1	C	267	VAL	3.1
1	A	282	ASN	3.1
1	D	252	ILE	3.1
1	D	250	ASP	3.0
1	D	277	ARG	3.0
1	B	254	PHE	3.0
1	A	214	VAL	3.0
1	C	216	VAL	3.0
1	C	273	SER	3.0
1	A	249	SER	3.0
1	A	221	ASN	3.0
1	A	271	THR	3.0
1	C	214	VAL	3.0
1	A	213	TYR	2.9
1	C	265	VAL	2.9
1	C	225	ARG	2.9
1	C	57	PRO	2.9
1	A	256	GLN	2.9
1	D	109	LYS	2.9
1	B	292	PHE	2.9
1	C	222	ASP	2.8
1	D	279	ILE	2.8
1	A	215	ASP	2.8
1	D	54	THR	2.8
1	D	91	VAL	2.8
1	A	273	SER	2.8
1	B	219	SER	2.8
1	D	88	GLU	2.8
1	B	284	ASP	2.7
1	B	169	ILE	2.7
1	C	266	THR	2.7
1	A	247	ILE	2.7
1	D	149	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	241	LYS	2.7
1	B	281	PRO	2.7
1	A	208	GLN	2.6
1	D	249	SER	2.6
1	C	217	THR	2.6
1	A	293	VAL	2.6
1	B	189	VAL	2.6
1	D	62	ALA	2.6
1	D	141	GLN	2.6
1	A	84	GLY	2.6
1	A	251	GLY	2.6
1	C	272	GLY	2.6
1	D	214	VAL	2.6
1	A	254	PHE	2.6
1	D	213	TYR	2.6
1	A	89	ALA	2.6
1	C	293	VAL	2.6
1	A	280	PHE	2.5
1	C	148	ALA	2.5
1	D	190	THR	2.5
1	B	100	THR	2.5
1	D	245	SER	2.5
1	C	257	ASP	2.4
1	C	229	GLU	2.4
1	A	272	GLY	2.4
1	D	254	PHE	2.4
1	D	262	PHE	2.4
1	A	270	THR	2.4
1	C	270	THR	2.4
1	C	298	GLU	2.4
1	C	236	LYS	2.4
1	D	246	LEU	2.4
1	D	111	ASP	2.4
1	A	277	ARG	2.3
1	B	103	ALA	2.3
1	D	64	ARG	2.3
1	D	84	GLY	2.3
1	A	285	HIS	2.3
1	D	270	THR	2.3
1	A	218	GLN	2.3
1	B	256	GLN	2.3
1	C	237	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	THR	2.2
1	D	63	TYR	2.2
1	D	57	PRO	2.2
1	D	219	SER	2.2
1	C	254	PHE	2.2
1	A	103	ALA	2.2
1	A	162	ALA	2.2
1	A	278	ALA	2.2
1	D	280	PHE	2.2
1	A	242	ALA	2.2
1	C	221	ASN	2.2
1	D	208	GLN	2.2
1	A	138	ILE	2.2
1	D	138	ILE	2.2
1	D	164	VAL	2.2
1	D	189	VAL	2.2
1	C	262	PHE	2.2
1	C	277	ARG	2.1
1	A	246	LEU	2.1
1	A	281	PRO	2.1
1	D	133	LEU	2.1
1	C	215	ASP	2.1
1	D	265	VAL	2.1
1	C	253	LYS	2.1
1	C	218	GLN	2.1
1	C	54	THR	2.1
1	D	116	GLN	2.1
1	D	275	THR	2.0
1	B	56	LEU	2.0
1	D	216	VAL	2.0
1	D	102	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.