



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:30 PM UTC

PDB ID : 5X5L / pdb_00005x5l
Title : Crystal structure of response regulator AdeR DNA binding domain in complex with an intercistronic region
Authors : Wen, Y.
Deposited on : 2017-02-16
Resolution : 2.75 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

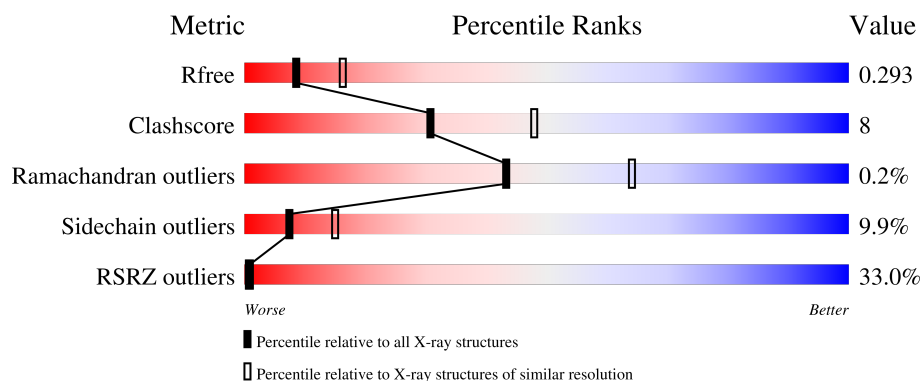
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	109	22% 61% 22% 5% 13%
1	B	109	29% 66% 16% 6% 13%
1	E	109	32% 70% 17% • 10%
1	H	109	33% 68% 17% • 13%
1	M	109	27% 67% 15% • 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N	109	28%56%22%••18%
2	C	25	32%68%24%••
2	F	25	28%72%20%••
3	D	25	20%84%8%8%
3	G	25	52%72%20%8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6667 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 AdeR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			782	497	137	143	5			
1	B	95	Total	C	N	O	S	0	0	0
			775	491	135	144	5			
1	E	98	Total	C	N	O	S	0	0	0
			809	511	143	150	5			
1	H	95	Total	C	N	O	S	0	0	0
			779	494	136	144	5			
1	M	93	Total	C	N	O	S	0	0	0
			767	487	135	140	5			
1	N	89	Total	C	N	O	S	0	0	0
			741	471	130	135	5			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*AP*AP*GP*TP*GP*TP*GP*GP*AP*GP*TP*AP*AP*GP*TP*GP*TP*GP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	24	Total	C	N	O	P	0	0	0
			508	240	102	142	24			
2	F	24	Total	C	N	O	P	0	0	0
			508	240	102	142	24			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*CP*TP*CP*CP*AP*CP*AP*CP*TP*TP*AP*CP*TP*CP*CP*AP*CP*AP*CP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	25	Total	C	N	O	P	0	0	0
			496	240	78	153	25			
3	G	25	Total	C	N	O	P	0	0	0
			495	240	78	152	25			

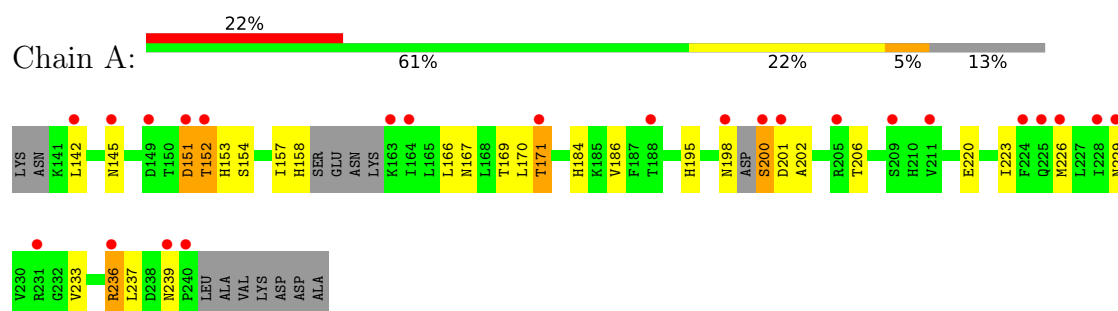
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	O 2	0	0
4	M	1	Total 1	O 1	0	0
4	N	2	Total 2	O 2	0	0
4	C	2	Total 2	O 2	0	0

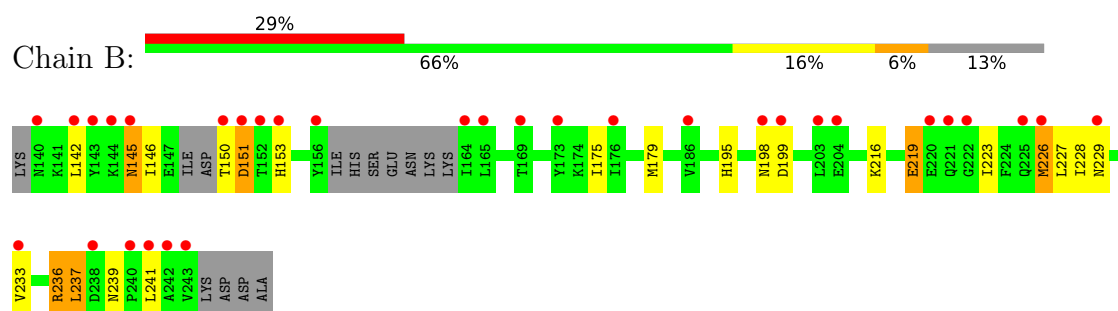
3 Residue-property plots [i](#)

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.

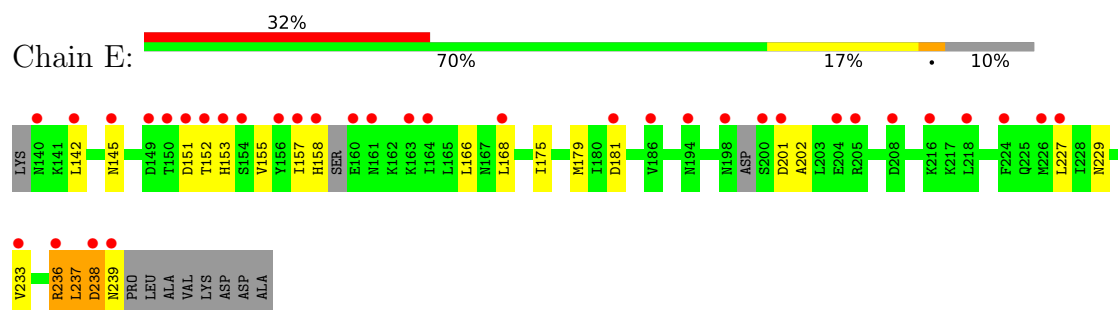
• Molecule 1: AdeR



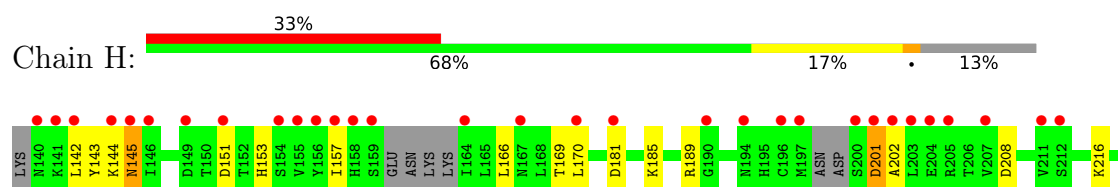
• Molecule 1: AdeR

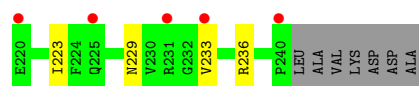


• Molecule 1: AdeR

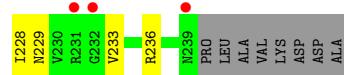
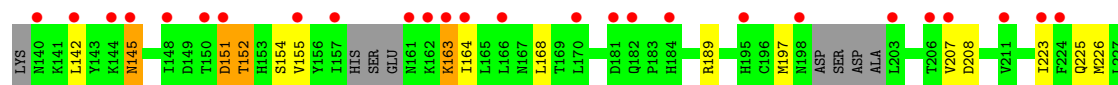


• Molecule 1: AdeR

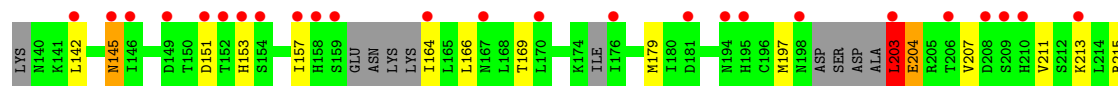




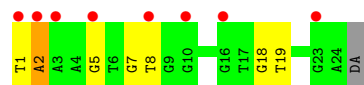
• Molecule 1: AdeR



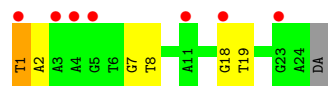
• Molecule 1: AdeR



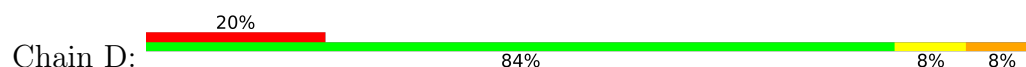
• Molecule 2: DNA (5'-D(P*TP*AP*AP*AP*GP*TP*GP*TP*GP*GP*AP*GP*TP*AP*AP*G
P*TP*GP*TP*GP*GP*AP*GP*A)-3')



• Molecule 2: DNA (5'-D(P*TP*AP*AP*AP*GP*TP*GP*TP*GP*GP*AP*GP*TP*AP*AP*G
P*TP*GP*TP*GP*GP*AP*GP*A)-3')

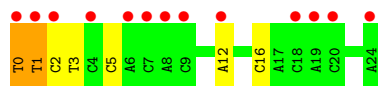


• Molecule 3: DNA (5'-D(P*TP*CP*TP*CP*CP*AP*CP*AP*CP*TP*TP*AP*CP*TP*CP*C
P*AP*CP*AP*CP*TP*TP*TP*A)-3')



- Molecule 3: DNA (5'-D(P*TP*CP*TP*CP*CP*AP*CP*AP*CP*TP*TP*AP*CP*TP*CP*CP*AP*CP*AP*CP*TP*TP*TP*A)-3')

Chain G: 52% 72% 20% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.51Å 71.38Å 78.36Å 101.96° 104.53° 101.86°	Depositor
Resolution (Å)	43.82 – 2.75 43.82 – 2.75	Depositor EDS
% Data completeness (in resolution range)	83.0 (43.82-2.75) 83.0 (43.82-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0171	Depositor
R, R_{free}	0.278 , 0.296 0.274 , 0.293	Depositor DCC
R_{free} test set	2000 reflections (7.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.921	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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

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	0.79	0/793	1.10	5/1063 (0.5%)
1	B	0.73	1/785 (0.1%)	0.97	3/1054 (0.3%)
1	E	0.68	0/819	0.90	0/1096
1	H	0.66	0/790	0.91	1/1060 (0.1%)
1	M	0.74	0/776	1.00	1/1039 (0.1%)
1	N	0.71	0/749	0.99	2/1000 (0.2%)
2	C	0.40	0/573	0.86	1/886 (0.1%)
2	F	0.39	0/573	0.87	1/886 (0.1%)
3	D	0.43	0/551	0.89	2/844 (0.2%)
3	G	0.58	1/550 (0.2%)	0.93	2/841 (0.2%)
All	All	0.65	2/6959 (0.0%)	0.95	18/9769 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	0	DT	P-OP2	8.44	1.65	1.48
1	B	226	MET	C-O	-7.09	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	CA-CB-CG	9.96	134.02	114.10
1	M	163	LYS	N-CA-C	-8.95	85.94	111.00
1	H	201	ASP	N-CA-CB	7.82	120.07	110.53
1	B	226	MET	CA-C-O	-7.74	112.20	120.71
1	B	219	GLU	CA-CB-CG	7.19	128.48	114.10
2	F	1	DT	C4'-C3'-O3'	7.02	120.53	110.00
1	N	203	LEU	CB-CA-C	6.90	123.22	110.10
2	C	2	DA	C4'-C3'-O3'	6.74	120.11	110.00
1	A	200	SER	CB-CA-C	6.19	121.87	110.10
3	D	1	DT	C4'-C3'-O3'	6.01	119.02	110.00
3	G	1	DT	C4'-C3'-O3'	5.79	118.69	110.00
3	G	12	DA	C2'-C3'-O3'	-5.59	103.11	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	203	LEU	N-CA-C	-5.30	96.15	111.00
1	A	152	THR	CA-C-N	5.27	131.61	121.54
1	A	152	THR	C-N-CA	5.27	131.61	121.54
1	A	171	THR	CA-CB-CG2	5.19	119.32	110.50
1	B	151	ASP	N-CA-C	-5.14	105.37	111.69
3	D	0	DT	N1-C1'-C2'	5.04	121.06	113.50

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	782	0	797	27	0
1	B	775	0	786	15	0
1	E	809	0	821	18	0
1	H	779	0	789	16	0
1	M	767	0	783	11	0
1	N	741	0	752	15	0
2	C	508	0	271	5	0
2	F	508	0	271	3	0
3	D	496	0	285	7	0
3	G	495	0	285	9	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
All	All	6667	0	5840	104	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 8.

All (104) 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:N:226:MET:O	1:N:237:LEU:O	1.79	1.00
1:A:151:ASP:HA	1:A:152:THR:CG2	2.02	0.89
1:H:169:THR:HG21	3:D:14:DT:OP2	1.73	0.89
1:A:169:THR:HG21	3:G:3:DT:OP2	1.73	0.89
1:B:146:ILE:HD12	1:B:226:MET:HE2	1.57	0.86
1:A:151:ASP:HA	1:A:152:THR:HG23	1.58	0.84
1:E:166:LEU:HB3	1:E:168:LEU:CD1	2.14	0.78
1:A:186:VAL:HG22	1:A:236:ARG:HG3	1.66	0.75
1:B:226:MET:O	1:B:228:ILE:HD12	1.87	0.74
1:A:198:ASN:HB3	1:H:185:LYS:HE3	1.70	0.72
1:N:179:MET:HE1	1:N:227:LEU:HD22	1.72	0.71
1:A:151:ASP:CA	1:A:152:THR:HG23	2.22	0.70
1:H:169:THR:HG21	3:D:14:DT:P	2.31	0.70
1:N:203:LEU:HG	1:N:204:GLU:H	1.58	0.68
1:M:223:ILE:CG2	1:M:226:MET:HG3	2.26	0.65
1:M:151:ASP:OD1	1:M:152:THR:N	2.30	0.65
1:E:179:MET:HE1	1:E:227:LEU:CD2	2.28	0.64
1:M:197:MET:HE1	1:M:207:VAL:HG13	1.80	0.64
1:A:223:ILE:CG2	1:A:226:MET:HG3	2.28	0.64
1:B:146:ILE:CD1	1:B:226:MET:HE2	2.26	0.64
1:H:143:TYR:CZ	1:H:144:LYS:HD3	2.32	0.63
1:B:179:MET:HE1	1:B:227:LEU:HD22	1.80	0.63
1:N:197:MET:HE1	1:N:207:VAL:HG13	1.80	0.63
1:A:169:THR:HG21	3:G:3:DT:P	2.40	0.61
1:H:169:THR:CG2	3:D:14:DT:P	2.89	0.61
1:M:189:ARG:NH1	1:M:208:ASP:OD1	2.34	0.61
1:A:169:THR:CG2	3:G:3:DT:P	2.89	0.60
1:E:236:ARG:HD3	1:E:239:ASN:ND2	2.17	0.60
1:H:189:ARG:NH1	1:H:208:ASP:OD1	2.34	0.59
1:N:215:ARG:NH1	1:N:227:LEU:O	2.36	0.59
1:A:151:ASP:HA	1:A:152:THR:HG22	1.83	0.59
1:N:164:ILE:HD12	1:N:164:ILE:N	2.19	0.58
2:F:1:DT:H4'	2:F:2:DA:OP1	2.03	0.57
1:A:198:ASN:HB3	1:H:185:LYS:CE	2.35	0.56
1:A:200:SER:HB2	1:A:202:ALA:N	2.21	0.56
1:E:155:VAL:HG23	1:E:166:LEU:HB2	1.87	0.56
1:B:216:LYS:HA	1:B:219:GLU:HG2	1.89	0.55
1:E:175:ILE:CG2	1:E:179:MET:HE2	2.38	0.54
1:A:167:ASN:HD22	1:N:169:THR:HA	1.73	0.54
1:A:184:HIS:O	1:E:152:THR:HG22	2.07	0.54
1:A:169:THR:HG23	3:G:2:DC:H3'	1.89	0.53
1:A:200:SER:HB3	1:A:201:ASP:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:LYS:NZ	2:C:8:DT:OP1	2.41	0.53
1:B:175:ILE:CG2	1:B:179:MET:HE2	2.39	0.52
1:M:223:ILE:HG22	1:M:226:MET:HG3	1.91	0.52
1:B:175:ILE:HG22	1:B:179:MET:HE2	1.93	0.51
1:H:169:THR:HG22	1:H:170:LEU:N	2.26	0.50
1:B:179:MET:HE1	1:B:227:LEU:CD2	2.41	0.50
1:B:226:MET:HE3	1:B:237:LEU:HD22	1.94	0.48
1:B:226:MET:HE3	1:B:237:LEU:CD2	2.43	0.48
1:N:221:GLN:CG	1:N:223:ILE:N	2.77	0.48
3:G:0:DT:H2'	3:G:1:DT:C2	2.49	0.48
1:A:200:SER:HB3	1:A:201:ASP:C	2.38	0.48
1:E:145:ASN:OD1	1:E:158:HIS:HB2	2.13	0.48
1:M:225:GLN:O	1:M:228:ILE:HD11	2.14	0.48
1:E:237:LEU:O	1:E:238:ASP:C	2.57	0.47
1:A:145:ASN:OD1	1:A:158:HIS:HB2	2.14	0.47
1:E:157:ILE:HG12	1:E:166:LEU:HD11	1.96	0.47
1:H:145:ASN:HD21	1:H:223:ILE:HD11	1.79	0.47
3:D:0:DT:H2'	3:D:1:DT:C2	2.49	0.47
1:A:169:THR:HG22	1:A:170:LEU:N	2.28	0.47
1:A:157:ILE:HG12	1:A:166:LEU:HD11	1.97	0.47
1:E:179:MET:HE1	1:E:227:LEU:HD21	1.97	0.47
2:C:1:DT:H2''	2:C:2:DA:C8	2.50	0.47
2:F:18:DG:H2''	2:F:19:DT:H72	1.96	0.46
1:M:145:ASN:HD21	1:M:223:ILE:HD11	1.80	0.46
1:E:155:VAL:HG23	1:E:155:VAL:O	2.15	0.46
1:H:157:ILE:HG12	1:H:166:LEU:HD11	1.97	0.46
1:E:236:ARG:HD3	1:E:239:ASN:HD21	1.80	0.46
1:H:189:ARG:NH2	2:C:5:DG:OP1	2.50	0.45
1:N:221:GLN:HG3	1:N:223:ILE:N	2.31	0.45
1:B:236:ARG:HD2	1:B:239:ASN:HA	1.98	0.45
1:E:202:ALA:HB1	3:G:16:DC:OP2	2.16	0.45
1:A:200:SER:CB	1:A:202:ALA:N	2.80	0.45
1:B:145:ASN:HD21	1:B:223:ILE:HD11	1.81	0.45
1:H:169:THR:CG2	3:D:14:DT:OP1	2.65	0.45
1:B:195:HIS:NE2	1:E:181:ASP:OD1	2.50	0.44
1:N:145:ASN:HD21	1:N:223:ILE:HD11	1.83	0.44
1:A:198:ASN:HB2	1:A:200:SER:N	2.33	0.44
1:A:202:ALA:HB1	3:G:5:DC:OP2	2.18	0.44
1:N:225:GLN:O	1:N:228:ILE:HD11	2.18	0.44
1:M:151:ASP:OD1	1:M:151:ASP:C	2.61	0.44
1:N:211:VAL:HG11	1:N:235:TYR:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:DG:H2''	2:F:8:DT:H72	1.99	0.43
1:B:226:MET:HG3	1:B:237:LEU:HD22	1.98	0.43
1:E:155:VAL:CG2	1:E:166:LEU:HB2	2.49	0.43
1:H:202:ALA:HB1	3:D:16:DC:OP2	2.19	0.42
1:A:195:HIS:NE2	1:H:181:ASP:OD1	2.53	0.42
1:N:233:VAL:HG22	1:N:234:GLY:N	2.34	0.42
1:N:157:ILE:HG12	1:N:166:LEU:HD11	2.02	0.42
1:E:175:ILE:HG22	1:E:179:MET:HE2	2.02	0.42
1:M:152:THR:HB	1:M:154:SER:OG	2.20	0.41
2:C:7:DG:H2''	2:C:8:DT:H72	2.01	0.41
1:N:233:VAL:CG2	1:N:234:GLY:N	2.83	0.41
1:A:206:THR:OG1	3:G:5:DC:OP2	2.35	0.41
1:H:169:THR:HG22	3:D:14:DT:OP1	2.20	0.41
1:E:236:ARG:HG3	1:E:237:LEU:O	2.20	0.41
1:A:169:THR:CG2	3:G:2:DC:H3'	2.51	0.41
1:A:223:ILE:HG22	1:A:226:MET:HG3	2.01	0.41
1:M:155:VAL:HG21	1:M:168:LEU:HD11	2.02	0.41
2:C:18:DG:H2''	2:C:19:DT:H72	2.03	0.41
1:E:237:LEU:O	1:E:238:ASP:O	2.39	0.41
1:M:163:LYS:H	1:M:164:ILE:HD12	1.85	0.40
1:B:198:ASN:O	1:B:199:ASP:C	2.63	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	89/109 (82%)	86 (97%)	3 (3%)	0	100	100
1	B	89/109 (82%)	85 (96%)	4 (4%)	0	100	100
1	E	92/109 (84%)	87 (95%)	4 (4%)	1 (1%)	11	22
1	H	89/109 (82%)	85 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	87/109 (80%)	83 (95%)	4 (5%)	0	100	100
1	N	79/109 (72%)	75 (95%)	4 (5%)	0	100	100
All	All	525/654 (80%)	501 (95%)	23 (4%)	1 (0%)	43	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	238	ASP

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	90/102 (88%)	80 (89%)	10 (11%)	6	11
1	B	89/102 (87%)	79 (89%)	10 (11%)	6	11
1	E	93/102 (91%)	85 (91%)	8 (9%)	10	18
1	H	90/102 (88%)	82 (91%)	8 (9%)	9	17
1	M	88/102 (86%)	81 (92%)	7 (8%)	11	20
1	N	86/102 (84%)	76 (88%)	10 (12%)	5	10
All	All	536/612 (88%)	483 (90%)	53 (10%)	7	15

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	A	151	ASP
1	A	153	HIS
1	A	154	SER
1	A	171	THR
1	A	220	GLU
1	A	229	ASN
1	A	233	VAL
1	A	237	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	ASN
1	B	142	LEU
1	B	145	ASN
1	B	150	THR
1	B	151	ASP
1	B	153	HIS
1	B	229	ASN
1	B	233	VAL
1	B	236	ARG
1	B	237	LEU
1	B	241	LEU
1	E	142	LEU
1	E	151	ASP
1	E	153	HIS
1	E	201	ASP
1	E	229	ASN
1	E	233	VAL
1	E	236	ARG
1	E	237	LEU
1	H	142	LEU
1	H	145	ASN
1	H	151	ASP
1	H	153	HIS
1	H	201	ASP
1	H	229	ASN
1	H	233	VAL
1	H	236	ARG
1	M	142	LEU
1	M	145	ASN
1	M	151	ASP
1	M	152	THR
1	M	229	ASN
1	M	233	VAL
1	M	236	ARG
1	N	142	LEU
1	N	145	ASN
1	N	151	ASP
1	N	153	HIS
1	N	203	LEU
1	N	204	GLU
1	N	213	LYS
1	N	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	233	VAL
1	N	236	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	198	ASN
1	B	145	ASN
1	B	239	ASN
1	E	140	ASN
1	E	239	ASN
1	H	145	ASN
1	H	239	ASN
1	M	145	ASN
1	M	153	HIS
1	N	145	ASN

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 ⓘ

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	95/109 (87%)	1.62	24 (25%) 1 1	41, 50, 66, 76	0
1	B	95/109 (87%)	1.86	32 (33%) 1 0	43, 52, 73, 87	0
1	E	98/109 (89%)	1.66	35 (35%) 1 0	43, 52, 65, 82	0
1	H	95/109 (87%)	1.75	36 (37%) 1 0	45, 58, 73, 92	0
1	M	93/109 (85%)	1.75	29 (31%) 1 1	45, 55, 68, 75	0
1	N	89/109 (81%)	1.81	30 (33%) 1 0	40, 52, 66, 72	0
2	C	24/25 (96%)	1.65	8 (33%) 1 0	50, 62, 73, 83	0
2	F	24/25 (96%)	1.72	7 (29%) 1 1	50, 61, 72, 79	0
3	D	25/25 (100%)	1.40	5 (20%) 3 2	48, 58, 77, 86	0
3	G	25/25 (100%)	2.07	13 (52%) 0 0	60, 71, 85, 88	0
All	All	663/754 (87%)	1.73	219 (33%) 1 1	40, 55, 73, 92	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	203	LEU	6.5
1	H	159	SER	5.5
1	B	242	ALA	5.3
1	A	145	ASN	5.0
1	B	164	ILE	5.0
1	A	198	ASN	4.8
1	B	145	ASN	4.7
1	B	243	VAL	4.7
1	A	240	PRO	4.6
1	H	156	TYR	4.2
1	N	221	GLN	4.1
3	G	1	DT	4.1
1	M	181	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	164	ILE	4.0
1	B	165	LEU	3.9
1	B	150	THR	3.8
1	M	203	LEU	3.8
1	E	198	ASN	3.8
1	E	158	HIS	3.8
1	B	140	ASN	3.7
1	M	161	ASN	3.7
1	N	176	ILE	3.7
1	E	149	ASP	3.7
1	H	140	ASN	3.6
1	E	224	PHE	3.6
1	M	198	ASN	3.6
1	B	226	MET	3.5
1	M	162	LYS	3.5
1	M	164	ILE	3.5
1	E	145	ASN	3.5
1	M	151	ASP	3.5
1	H	204	GLU	3.5
3	G	8	DA	3.5
1	A	201	ASP	3.4
3	D	1	DT	3.4
1	B	241	LEU	3.4
1	E	233	VAL	3.4
1	N	224	PHE	3.4
1	M	231	ARG	3.3
1	N	158	HIS	3.3
1	H	157	ILE	3.3
1	B	142	LEU	3.2
1	A	163	LYS	3.2
1	M	145	ASN	3.2
1	H	158	HIS	3.2
1	H	142	LEU	3.2
1	N	225	GLN	3.2
1	M	207	VAL	3.2
1	N	159	SER	3.1
1	M	140	ASN	3.1
3	G	9	DC	3.1
1	N	145	ASN	3.1
1	A	239	ASN	3.1
1	B	238	ASP	3.1
1	M	195	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	144	LYS	3.1
1	E	156	TYR	3.0
1	E	239	ASN	3.0
1	A	151	ASP	3.0
1	N	213	LYS	3.0
1	A	231	ARG	3.0
1	B	156	TYR	3.0
1	A	149	ASP	3.0
1	E	160	GLU	3.0
1	B	186	VAL	2.9
1	N	198	ASN	2.9
1	E	204	GLU	2.9
1	A	225	GLN	2.9
1	N	149	ASP	2.9
1	A	142	LEU	2.9
1	N	153	HIS	2.9
1	H	202	ALA	2.9
1	M	142	LEU	2.9
1	B	176	ILE	2.8
1	H	233	VAL	2.8
1	H	145	ASN	2.8
1	B	144	LYS	2.8
1	E	201	ASP	2.8
1	H	155	VAL	2.8
1	M	184	HIS	2.8
1	B	222	GLY	2.8
3	G	24	DA	2.8
1	N	164	ILE	2.7
1	N	142	LEU	2.7
1	E	164	ILE	2.7
1	H	170	LEU	2.7
1	M	166	LEU	2.7
1	A	209	SER	2.7
1	M	239	ASN	2.7
1	E	157	ILE	2.7
1	E	161	ASN	2.7
1	N	157	ILE	2.6
3	G	20	DC	2.6
1	H	194	ASN	2.6
1	A	152	THR	2.6
1	B	199	ASP	2.6
2	F	23	DG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	205	ARG	2.6
1	H	205	ARG	2.6
3	G	7	DC	2.6
1	B	233	VAL	2.6
1	N	209	SER	2.6
1	B	169	THR	2.6
2	C	16	DG	2.6
1	B	225	GLN	2.6
1	H	200	SER	2.6
1	N	208	ASP	2.6
1	E	216	LYS	2.6
1	A	171	THR	2.5
1	E	151	ASP	2.5
1	A	164	ILE	2.5
1	E	153	HIS	2.5
1	E	140	ASN	2.5
1	H	212	SER	2.5
2	F	5	DG	2.5
1	E	181	ASP	2.5
1	N	146	ILE	2.5
3	D	8	DA	2.5
2	F	1	DT	2.5
1	H	196	CYS	2.5
1	H	203	LEU	2.5
1	M	223	ILE	2.5
3	D	18	DC	2.5
1	B	152	THR	2.4
1	H	146	ILE	2.4
1	N	154	SER	2.4
1	N	151	ASP	2.4
1	N	210	HIS	2.4
2	C	23	DG	2.4
1	N	152	THR	2.4
1	N	223	ILE	2.4
1	H	201	ASP	2.4
1	A	211	VAL	2.4
2	C	10	DG	2.4
1	N	238	ASP	2.4
1	B	221	GLN	2.4
1	M	182	GLN	2.4
1	H	207	VAL	2.4
1	A	236	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	2	DC	2.4
1	H	240	PRO	2.4
3	G	0	DT	2.4
1	B	173	TYR	2.3
1	M	157	ILE	2.3
1	E	200	SER	2.3
1	H	141	LYS	2.3
1	H	190	GLY	2.3
1	E	227	LEU	2.3
1	N	167	ASN	2.3
1	M	155	VAL	2.3
1	M	150	THR	2.3
1	H	167	ASN	2.3
1	H	151	ASP	2.3
2	C	8	DT	2.3
1	E	163	LYS	2.3
1	E	226	MET	2.3
1	H	149	ASP	2.3
1	H	181	ASP	2.3
1	N	206	THR	2.2
2	C	3	DA	2.2
1	A	205	ARG	2.2
1	M	224	PHE	2.2
2	C	2	DA	2.2
3	G	6	DA	2.2
1	E	208	ASP	2.2
1	M	232	GLY	2.2
1	E	168	LEU	2.2
1	M	163	LYS	2.2
1	A	188	THR	2.2
1	B	220	GLU	2.2
1	M	206	THR	2.2
3	G	19	DA	2.2
1	B	203	LEU	2.2
3	D	20	DC	2.2
1	A	228	ILE	2.2
2	F	11	DA	2.2
3	D	24	DA	2.2
3	G	12	DA	2.2
1	E	150	THR	2.1
2	F	18	DG	2.1
1	B	198	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	204	GLU	2.1
1	E	218	LEU	2.1
1	N	170	LEU	2.1
1	N	181	ASP	2.1
1	A	224	PHE	2.1
1	H	154	SER	2.1
1	H	231	ARG	2.1
3	G	18	DC	2.1
2	F	3	DA	2.1
1	M	144	LYS	2.1
1	H	197	MET	2.1
1	E	142	LEU	2.1
1	N	194	ASN	2.1
1	B	153	HIS	2.1
2	C	5	DG	2.1
1	B	151	ASP	2.1
1	A	200	SER	2.1
1	E	152	THR	2.1
1	A	226	MET	2.1
1	M	170	LEU	2.1
1	B	143	TYR	2.1
1	E	238	ASP	2.0
1	H	220	GLU	2.0
1	E	154	SER	2.0
2	C	1	DT	2.0
2	F	4	DA	2.0
1	A	229	ASN	2.0
1	B	229	ASN	2.0
1	E	194	ASN	2.0
1	M	148	ILE	2.0
1	E	236	ARG	2.0
1	B	240	PRO	2.0
1	H	225	GLN	2.0
1	N	195	HIS	2.0
1	E	186	VAL	2.0
1	H	211	VAL	2.0
1	M	211	VAL	2.0
3	G	4	DC	2.0

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

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.