



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:00 PM UTC

PDB ID : 7RAH / pdb_00007rah
Title : Adenylate cyclase toxin RTX domain fragment bound to M1H5 Fab and M2B10 Fab
Authors : Goldsmith, J.A.; McLellan, J.S.
Deposited on : 2021-07-01
Resolution : 2.60 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

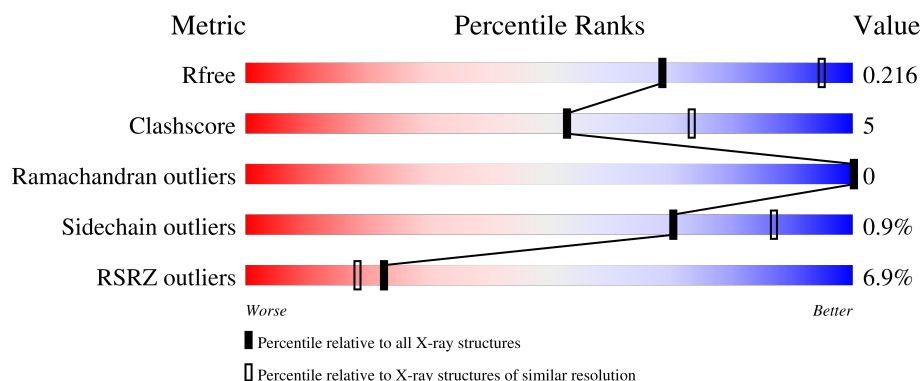
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	215	% 87% 13%
2	B	233	% 90% 6%
3	C	214	12% 77% 10% 14%
4	D	235	20% 69% 16% 15%
5	E	458	% 71% 8% 21%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9183 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 M1H5 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1671	1035	282	347	7			

- Molecule 2 is a protein called M1H5 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1680	1060	278	333	9			

- Molecule 3 is a protein called M2B10 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	185	Total	C	N	O	S	0	0	0
			1395	870	232	286	7			

- Molecule 4 is a protein called M2B10 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1499	948	252	294	5			

- Molecule 5 is a protein called Bifunctional adenylate cyclase toxin/hemolysin CyaA,Bifunctional adenylate cyclase toxin/hemolysin CyaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	360	Total	C	N	O	S	0	0	0
			2726	1664	484	573	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1011	GLY	-	expression tag	UNP A0A380ZZA1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1012	PRO	-	expression tag	UNP A0A380ZZA1
E	1013	GLY	-	expression tag	UNP A0A380ZZA1
E	1014	SER	-	expression tag	UNP A0A380ZZA1

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	19	Total	Ca	0	0
			19	19		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	48	Total	O	0	0
			48	48		
8	B	44	Total	O	0	0
			44	44		
8	C	18	Total	O	0	0
			18	18		

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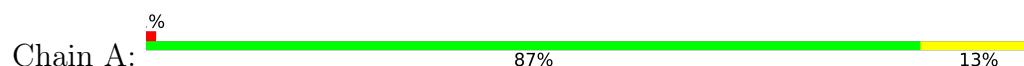
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	10	Total	O	0	0
			10	10		
8	E	68	Total	O	0	0
			68	68		

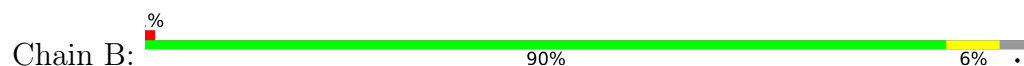
3 Residue-property plots [i](#)

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.

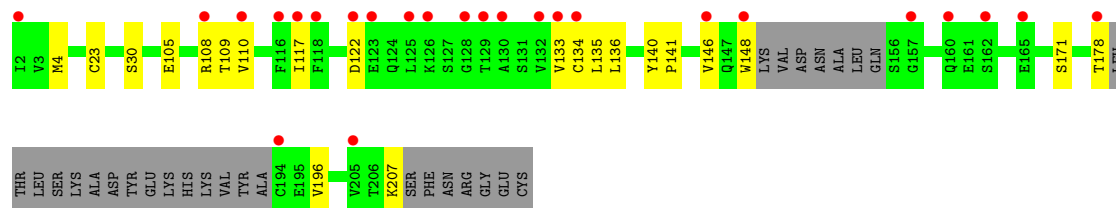
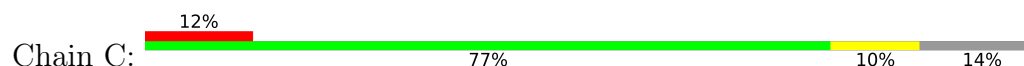
- Molecule 1: M1H5 Fab Light Chain



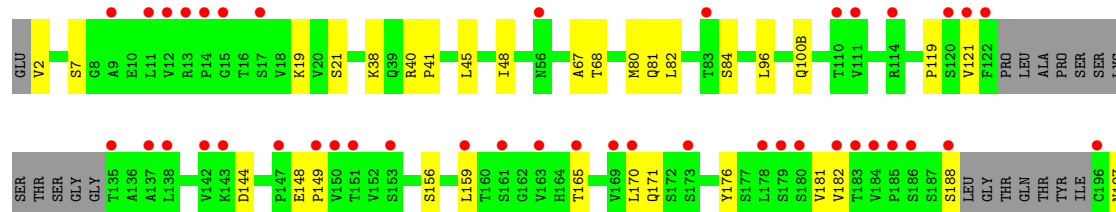
- Molecule 2: M1H5 Fab Heavy Chain

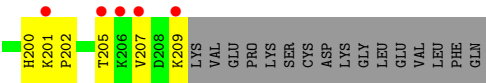


- Molecule 3: M2B10 Fab Light Chain

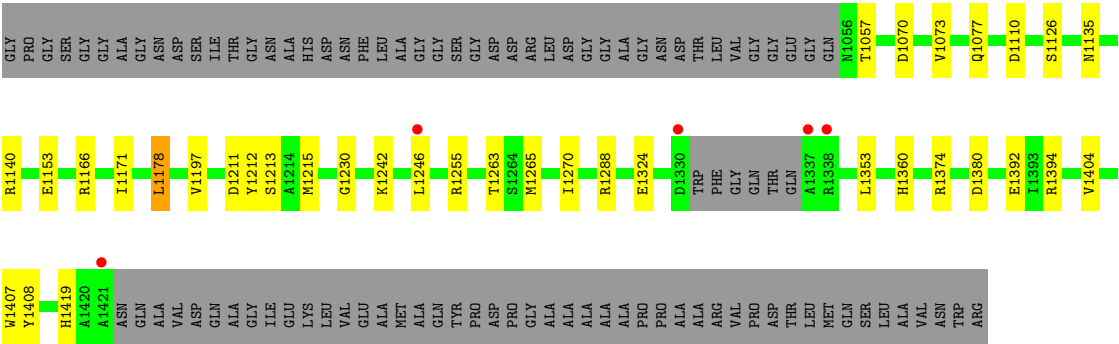


- Molecule 4: M2B10 Fab Heavy Chain





● Molecule 5: Bifunctional adenylate cyclase toxin/hemolysin CyaA, Bifunctional adenylate cyclase toxin/hemolysin CyaA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.56Å 117.02Å 254.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.81 – 2.60 55.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.81-2.60) 99.7 (55.81-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.195 , 0.218 0.194 , 0.216	Depositor DCC
R_{free} test set	3077 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	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	0.94	EDS
Total number of atoms	9183	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: PO4, CA

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	0.09	0/1705	0.29	0/2314
2	B	0.10	0/1721	0.31	0/2339
3	C	0.11	0/1427	0.30	0/1940
4	D	0.11	0/1534	0.33	0/2087
5	E	0.08	0/2772	0.28	0/3756
All	All	0.10	0/9159	0.30	0/12436

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 [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	1671	0	1597	19	0
2	B	1680	0	1644	8	0
3	C	1395	0	1339	12	0
4	D	1499	0	1458	28	0
5	E	2726	0	2493	23	0
6	A	5	0	0	0	0
7	E	19	0	0	0	0
8	A	48	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	44	0	0	3	0
8	C	18	0	0	1	0
8	D	10	0	0	2	0
8	E	68	0	0	6	1
All	All	9183	0	8531	87	1

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 5.

All (87) 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)
5:E:1288:ARG:NH1	8:E:1601:HOH:O	2.00	0.95
1:A:132:SER:O	8:A:401:HOH:O	1.89	0.88
4:D:121:VAL:HG21	4:D:207:VAL:HG11	1.56	0.84
5:E:1360:HIS:ND1	8:E:1603:HOH:O	2.10	0.82
5:E:1324:GLU:OE1	8:E:1602:HOH:O	2.01	0.78
1:A:156:ARG:NH1	8:A:403:HOH:O	2.18	0.73
3:C:105:GLU:OE2	3:C:140:TYR:OH	2.08	0.70
1:A:38:GLN:HG3	1:A:44:VAL:HG22	1.72	0.69
2:B:13:LYS:HG3	8:B:311:HOH:O	1.95	0.66
1:A:166:ASP:OD1	8:A:402:HOH:O	2.13	0.66
4:D:2:VAL:N	8:D:302:HOH:O	2.29	0.65
1:A:191:ASN:HD21	1:A:213:ASN:H	1.47	0.62
4:D:19:LYS:NZ	4:D:81:GLN:HB2	2.14	0.62
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.82	0.60
3:C:171:SER:OG	8:C:301:HOH:O	2.16	0.60
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.68	0.58
1:A:191:ASN:ND2	1:A:213:ASN:H	2.01	0.58
4:D:200:HIS:CD2	4:D:202:PRO:HD2	2.37	0.58
5:E:1324:GLU:HG3	5:E:1353:LEU:HB2	1.85	0.57
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.20	0.57
1:A:29:ILE:HA	1:A:92:ASN:HD22	1.70	0.57
1:A:115:THR:HG23	1:A:138:ASN:HB3	1.87	0.57
3:C:136:LEU:HD21	3:C:196:VAL:HG21	1.88	0.55
4:D:209:LYS:HB2	4:D:209:LYS:NZ	2.21	0.55
4:D:45:LEU:N	8:D:301:HOH:O	2.05	0.54
5:E:1153:GLU:HG2	5:E:1171:ILE:HB	1.89	0.54
4:D:148:GLU:HG2	4:D:149:PRO:HA	1.89	0.54
5:E:1140:ARG:N	8:E:1604:HOH:O	2.15	0.53
5:E:1178:LEU:HD12	5:E:1197:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:SER:HG	4:D:21:SER:H	1.54	0.53
4:D:80:MET:HE3	4:D:82:LEU:HD21	1.90	0.52
1:A:156:ARG:NH1	1:A:182:LEU:HD21	2.24	0.52
4:D:40:ARG:HG2	4:D:41:PRO:HD2	1.92	0.52
5:E:1215:MET:HE2	5:E:1242:LYS:HB2	1.92	0.51
3:C:117:ILE:HD11	3:C:207:LYS:HB3	1.93	0.50
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.94	0.50
3:C:110:VAL:HG12	3:C:141:PRO:HD3	1.93	0.50
4:D:19:LYS:NZ	4:D:81:GLN:OE1	2.45	0.50
1:A:185:ASP:O	1:A:189:ARG:HG3	2.12	0.49
4:D:19:LYS:CE	4:D:81:GLN:HB2	2.42	0.49
3:C:135:LEU:HD22	4:D:181:VAL:HG11	1.95	0.49
5:E:1135:ASN:CG	5:E:1153:GLU:HB2	2.38	0.49
5:E:1211:ASP:OD1	5:E:1213:SER:OG	2.29	0.49
4:D:159:LEU:HD11	4:D:182:VAL:HG11	1.96	0.48
5:E:1057:THR:HG23	5:E:1077:GLN:HB2	1.96	0.48
1:A:191:ASN:OD1	1:A:211:ASN:ND2	2.38	0.47
4:D:68:THR:HB	4:D:81:GLN:HB3	1.95	0.47
2:B:155:ASN:O	8:B:301:HOH:O	2.20	0.47
2:B:165:THR:OG1	8:B:302:HOH:O	2.21	0.46
1:A:124:GLU:N	1:A:124:GLU:OE1	2.47	0.46
4:D:38:LYS:HB2	4:D:48:ILE:HD11	1.97	0.46
3:C:134:CYS:HB2	3:C:148:TRP:CH2	2.51	0.46
4:D:201:LYS:HB3	4:D:202:PRO:HD3	1.98	0.46
3:C:135:LEU:CD2	4:D:181:VAL:HG11	2.47	0.45
5:E:1404:VAL:HG11	5:E:1407:TRP:HD1	1.81	0.45
5:E:1374:ARG:HG2	5:E:1419:HIS:HB2	1.98	0.45
4:D:156:SER:H	4:D:197:ASN:HD21	1.65	0.45
1:A:18:ARG:HG3	1:A:76:SER:HA	1.99	0.45
4:D:96:LEU:HD11	4:D:100(B):GLN:HB3	1.99	0.45
4:D:119:PRO:HD3	4:D:200:HIS:ND1	2.32	0.45
4:D:170:LEU:HB2	4:D:176:TYR:HE1	1.82	0.45
3:C:4:MET:HE3	3:C:23:CYS:SG	2.56	0.44
1:A:24:ARG:NH1	1:A:70:ASP:OD1	2.51	0.43
4:D:119:PRO:HA	4:D:144:ASP:O	2.18	0.43
5:E:1392:GLU:OE2	5:E:1394:ARG:NE	2.48	0.43
5:E:1255:ARG:NE	8:E:1605:HOH:O	2.17	0.43
3:C:133:VAL:HG22	3:C:178:THR:HG23	2.00	0.43
5:E:1073:VAL:HA	5:E:1126:SER:HB2	1.99	0.43
3:C:122:ASP:N	3:C:122:ASP:OD1	2.52	0.43
1:A:14:SER:O	1:A:17:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1070:ASP:OD1	5:E:1070:ASP:C	2.61	0.43
4:D:171:GLN:H	4:D:171:GLN:HG2	1.70	0.42
5:E:1110:ASP:OD1	5:E:1166:ARG:NH1	2.51	0.42
3:C:108:ARG:HG2	3:C:109:THR:N	2.34	0.42
5:E:1212:TYR:O	5:E:1263:THR:HG22	2.20	0.42
2:B:199:ASN:HD22	2:B:206:LYS:HE2	1.85	0.41
4:D:40:ARG:NH2	4:D:84:SER:O	2.53	0.41
2:B:168:ALA:HA	2:B:178:LEU:HB3	2.02	0.41
4:D:67:ALA:HA	4:D:81:GLN:O	2.19	0.41
4:D:119:PRO:HD2	4:D:205:THR:OG1	2.21	0.41
2:B:12:VAL:HG21	2:B:82(C):LEU:HD13	2.02	0.41
4:D:144:ASP:OD1	4:D:171:GLN:NE2	2.54	0.41
5:E:1380:ASP:OD1	5:E:1380:ASP:N	2.49	0.41
1:A:121:PRO:HD3	1:A:133:VAL:HG22	2.03	0.41
5:E:1230:GLY:HA2	5:E:1265:MET:HE3	2.04	0.40
2:B:100:GLY:HA2	5:E:1270:ILE:HD11	2.04	0.40
5:E:1408:TYR:O	8:E:1606:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:1619:HOH:O	8:E:1636:HOH:O[3_555]	2.14	0.06

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	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
2	B	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
3	C	179/214 (84%)	174 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	193/235 (82%)	188 (97%)	5 (3%)	0	100	100
5	E	356/458 (78%)	339 (95%)	17 (5%)	0	100	100
All	All	1162/1355 (86%)	1128 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	193/193 (100%)	192 (100%)	1 (0%)	81	92
2	B	191/200 (96%)	189 (99%)	2 (1%)	68	86
3	C	161/186 (87%)	159 (99%)	2 (1%)	63	83
4	D	169/200 (84%)	167 (99%)	2 (1%)	63	83
5	E	277/341 (81%)	275 (99%)	2 (1%)	76	89
All	All	991/1120 (88%)	982 (99%)	9 (1%)	70	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
2	B	92	CYS
2	B	138	LEU
3	C	30	SER
3	C	146	VAL
4	D	165	THR
4	D	188	SER
5	E	1178	LEU
5	E	1246	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	77	ASN
1	A	138	ASN
2	B	164	HIS
2	B	199	ASN
4	D	100(C)	HIS
4	D	164	HIS
5	E	1056	ASN
5	E	1329	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](#)

Of 20 ligands modelled in this entry, 19 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
6	PO4	A	301	-	4,4,4	0.96	0	6,6,6	0.46	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.

No monomer is involved in short contacts.

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	215/215 (100%)	-0.08	2 (0%) 81 78	38, 53, 74, 86	0
2	B	223/233 (95%)	-0.24	3 (1%) 75 71	37, 49, 64, 93	0
3	C	185/214 (86%)	0.56	25 (13%) 7 5	46, 65, 142, 164	0
4	D	199/235 (84%)	1.21	47 (23%) 2 1	49, 100, 142, 238	0
5	E	360/458 (78%)	-0.20	5 (1%) 73 69	40, 52, 71, 85	0
All	All	1182/1355 (87%)	0.17	82 (6%) 23 18	37, 56, 125, 238	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	56	ASN	4.8
4	D	138	LEU	4.5
5	E	1337	ALA	3.8
3	C	132	VAL	3.8
4	D	143	LYS	3.6
4	D	209	LYS	3.6
4	D	120	SER	3.6
4	D	121	VAL	3.6
4	D	135	THR	3.4
4	D	122	PHE	3.4
4	D	165	THR	3.4
3	C	117	ILE	3.4
4	D	183	THR	3.3
3	C	125	LEU	3.3
4	D	150	VAL	3.3
3	C	194	CYS	3.3
4	D	188	SER	3.3
4	D	137	ALA	3.3
3	C	2	ILE	3.3
2	B	216	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	178	THR	3.2
5	E	1338	ARG	3.2
4	D	149	PRO	3.2
4	D	114	ARG	3.1
3	C	148	TRP	3.0
3	C	134	CYS	3.0
4	D	159	LEU	3.0
4	D	196	CYS	3.0
3	C	126	LYS	3.0
4	D	185	PRO	3.0
4	D	110	THR	3.0
3	C	116	PHE	3.0
4	D	205	THR	2.9
5	E	1421	ALA	2.9
4	D	206	LYS	2.8
3	C	129	THR	2.8
3	C	157	GLY	2.8
4	D	111	VAL	2.8
3	C	130	ALA	2.7
4	D	142	VAL	2.7
3	C	118	PHE	2.7
3	C	110	VAL	2.7
1	A	215	CYS	2.6
5	E	1330	ASP	2.6
3	C	165	GLU	2.6
3	C	160	GLN	2.6
4	D	83	THR	2.5
1	A	122	SER	2.5
4	D	11	LEU	2.5
3	C	128	GLY	2.5
4	D	169	VAL	2.5
4	D	201	LYS	2.5
4	D	14	PRO	2.4
4	D	178	LEU	2.4
4	D	15	GLY	2.4
4	D	184	VAL	2.4
4	D	17	SER	2.3
4	D	182	VAL	2.3
3	C	122	ASP	2.3
4	D	161	SER	2.3
4	D	147	PRO	2.3
3	C	133	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	153	SER	2.3
4	D	180	SER	2.3
4	D	163	VAL	2.3
3	C	123	GLU	2.2
2	B	2	VAL	2.2
3	C	108	ARG	2.2
4	D	12	VAL	2.2
4	D	179	SER	2.2
3	C	162	SER	2.1
3	C	205	VAL	2.1
4	D	207	VAL	2.1
2	B	215	SER	2.1
5	E	1246	LEU	2.1
4	D	13	ARG	2.0
4	D	173	SER	2.0
4	D	151	THR	2.0
4	D	170	LEU	2.0
4	D	9	ALA	2.0
4	D	186	SER	2.0
3	C	146	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	A	301	5/5	0.89	0.17	74,81,94,106	0
7	CA	E	1519	1/1	0.89	0.15	79,79,79,79	0
7	CA	E	1517	1/1	0.95	0.17	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	E	1503	1/1	0.98	0.04	53,53,53,53	0
7	CA	E	1507	1/1	0.98	0.11	35,35,35,35	0
7	CA	E	1501	1/1	0.98	0.10	76,76,76,76	0
7	CA	E	1502	1/1	0.98	0.09	76,76,76,76	0
7	CA	E	1511	1/1	0.99	0.07	31,31,31,31	0
7	CA	E	1514	1/1	0.99	0.03	37,37,37,37	0
7	CA	E	1516	1/1	0.99	0.02	44,44,44,44	0
7	CA	E	1504	1/1	0.99	0.02	39,39,39,39	0
7	CA	E	1518	1/1	0.99	0.03	48,48,48,48	0
7	CA	E	1508	1/1	0.99	0.03	44,44,44,44	0
7	CA	E	1513	1/1	1.00	0.02	33,33,33,33	0
7	CA	E	1506	1/1	1.00	0.07	36,36,36,36	0
7	CA	E	1515	1/1	1.00	0.01	47,47,47,47	0
7	CA	E	1509	1/1	1.00	0.03	48,48,48,48	0
7	CA	E	1510	1/1	1.00	0.07	41,41,41,41	0
7	CA	E	1505	1/1	1.00	0.04	37,37,37,37	0
7	CA	E	1512	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.