



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 10:29 AM EST

PDB ID : 6XJY
Title : Crystal structure of a self-alkylating ribozyme - short time incubation with the epoxide substrate
Authors : Koirala, D.; Piccirilli, J.A.
Deposited on : 2020-06-24
Resolution : 2.16 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.25
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.25

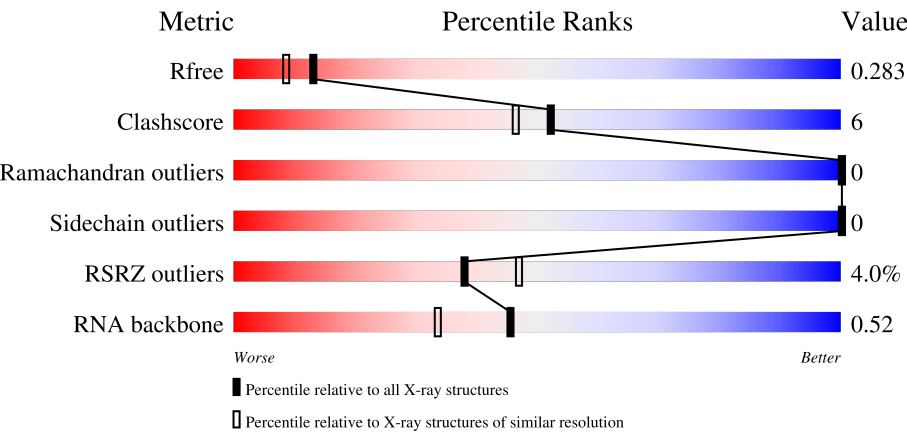
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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.



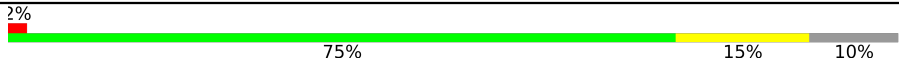

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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	58	<div><div>69%</div><div>24%</div><div>5%</div></div>
1	B	58	<div><div>60%</div><div>34%</div><div>5%</div></div>
2	C	258	<div><div>5%</div><div>78%</div><div>10%</div><div>13%</div></div>
2	H	258	<div><div>6%</div><div>79%</div><div>8%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
3	D	238	 2% 75% 15% 10%
3	L	238	 3% 81% 9% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 RNA chain called Self-alkylating ribozyme (58-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	58	Total	C	N	O	P	0	0	0
			1237	550	220	409	58			
1	B	58	Total	C	N	O	P	0	0	0
			1237	550	220	409	58			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	225	Total	C	N	O	S	0	0	0
			1686	1067	281	332	6			
2	H	225	Total	C	N	O	S	0	0	0
			1686	1067	281	332	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1668	1046	283	334	5			
3	L	214	Total	C	N	O	S	0	0	0
			1668	1046	283	334	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	42	Total	O	0	0
			42	42		
4	C	46	Total	O	0	0
			46	46		
4	D	51	Total	O	0	0
			51	51		

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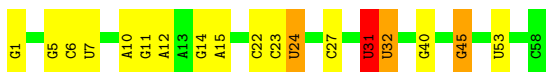
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	45	Total	O	0	0
			45	45		
4	L	49	Total	O	0	0
			49	49		

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: Self-alkylating ribozyme (58-MER)

Chain A: 




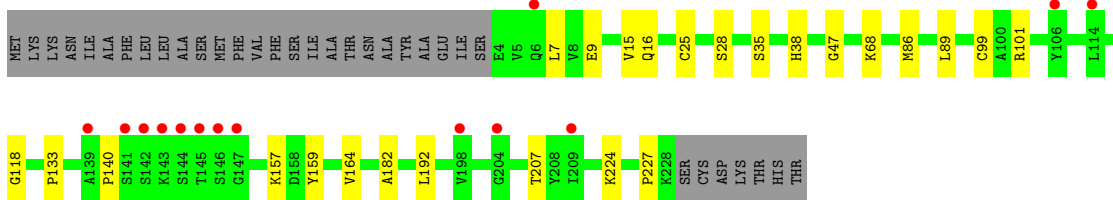
- Molecule 1: Self-alkylating ribozyme (58-MER)

Chain B: 




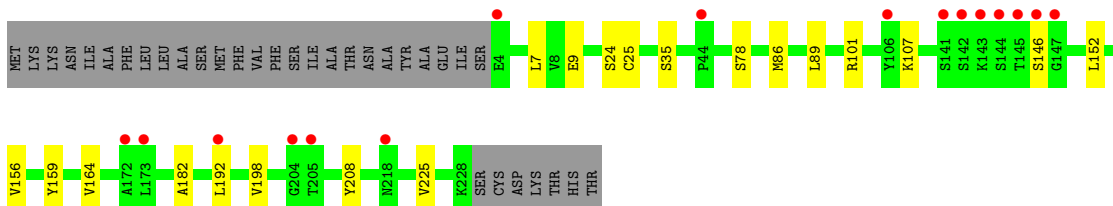
- Molecule 2: Fab HAVx Heavy Chain

Chain C: 

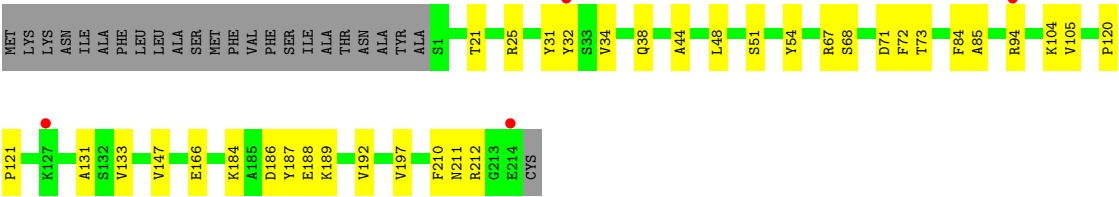
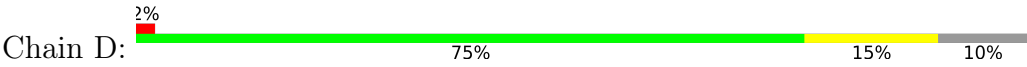


- Molecule 2: Fab HAVx Heavy Chain

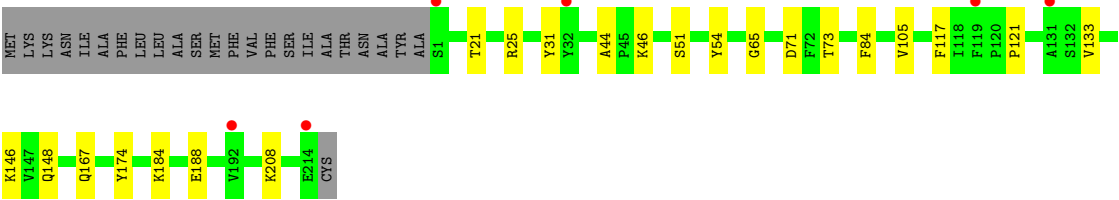
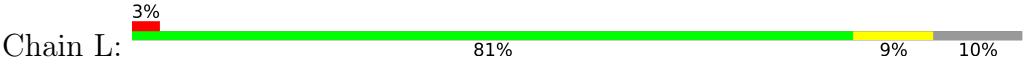
Chain H: 



- Molecule 3: Fab HAVx Light Chain



• Molecule 3: Fab HAVx Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.60Å 79.38Å 106.07Å 90.00° 111.52° 90.00°	Depositor
Resolution (Å)	61.85 – 2.16 77.38 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.3 (61.85-2.16) 85.0 (77.38-2.16)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.227 , 0.285 0.229 , 0.283	Depositor DCC
R_{free} test set	2007 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.96% 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	0/1380	1.16	3/2150 (0.1%)
1	B	0.56	0/1380	1.06	2/2150 (0.1%)
2	C	0.46	0/1731	0.62	0/2361
2	H	0.45	0/1731	0.64	0/2361
3	D	0.52	0/1705	0.62	1/2313 (0.0%)
3	L	0.45	0/1705	0.63	0/2313
All	All	0.50	0/9632	0.81	6/13648 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	U	O5'-P-OP2	-8.92	97.67	105.70
1	B	11	G	O4'-C1'-N9	6.07	113.06	108.20
1	A	45	G	C4-N9-C1'	5.38	133.49	126.50
1	A	40	G	C5-C6-O6	-5.17	125.50	128.60
3	D	31	TYR	N-CA-C	-5.09	97.25	111.00
1	B	5	G	N1-C6-O6	-5.07	116.86	119.90

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	1237	0	629	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1237	0	629	9	0
2	C	1686	0	1640	23	0
2	H	1686	0	1640	17	0
3	D	1668	0	1628	24	0
3	L	1668	0	1628	17	0
4	A	39	0	0	2	0
4	B	42	0	0	4	0
4	C	46	0	0	5	0
4	D	51	0	0	4	0
4	H	45	0	0	1	0
4	L	49	0	0	2	0
All	All	9454	0	7794	92	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 (92) 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)
3:D:32:TYR:CE1	3:D:67:ARG:HD3	2.14	0.83
2:C:182:ALA:HB2	2:C:192:LEU:HD12	1.59	0.82
2:H:159:TYR:OH	2:H:192:LEU:HD23	1.79	0.82
2:C:159:TYR:CE2	2:C:164:VAL:HG23	2.19	0.77
1:B:58:C:OP1	4:B:101:HOH:O	2.08	0.72
3:D:104:LYS:NZ	3:D:166:GLU:OE1	2.22	0.71
1:A:1:G:OP1	4:A:101:HOH:O	2.08	0.70
2:C:182:ALA:CB	2:C:192:LEU:HD12	2.23	0.68
2:C:182:ALA:CA	2:C:192:LEU:HD12	2.27	0.65
3:L:25:ARG:NE	3:L:71:ASP:OD1	2.24	0.65
1:B:49:G:N3	4:B:105:HOH:O	2.30	0.64
3:D:25:ARG:NE	3:D:71:ASP:OD1	2.31	0.62
2:H:146:SER:HB2	3:L:117:PHE:CZ	2.34	0.61
2:H:86:MET:HB3	2:H:89:LEU:HD21	1.83	0.61
2:H:198:VAL:HG11	2:H:208:TYR:CZ	2.35	0.61
2:C:28:SER:HB3	2:H:78:SER:HB3	1.85	0.59
3:L:146:LYS:HZ3	3:L:148:GLN:HG3	1.68	0.59
1:A:24:U:H5'	3:L:31:TYR:OH	2.03	0.58
2:C:15:VAL:HG11	2:C:89:LEU:HD13	1.84	0.58
1:B:43:A:N6	4:B:108:HOH:O	2.37	0.58
3:D:184:LYS:O	3:D:188:GLU:HG2	2.04	0.57
2:C:182:ALA:HB2	2:C:192:LEU:CD1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TYR:OH	2:H:192:LEU:CD2	2.52	0.57
2:H:159:TYR:CE1	2:H:164:VAL:HG23	2.41	0.55
3:D:32:TYR:CE1	3:D:67:ARG:CD	2.89	0.55
2:H:152:LEU:HD13	2:H:225:VAL:HG21	1.88	0.55
2:H:35:SER:HB2	2:H:101:ARG:HG3	1.88	0.55
3:L:184:LYS:O	3:L:188:GLU:HG2	2.08	0.54
3:D:147:VAL:O	4:D:301:HOH:O	2.17	0.54
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.89	0.53
3:L:146:LYS:NZ	4:L:308:HOH:O	2.38	0.52
2:C:35:SER:HB2	2:C:101:ARG:HG3	1.92	0.52
3:D:84:PHE:HA	3:D:105:VAL:HG23	1.93	0.51
3:D:186:ASP:OD1	3:D:189:LYS:NZ	2.39	0.51
1:A:31:U:H3'	1:A:32:U:H5''	1.93	0.49
3:D:187:TYR:CE2	3:D:212:ARG:HD3	2.48	0.49
3:D:21:THR:HG23	3:D:73:THR:HG23	1.94	0.48
3:L:21:THR:HG23	3:L:73:THR:HG23	1.94	0.48
3:D:192:VAL:HG22	3:D:211:ASN:OD1	2.13	0.48
2:C:38:HIS:O	2:C:99:CYS:HA	2.12	0.48
3:D:147:VAL:HG23	4:D:301:HOH:O	2.12	0.48
2:C:68:LYS:CE	4:C:343:HOH:O	2.61	0.47
2:H:9:GLU:HA	2:H:24:SER:O	2.14	0.47
2:C:133:PRO:HB3	2:C:159:TYR:HB3	1.96	0.47
3:L:51:SER:HB3	3:L:54:TYR:CD2	2.50	0.47
2:C:86:MET:HB3	2:C:89:LEU:HD21	1.97	0.46
3:D:34:VAL:HG21	3:D:72:PHE:CD2	2.51	0.46
2:C:118:GLY:O	3:D:44:ALA:HB2	2.16	0.46
2:C:16:GLN:OE1	4:C:302:HOH:O	2.21	0.46
2:C:68:LYS:HE3	4:C:344:HOH:O	2.16	0.46
2:C:157:LYS:NZ	4:D:308:HOH:O	2.50	0.45
3:D:121:PRO:HD3	3:D:133:VAL:HG22	1.98	0.45
2:H:107:LYS:O	2:H:107:LYS:HD3	2.16	0.45
3:D:38:GLN:HB2	3:D:48:LEU:HD11	1.98	0.45
3:D:121:PRO:HG3	3:D:131:ALA:HB1	1.99	0.45
1:B:25:U:H4'	1:B:26:G:O5'	2.17	0.45
1:B:46:C:H2'	1:B:47:U:C6	2.51	0.45
3:D:68:SER:O	3:D:71:ASP:HB2	2.17	0.45
2:H:198:VAL:CG1	2:H:208:TYR:OH	2.65	0.44
2:C:9:GLU:N	2:C:9:GLU:OE1	2.50	0.44
1:B:46:C:H2'	1:B:47:U:H6	1.81	0.44
3:D:120:PRO:HG3	3:D:210:PHE:CD2	2.53	0.43
1:A:1:G:OP1	4:A:102:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:84:PHE:HA	3:L:105:VAL:HG23	2.00	0.43
1:B:2:G:H2'	1:B:3:C:C6	2.54	0.43
3:D:51:SER:HB3	3:D:54:TYR:CD2	2.54	0.43
2:H:146:SER:HB2	3:L:117:PHE:HZ	1.80	0.43
3:D:94:ARG:NH2	4:D:315:HOH:O	2.51	0.43
2:H:182:ALA:HA	2:H:192:LEU:HB3	2.01	0.43
1:B:33:A:OP1	4:B:102:HOH:O	2.21	0.43
3:D:32:TYR:CE2	3:D:67:ARG:NH1	2.87	0.43
2:C:140:PRO:HG2	2:C:227:PRO:HA	2.01	0.42
2:H:156:VAL:HG11	2:H:164:VAL:HG11	2.01	0.42
2:C:68:LYS:HE3	4:C:343:HOH:O	2.18	0.42
4:H:313:HOH:O	3:L:46:LYS:HD2	2.19	0.42
3:L:208:LYS:HA	3:L:208:LYS:HD3	1.89	0.42
3:D:85:ALA:H	3:D:105:VAL:HG22	1.84	0.42
2:C:207:THR:HG23	2:C:224:LYS:HE3	2.02	0.42
1:B:31:U:H3'	1:B:32:U:H5''	2.02	0.42
3:L:44:ALA:O	4:L:302:HOH:O	2.22	0.42
1:A:22:C:H2'	1:A:23:C:C6	2.55	0.41
2:H:7:LEU:HD22	2:H:25:CYS:SG	2.61	0.41
1:A:5:G:O2'	1:A:6:C:H5'	2.20	0.41
3:L:146:LYS:HZ3	3:L:148:GLN:CG	2.32	0.41
2:C:7:LEU:HD22	2:C:25:CYS:SG	2.60	0.41
2:H:198:VAL:HG11	2:H:208:TYR:CE2	2.55	0.41
2:C:47:GLY:HA3	4:C:305:HOH:O	2.19	0.41
1:A:10:A:O2'	1:A:11:G:H5'	2.20	0.41
3:D:147:VAL:HG12	3:D:197:VAL:HG22	2.03	0.41
3:L:167:GLN:HG3	3:L:174:TYR:CZ	2.56	0.41
2:C:159:TYR:CE2	2:C:164:VAL:CG2	2.98	0.41
3:L:65:GLY:HA2	3:L:73:THR:O	2.21	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	
2	C	223/258 (86%)	217 (97%)	6 (3%)	0	100	100
2	H	223/258 (86%)	216 (97%)	7 (3%)	0	100	100
3	D	212/238 (89%)	206 (97%)	6 (3%)	0	100	100
3	L	212/238 (89%)	205 (97%)	7 (3%)	0	100	100
All	All	870/992 (88%)	844 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	C	188/216 (87%)	188 (100%)	0	100	100
2	H	188/216 (87%)	188 (100%)	0	100	100
3	D	190/209 (91%)	190 (100%)	0	100	100
3	L	190/209 (91%)	190 (100%)	0	100	100
All	All	756/850 (89%)	756 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/58 (98%)	10 (17%)	0
1	B	57/58 (98%)	12 (21%)	0
All	All	114/116 (98%)	22 (19%)	0

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	U
1	A	12	A
1	A	14	G
1	A	15	A
1	A	24	U
1	A	27	C
1	A	31	U
1	A	32	U
1	A	45	G
1	A	53	U
1	B	7	U
1	B	11	G
1	B	12	A
1	B	13	A
1	B	15	A
1	B	24	U
1	B	27	C
1	B	31	U
1	B	32	U
1	B	34	U
1	B	44	G
1	B	53	U

There are no RNA pucker outliers to report.

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 monosaccharides 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	58/58 (100%)	-0.58	0	100	100	35, 52, 66, 83	0
1	B	58/58 (100%)	-0.45	0	100	100	35, 58, 75, 84	0
2	C	225/258 (87%)	0.76	14 (6%)	20	27	32, 43, 61, 115	0
2	H	225/258 (87%)	0.68	16 (7%)	16	22	31, 44, 64, 92	0
3	D	214/238 (89%)	0.49	4 (1%)	66	74	31, 43, 59, 84	0
3	L	214/238 (89%)	0.56	6 (2%)	53	62	33, 44, 62, 89	0
All	All	994/1108 (89%)	0.49	40 (4%)	38	47	31, 44, 64, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	144	SER	19.7
2	C	145	THR	12.2
2	H	144	SER	12.0
2	C	147	GLY	11.4
2	H	143	LYS	6.2
3	L	214	GLU	5.7
2	H	145	THR	5.6
2	C	143	LYS	5.4
2	C	142	SER	4.8
2	C	146	SER	4.5
2	H	147	GLY	3.8
3	D	214	GLU	3.7
2	H	146	SER	3.6
2	H	204	GLY	3.3
2	C	106	TYR	3.1
2	H	142	SER	3.1
2	H	205	THR	3.1
2	H	218	ASN	3.1
2	H	173	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	172	ALA	3.0
2	H	4	GLU	2.9
2	C	198	VAL	2.7
2	C	141	SER	2.6
2	H	106	TYR	2.6
3	L	192	VAL	2.6
2	C	6	GLN	2.5
2	C	204	GLY	2.4
3	D	32	TYR	2.4
3	L	131	ALA	2.4
3	D	127	LYS	2.4
2	H	192	LEU	2.3
2	C	209	ILE	2.3
2	H	44	PRO	2.3
3	L	1	SER	2.3
2	C	114	LEU	2.2
3	L	32	TYR	2.2
2	H	141	SER	2.2
3	D	94	ARG	2.1
2	C	139	ALA	2.1
3	L	119	PHE	2.1

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 monosaccharides 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.