



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:54 PM GMT

PDB ID : 4U7B
Title : Crystal structure of a pre-cleavage Mos1 transpososome
Authors : Richardson, J.M.
Deposited on : 2014-07-30
Resolution : 3.09 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

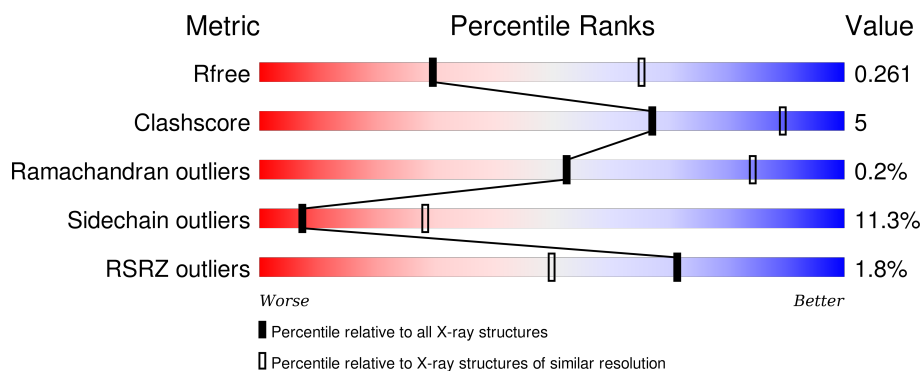
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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.






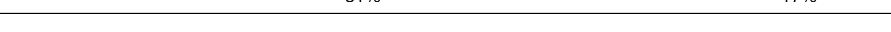
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	C	25	<div> <div>48%</div> <div>48%</div> <div>.</div> </div>
1	E	25	<div> <div>56%</div> <div>44%</div> </div>
1	H	25	<div> <div>56%</div> <div>44%</div> </div>
2	D	31	<div> <div>6%</div> <div>71%</div> <div>29%</div> </div>
2	F	31	<div> <div>65%</div> <div>35%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	31	 71% 29%
3	A	342	 3% 82% 17% •
3	B	342	 2% 81% 17% •
3	G	342	 82% 15% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	101	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12039 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 DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			
1	E	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			
1	H	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			

- Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	31	Total	C	N	O	P	0	0	0
			629	303	114	182	30			
2	F	31	Total	C	N	O	P	0	0	0
			629	303	114	182	30			
2	I	31	Total	C	N	O	P	0	0	0
			629	303	114	182	30			

- Molecule 3 is a protein called Mariner Mos1 transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	342	Total	C	N	O	S	0	0	0
			2858	1814	521	513	10			
3	B	342	Total	C	N	O	S	0	0	0
			2859	1814	521	514	10			
3	G	342	Total	C	N	O	S	0	0	0
			2858	1814	521	513	10			

There are 18 discrepancies between the modelled and reference sequences:

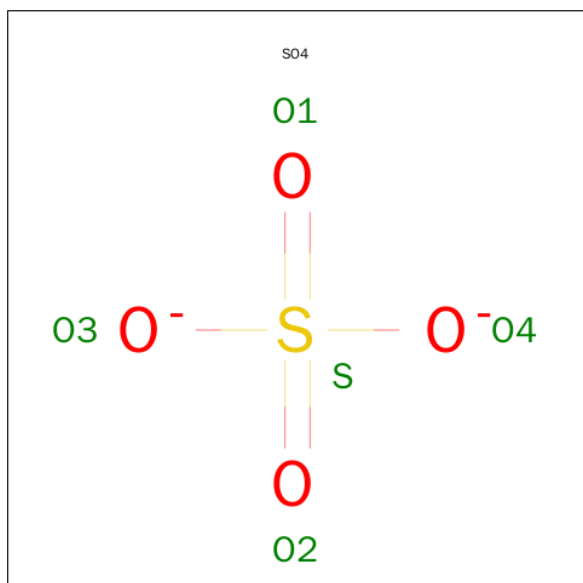
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	THR	LYS	conflict	UNP Q7JQ07
A	164	ASN	SER	conflict	UNP Q7JQ07

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	PRO	ARG	conflict	UNP Q7JQ07
A	216	ALA	THR	conflict	UNP Q7JQ07
A	249	ALA	ASP	conflict	UNP Q7JQ07
A	344	PHE	LEU	conflict	UNP Q7JQ07
B	45	THR	LYS	conflict	UNP Q7JQ07
B	164	ASN	SER	conflict	UNP Q7JQ07
B	210	PRO	ARG	conflict	UNP Q7JQ07
B	216	ALA	THR	conflict	UNP Q7JQ07
B	249	ALA	ASP	conflict	UNP Q7JQ07
B	344	PHE	LEU	conflict	UNP Q7JQ07
G	45	THR	LYS	conflict	UNP Q7JQ07
G	164	ASN	SER	conflict	UNP Q7JQ07
G	210	PRO	ARG	conflict	UNP Q7JQ07
G	216	ALA	THR	conflict	UNP Q7JQ07
G	249	ALA	ASP	conflict	UNP Q7JQ07
G	344	PHE	LEU	conflict	UNP Q7JQ07

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

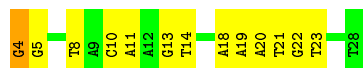
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

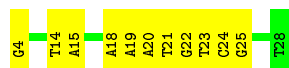
- Molecule 1: DNA (25-MER)

Chain C: 



- Molecule 1: DNA (25-MER)

Chain E: 




- Molecule 1: DNA (25-MER)

Chain H: 



- Molecule 2: DNA (31-MER)

Chain D: 



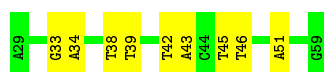
- Molecule 2: DNA (31-MER)

Chain F: 

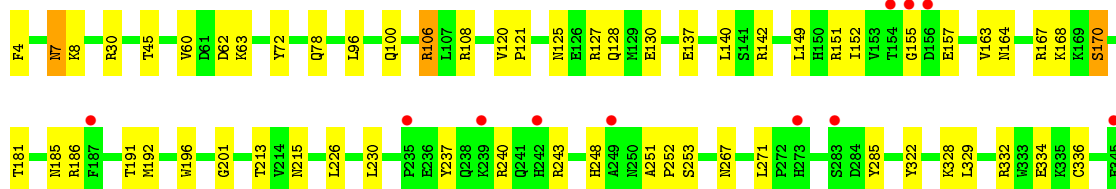
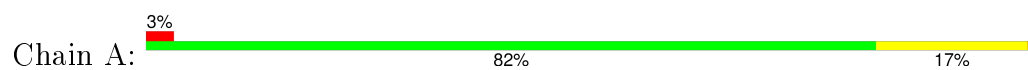


- Molecule 2: DNA (31-MER)

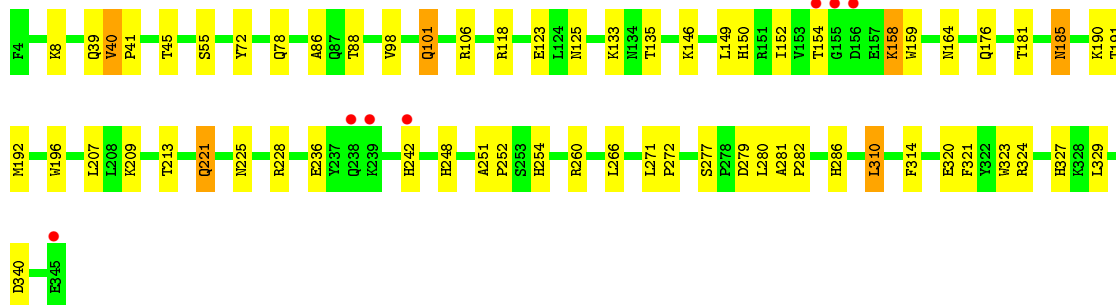
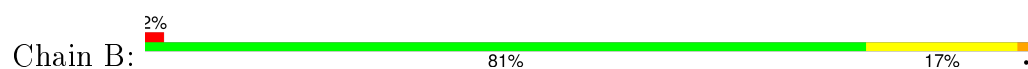
Chain I: 



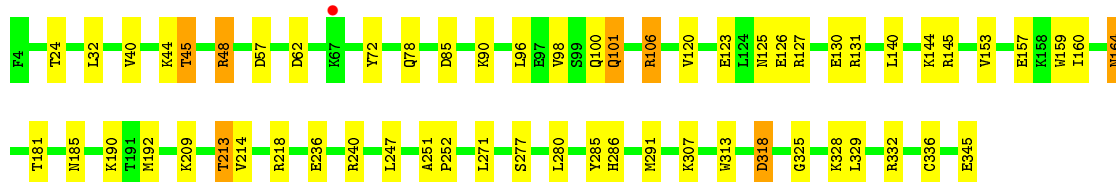
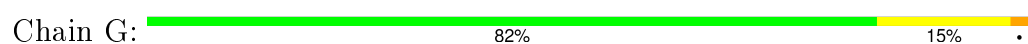
• Molecule 3: Mariner Mos1 transposase



• Molecule 3: Mariner Mos1 transposase



• Molecule 3: Mariner Mos1 transposase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.47Å 340.09Å 160.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.09 29.73 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.75-3.09) 98.8 (29.73-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.228 , 0.261 0.224 , 0.261	Depositor DCC
R_{free} test set	2447 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 48326 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12039	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	C	0.50	1/583 (0.2%)	0.71	0/898
1	E	0.52	1/583 (0.2%)	0.77	0/898
1	H	0.51	1/583 (0.2%)	0.76	0/898
2	D	0.36	0/705	0.73	0/1085
2	F	0.36	0/705	0.73	0/1085
2	I	0.31	0/705	0.71	0/1085
3	A	0.31	0/2934	0.52	0/3960
3	B	0.32	0/2935	0.55	0/3960
3	G	0.32	0/2934	0.53	0/3960
All	All	0.36	3/12667 (0.0%)	0.61	0/17829

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4	DG	OP3-P	-10.08	1.49	1.61
1	C	4	DG	OP3-P	-9.91	1.49	1.61
1	H	4	DG	OP3-P	-9.88	1.49	1.61

There are no bond angle outliers.

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	C	520	0	285	13	0
1	E	520	0	285	9	0
1	H	520	0	285	9	0
2	D	629	0	352	11	0
2	F	629	0	352	8	0
2	I	629	0	352	7	0
3	A	2858	0	2799	26	0
3	B	2859	0	2799	22	0
3	G	2858	0	2799	24	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	12039	0	10308	107	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 5.

All (107) 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:C:4:DG:C6	2:D:54:DT:H72	2.05	0.92
3:G:72:TYR:O	3:G:106:ARG:NH1	2.13	0.82
3:A:130:GLU:HB2	3:G:127:ARG:HD2	1.63	0.80
3:A:130:GLU:OE1	3:G:127:ARG:NH2	2.24	0.71
3:A:267:ASN:OD1	3:G:145:ARG:NH1	2.24	0.70
3:A:251:ALA:HB1	3:A:252:PRO:HD2	1.74	0.70
2:D:30:DA:OP1	3:A:30:ARG:NH2	2.24	0.69
2:F:47:DG:H2''	2:F:48:DT:O4'	1.93	0.68
1:C:4:DG:O6	2:D:54:DT:H72	1.94	0.67
1:C:10:DC:OP1	3:A:108:ARG:NH2	2.30	0.65
1:E:24:DC:H2''	1:E:25:DG:C8	2.32	0.64
3:B:251:ALA:HB1	3:B:252:PRO:HD2	1.80	0.64
1:C:4:DG:N3	1:C:4:DG:H2'	2.13	0.63
2:I:46:DT:O4	3:G:101:GLN:HG2	2.00	0.61
3:G:160:ILE:HD11	3:G:291:MET:HE1	1.85	0.57
2:F:41:DA:H2''	2:F:42:DT:H5''	1.87	0.57
2:I:33:DG:H2''	2:I:34:DA:C8	2.40	0.57
3:A:230:LEU:HD21	3:A:237:TYR:CD2	2.41	0.56
3:A:127:ARG:NH2	3:G:130:GLU:OE2	2.39	0.54
3:A:125:ASN:OD1	3:A:128:GLN:NE2	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:DT:H4'	2:D:43:DA:OP1	2.07	0.54
1:E:18:DA:H2''	1:E:19:DA:OP2	2.07	0.53
1:C:22:DG:H2''	1:C:23:DT:H5'	1.90	0.53
2:F:48:DT:H2'	2:F:49:DA:C8	2.43	0.53
2:F:58:DA:H2''	2:F:59:DG:C8	2.43	0.53
2:I:38:DT:H2''	2:I:39:DT:H5'	1.90	0.52
3:G:251:ALA:HB1	3:G:252:PRO:HD2	1.91	0.52
3:G:291:MET:HG3	3:G:313:TRP:CH2	2.45	0.52
1:H:23:DT:H73	3:G:44:LYS:HG2	1.92	0.51
3:G:318:ASP:N	3:G:318:ASP:OD1	2.44	0.51
3:B:251:ALA:HB3	3:B:254:HIS:ND1	2.26	0.51
1:C:18:DA:H2''	1:C:19:DA:O5'	2.10	0.51
3:A:151:ARG:HD2	3:A:243:ARG:HH21	1.76	0.50
3:B:310:LEU:HD12	3:B:314:PHE:CE2	2.47	0.50
3:A:72:TYR:O	3:A:106:ARG:NH1	2.44	0.50
3:A:155:GLY:HA3	3:A:196:TRP:CD1	2.47	0.50
3:B:323:TRP:CE2	3:B:327:HIS:CD2	3.00	0.50
2:D:42:DT:H2'	2:D:43:DA:C8	2.48	0.49
1:H:21:DT:H3'	3:G:45:THR:HG21	1.94	0.49
2:I:45:DT:H2'	2:I:46:DT:C6	2.47	0.49
2:I:42:DT:H4'	2:I:43:DA:OP1	2.12	0.49
3:B:286:HIS:NE2	3:B:321:PHE:CE1	2.81	0.49
3:A:201:GLY:HA2	3:A:322:TYR:CD2	2.48	0.49
2:F:47:DG:O6	3:B:101:GLN:NE2	2.44	0.48
3:G:72:TYR:OH	3:G:106:ARG:HG3	2.13	0.48
3:A:201:GLY:HA2	3:A:322:TYR:CG	2.48	0.48
3:A:251:ALA:HB1	3:A:252:PRO:CD	2.42	0.48
3:B:221:GLN:O	3:B:225:ASN:ND2	2.47	0.48
2:D:32:DC:H2''	2:D:33:DG:H5'	1.95	0.48
2:D:54:DT:H73	3:B:118:ARG:HH22	1.79	0.48
3:B:72:TYR:O	3:B:106:ARG:NH1	2.40	0.47
1:C:4:DG:C6	2:D:54:DT:C7	2.87	0.47
3:A:137:GLU:OE2	3:G:131:ARG:NH2	2.48	0.47
3:A:7:ASN:C	3:A:7:ASN:OD1	2.54	0.46
1:E:22:DG:C2	2:F:36:DA:C2	3.04	0.46
1:H:19:DA:H2'	1:H:20:DA:C8	2.50	0.46
3:G:328:LYS:O	3:G:332:ARG:HG2	2.16	0.46
1:E:23:DT:H2''	1:E:24:DC:H5''	1.97	0.46
3:B:40:VAL:HG13	3:B:41:PRO:HD2	1.97	0.46
3:B:39:GLN:OE1	3:B:39:GLN:N	2.49	0.46
1:C:20:DA:H2''	1:C:21:DT:H5'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:72:TYR:OH	3:A:106:ARG:HG3	2.16	0.45
3:G:277:SER:HB3	3:G:280:LEU:HD23	1.98	0.45
2:D:29:DA:H2''	2:D:30:DA:H5'	1.97	0.45
1:E:14:DT:H2'	1:E:15:DA:C8	2.52	0.45
1:H:9:DA:N6	3:G:101:GLN:OE1	2.49	0.45
2:D:52:DC:H2''	2:D:53:DC:OP2	2.16	0.45
3:A:120:VAL:HG22	3:A:121:PRO:HD2	1.98	0.45
1:E:19:DA:H2'	1:E:20:DA:C8	2.52	0.44
3:B:277:SER:HB3	3:B:280:LEU:HD23	1.99	0.44
1:E:24:DC:C2'	1:E:25:DG:C8	3.00	0.43
3:G:213:THR:OG1	3:G:214:VAL:N	2.51	0.43
1:E:21:DT:H3'	3:B:45:THR:HG21	2.01	0.43
3:G:286:HIS:CD2	3:G:325:GLY:HA2	2.53	0.43
1:E:18:DA:C2'	1:E:19:DA:OP2	2.66	0.43
3:A:285:TYR:CD1	3:A:332:ARG:NH1	2.87	0.43
3:B:158:LYS:HE3	3:B:159:TRP:O	2.19	0.43
1:H:7:DG:C2	2:I:51:DA:C2	3.07	0.42
2:D:32:DC:H2''	2:D:33:DG:C8	2.53	0.42
3:B:279:ASP:OD1	3:B:279:ASP:N	2.52	0.42
2:I:42:DT:H2'	2:I:43:DA:C8	2.54	0.42
3:A:328:LYS:O	3:A:332:ARG:HG3	2.19	0.42
1:H:18:DA:H2''	1:H:19:DA:O5'	2.19	0.42
3:B:135:THR:HG23	3:B:272:PRO:HB2	2.01	0.42
3:G:159:TRP:CZ3	3:G:190:LYS:HG3	2.54	0.42
3:A:127:ARG:HG3	3:G:126:GLU:HB3	2.00	0.42
3:A:170:SER:HA	3:B:86:ALA:HA	2.02	0.42
3:A:8:LYS:H	3:A:8:LYS:HD2	1.85	0.42
3:B:154:THR:O	3:B:196:TRP:HA	2.20	0.41
1:C:8:DT:H73	3:A:100:GLN:CD	2.40	0.41
3:A:226:LEU:O	3:A:230:LEU:N	2.52	0.41
3:G:164:ASN:OD1	3:G:164:ASN:N	2.53	0.41
3:G:45:THR:HA	3:G:48:ARG:HG3	2.02	0.41
2:F:45:DT:H2'	2:F:46:DT:C6	2.55	0.41
3:G:285:TYR:C	3:G:285:TYR:CD1	2.93	0.41
1:C:4:DG:N2	1:C:5:DG:C4	2.89	0.41
3:B:191:THR:HB	3:B:207:LEU:HD11	2.02	0.41
1:C:10:DC:N4	1:C:11:DA:N6	2.69	0.41
1:C:19:DA:H2'	1:C:20:DA:C8	2.56	0.41
1:C:13:DG:H2''	1:C:14:DT:C5'	2.50	0.41
1:H:21:DT:H2''	1:H:22:DG:H5'	2.01	0.40
3:B:185:ASN:O	3:B:185:ASN:ND2	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:133:LYS:HD2	3:B:340:ASP:HA	2.03	0.40
1:H:22:DG:H2''	1:H:23:DT:H5'	2.03	0.40
2:F:44:DC:H2'	2:F:45:DT:C6	2.57	0.40
3:B:281:ALA:O	3:B:282:PRO:C	2.59	0.40
1:H:12:DA:H2''	1:H:13:DG:OP2	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	
3	A	340/342 (99%)	312 (92%)	27 (8%)	1 (0%)	46	80
3	B	340/342 (99%)	314 (92%)	25 (7%)	1 (0%)	46	80
3	G	340/342 (99%)	325 (96%)	15 (4%)	0	100	100
All	All	1020/1026 (99%)	951 (93%)	67 (7%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	7	ASN
3	B	236	GLU

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	
3	A	303/303 (100%)	271 (89%)	32 (11%)	8	31
3	B	303/303 (100%)	270 (89%)	33 (11%)	8	30
3	G	303/303 (100%)	265 (88%)	38 (12%)	6	22
All	All	909/909 (100%)	806 (89%)	103 (11%)	7	28

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4	PHE
3	A	45	THR
3	A	60	VAL
3	A	62	ASP
3	A	63	LYS
3	A	78	GLN
3	A	96	LEU
3	A	106	ARG
3	A	140	LEU
3	A	142	ARG
3	A	149	LEU
3	A	152	ILE
3	A	157	GLU
3	A	163	VAL
3	A	164	ASN
3	A	167	ARG
3	A	168	LYS
3	A	170	SER
3	A	181	THR
3	A	185	ASN
3	A	186	ARG
3	A	191	THR
3	A	192	MET
3	A	213	THR
3	A	215	ASN
3	A	240	ARG
3	A	248	HIS
3	A	253	SER
3	A	271	LEU
3	A	329	LEU
3	A	334	GLU
3	A	336	CYS
3	B	8	LYS
3	B	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	55	SER
3	B	78	GLN
3	B	88	THR
3	B	98	VAL
3	B	101	GLN
3	B	123	GLU
3	B	125	ASN
3	B	146	LYS
3	B	149	LEU
3	B	150	HIS
3	B	152	ILE
3	B	158	LYS
3	B	164	ASN
3	B	176	GLN
3	B	181	THR
3	B	185	ASN
3	B	190	LYS
3	B	192	MET
3	B	209	LYS
3	B	213	THR
3	B	221	GLN
3	B	228	ARG
3	B	242	HIS
3	B	248	HIS
3	B	260	ARG
3	B	266	LEU
3	B	271	LEU
3	B	310	LEU
3	B	320	GLU
3	B	324	ARG
3	B	329	LEU
3	G	24	THR
3	G	32	LEU
3	G	40	VAL
3	G	45	THR
3	G	48	ARG
3	G	57	ASP
3	G	62	ASP
3	G	78	GLN
3	G	85	ASP
3	G	90	LYS
3	G	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	98	VAL
3	G	100	GLN
3	G	101	GLN
3	G	106	ARG
3	G	120	VAL
3	G	123	GLU
3	G	125	ASN
3	G	140	LEU
3	G	144	LYS
3	G	153	VAL
3	G	157	GLU
3	G	164	ASN
3	G	181	THR
3	G	185	ASN
3	G	192	MET
3	G	209	LYS
3	G	213	THR
3	G	218	ARG
3	G	236	GLU
3	G	240	ARG
3	G	247	LEU
3	G	271	LEU
3	G	307	LYS
3	G	318	ASP
3	G	329	LEU
3	G	336	CYS
3	G	345	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	10	GLN
3	B	29	HIS
3	B	176	GLN
3	B	225	ASN
3	B	293	HIS
3	B	327	HIS
3	G	100	GLN
3	G	125	ASN
3	G	128	GLN
3	G	134	ASN
3	G	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	185	ASN
3	G	227	ASN
3	G	267	ASN
3	G	286	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
4	SO4	C	101	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SO4	D	101	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	E	101	-	4,4,4	0.37	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	101	-	-	0/0/0/0	0/0/0/0
4	SO4	D	101	-	-	0/0/0/0	0/0/0/0
4	SO4	E	101	-	-	0/0/0/0	0/0/0/0

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

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	C	25/25 (100%)	-0.54	0 100 100	73, 98, 108, 118	0
1	E	25/25 (100%)	-0.24	0 100 100	69, 93, 153, 169	0
1	H	25/25 (100%)	-0.48	0 100 100	80, 101, 124, 130	0
2	D	31/31 (100%)	-0.23	2 (6%) 22 8	82, 96, 145, 211	0
2	F	31/31 (100%)	-0.20	0 100 100	74, 88, 136, 193	0
2	I	31/31 (100%)	-0.33	0 100 100	84, 99, 123, 179	0
3	A	342/342 (100%)	-0.04	11 (3%) 51 27	66, 108, 158, 218	0
3	B	342/342 (100%)	-0.08	7 (2%) 68 46	70, 109, 150, 218	0
3	G	342/342 (100%)	-0.12	1 (0%) 94 88	61, 104, 149, 175	0
All	All	1194/1194 (100%)	-0.11	21 (1%) 71 50	61, 105, 154, 218	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	345	GLU	3.7
3	A	155	GLY	3.5
3	B	345	GLU	3.1
3	B	155	GLY	3.1
3	B	242	HIS	3.0
3	A	156	ASP	2.9
2	D	59	DG	2.9
3	B	239	LYS	2.9
3	B	156	ASP	2.7
3	A	239	LYS	2.6
3	A	187	PHE	2.5
3	A	249	ALA	2.4
3	A	235	PRO	2.3
3	A	283	SER	2.2
3	B	154	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	58	DA	2.2
3	G	67	LYS	2.2
3	A	273	HIS	2.1
3	B	238	GLN	2.1
3	A	242	HIS	2.1
3	A	154	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	C	101	5/5	0.90	0.41	24.39	150,154,157,160	0
4	SO4	D	101	5/5	0.84	0.42	-	191,191,193,193	0
4	SO4	E	101	5/5	0.92	0.27	-	155,156,161,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.