Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2022 – 11:00 am BST

PDB ID	:	7QQR
Title	:	SpCas9 bound to AAVS1 off-target5 DNA substrate
Authors	:	Pacesa, M.; Jinek, M.
Deposited on	:	2022-01-10
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 (i) 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 (1)) were used in the production of this report:

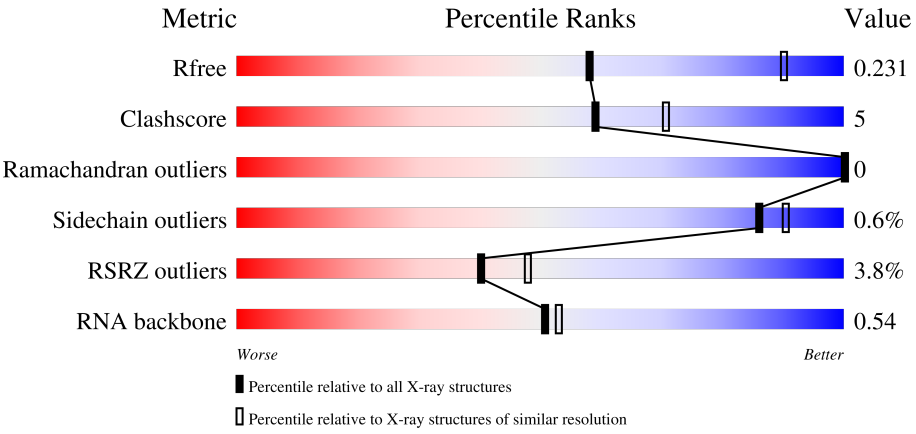
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

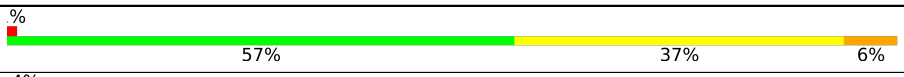
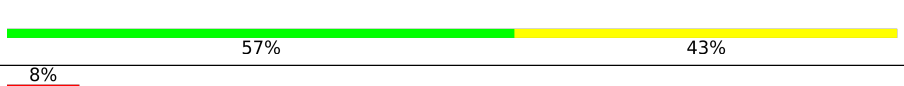
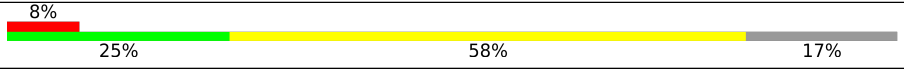
The reported resolution of this entry is 2.75 Å.

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 <=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	84	
2	B	1368	
3	C	28	
4	D	12	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13710 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 AAVS1 sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	P	0	0	1
			1788	799	334	572	83			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1334	Total	C	N	O	S	0	0	0
			10905	6948	1892	2043	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called AAVS1 off-target5 target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			562	268	101	166	27			

- Molecule 4 is a DNA chain called AAVS1 off-target5 non-target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			

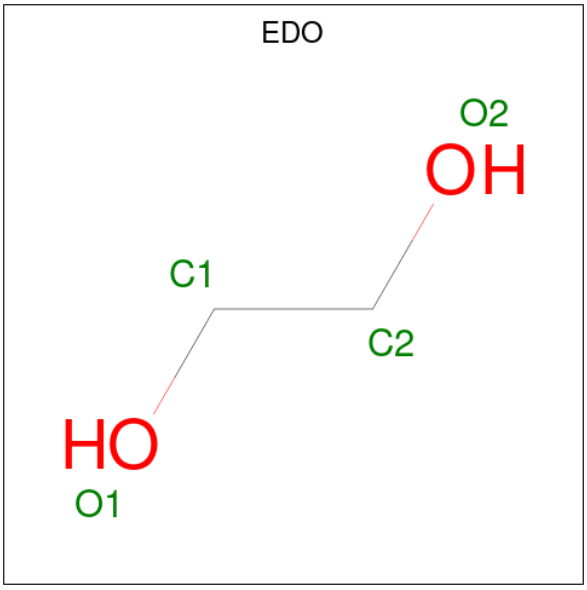
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total K 5 5	0	0
6	B	7	Total K 7 7	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	76	Total O 76 76	0	0

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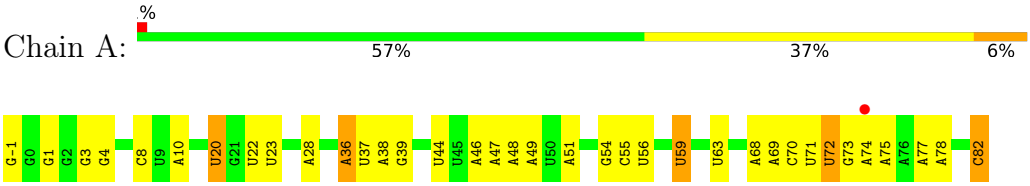
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	124	Total O 124 124	0	0
8	C	14	Total O 14 14	0	0
8	D	4	Total O 4 4	0	0

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.

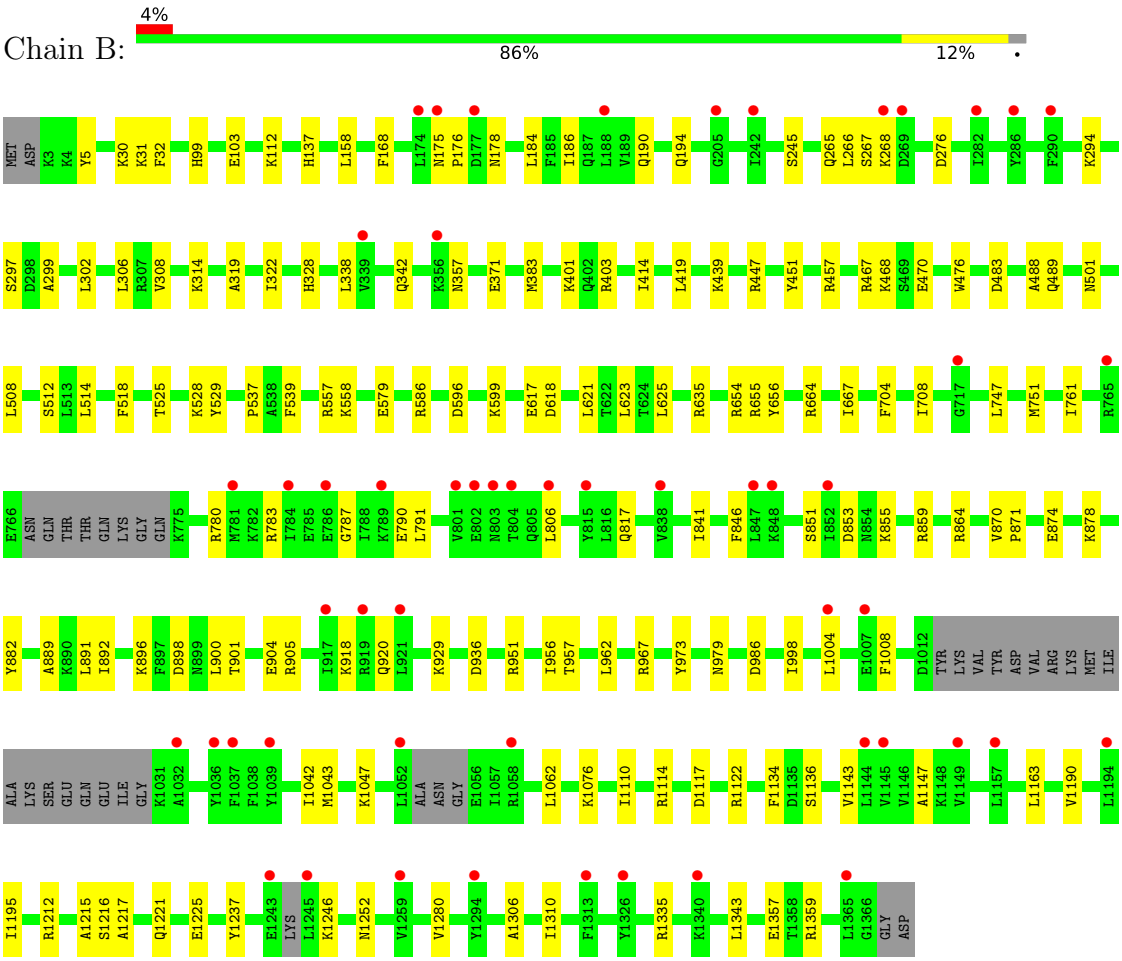
• Molecule 1: AAVS1 sgRNA

Chain A:



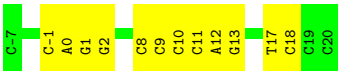
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

Chain B:



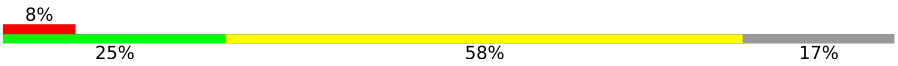
• Molecule 3: AAVS1 off-target5 target strand

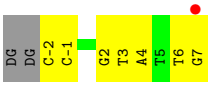
Chain C:



• Molecule 4: AAVS1 off-target5 non-target strand

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	178.64Å 67.03Å 187.80Å 90.00° 111.34° 90.00°	Depositor
Resolution (Å)	47.70 – 2.75 47.70 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.70-2.75) 99.2 (47.70-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.189 , 0.231 0.189 , 0.231	Depositor DCC
R_{free} test set	2704 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13710	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, K

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	0.36	0/2005	0.91	0/3127
2	B	0.28	0/11096	0.45	0/14907
3	C	0.70	0/628	0.91	0/965
4	D	0.63	0/225	1.02	0/346
All	All	0.33	0/13954	0.59	0/19345

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

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	1788	0	895	23	0
2	B	10905	0	11080	94	0
3	C	562	0	315	9	0
4	D	202	0	116	6	0
5	A	2	0	0	0	0
6	A	5	0	0	0	0
6	B	7	0	0	0	0
6	C	1	0	0	0	0
7	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	0	12	0	0
7	C	4	0	6	0	0
8	A	76	0	0	0	0
8	B	124	0	0	2	0
8	C	14	0	0	0	0
8	D	4	0	0	0	0
All	All	13710	0	12436	121	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 (121) 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:A:1:G:OP1	2:B:929:LYS:NZ	2.21	0.73
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.27	0.68
1:A:20:U:OP2	2:B:403:ARG:NH1	2.28	0.66
4:D:6:DT:H2"	4:D:7:DG:H5"	1.80	0.61
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.83	0.60
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.82	0.60
2:B:1246:LYS:HB3	2:B:1252:ASN:OD1	2.01	0.60
1:A:77:A:H2'	1:A:78:A:C8	2.36	0.60
2:B:158:LEU:HD22	2:B:419:LEU:HD12	1.84	0.58
2:B:168:PHE:CG	2:B:447:ARG:HD2	2.39	0.58
2:B:1114:ARG:NH1	4:D:4:DA:OP1	2.37	0.57
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.86	0.57
1:A:-1:G:O3'	2:B:918:LYS:NZ	2.37	0.57
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.85	0.57
2:B:936:ASP:OD1	2:B:951:ARG:NH1	2.38	0.56
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.86	0.56
1:A:82:C:N3	2:B:30:LYS:HD3	2.22	0.55
1:A:46:A:H2'	1:A:47:A:C8	2.43	0.54
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.41	0.54
3:C:17:DT:H2'	3:C:18:DC:C6	2.42	0.54
2:B:874:GLU:HG2	2:B:878:LYS:HE3	1.90	0.54
2:B:306:LEU:HD21	2:B:414:ILE:HD13	1.90	0.54
2:B:529:TYR:HA	2:B:579:GLU:O	2.07	0.53
2:B:654:ARG:HD2	2:B:656:TYR:CZ	2.43	0.53
2:B:956:ILE:HD11	2:B:998:ILE:HD13	1.91	0.53
1:A:71:U:H2'	1:A:72:U:C6	2.43	0.53
2:B:457:ARG:HD2	2:B:470:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:TYR:CZ	2:B:751:MET:HG3	2.44	0.53
2:B:245:SER:HA	2:B:297:SER:HB2	1.90	0.52
2:B:1047:LYS:O	2:B:1076:LYS:NZ	2.30	0.52
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.91	0.52
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.42	0.52
2:B:956:ILE:HA	2:B:1008:PHE:O	2.10	0.52
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.45	0.51
1:A:70:C:H2'	1:A:71:U:C6	2.46	0.51
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.93	0.51
3:C:1:DG:H2"	3:C:2:DG:O4'	2.11	0.50
1:A:59:U:OP1	2:B:467:ARG:NH2	2.44	0.50
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.45	0.50
1:A:22:U:H2'	1:A:23:U:C6	2.47	0.50
2:B:468:LYS:HG3	2:B:483:ASP:HB2	1.94	0.50
2:B:973:TYR:HB3	2:B:1237:TYR:CD2	2.46	0.50
1:A:10:A:OP1	2:B:783:ARG:NH2	2.44	0.49
4:D:-2:DC:H2"	4:D:-1:DC:H5"	1.94	0.49
2:B:1122:ARG:HG2	2:B:1134:PHE:CE2	2.48	0.49
3:C:8:DC:H2'	3:C:9:DC:C6	2.47	0.49
2:B:1216:SER:OG	2:B:1217:ALA:N	2.45	0.48
2:B:898:ASP:O	2:B:905:ARG:NH2	2.46	0.48
1:A:54:G:H2'	1:A:55:C:C6	2.49	0.48
2:B:265:GLN:HG2	2:B:267:SER:H	1.80	0.47
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.96	0.47
2:B:518:PHE:CD1	2:B:667:ILE:HD12	2.49	0.47
2:B:99:HIS:O	2:B:103:GLU:HG2	2.15	0.47
2:B:870:VAL:HG13	2:B:871:PRO:HD2	1.97	0.47
2:B:892:ILE:HB	2:B:896:LYS:HD3	1.97	0.47
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.95	0.47
2:B:401:LYS:NZ	8:B:1508:HOH:O	2.48	0.46
2:B:841:ILE:O	2:B:864:ARG:NH2	2.48	0.46
1:A:82:C:N4	2:B:32:PHE:CE1	2.82	0.46
1:A:74:A:OP1	1:A:74:A:H8	1.97	0.46
3:C:8:DC:H2'	3:C:9:DC:H6	1.81	0.46
2:B:956:ILE:HG23	2:B:1008:PHE:HB3	1.96	0.46
2:B:851:SER:O	2:B:855:LYS:HG3	2.16	0.46
2:B:439:LYS:HG2	2:B:476:TRP:CD1	2.50	0.46
1:A:72:U:H2'	1:A:73:G:O4'	2.16	0.46
2:B:501:ASN:HB3	2:B:708:ILE:HD12	1.96	0.46
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.97	0.46
3:C:10:DC:H2'	3:C:11:DC:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:PHE:CD2	2:B:447:ARG:HD2	2.52	0.45
2:B:1136:SER:HA	4:D:2:DG:O3'	2.16	0.45
2:B:276:ASP:HB3	2:B:599:LYS:NZ	2.31	0.45
1:A:3:G:H2'	1:A:4:G:H8	1.81	0.45
2:B:338:LEU:HB3	2:B:383:MET:HE2	1.98	0.45
3:C:12:DA:H2"	3:C:13:DG:H8	1.81	0.45
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.99	0.45
2:B:175:ASN:N	2:B:176:PRO:HD3	2.32	0.45
1:A:44:U:H3	2:B:328:HIS:HB3	1.82	0.44
2:B:342:GLN:HB2	2:B:383:MET:HE3	1.99	0.44
1:A:3:G:H2'	1:A:4:G:C8	2.53	0.44
2:B:704:PHE:O	2:B:708:ILE:HG12	2.18	0.44
2:B:1117:ASP:N	2:B:1117:ASP:OD1	2.51	0.44
2:B:901:THR:O	2:B:904:GLU:HG2	2.17	0.44
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	2.00	0.44
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.99	0.44
3:C:1:DG:H2'	3:C:2:DG:C8	2.53	0.43
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.51	0.43
4:D:3:DT:H2"	4:D:4:DA:C8	2.52	0.43
2:B:112:LYS:HA	2:B:112:LYS:HD3	1.82	0.43
2:B:761:ILE:HD11	2:B:957:THR:HG22	1.99	0.43
1:A:69:A:H2'	1:A:70:C:C6	2.54	0.43
1:A:38:A:H2'	1:A:39:G:C8	2.54	0.43
2:B:841:ILE:HD13	2:B:900:LEU:HG	2.00	0.43
2:B:178:ASN:HA	2:B:184:LEU:HD11	2.01	0.42
2:B:186:ILE:O	2:B:190:GLN:HG2	2.19	0.42
2:B:266:LEU:HD22	2:B:294:LYS:HD2	2.02	0.42
2:B:962:LEU:HD23	2:B:962:LEU:HA	1.89	0.42
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.18	0.42
3:C:1:DG:H2'	3:C:2:DG:H8	1.84	0.42
1:A:36:A:H8	1:A:36:A:O5'	2.02	0.42
2:B:31:LYS:HD3	2:B:31:LYS:HA	1.88	0.42
2:B:780:ARG:NH1	2:B:806:LEU:O	2.51	0.42
2:B:314:LYS:HE2	2:B:314:LYS:HB3	1.81	0.42
2:B:512:SER:OG	2:B:617:GLU:OE1	2.28	0.42
2:B:451:TYR:CD1	2:B:488:ALA:HB2	2.55	0.41
2:B:747:LEU:HD23	2:B:747:LEU:HA	1.91	0.41
2:B:537:PRO:HG2	8:B:1576:HOH:O	2.21	0.41
2:B:618:ASP:O	2:B:621:LEU:HB3	2.20	0.41
2:B:302:LEU:HD13	2:B:302:LEU:HA	1.82	0.41
2:B:558:LYS:HE2	2:B:586:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:787:GLY:O	2:B:791:LEU:HB2	2.20	0.41
2:B:357:ASN:ND2	2:B:371:GLU:HB3	2.35	0.41
2:B:623:LEU:HD13	2:B:654:ARG:HG3	2.02	0.41
2:B:817:GLN:O	2:B:882:TYR:OH	2.38	0.41
1:A:48:A:H2'	1:A:49:A:C8	2.56	0.41
1:A:82:C:H6	1:A:82:C:H2'	1.62	0.41
3:C:-1:DC:H2'	3:C:0:DA:C8	2.56	0.40
2:B:979:ASN:HB2	2:B:1225:GLU:OE1	2.22	0.40
2:B:265:GLN:HB3	2:B:268:LYS:HG2	2.04	0.40
2:B:654:ARG:HD3	2:B:655:ARG:N	2.36	0.40
2:B:787:GLY:HA3	2:B:891:LEU:HD21	2.04	0.40
2:B:846:PHE:O	2:B:920:GLN:NE2	2.54	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	B	1324/1368 (97%)	1281 (97%)	43 (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
2	B	1197/1225 (98%)	1190 (99%)	7 (1%)	86 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	194	GLN
2	B	514	LEU
2	B	525	THR
2	B	635	ARG
2	B	853	ASP
2	B	859	ARG
2	B	1062	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	281	GLN
2	B	826	GLN
2	B	980	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	82/84 (97%)	13 (15%)	0

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	C
1	A	20	U
1	A	28	A
1	A	36	A
1	A	37	U
1	A	51	A
1	A	56	U
1	A	59	U
1	A	63	U
1	A	68	A
1	A	72	U
1	A	75	A

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Mol	Chain	Res	Type
1	A	82	C

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)

Of 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
7	EDO	B	1409	-	3,3,3	0.54	0	2,2,2	0.10	0
7	EDO	B	1408	-	3,3,3	0.46	0	2,2,2	0.17	0
7	EDO	A	108	-	3,3,3	0.46	0	2,2,2	0.38	0
7	EDO	C	102	-	3,3,3	0.54	0	2,2,2	0.01	0
7	EDO	A	109	-	3,3,3	0.51	0	2,2,2	0.23	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
7	EDO	B	1409	-	-	1/1/1/1	-
7	EDO	B	1408	-	-	1/1/1/1	-
7	EDO	A	108	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	102	-	-	1/1/1/1	-
7	EDO	A	109	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1408	EDO	O1-C1-C2-O2
7	C	102	EDO	O1-C1-C2-O2
7	A	108	EDO	O1-C1-C2-O2
7	B	1409	EDO	O1-C1-C2-O2

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, 95^{th} 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	84/84 (100%)	-0.26	1 (1%) 79 85	49, 70, 166, 219	0
2	B	1334/1368 (97%)	0.26	53 (3%) 38 45	42, 76, 126, 165	0
3	C	28/28 (100%)	-0.15	0 100 100	55, 71, 135, 160	0
4	D	10/12 (83%)	0.16	1 (10%) 7 7	59, 96, 150, 163	0
All	All	1456/1492 (97%)	0.22	55 (3%) 40 48	42, 76, 130, 219	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1245	LEU	6.2
2	B	1032	ALA	5.1
2	B	802	GLU	4.8
2	B	1039	TYR	3.8
2	B	801	VAL	3.7
2	B	177	ASP	3.5
2	B	1243	GLU	3.4
2	B	1036	TYR	3.3
2	B	1052	LEU	3.2
2	B	188	LEU	3.2
2	B	848	LYS	3.2
2	B	847	LEU	3.2
2	B	804	THR	3.1
2	B	1004	LEU	3.0
2	B	1058	ARG	3.0
2	B	806	LEU	3.0
2	B	784	ILE	2.9
2	B	1149	VAL	2.9
2	B	339	VAL	2.9
2	B	1157	LEU	2.7
2	B	789	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	781	MET	2.6
2	B	269	ASP	2.6
2	B	290	PHE	2.6
2	B	765	ARG	2.6
2	B	282	ILE	2.5
2	B	917	ILE	2.5
2	B	838	VAL	2.5
2	B	803	ASN	2.5
4	D	7	DG	2.5
2	B	1294	TYR	2.4
1	A	74	A	2.4
2	B	356	LYS	2.3
2	B	852	ILE	2.3
2	B	1194	LEU	2.3
2	B	1144	LEU	2.3
2	B	786	GLU	2.3
2	B	1259	VAL	2.3
2	B	919	ARG	2.2
2	B	268	LYS	2.2
2	B	205	GLY	2.2
2	B	1037	PHE	2.2
2	B	174	LEU	2.2
2	B	175	ASN	2.1
2	B	242	ILE	2.1
2	B	286	TYR	2.1
2	B	815	TYR	2.1
2	B	717	GLY	2.1
2	B	1007	GLU	2.1
2	B	1313	PHE	2.1
2	B	1326	TYR	2.1
2	B	1340	LYS	2.1
2	B	921	LEU	2.0
2	B	1365	LEU	2.0
2	B	1145	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 monosaccharides 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, 95^{th} 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	K	B	1404	1/1	0.73	0.09	144,144,144,144	0
7	EDO	C	102	4/4	0.77	0.33	79,85,86,88	0
6	K	A	107	1/1	0.82	0.22	128,128,128,128	0
6	K	B	1406	1/1	0.85	0.15	118,118,118,118	0
7	EDO	B	1409	4/4	0.86	0.29	65,66,68,72	0
6	K	B	1401	1/1	0.89	0.42	132,132,132,132	0
7	EDO	B	1408	4/4	0.89	0.34	78,82,86,88	0
7	EDO	A	109	4/4	0.90	0.11	67,75,80,81	0
6	K	A	103	1/1	0.91	0.15	82,82,82,82	0
5	MG	A	102	1/1	0.92	0.11	83,83,83,83	0
7	EDO	A	108	4/4	0.92	0.16	89,90,94,98	0
6	K	A	106	1/1	0.96	0.17	120,120,120,120	0
6	K	B	1402	1/1	0.96	0.24	85,85,85,85	0
6	K	A	104	1/1	0.96	0.08	62,62,62,62	0
6	K	C	101	1/1	0.97	0.12	83,83,83,83	0
6	K	A	105	1/1	0.97	0.21	94,94,94,94	0
6	K	B	1407	1/1	0.97	0.07	75,75,75,75	0
6	K	B	1403	1/1	0.98	0.10	117,117,117,117	0
5	MG	A	101	1/1	0.99	0.11	57,57,57,57	0
6	K	B	1405	1/1	0.99	0.07	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.