Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2022 – 01:58 pm BST

PDB ID	:	7QQZ
Title	:	SpCas9 bound to FANCF off-target7 DNA substrate
Authors	:	Pacesa, M.; Jinek, M.
Deposited on	:	2022-01-10
Resolution	:	2.25 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 (i)) were used in the production of this report:

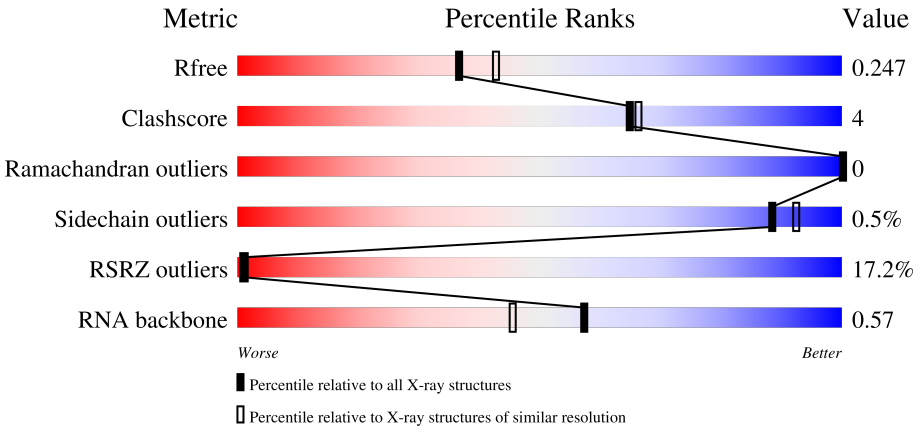
MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)
RNA backbone	3102	1016 (2.66-1.86)

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	15% 67% 27% 6%
2	B	1368	17% 86% 11% .
3	C	28	7% 75% 25%
4	D	12	17% 67% 17% 17%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13949 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 FANCF sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	P	0	0	1
			1755	784	317	571	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1335	Total	C	N	O	S	0	0	0
			10910	6947	1895	2046	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 FANCF off-target7 target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			571	274	104	166	27			

- Molecule 4 is a DNA chain called FANCF off-target7 non-target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			203	98	37	59	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	4	Total K 4 4	0	0
6	B	7	Total K 7 7	0	0

- Molecule 7 is water.

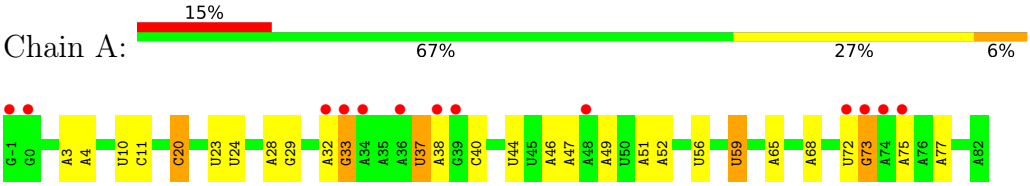
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	131	Total O 131 131	0	0
7	B	325	Total O 325 325	0	0
7	C	32	Total O 32 32	0	0
7	D	9	Total O 9 9	0	0

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.

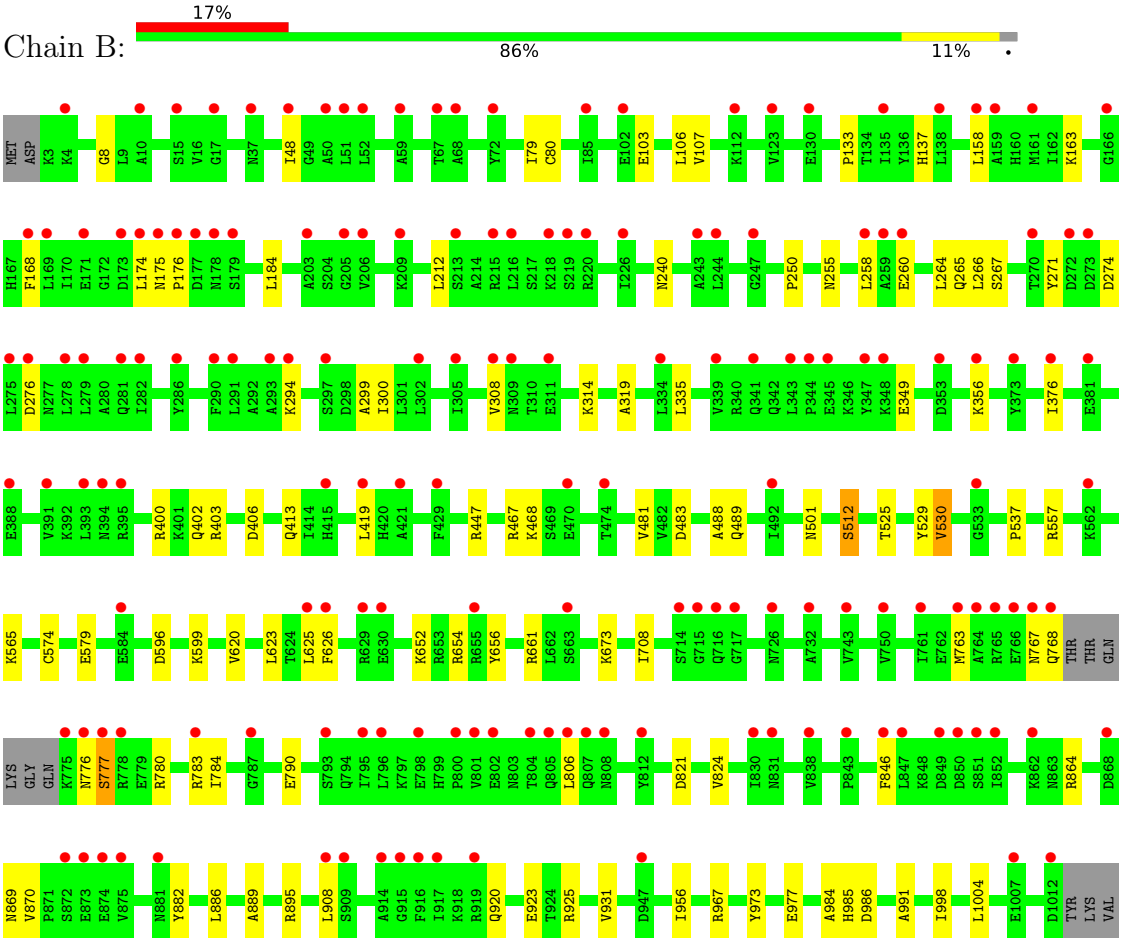
• Molecule 1: FANCF sgRNA

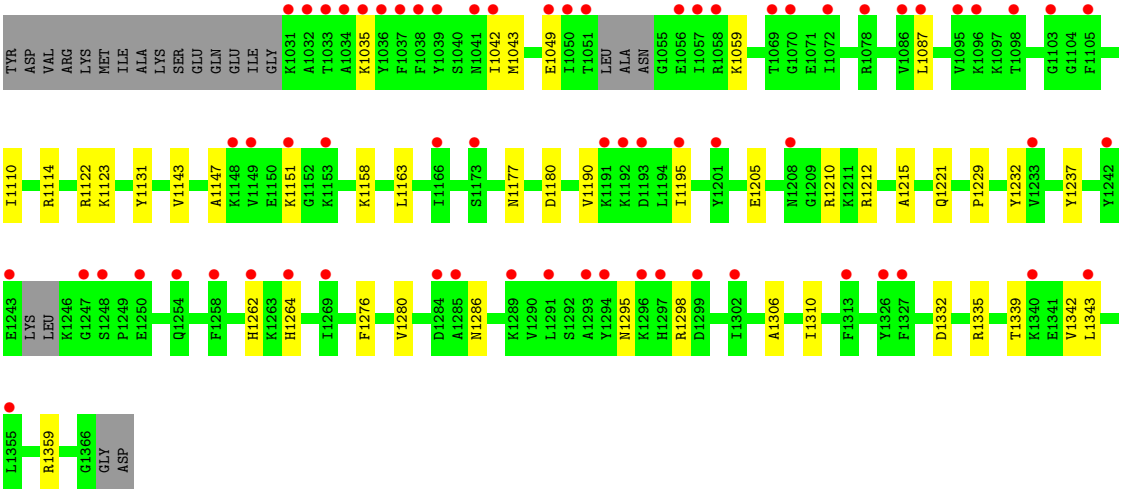
Chain A:



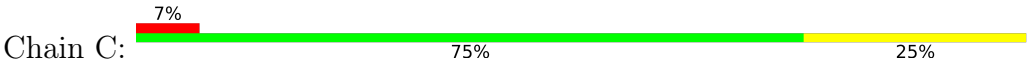
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

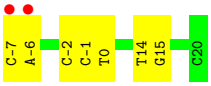
Chain B:



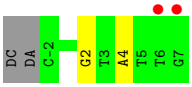


• Molecule 3: FANCF off-target7 target strand





• Molecule 4: FANCF off-target7 non-target strand



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.80Å 66.69Å 187.61Å 90.00° 110.83° 90.00°	Depositor
Resolution (Å)	47.67 – 2.25 47.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.67-2.25) 99.2 (47.67-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.217 , 0.247 0.217 , 0.247	Depositor DCC
R_{free} test set	4857 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13949	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: 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	0.26	0/1964	0.76	0/3060
2	B	0.25	0/11101	0.41	0/14913
3	C	0.57	0/640	1.00	0/986
4	D	0.59	0/227	0.93	0/349
All	All	0.28	0/13932	0.54	0/19308

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	1755	0	881	16	0
2	B	10910	0	11075	93	0
3	C	571	0	318	6	0
4	D	203	0	115	2	0
5	A	2	0	0	0	0
6	A	4	0	0	0	0
6	B	7	0	0	0	0
7	A	131	0	0	1	0
7	B	325	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	32	0	0	0	0
7	D	9	0	0	0	0
All	All	13949	0	12389	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 4.

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)
2:B:80:CYS:SG	7:B:1778:HOH:O	2.42	0.78
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.21	0.72
1:A:49:A:N3	2:B:1122:ARG:NH2	2.39	0.70
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.75	0.68
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.29	0.66
2:B:574:CYS:SG	7:B:1698:HOH:O	2.54	0.65
2:B:1210:ARG:HG3	2:B:1280:VAL:HG23	1.81	0.62
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.82	0.61
2:B:967:ARG:NH2	7:B:1505:HOH:O	2.33	0.60
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.85	0.59
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.30	0.58
2:B:294:LYS:NZ	7:B:1508:HOH:O	2.36	0.58
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.37	0.58
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.85	0.57
2:B:870:VAL:HG13	2:B:908:LEU:HG	1.85	0.57
2:B:1035:LYS:NZ	7:B:1514:HOH:O	2.38	0.55
3:C:-7:DC:H2"	3:C:-6:DA:H5"	1.88	0.55
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.39	0.55
2:B:864:ARG:NH1	2:B:869:ASN:O	2.37	0.55
2:B:266:LEU:HD22	2:B:294:LYS:HD2	1.89	0.55
1:A:3:A:H2'	1:A:4:A:C8	2.42	0.54
2:B:1276:PHE:O	2:B:1280:VAL:HG12	2.08	0.54
2:B:501:ASN:HB3	2:B:708:ILE:HD12	1.88	0.54
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.88	0.54
2:B:240:ASN:ND2	2:B:255:ASN:OD1	2.37	0.54
1:A:52:A:OP1	2:B:1123:LYS:NZ	2.40	0.53
2:B:512:SER:HA	2:B:620:VAL:HG11	1.89	0.53
2:B:1151:LYS:HD2	2:B:1158:LYS:HD2	1.91	0.53
2:B:846:PHE:O	2:B:920:GLN:NE2	2.40	0.53
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.90	0.53
3:C:14:DT:H2'	3:C:15:DG:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1114:ARG:NH1	4:D:4:DA:OP1	2.42	0.52
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.43	0.52
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.93	0.50
3:C:14:DT:H2'	3:C:15:DG:C8	2.47	0.50
1:A:59:U:OP1	2:B:467:ARG:NH2	2.44	0.50
2:B:168:PHE:CG	2:B:447:ARG:HD2	2.47	0.49
2:B:488:ALA:HB3	2:B:626:PHE:HE1	1.77	0.49
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.94	0.49
2:B:623:LEU:HD13	2:B:654:ARG:HG3	1.94	0.49
1:A:3:A:H2'	1:A:4:A:H8	1.77	0.48
2:B:79:ILE:HD11	2:B:163:LYS:HB2	1.95	0.48
2:B:1295:ASN:HA	2:B:1298:ARG:HD2	1.96	0.48
2:B:565:LYS:NZ	7:B:1528:HOH:O	2.46	0.48
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.96	0.47
1:A:20:C:OP2	2:B:403:ARG:NH1	2.48	0.47
2:B:447:ARG:NH2	7:B:1513:HOH:O	2.37	0.47
1:A:32:A:H2'	1:A:33:G:O4'	2.14	0.47
2:B:271:TYR:HA	2:B:274:ASP:HB2	1.96	0.47
2:B:654:ARG:HD2	2:B:656:TYR:CZ	2.50	0.47
2:B:784:ILE:HD12	2:B:806:LEU:HD13	1.97	0.46
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.49	0.46
2:B:212:LEU:HD13	2:B:300:ILE:HD11	1.98	0.46
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.97	0.46
2:B:776:ASN:OD1	2:B:777:SER:N	2.48	0.46
2:B:780:ARG:NH1	2:B:806:LEU:O	2.47	0.46
3:C:-2:DC:H2'	3:C:-1:DC:C6	2.50	0.46
2:B:158:LEU:HD22	2:B:419:LEU:HD12	1.99	0.45
1:A:10:U:OP1	2:B:783:ARG:NH2	2.44	0.45
1:A:65:A:N6	7:A:217:HOH:O	2.48	0.45
2:B:985:HIS:CG	2:B:1087:LEU:HD22	2.52	0.45
1:A:46:A:H2'	1:A:47:A:C8	2.52	0.45
2:B:468:LYS:HG3	2:B:483:ASP:HB2	1.99	0.44
2:B:276:ASP:HB3	2:B:599:LYS:NZ	2.32	0.44
2:B:1049:GLU:OE1	2:B:1059:LYS:NZ	2.49	0.44
2:B:1210:ARG:HA	2:B:1280:VAL:HG23	1.98	0.44
1:A:73:G:H5"	1:A:73:G:H8	1.82	0.44
2:B:895:ARG:NE	3:C:14:DT:O2	2.38	0.43
1:A:44:U:O2'	2:B:402:GLN:OE1	2.28	0.43
2:B:103:GLU:HB2	2:B:106:LEU:HD12	1.99	0.43
1:A:37:U:H2'	1:A:38:A:C8	2.54	0.43
2:B:973:TYR:HB3	2:B:1237:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:A:OP1	2:B:661:ARG:NE	2.30	0.43
2:B:8:GLY:HA3	2:B:991:ALA:HB2	2.00	0.43
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.83	0.43
2:B:821:ASP:HB3	2:B:824:VAL:O	2.19	0.43
2:B:133:PRO:HG2	2:B:137:HIS:CE1	2.54	0.42
3:C:-1:DC:H2'	3:C:0:DT:C6	2.54	0.42
2:B:107:VAL:HG23	2:B:1131:TYR:CZ	2.54	0.42
2:B:1122:ARG:HD3	7:B:1608:HOH:O	2.18	0.42
2:B:174:LEU:HD22	2:B:413:GLN:HB2	2.01	0.42
2:B:250:PRO:HD2	2:B:264:LEU:O	2.20	0.42
2:B:1262:HIS:HA	2:B:1264:HIS:CE1	2.55	0.42
1:A:10:U:H2'	1:A:11:C:C6	2.55	0.42
2:B:489:GLN:HG3	2:B:625:LEU:HD21	2.01	0.42
2:B:529:TYR:HA	2:B:579:GLU:O	2.20	0.42
2:B:923:GLU:OE1	2:B:925:ARG:HD3	2.20	0.42
2:B:175:ASN:N	2:B:176:PRO:HD3	2.35	0.41
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.53	0.41
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.55	0.41
2:B:265:GLN:HG2	2:B:267:SER:H	1.86	0.41
2:B:335:LEU:HD21	2:B:376:ILE:HD11	2.02	0.41
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	2.03	0.41
2:B:349:GLU:OE2	2:B:356:LYS:HE2	2.21	0.41
1:A:23:U:H2'	1:A:24:U:C6	2.56	0.41
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.20	0.41
2:B:767:ASN:O	2:B:768:GLN:HB3	2.20	0.41
2:B:48:ILE:HG12	2:B:984:ALA:HB1	2.03	0.41
2:B:314:LYS:HE2	2:B:314:LYS:HB3	1.84	0.41
2:B:673:LYS:HE3	2:B:673:LYS:HB2	1.95	0.41
2:B:763:MET:HE1	2:B:931:VAL:HG21	2.03	0.41
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.87	0.40
2:B:468:LYS:N	2:B:481:VAL:O	2.39	0.40
2:B:956:ILE:HD11	2:B:998:ILE:HD13	2.03	0.40
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.21	0.40
2:B:652:LYS:HE2	2:B:652:LYS:HB3	1.83	0.40
2:B:977:GLU:OE2	2:B:977:GLU:N	2.49	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	1325/1368 (97%)	1293 (98%)	32 (2%)	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%)	1191 (100%)	6 (0%)	88 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	258	LEU
2	B	260	GLU
2	B	512	SER
2	B	525	THR
2	B	530	VAL
2	B	777	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	HIS
2	B	511	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	81/84 (96%)	14 (17%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	20	C
1	A	28	A
1	A	29	G
1	A	33	G
1	A	37	U
1	A	40	C
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	72	U
1	A	73	G
1	A	75	A
1	A	77	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers

Mogul failed to run properly - this section is therefore empty.

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%)	1.51	13 (15%) 2 1	44, 60, 145, 186	0
2	B	1335/1368 (97%)	1.25	233 (17%) 1 1	40, 65, 107, 133	0
3	C	28/28 (100%)	0.90	2 (7%) 16 17	50, 63, 126, 156	0
4	D	10/12 (83%)	1.28	2 (20%) 1 1	57, 76, 124, 155	0
All	All	1457/1492 (97%)	1.26	250 (17%) 1 1	40, 64, 111, 186	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	G	20.8
1	A	74	A	9.9
2	B	1057	ILE	8.4
2	B	1037	PHE	7.4
2	B	767	ASN	7.4
2	B	206	VAL	7.2
2	B	775	LYS	7.1
2	B	1050	ILE	6.8
2	B	259	ALA	6.5
2	B	388	GLU	6.2
3	C	-7	DC	6.1
2	B	802	GLU	5.8
2	B	175	ASN	5.5
2	B	394	ASN	5.4
2	B	765	ARG	5.2
2	B	872	SER	5.1
4	D	7	DG	5.1
2	B	776	ASN	5.1
1	A	0	G	5.1
2	B	1243	GLU	5.0
2	B	868	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	947	ASP	5.0
2	B	766	GLU	5.0
2	B	1069	THR	4.9
2	B	1031	LYS	4.9
2	B	714	SER	4.7
2	B	1293	ALA	4.7
2	B	308	VAL	4.7
2	B	846	PHE	4.7
2	B	1192	LYS	4.7
2	B	171	GLU	4.6
2	B	356	LYS	4.5
2	B	176	PRO	4.4
2	B	281	GLN	4.4
2	B	849	ASP	4.3
2	B	1078	ARG	4.3
2	B	177	ASP	4.3
2	B	279	LEU	4.2
2	B	764	ALA	4.1
2	B	1032	ALA	4.1
2	B	339	VAL	4.1
2	B	1038	PHE	4.1
2	B	851	SER	4.0
2	B	873	GLU	4.0
2	B	347	TYR	4.0
2	B	1051	THR	3.9
2	B	850	ASP	3.9
2	B	205	GLY	3.8
2	B	216	LEU	3.8
2	B	470	GLU	3.8
2	B	1269	ILE	3.8
2	B	1036	TYR	3.7
2	B	1041	ASN	3.7
2	B	309	ASN	3.7
2	B	914	ALA	3.7
2	B	716	GLN	3.7
2	B	290	PHE	3.7
2	B	804	THR	3.6
2	B	917	ILE	3.6
2	B	838	VAL	3.6
2	B	777	SER	3.6
2	B	852	ILE	3.5
2	B	1264	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	213	SER	3.5
2	B	768	GLN	3.5
2	B	847	LEU	3.4
2	B	881	ASN	3.4
2	B	1070	GLY	3.4
2	B	258	LEU	3.4
2	B	348	LYS	3.4
2	B	798	GLU	3.4
2	B	1148	LYS	3.4
2	B	244	LEU	3.4
2	B	334	LEU	3.4
1	A	36	A	3.3
2	B	1326	TYR	3.3
2	B	862	LYS	3.3
2	B	1042	ILE	3.3
2	B	1250	GLU	3.3
2	B	273	ASP	3.3
2	B	278	LEU	3.3
2	B	800	PRO	3.3
2	B	533	GLY	3.2
2	B	1291	LEU	3.2
3	C	-6	DA	3.2
2	B	220	ARG	3.2
2	B	715	GLY	3.2
1	A	73	G	3.2
2	B	1297	HIS	3.2
1	A	33	G	3.1
2	B	305	ILE	3.1
2	B	286	TYR	3.1
2	B	1039	TYR	3.1
4	D	6	DT	3.1
2	B	1151	LYS	3.1
2	B	275	LEU	3.1
2	B	474	THR	3.1
2	B	311	GLU	3.1
2	B	1056	GLU	3.1
2	B	1033	THR	3.0
2	B	343	LEU	3.0
2	B	1296	LYS	3.0
1	A	75	A	3.0
2	B	344	PRO	3.0
2	B	294	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	1034	ALA	2.9
2	B	272	ASP	2.9
2	B	219	SER	2.9
2	B	215	ARG	2.9
2	B	297	SER	2.8
2	B	1327	PHE	2.8
2	B	801	VAL	2.8
2	B	843	PRO	2.8
2	B	178	ASN	2.8
2	B	1149	VAL	2.8
2	B	1095	VAL	2.8
2	B	874	GLU	2.8
2	B	732	ALA	2.7
2	B	270	THR	2.7
2	B	1072	ILE	2.7
2	B	276	ASP	2.7
2	B	138	LEU	2.7
2	B	243	ALA	2.7
2	B	291	LEU	2.7
2	B	376	ILE	2.7
1	A	38	A	2.7
2	B	763	MET	2.7
2	B	395	ARG	2.6
1	A	32	A	2.6
2	B	52	LEU	2.6
2	B	341	GLN	2.6
2	B	743	VAL	2.6
2	B	831	ASN	2.6
2	B	209	LYS	2.6
2	B	663	SER	2.6
2	B	875	VAL	2.6
2	B	1343	LEU	2.6
2	B	1355	LEU	2.6
2	B	1299	ASP	2.6
2	B	1289	LYS	2.5
2	B	37	ASN	2.5
2	B	1058	ARG	2.5
2	B	795	ILE	2.5
2	B	1248	SER	2.5
2	B	778	ARG	2.5
2	B	226	ILE	2.5
2	B	10	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	159	ALA	2.5
2	B	1242	TYR	2.5
2	B	726	ASN	2.5
2	B	806	LEU	2.5
2	B	373	TYR	2.5
2	B	17	GLY	2.5
2	B	1285	ALA	2.4
2	B	260	GLU	2.4
2	B	381	GLU	2.4
2	B	391	VAL	2.4
2	B	130	GLU	2.4
2	B	302	LEU	2.4
2	B	1340	LYS	2.4
2	B	393	LEU	2.4
2	B	625	LEU	2.4
2	B	1103	GLY	2.4
2	B	915	GLY	2.4
2	B	1195	ILE	2.4
2	B	717	GLY	2.4
2	B	293	ALA	2.4
2	B	1302	ILE	2.3
2	B	812	TYR	2.3
2	B	1262	HIS	2.3
2	B	59	ALA	2.3
1	A	34	A	2.3
2	B	345	GLU	2.3
2	B	169	LEU	2.3
2	B	655	ARG	2.3
2	B	173	ASP	2.3
2	B	247	GLY	2.3
2	B	1153	LYS	2.3
2	B	1247	GLY	2.3
2	B	421	ALA	2.3
2	B	1313	PHE	2.3
2	B	112	LYS	2.3
2	B	50	ALA	2.3
2	B	805	GLN	2.3
2	B	85	ILE	2.3
2	B	179	SER	2.3
2	B	174	LEU	2.2
2	B	353	ASP	2.2
2	B	1086	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	282	ILE	2.2
1	A	72	U	2.2
2	B	48	ILE	2.2
2	B	51	LEU	2.2
2	B	102	GLU	2.2
2	B	218	LYS	2.2
2	B	1096	LYS	2.2
2	B	1098	THR	2.2
2	B	562	LYS	2.2
2	B	15	SER	2.2
2	B	1105	PHE	2.2
2	B	584	GLU	2.2
2	B	1007	GLU	2.2
2	B	1284	ASP	2.2
2	B	1208	ASN	2.2
2	B	135	ILE	2.2
2	B	1035	LYS	2.2
2	B	1173	SER	2.2
2	B	787	GLY	2.2
2	B	168	PHE	2.2
2	B	429	PHE	2.2
2	B	1258	PHE	2.2
2	B	4	LYS	2.2
2	B	1166	ILE	2.2
2	B	419	LEU	2.2
2	B	161	MET	2.2
2	B	1193	ASP	2.2
2	B	1294	TYR	2.1
2	B	203	ALA	2.1
2	B	761	ILE	2.1
2	B	1087	LEU	2.1
2	B	72	TYR	2.1
2	B	123	VAL	2.1
2	B	67	THR	2.1
2	B	158	LEU	2.1
2	B	796	LEU	2.1
2	B	1201	TYR	2.1
2	B	783	ARG	2.1
2	B	919	ARG	2.1
2	B	68	ALA	2.1
2	B	1233	VAL	2.1
2	B	916	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	909	SER	2.1
2	B	492	ILE	2.1
2	B	1049	GLU	2.1
2	B	166	GLY	2.1
2	B	793	SER	2.1
2	B	630	GLU	2.0
2	B	415	HIS	2.0
2	B	629	ARG	2.0
2	B	908	LEU	2.0
1	A	48	A	2.0
2	B	808	ASN	2.0
2	B	807	GLN	2.0
2	B	1191	LYS	2.0
2	B	830	ILE	2.0
2	B	1254	GLN	2.0
2	B	750	VAL	2.0
2	B	626	PHE	2.0
1	A	39	G	2.0
2	B	1012	ASP	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	A	106	1/1	0.62	0.15	122,122,122,122	0
6	K	B	1401	1/1	0.79	0.17	104,104,104,104	0
6	K	A	103	1/1	0.80	0.70	110,110,110,110	0
6	K	B	1403	1/1	0.82	0.23	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	K	A	105	1/1	0.83	0.28	86,86,86,86	0
6	K	B	1404	1/1	0.87	0.16	91,91,91,91	0
6	K	B	1405	1/1	0.88	0.11	82,82,82,82	0
5	MG	A	102	1/1	0.91	0.15	46,46,46,46	0
5	MG	A	101	1/1	0.92	0.42	68,68,68,68	0
6	K	B	1406	1/1	0.92	0.11	90,90,90,90	0
6	K	B	1407	1/1	0.94	0.09	56,56,56,56	0
6	K	B	1402	1/1	0.97	0.14	62,62,62,62	0
6	K	A	104	1/1	0.98	0.19	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.