Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2022 – 10:47 am BST

PDB ID	:	7QQU
Title	:	SpCas9 bound to FANCF off-target2 DNA substrate
Authors	:	Pacesa, M.; Jinek, M.
Deposited on	:	2022-01-10
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

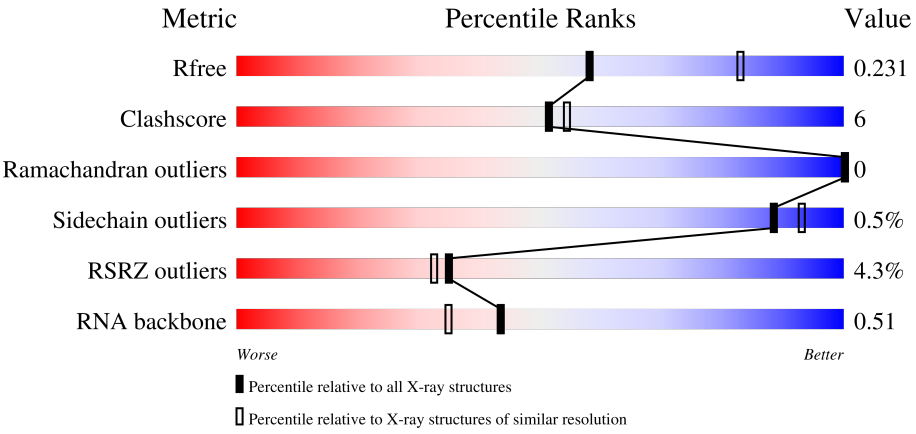
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	4% 50% 43% 7%
2	B	1368	4% 84% 13% .
3	C	28	57% 43%
4	D	12	17% 58% 33% 8%

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
6	K	B	1408	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14010 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	1327	Total	C	N	O	S	0	0	0
			10846	6911	1882	2031	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-target2 target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			574	273	108	166	27			

- Molecule 4 is a DNA chain called FANCF off-target2 non-target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- 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	8	Total K 8 8	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is water.

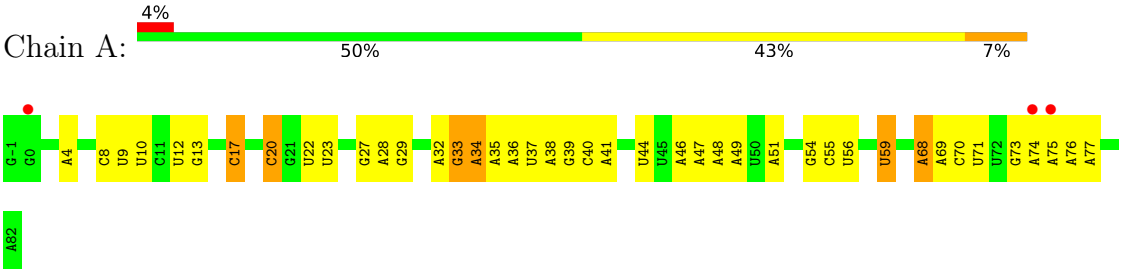
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	152	Total O 152 152	0	0
7	B	397	Total O 397 397	0	0
7	C	36	Total O 36 36	0	0
7	D	11	Total O 11 11	0	0

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.

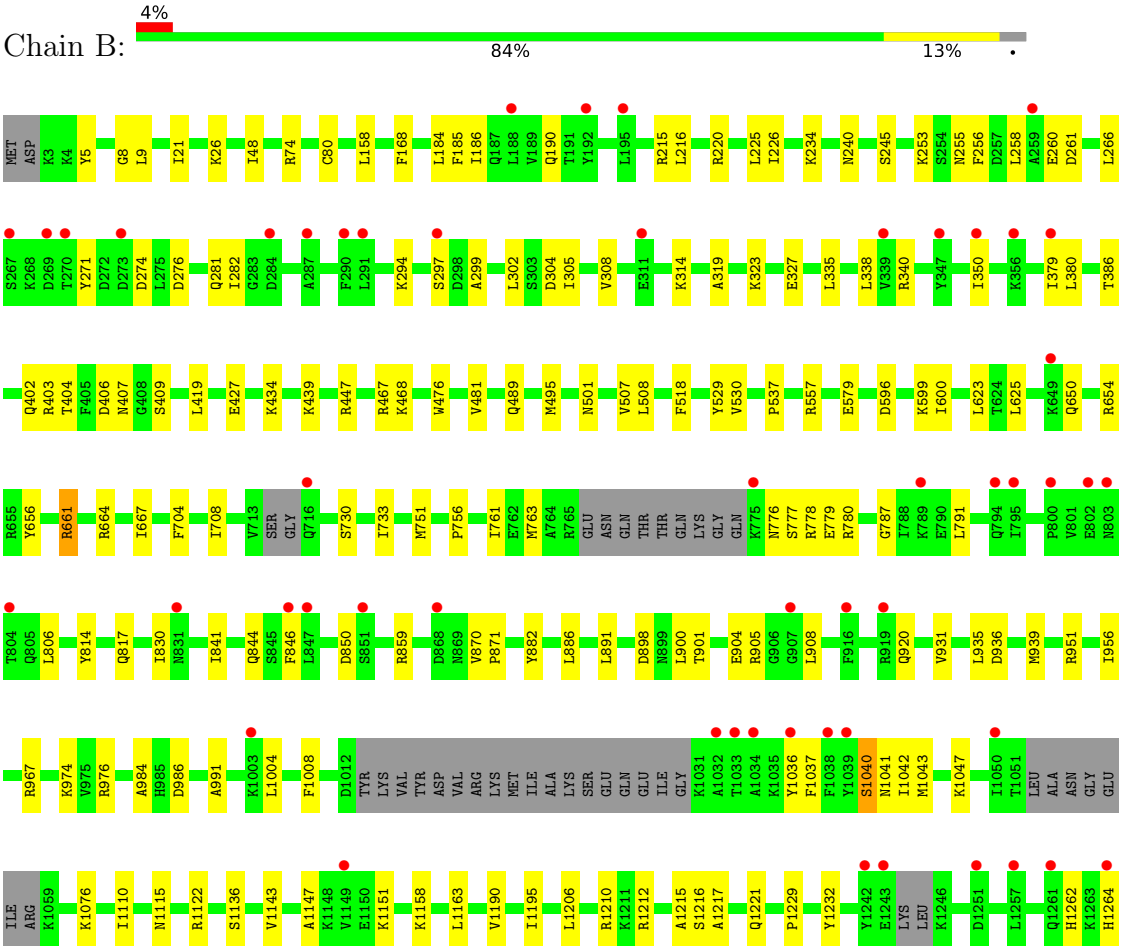
• Molecule 1: FANCF sgRNA

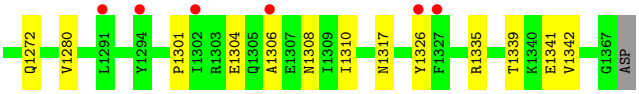
Chain A:



• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

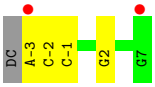
Chain B:





• Molecule 3: FANCF off-target2 target strand

• Molecule 4: FANCF off-target2 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	177.44Å 67.49Å 187.11Å 90.00° 111.17° 90.00°	Depositor
Resolution (Å)	47.81 – 2.45 47.81 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.81-2.45) 99.7 (47.81-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.202 , 0.231 0.202 , 0.231	Depositor DCC
R_{free} test set	3807 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: K, MG

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	0.28	0/1964	0.82	0/3060
2	B	0.25	0/11036	0.42	0/14825
3	C	0.62	0/644	1.00	1/993 (0.1%)
4	D	0.62	0/251	0.93	0/386
All	All	0.29	0/13895	0.56	1/19264 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	DG	O4'-C4'-C3'	-6.03	102.09	104.50

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	29	0
2	B	10846	0	11016	112	0
3	C	574	0	316	10	0
4	D	224	0	126	5	0
5	A	2	0	0	0	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	0	0	0
6	C	1	0	0	0	0
7	A	152	0	0	0	0
7	B	397	0	0	5	0
7	C	36	0	0	0	0
7	D	11	0	0	0	0
All	All	14010	0	12339	144	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 (144) 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:158:LEU:HD22	2:B:419:LEU:HD12	1.69	0.75
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.72	0.72
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.73	0.71
2:B:216:LEU:HD22	2:B:220:ARG:HG2	1.74	0.69
1:A:46:A:H2'	1:A:47:A:H8	1.57	0.69
2:B:260:GLU:HB3	2:B:281:GLN:HE22	1.56	0.69
2:B:256:PHE:HB3	2:B:282:ILE:HD11	1.74	0.68
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.29	0.66
1:A:46:A:H2'	1:A:47:A:C8	2.31	0.65
2:B:266:LEU:HD22	2:B:294:LYS:HD2	1.80	0.64
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.80	0.63
1:A:4:A:OP1	2:B:661:ARG:HD3	1.98	0.63
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.33	0.62
1:A:41:A:OP2	2:B:340:ARG:NH2	2.31	0.61
2:B:661:ARG:NH1	3:C:11:DG:OP2	2.34	0.61
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.34	0.60
2:B:168:PHE:CG	2:B:447:ARG:HD2	2.37	0.59
2:B:763:MET:HE1	2:B:931:VAL:HG21	1.84	0.59
2:B:215:ARG:NH1	2:B:304:ASP:O	2.36	0.58
2:B:258:LEU:HD21	2:B:282:ILE:HD11	1.86	0.58
1:A:59:U:OP1	2:B:467:ARG:NH2	2.36	0.57
2:B:271:TYR:HA	2:B:274:ASP:HB2	1.87	0.57
1:A:49:A:N3	2:B:1122:ARG:NH2	2.49	0.56
3:C:-2:DC:H2'	3:C:-1:DC:C6	2.40	0.56
3:C:-2:DC:H2"	3:C:-1:DC:H5'	1.87	0.56
2:B:898:ASP:O	2:B:905:ARG:NH2	2.39	0.56
2:B:844:GLN:NE2	2:B:850:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:G:H5'	1:A:34:A:OP2	2.06	0.56
1:A:44:U:O2'	2:B:402:GLN:OE1	2.22	0.55
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.88	0.55
2:B:1151:LYS:HD2	2:B:1158:LYS:HD2	1.88	0.55
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	1.89	0.55
2:B:80:CYS:SG	7:B:1862:HOH:O	2.58	0.55
2:B:654:ARG:HD2	2:B:656:TYR:CZ	2.42	0.55
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.87	0.54
1:A:54:G:H2'	1:A:55:C:C6	2.43	0.54
1:A:27:G:N2	1:A:44:U:OP2	2.41	0.54
1:A:17:C:OP2	2:B:74:ARG:NH1	2.42	0.53
4:D:-2:DC:H2'	4:D:-1:DC:C6	2.44	0.53
1:A:34:A:H8	1:A:34:A:O5'	1.91	0.53
2:B:967:ARG:NH2	7:B:1520:HOH:O	2.36	0.53
3:C:-7:DC:H2'	3:C:-7:DC:O2	2.08	0.53
2:B:245:SER:HA	2:B:297:SER:HB2	1.90	0.53
2:B:859:ARG:NH2	7:B:1504:HOH:O	2.39	0.52
2:B:276:ASP:HB3	2:B:599:LYS:NZ	2.23	0.52
3:C:9:DA:H2'	3:C:10:DG:H8	1.73	0.52
2:B:338:LEU:HD13	2:B:386:THR:HG22	1.91	0.51
3:C:-5:DA:H1'	3:C:-4:DT:H5'	1.92	0.51
3:C:-6:DA:H2"	3:C:-5:DA:C8	2.46	0.51
1:A:22:U:H2'	1:A:23:U:C6	2.46	0.51
1:A:70:C:H2'	1:A:71:U:H6	1.76	0.51
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.93	0.50
2:B:240:ASN:ND2	2:B:255:ASN:OD1	2.30	0.50
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.94	0.49
1:A:74:A:OP1	1:A:74:A:H8	1.96	0.49
2:B:870:VAL:HG23	2:B:908:LEU:HG	1.94	0.49
1:A:38:A:H2'	1:A:39:G:C8	2.48	0.49
1:A:70:C:H2'	1:A:71:U:C6	2.48	0.48
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.95	0.48
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.94	0.48
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.14	0.48
2:B:787:GLY:O	2:B:791:LEU:HB2	2.15	0.47
2:B:529:TYR:HA	2:B:579:GLU:O	2.14	0.47
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.47	0.47
2:B:1262:HIS:HA	2:B:1264:HIS:CE1	2.50	0.47
1:A:20:C:OP2	2:B:403:ARG:NH1	2.48	0.47
2:B:1317:ASN:ND2	7:B:1508:HOH:O	2.32	0.46
2:B:350:ILE:HD11	2:B:379:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:ILE:HD13	2:B:900:LEU:HG	1.97	0.46
1:A:69:A:H2'	1:A:70:C:C6	2.50	0.46
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.97	0.46
2:B:501:ASN:HB3	2:B:708:ILE:HD12	1.97	0.46
2:B:1136:SER:HA	4:D:2:DG:O3'	2.15	0.46
3:C:8:DT:H2'	3:C:9:DA:C8	2.51	0.46
1:A:69:A:H2'	1:A:70:C:H6	1.81	0.46
2:B:323:LYS:HE2	2:B:327:GLU:OE2	2.16	0.46
2:B:600:ILE:HG23	2:B:650:GLN:HB3	1.98	0.45
2:B:936:ASP:OD1	2:B:951:ARG:NH1	2.49	0.45
2:B:185:PHE:HE1	2:B:225:LEU:HD21	1.81	0.45
2:B:935:LEU:O	2:B:939:MET:HG2	2.15	0.45
2:B:404:THR:H	2:B:407:ASN:ND2	2.15	0.45
2:B:704:PHE:O	2:B:708:ILE:HG12	2.16	0.45
2:B:5:TYR:CZ	2:B:751:MET:HG3	2.51	0.45
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.99	0.45
2:B:1036:TYR:O	2:B:1040:SER:OG	2.25	0.45
2:B:776:ASN:OD1	2:B:777:SER:N	2.49	0.45
1:A:9:U:H2'	1:A:10:U:O4'	2.17	0.45
2:B:1216:SER:OG	2:B:1217:ALA:N	2.49	0.45
1:A:33:G:H5"	1:A:33:G:H8	1.82	0.45
2:B:335:LEU:HA	2:B:338:LEU:HD12	1.99	0.44
3:C:9:DA:H2'	3:C:10:DG:C8	2.51	0.44
2:B:168:PHE:CD1	2:B:447:ARG:HD2	2.53	0.44
2:B:186:ILE:O	2:B:190:GLN:HG3	2.18	0.44
2:B:276:ASP:HB3	2:B:599:LYS:HZ1	1.82	0.44
4:D:-3:DA:H2"	4:D:-2:DC:C5'	2.47	0.44
2:B:1206:LEU:HD22	2:B:1210:ARG:HH12	1.82	0.44
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.83	0.44
1:A:32:A:H2'	1:A:33:G:O4'	2.17	0.44
2:B:380:LEU:O	2:B:386:THR:OG1	2.28	0.44
2:B:623:LEU:HD13	2:B:654:ARG:HG3	1.99	0.44
2:B:956:ILE:HG23	2:B:1008:PHE:HB3	1.99	0.44
2:B:253:LYS:HD2	2:B:261:ASP:OD1	2.18	0.43
2:B:901:THR:O	2:B:904:GLU:HG2	2.18	0.43
2:B:1210:ARG:NH2	2:B:1341:GLU:OE2	2.51	0.43
2:B:778:ARG:HD3	3:C:4:DG:OP1	2.18	0.43
2:B:256:PHE:HB3	2:B:282:ILE:CD1	2.46	0.43
2:B:468:LYS:N	2:B:481:VAL:O	2.42	0.43
1:A:33:G:N2	1:A:36:A:OP2	2.44	0.43
2:B:447:ARG:NH2	7:B:1549:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:LYS:O	2:B:1076:LYS:NZ	2.34	0.43
1:A:37:U:H2'	1:A:38:A:C8	2.54	0.43
2:B:226:ILE:HG13	2:B:234:LYS:HA	2.01	0.43
2:B:518:PHE:CD1	2:B:667:ILE:HD12	2.53	0.42
2:B:21:ILE:HA	2:B:26:LYS:O	2.20	0.42
2:B:439:LYS:HG2	2:B:476:TRP:CD1	2.55	0.42
2:B:530:VAL:HG22	2:B:537:PRO:HB3	2.01	0.42
1:A:48:A:H2'	1:A:49:A:C8	2.54	0.42
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	2.02	0.42
2:B:1308:ASN:HB3	2:B:1326:TYR:CD1	2.54	0.42
4:D:-3:DA:H2"	4:D:-2:DC:H5"	2.01	0.42
2:B:406:ASP:OD1	2:B:406:ASP:N	2.47	0.42
2:B:817:GLN:O	2:B:882:TYR:OH	2.34	0.42
2:B:8:GLY:HA3	2:B:991:ALA:HB2	2.02	0.41
2:B:302:LEU:HD13	2:B:302:LEU:HA	1.91	0.41
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.20	0.41
2:B:846:PHE:O	2:B:920:GLN:NE2	2.53	0.41
1:A:68:A:C4	1:A:69:A:C8	3.09	0.41
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.55	0.41
1:A:76:A:H8	1:A:76:A:O5'	2.03	0.41
2:B:814:TYR:CZ	2:B:830:ILE:HG12	2.55	0.41
2:B:185:PHE:CE1	2:B:225:LEU:HD21	2.56	0.41
2:B:870:VAL:HG13	2:B:871:PRO:HD2	2.02	0.41
2:B:305:ILE:HD11	2:B:409:SER:HB3	2.03	0.41
2:B:314:LYS:HE2	2:B:314:LYS:HB3	1.85	0.41
2:B:427:GLU:HB2	2:B:434:LYS:HB2	2.02	0.41
2:B:787:GLY:HA3	2:B:891:LEU:HD21	2.03	0.41
2:B:974:LYS:HD2	2:B:976:ARG:NH1	2.36	0.41
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.91	0.41
2:B:780:ARG:NH1	2:B:806:LEU:O	2.52	0.41
2:B:756:PRO:HD2	2:B:939:MET:CE	2.51	0.40
1:A:13:G:N2	2:B:495:MET:SD	2.95	0.40
2:B:730:SER:O	2:B:733:ILE:HG22	2.22	0.40
2:B:1301:PRO:HB2	2:B:1304:GLU:HG2	2.04	0.40
2:B:1037:PHE:O	2:B:1041:ASN:ND2	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	1315/1368 (96%)	1269 (96%)	46 (4%)	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	1190/1225 (97%)	1184 (100%)	6 (0%)	88 93

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

Mol	Chain	Res	Type
2	B	507	VAL
2	B	661	ARG
2	B	779	GLU
2	B	1040	SER
2	B	1115	ASN
2	B	1272	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	281	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	81/84 (96%)	17 (20%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	C
1	A	12	U
1	A	17	C
1	A	20	C
1	A	28	A
1	A	29	G
1	A	33	G
1	A	34	A
1	A	35	A
1	A	40	C
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.04	3 (3%) 42 39	35, 53, 145, 192	0
2	B	1327/1368 (97%)	0.31	58 (4%) 34 32	29, 61, 107, 155	0
3	C	28/28 (100%)	0.01	0 100 100	43, 55, 108, 119	0
4	D	11/12 (91%)	0.64	2 (18%) 1 0	44, 64, 131, 140	0
All	All	1450/1492 (97%)	0.29	63 (4%) 35 32	29, 60, 108, 192	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	804	THR	4.6
2	B	802	GLU	4.3
2	B	1036	TYR	4.3
2	B	287	ALA	4.2
1	A	74	A	4.1
2	B	1039	TYR	4.0
2	B	259	ALA	3.9
2	B	188	LEU	3.6
2	B	195	LEU	3.5
1	A	0	G	3.5
2	B	297	SER	3.5
2	B	290	PHE	3.4
2	B	1291	LEU	3.4
2	B	795	ILE	3.3
2	B	1032	ALA	3.3
2	B	379	ILE	3.3
4	D	-3	DA	3.0
2	B	1038	PHE	2.9
2	B	847	LEU	2.9
4	D	7	DG	2.8
2	B	1050	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	270	THR	2.7
2	B	800	PRO	2.7
2	B	356	LYS	2.6
2	B	846	PHE	2.6
2	B	350	ILE	2.6
2	B	267	SER	2.6
2	B	269	ASP	2.5
2	B	1294	TYR	2.4
2	B	868	ASP	2.4
2	B	1257	LEU	2.4
2	B	1302	ILE	2.4
2	B	1033	THR	2.4
2	B	907	GLY	2.4
2	B	775	LYS	2.4
2	B	1327	PHE	2.4
2	B	716	GLN	2.4
2	B	649	LYS	2.3
2	B	1034	ALA	2.3
2	B	1243	GLU	2.3
2	B	311	GLU	2.3
2	B	803	ASN	2.3
2	B	284	ASP	2.3
2	B	1326	TYR	2.2
2	B	1264	HIS	2.2
2	B	794	GLN	2.2
2	B	192	TYR	2.2
2	B	291	LEU	2.2
2	B	1306	ALA	2.2
1	A	75	A	2.2
2	B	347	TYR	2.1
2	B	1242	TYR	2.1
2	B	1251	ASP	2.1
2	B	831	ASN	2.1
2	B	1149	VAL	2.1
2	B	916	PHE	2.1
2	B	273	ASP	2.1
2	B	789	LYS	2.1
2	B	851	SER	2.1
2	B	1261	GLN	2.1
2	B	919	ARG	2.0
2	B	339	VAL	2.0
2	B	1003	LYS	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	1408	1/1	0.76	1.01	138,138,138,138	0
6	K	A	106	1/1	0.80	0.14	109,109,109,109	0
6	K	B	1401	1/1	0.84	0.32	100,100,100,100	0
6	K	B	1405	1/1	0.85	0.09	95,95,95,95	0
6	K	B	1406	1/1	0.90	0.14	113,113,113,113	0
6	K	B	1404	1/1	0.92	0.12	86,86,86,86	0
6	K	A	105	1/1	0.92	0.25	81,81,81,81	0
6	K	A	103	1/1	0.95	0.16	75,75,75,75	0
6	K	B	1402	1/1	0.96	0.13	62,62,62,62	0
6	K	B	1403	1/1	0.96	0.08	75,75,75,75	0
5	MG	A	102	1/1	0.96	0.14	33,33,33,33	0
6	K	C	101	1/1	0.96	0.26	74,74,74,74	0
5	MG	A	101	1/1	0.97	0.28	58,58,58,58	0
6	K	B	1407	1/1	0.97	0.14	80,80,80,80	0
6	K	A	104	1/1	0.99	0.12	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.