Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 12:15 pm GMT

PDB ID	:	6I1K
Title	:	Crystal structure of catalytically inactive FnCas12a in complex with a crRNA guide and a dsDNA target
Authors	:	Jinek, M.; Swarts, D.C.
Deposited on	:	2018-10-29
Resolution	:	2.65 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:

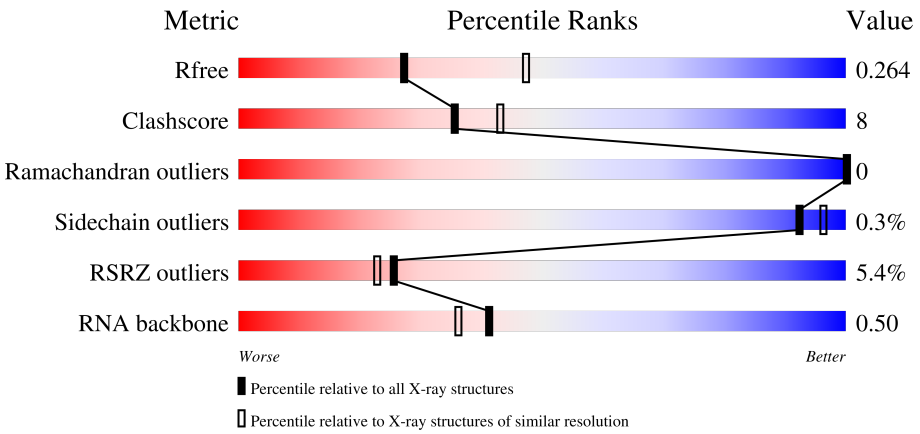
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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	1302	6% 79% 20% ·
2	B	40	35% 40% 25%
3	C	38	53% 47%
4	D	38	3% 42% 42% · 13%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12982 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 protein called CRISPR-associated endonuclease Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1282	10578	6801	1744	2012	21	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0Q7Q2
A	0	ASN	-	expression tag	UNP A0Q7Q2
A	1	ALA	-	expression tag	UNP A0Q7Q2

- Molecule 2 is a RNA chain called crRNA (40-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	40	827	371	141	276	39	0	0	0

- Molecule 3 is a DNA chain called DNA target strand (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	38	774	374	136	227	37	0	0	0

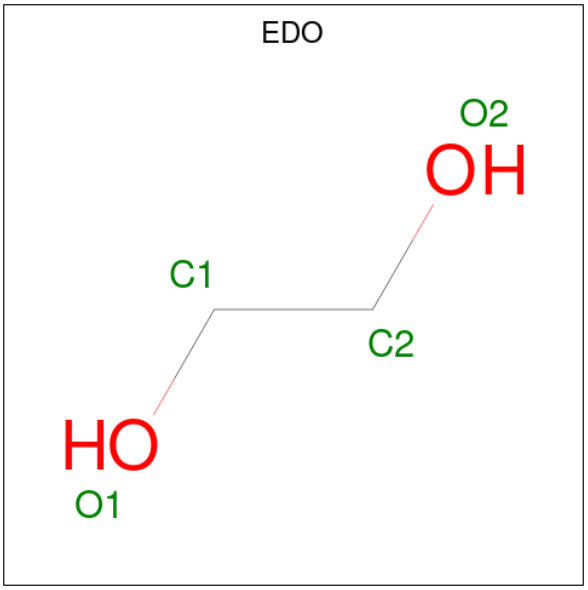
- Molecule 4 is a DNA chain called DNA non-target strand (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	33	665	323	109	201	32	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	9	9	9	0	0
			Total	Mg		
5	B	2	2	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 7 is water.

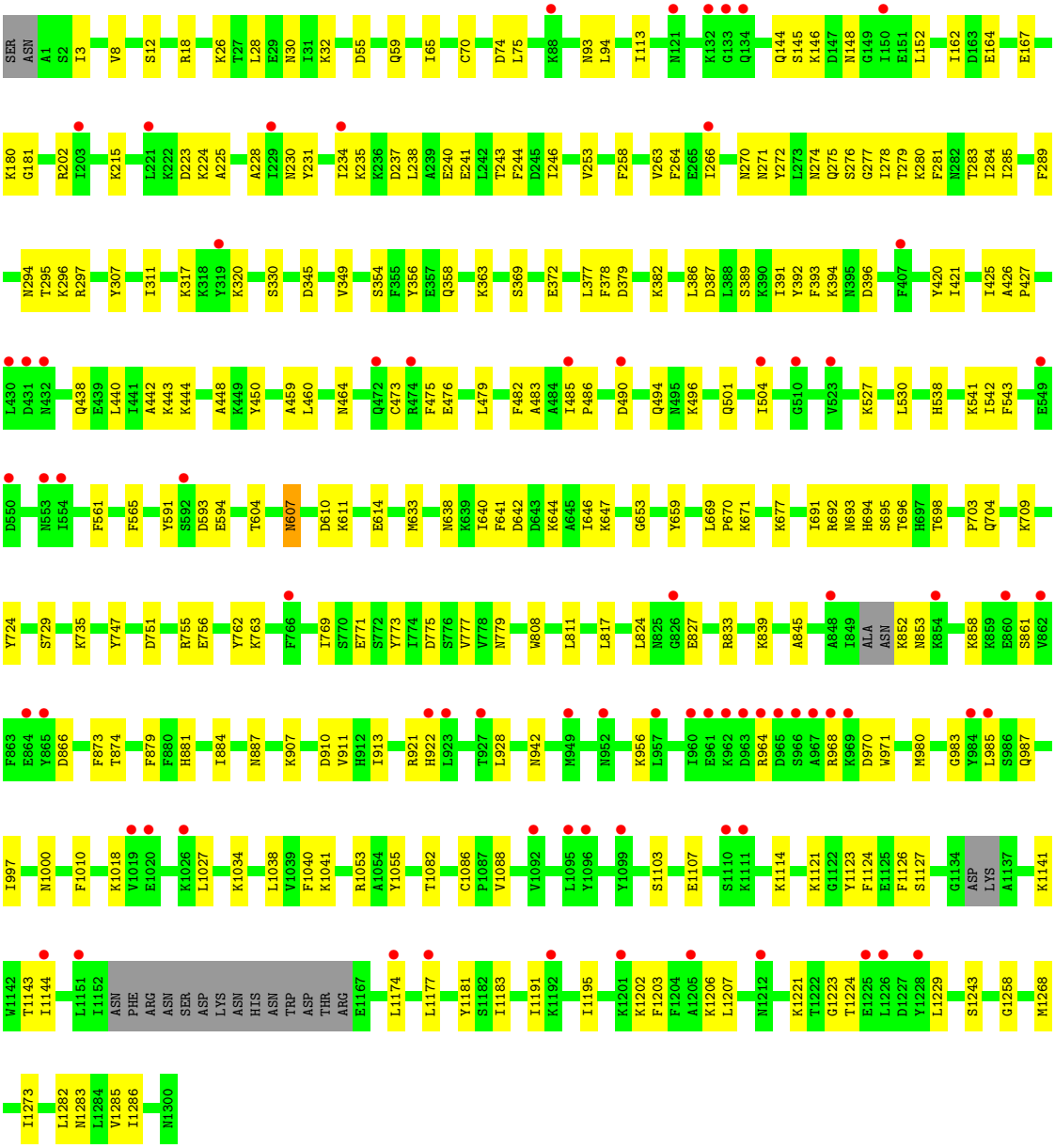
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	46	46	46	0	0
7	B	16	16	16	0	0
7	C	3	3	3	0	0
7	D	6	6	6	0	0

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: CRISPR-associated endonuclease Cas12a

Chain A:

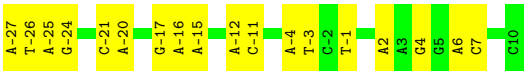


- Molecule 2: crRNA (40-MER)

Chain B:

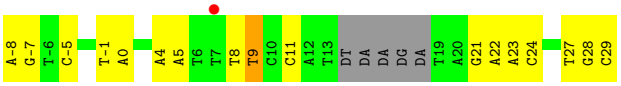
- Molecule 3: DNA target strand (38-MER)

Chain C:



- Molecule 4: DNA non-target strand (33-MER)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.17Å 141.68Å 89.48Å 90.00° 97.43° 90.00°	Depositor
Resolution (Å)	47.61 – 2.65 47.61 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.61-2.65) 99.6 (47.61-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, R_{free}	0.248 , 0.264 0.248 , 0.264	Depositor DCC
R_{free} test set	2926 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 (i)

5.1 Standard geometry (i)

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

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	0/10787	0.41	0/14480
2	B	0.33	0/924	0.97	2/1437 (0.1%)
3	C	0.57	0/867	1.00	0/1336
4	D	0.65	1/741 (0.1%)	1.09	0/1138
All	All	0.33	1/13319 (0.0%)	0.60	2/18391 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	9	DT	C1'-N1	5.07	1.55	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-10	C	C2-N1-C1'	5.63	124.99	118.80
2	B	13	A	N1-C6-N6	5.02	121.61	118.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10578	0	10568	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	827	0	414	25	0
3	C	774	0	434	17	0
4	D	665	0	380	14	0
5	A	9	0	0	0	0
5	B	2	0	0	0	0
6	A	20	0	30	3	0
6	B	24	0	36	0	0
6	C	12	0	18	0	0
7	A	46	0	0	1	0
7	B	16	0	0	0	0
7	C	3	0	0	0	0
7	D	6	0	0	0	0
All	All	12982	0	11880	197	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 8.

All (197) 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:382:LYS:HE2	1:A:483:ALA:HB1	1.69	0.75
1:A:671:LYS:NZ	3:C:2:DA:N3	2.38	0.72
3:C:-24:DG:H1	4:D:24:DC:H42	1.40	0.69
4:D:4:DA:H2'	4:D:5:DA:C8	2.28	0.69
1:A:238:LEU:HD13	1:A:284:ILE:HA	1.75	0.68
3:C:-12:DA:H2'	3:C:-11:DC:C6	2.30	0.66
1:A:980:MET:HA	2:B:-12:U:H4'	1.76	0.66
1:A:223:ASP:OD1	1:A:224:LYS:N	2.29	0.65
1:A:703:PRO:HD3	1:A:709:LYS:HG2	1.77	0.64
1:A:591:TYR:HD1	1:A:593:ASP:H	1.45	0.64
1:A:839:LYS:HG2	1:A:874:THR:HB	1.78	0.64
1:A:1121:LYS:HD3	1:A:1123:TYR:HE2	1.63	0.64
1:A:852:LYS:N	2:B:-9:U:OP2	2.31	0.62
4:D:-8:DA:H2'	4:D:-7:DG:C8	2.34	0.62
4:D:8:DT:H1'	4:D:9:DT:H5'	1.80	0.61
3:C:-26:DT:H2'	3:C:-25:DA:H8	1.64	0.61
3:C:-26:DT:H2'	3:C:-25:DA:C8	2.34	0.61
1:A:644:LYS:HA	1:A:647:LYS:HE2	1.83	0.61
1:A:591:TYR:HE1	1:A:594:GLU:HG2	1.65	0.60
1:A:921:ARG:NH1	1:A:1224:THR:O	2.34	0.60
2:B:7:A:H2'	2:B:8:A:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LYS:HA	1:A:530:LEU:HD12	1.83	0.60
1:A:543:PHE:HB2	1:A:565:PHE:CZ	2.37	0.60
1:A:241:GLU:HG2	1:A:283:THR:HB	1.84	0.59
1:A:1273:ILE:HG12	1:A:1282:LEU:HD21	1.84	0.59
1:A:1221:LYS:HE2	1:A:1223:GLY:H	1.68	0.59
1:A:421:ILE:HD13	1:A:444:LYS:HB3	1.83	0.58
1:A:144:GLN:O	1:A:148:ASN:ND2	2.35	0.58
1:A:356:TYR:O	1:A:496:LYS:NZ	2.36	0.58
1:A:501:GLN:HA	1:A:504:ILE:HD12	1.85	0.58
1:A:641:PHE:HE2	1:A:769:ILE:HD13	1.69	0.57
1:A:12:SER:HA	1:A:887:ASN:HB2	1.86	0.57
1:A:638:ASN:ND2	4:D:-5:DC:OP2	2.37	0.57
1:A:460:LEU:HD12	1:A:475:PHE:HD2	1.68	0.57
1:A:922:HIS:HA	1:A:942:ASN:HD21	1.70	0.56
1:A:202:ARG:HH22	2:B:7:A:H4'	1.68	0.56
1:A:425:ILE:HG21	1:A:440:LEU:HD22	1.88	0.56
1:A:921:ARG:O	1:A:1018:LYS:NZ	2.37	0.56
1:A:762:TYR:O	1:A:763:LYS:HD2	2.05	0.56
1:A:464:ASN:ND2	1:A:473:CYS:O	2.36	0.56
1:A:476:GLU:HA	1:A:479:LEU:HD12	1.88	0.55
1:A:853:ASN:N	2:B:-9:U:OP2	2.38	0.55
1:A:490:ASP:O	1:A:494:GLN:HG2	2.07	0.55
1:A:827:GLU:HG3	3:C:-1:DT:H4'	1.88	0.55
1:A:858:LYS:NZ	2:B:-7:U:O4	2.40	0.54
1:A:1010:PHE:CE2	4:D:11:DC:H2'	2.42	0.54
1:A:237:ASP:HB3	1:A:297:ARG:HD3	1.90	0.54
1:A:225:ALA:HB1	1:A:228:ALA:HB2	1.90	0.54
1:A:93:ASN:OD1	1:A:94:LEU:N	2.41	0.53
1:A:956:LYS:NZ	2:B:-11:A:O3'	2.35	0.53
2:B:1:A:H1'	2:B:2:G:C8	2.43	0.53
2:B:-17:A:H3'	2:B:-16:U:H5'	1.91	0.53
1:A:541:LYS:NZ	7:A:1503:HOH:O	2.42	0.52
4:D:-1:DT:H2"	4:D:0:DA:C8	2.45	0.52
1:A:246:ILE:HG22	1:A:253:VAL:HG13	1.92	0.52
1:A:65:ILE:HD11	1:A:113:ILE:HA	1.91	0.52
1:A:693:ASN:HA	1:A:704:GLN:HG2	1.92	0.52
3:C:-27:DA:H2'	3:C:-26:DT:C6	2.45	0.52
1:A:356:TYR:HB3	1:A:496:LYS:HE3	1.92	0.52
1:A:633:MET:HB2	1:A:640:ILE:HD12	1.92	0.51
1:A:1103:SER:O	1:A:1107:GLU:HG3	2.10	0.51
1:A:659:TYR:HE1	1:A:824:LEU:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:GLY:HA3	1:A:771:GLU:HB2	1.93	0.51
4:D:27:DT:H2'	4:D:28:DG:C8	2.45	0.51
1:A:833:ARG:HH21	1:A:879:PHE:HZ	1.58	0.50
1:A:28:LEU:HG	1:A:32:LYS:HE2	1.92	0.50
1:A:231:TYR:O	1:A:235:LYS:HG2	2.11	0.50
1:A:145:SER:HB2	1:A:152:LEU:HD11	1.94	0.50
1:A:70:CYS:HA	1:A:270:ASN:ND2	2.27	0.50
1:A:32:LYS:HA	6:A:1412:EDO:H22	1.93	0.49
1:A:747:TYR:OH	1:A:756:GLU:OE1	2.27	0.49
2:B:-16:U:O2	2:B:-13:C:N4	2.44	0.49
3:C:-21:DC:H42	4:D:21:DG:H1	1.60	0.49
1:A:392:TYR:HB3	1:A:450:TYR:HB3	1.95	0.49
1:A:913:ILE:O	1:A:928:LEU:HA	2.12	0.49
1:A:378:PHE:HE1	1:A:485:ILE:HD12	1.78	0.49
1:A:180:LYS:HG3	1:A:181:GLY:H	1.77	0.49
1:A:833:ARG:HH12	1:A:873:PHE:HA	1.78	0.49
1:A:8:VAL:HG11	1:A:1053:ARG:HB3	1.94	0.49
1:A:692:ARG:HH21	1:A:704:GLN:NE2	2.11	0.49
2:B:-14:U:H2'	2:B:-13:C:H6	1.77	0.49
1:A:3:ILE:HD11	1:A:910:ASP:HB2	1.94	0.49
1:A:611:LYS:HA	1:A:614:GLU:HG3	1.95	0.49
3:C:-12:DA:H2'	3:C:-11:DC:H6	1.78	0.48
1:A:983:GLY:HA3	2:B:-12:U:H1'	1.95	0.48
1:A:354:SER:O	1:A:358:GLN:HG2	2.14	0.48
1:A:1082:THR:O	1:A:1258:GLY:HA2	2.13	0.48
1:A:1114:LYS:O	1:A:1127:SER:N	2.47	0.48
1:A:763:LYS:NZ	1:A:817:LEU:O	2.45	0.48
1:A:773:TYR:O	1:A:777:VAL:HG23	2.13	0.48
4:D:5:DA:O5'	4:D:5:DA:H8	1.96	0.48
6:A:1414:EDO:H21	2:B:-15:U:O2'	2.14	0.47
1:A:420:TYR:HB2	1:A:459:ALA:HA	1.96	0.47
1:A:1229:LEU:H	1:A:1243:SER:HG	1.62	0.47
1:A:26:LYS:O	1:A:30:ASN:ND2	2.46	0.47
1:A:1038:LEU:HB3	1:A:1055:TYR:HB2	1.96	0.47
2:B:-14:U:H2'	2:B:-13:C:C6	2.50	0.47
1:A:591:TYR:CE1	1:A:594:GLU:HG2	2.49	0.47
1:A:3:ILE:HD13	1:A:1000:ASN:HB3	1.95	0.47
1:A:180:LYS:HG3	1:A:181:GLY:N	2.30	0.47
3:C:-25:DA:H2'	3:C:-24:DG:C8	2.50	0.47
2:B:12:U:H2'	2:B:13:A:H8	1.80	0.47
1:A:146:LYS:HB2	1:A:162:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:G:H2'	2:B:3:A:H8	1.80	0.46
1:A:377:LEU:HD21	1:A:561:PHE:CE1	2.51	0.46
1:A:729:SER:HA	1:A:735:LYS:HD3	1.96	0.46
2:B:-17:A:C3'	2:B:-16:U:H5'	2.44	0.46
1:A:215:LYS:HD2	1:A:264:PHE:O	2.15	0.46
1:A:604:THR:HG22	1:A:607:ASN:HB2	1.98	0.46
4:D:8:DT:H6	4:D:9:DT:H71	1.79	0.46
1:A:443:LYS:O	1:A:448:ALA:HB2	2.16	0.46
3:C:-21:DC:O5'	3:C:-20:DA:H4'	2.15	0.46
1:A:1268:MET:HE3	1:A:1286:ILE:HD13	1.98	0.46
3:C:-17:DG:H2'	3:C:-16:DA:H8	1.80	0.46
1:A:1141:LYS:HE3	1:A:1141:LYS:HB2	1.76	0.46
2:B:16:U:H2'	2:B:17:C:O4'	2.16	0.45
1:A:695:SER:HB3	1:A:698:THR:OG1	2.16	0.45
1:A:230:ASN:O	1:A:234:ILE:HG12	2.16	0.45
1:A:164:GLU:HA	1:A:167:GLU:HG2	1.98	0.45
1:A:289:PHE:CZ	1:A:296:LYS:HB2	2.52	0.45
1:A:394:LYS:HG2	1:A:396:ASP:HB2	1.98	0.45
1:A:275:GLN:HA	1:A:278:ILE:HD12	1.98	0.45
1:A:691:ILE:HG23	1:A:696:THR:OG1	2.17	0.45
1:A:1010:PHE:HE2	4:D:11:DC:H2'	1.81	0.45
1:A:1181:TYR:CZ	1:A:1203:PHE:HB2	2.52	0.44
2:B:-8:G:H1'	2:B:-4:U:H1'	1.97	0.44
1:A:3:ILE:HD11	1:A:910:ASP:CB	2.47	0.44
1:A:538:HIS:NE2	2:B:15:U:OP1	2.49	0.44
1:A:1126:PHE:HB2	1:A:1144:ILE:HB	2.00	0.44
1:A:271:ASN:O	1:A:277:GLY:HA3	2.18	0.44
1:A:281:PHE:O	1:A:285:ILE:HG12	2.17	0.44
1:A:983:GLY:O	1:A:987:GLN:HG2	2.18	0.44
1:A:1195:ILE:HD13	1:A:1207:LEU:HD22	2.00	0.44
1:A:527:LYS:HG3	1:A:971:TRP:CE2	2.53	0.44
1:A:74:ASP:OD1	1:A:75:LEU:N	2.49	0.44
1:A:642:ASP:O	1:A:646:ILE:HG13	2.18	0.44
1:A:1183:ILE:HG21	1:A:1191:ILE:HG23	1.98	0.44
1:A:1034:LYS:HA	1:A:1034:LYS:HD2	1.87	0.44
1:A:907:LYS:O	1:A:911:VAL:HG23	2.18	0.44
1:A:320:LYS:HE3	3:C:-15:DA:OP1	2.18	0.43
1:A:1124:PHE:CG	1:A:1174:LEU:HD23	2.52	0.43
1:A:363:LYS:HD3	1:A:369:SER:HA	2.00	0.43
1:A:985:LEU:HD22	1:A:1027:LEU:HB2	1.99	0.43
1:A:296:LYS:HE2	3:C:-15:DA:H2"	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:TRP:O	1:A:811:LEU:HB2	2.18	0.43
3:C:-4:DA:H3'	3:C:-3:DT:H71	2.00	0.43
1:A:426:ALA:N	1:A:427:PRO:HD3	2.34	0.43
1:A:386:LEU:HD13	1:A:391:ILE:HD11	2.00	0.43
1:A:845:ALA:N	1:A:866:ASP:HB3	2.33	0.43
2:B:-9:U:H1'	2:B:-8:G:H2'	2.01	0.43
1:A:152:LEU:HD13	1:A:162:ILE:HD11	1.99	0.43
1:A:438:GLN:O	1:A:442:ALA:N	2.49	0.43
1:A:377:LEU:HD21	1:A:561:PHE:CZ	2.53	0.42
1:A:485:ILE:N	1:A:486:PRO:HD2	2.34	0.42
1:A:964:ARG:O	1:A:968:ARG:HG3	2.18	0.42
2:B:2:G:H2'	2:B:3:A:C8	2.53	0.42
1:A:275:GLN:HE21	1:A:279:THR:HG23	1.84	0.42
1:A:379:ASP:O	1:A:382:LYS:HB2	2.19	0.42
1:A:280:LYS:O	1:A:284:ILE:HG23	2.19	0.42
1:A:670:PRO:HG3	1:A:724:TYR:OH	2.19	0.42
3:C:6:DA:H2'	3:C:7:DC:C6	2.54	0.42
1:A:669:LEU:HB2	1:A:670:PRO:HD3	2.02	0.42
1:A:861:SER:OG	2:B:-7:U:O4	2.31	0.42
1:A:1041:LYS:NZ	2:B:-2:G:OP2	2.37	0.42
1:A:1086:CYS:SG	1:A:1088:VAL:HG22	2.59	0.42
1:A:751:ASP:O	1:A:755:ARG:HG2	2.19	0.42
1:A:275:GLN:HG2	1:A:330:SER:HB2	2.02	0.42
1:A:369:SER:N	1:A:372:GLU:HB2	2.34	0.42
1:A:997:ILE:HG13	1:A:1040:PHE:HE2	1.85	0.42
1:A:1283:ASN:OD1	1:A:1285:VAL:HG12	2.19	0.42
1:A:775:ASP:O	1:A:779:ASN:ND2	2.52	0.42
1:A:378:PHE:HD1	1:A:482:PHE:O	2.02	0.42
1:A:393:PHE:HB3	1:A:542:ILE:HD11	2.02	0.42
1:A:307:TYR:CE2	1:A:311:ILE:HG13	2.54	0.42
1:A:243:THR:O	1:A:280:LYS:NZ	2.36	0.41
1:A:244:PHE:HB2	1:A:258:PHE:CE2	2.55	0.41
1:A:1121:LYS:HB3	1:A:1123:TYR:CE2	2.56	0.41
1:A:345:ASP:O	1:A:349:VAL:HG23	2.20	0.41
1:A:18:ARG:HG2	1:A:881:HIS:CD2	2.56	0.41
1:A:294:ASN:OD1	1:A:295:THR:N	2.53	0.41
1:A:263:VAL:HG13	1:A:272:TYR:OH	2.21	0.41
1:A:997:ILE:HD13	1:A:997:ILE:HA	1.90	0.41
1:A:811:LEU:HD11	1:A:884:ILE:HG21	2.01	0.41
1:A:246:ILE:HG22	1:A:253:VAL:HA	2.03	0.40
1:A:240:GLU:O	1:A:243:THR:OG1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HG2	6:A:1413:EDO:H22	2.03	0.40
1:A:387:ASP:OD1	1:A:389:SER:HB3	2.21	0.40
1:A:694:HIS:O	1:A:696:THR:N	2.52	0.40
1:A:1177:LEU:HD22	1:A:1206:LYS:HG3	2.02	0.40
2:B:7:A:H2'	2:B:8:A:H8	1.83	0.40
4:D:22:DA:H2"	4:D:23:DA:C8	2.56	0.40
1:A:55:ASP:O	1:A:59:GLN:HG3	2.21	0.40
1:A:274:ASN:OD1	1:A:276:SER:N	2.47	0.40
1:A:610:ASP:HA	1:A:659:TYR:O	2.22	0.40
1:A:677:LYS:HB3	3:C:4:DG:OP2	2.21	0.40
1:A:215:LYS:NZ	1:A:266:ILE:HG13	2.37	0.40
1:A:1202:LYS:HE3	4:D:29:DC:OP1	2.22	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	
1	A	1274/1302 (98%)	1247 (98%)	27 (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
1	A	1166/1185 (98%)	1163 (100%)	3 (0%)	92 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	A	970	ASP
1	A	1143	THR

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

Mol	Chain	Res	Type
1	A	125	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	38/40 (95%)	12 (31%)	1 (2%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-17	A
2	B	-16	U
2	B	-15	U
2	B	-10	C
2	B	-9	U
2	B	-8	G
2	B	-7	U
2	B	-6	U
2	B	-5	G
2	B	1	A
2	B	12	U
2	B	18	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	-16	U

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 25 ligands modelled in this entry, 11 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	EDO	B	104	-	3,3,3	0.44	0	2,2,2	0.42	0
6	EDO	B	108	-	3,3,3	0.48	0	2,2,2	0.21	0
6	EDO	A	1414	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	C	101	-	3,3,3	0.46	0	2,2,2	0.41	0
6	EDO	B	103	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	B	105	-	3,3,3	0.42	0	2,2,2	0.45	0
6	EDO	B	106	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	B	107	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	C	103	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	A	1410	-	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	A	1412	-	3,3,3	0.43	0	2,2,2	0.34	0
6	EDO	A	1411	-	3,3,3	0.45	0	2,2,2	0.27	0
6	EDO	A	1413	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	C	102	-	3,3,3	0.49	0	2,2,2	0.19	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
6	EDO	B	104	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	108	-	-	0/1/1/1	-
6	EDO	A	1414	-	-	0/1/1/1	-
6	EDO	C	101	-	-	0/1/1/1	-
6	EDO	B	103	-	-	0/1/1/1	-
6	EDO	B	105	-	-	0/1/1/1	-
6	EDO	B	106	-	-	0/1/1/1	-
6	EDO	B	107	-	-	0/1/1/1	-
6	EDO	C	103	-	-	0/1/1/1	-
6	EDO	A	1410	-	-	0/1/1/1	-
6	EDO	A	1412	-	-	1/1/1/1	-
6	EDO	A	1411	-	-	0/1/1/1	-
6	EDO	A	1413	-	-	0/1/1/1	-
6	EDO	C	102	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	102	EDO	O1-C1-C2-O2
6	A	1412	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1414	EDO	1	0
6	A	1412	EDO	1	0
6	A	1413	EDO	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1282/1302 (98%)	0.35	74 (5%) 23 19	56, 108, 142, 162	0
2	B	40/40 (100%)	0.08	0 100 100	56, 89, 140, 145	0
3	C	38/38 (100%)	0.07	0 100 100	54, 88, 204, 205	0
4	D	33/38 (86%)	0.18	1 (3%) 50 47	83, 144, 225, 233	0
All	All	1393/1418 (98%)	0.33	75 (5%) 25 23	54, 108, 147, 233	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	ILE	7.3
1	A	961	GLU	7.3
1	A	963	ASP	7.1
1	A	962	LYS	6.9
1	A	592	SER	5.5
1	A	965	ASP	4.7
1	A	1225	GLU	4.6
1	A	407	PHE	4.4
1	A	964	ARG	4.3
1	A	968	ARG	4.1
1	A	1111	LYS	4.1
1	A	1226	LEU	4.0
1	A	854	LYS	3.7
1	A	549	GLU	3.6
1	A	550	ASP	3.4
1	A	553	ASN	3.4
1	A	1092	VAL	3.4
1	A	430	LEU	3.1
1	A	1151	LEU	2.9
1	A	1019	VAL	2.9
1	A	860	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1228	TYR	2.9
1	A	133	GLY	2.8
1	A	766	PHE	2.8
1	A	319	TYR	2.7
1	A	490	ASP	2.7
1	A	865	TYR	2.7
1	A	234	ILE	2.7
1	A	554	ILE	2.7
1	A	474	ARG	2.7
1	A	504	ILE	2.7
1	A	1110	SER	2.7
1	A	510	GLY	2.6
1	A	1144	ILE	2.6
1	A	969	LYS	2.5
1	A	922	HIS	2.5
1	A	1099	TYR	2.5
1	A	1192	LYS	2.5
1	A	923	LEU	2.5
1	A	952	ASN	2.5
1	A	134	GLN	2.4
1	A	1177	LEU	2.4
1	A	132	LYS	2.4
1	A	848	ALA	2.4
1	A	88	LYS	2.4
1	A	985	LEU	2.4
1	A	431	ASP	2.4
1	A	1201	LYS	2.3
1	A	523	VAL	2.3
4	D	7	DT	2.3
1	A	1026	LYS	2.3
1	A	967	ALA	2.2
1	A	229	ILE	2.2
1	A	1212	ASN	2.2
1	A	949	MET	2.2
1	A	864	GLU	2.2
1	A	862	VAL	2.2
1	A	1096	TYR	2.2
1	A	1174	LEU	2.2
1	A	957	LEU	2.1
1	A	1095	LEU	2.1
1	A	1020	GLU	2.1
1	A	121	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	826	GLY	2.1
1	A	266	ILE	2.1
1	A	221	LEU	2.1
1	A	203	ILE	2.1
1	A	1205	ALA	2.1
1	A	927	THR	2.1
1	A	485	ILE	2.0
1	A	472	GLN	2.0
1	A	984	TYR	2.0
1	A	966	SER	2.0
1	A	150	ILE	2.0
1	A	432	ASN	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, 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	B-factors(Å^2)	Q<0.9
5	MG	A	1406	1/1	0.32	0.12	88,88,88,88	0
5	MG	A	1407	1/1	0.44	0.11	107,107,107,107	0
5	MG	A	1401	1/1	0.52	0.31	107,107,107,107	0
5	MG	A	1404	1/1	0.53	0.11	76,76,76,76	0
5	MG	B	101	1/1	0.69	0.19	115,115,115,115	0
6	EDO	B	103	4/4	0.70	0.40	71,71,71,71	0
6	EDO	C	103	4/4	0.76	0.27	119,119,119,119	0
6	EDO	B	108	4/4	0.78	0.31	70,70,70,70	0
5	MG	A	1403	1/1	0.78	0.08	109,109,109,109	0
6	EDO	B	106	4/4	0.80	0.24	101,101,101,101	0
6	EDO	C	102	4/4	0.81	0.17	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1402	1/1	0.81	0.05	114,114,114,114	0
6	EDO	A	1414	4/4	0.86	0.28	80,80,80,80	0
5	MG	B	102	1/1	0.86	0.10	74,74,74,74	0
6	EDO	A	1411	4/4	0.86	0.28	65,65,65,65	0
6	EDO	B	104	4/4	0.88	0.22	72,72,72,72	0
6	EDO	A	1412	4/4	0.88	0.42	98,98,98,98	0
6	EDO	B	107	4/4	0.88	0.25	78,78,78,78	0
6	EDO	B	105	4/4	0.89	0.19	79,79,79,79	0
5	MG	A	1409	1/1	0.90	0.23	88,88,88,88	0
6	EDO	A	1413	4/4	0.91	0.36	82,82,82,82	0
5	MG	A	1405	1/1	0.93	0.15	105,105,105,105	0
6	EDO	A	1410	4/4	0.93	0.33	60,60,60,60	0
5	MG	A	1408	1/1	0.94	0.15	103,103,103,103	0
6	EDO	C	101	4/4	0.94	0.35	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.