



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:06 PM JST

PDB ID : 5B2O
Title : Crystal structure of Francisella novicida Cas9 in complex with sgRNA and target DNA (TGG PAM)
Authors : Hirano, H.; Nishimasu, H.; Nakane, T.; Ishitani, R.; Nureki, O.
Deposited on : 2016-02-01
Resolution : 1.70 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
Mogul : 1.8.5 (274361), 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

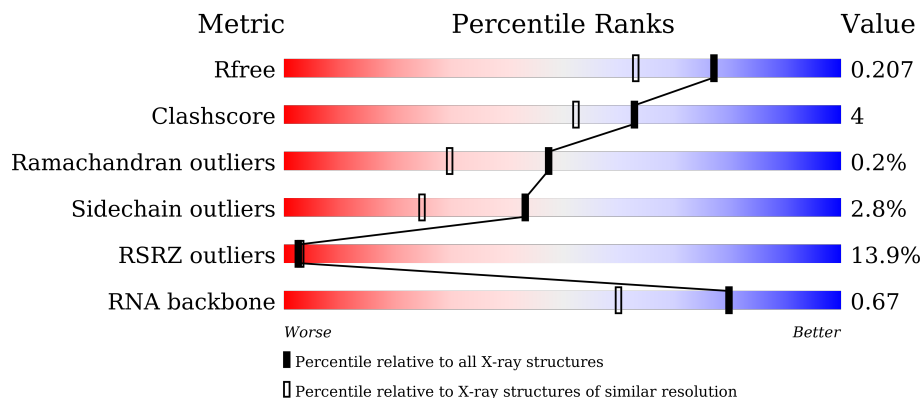
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)
RNA backbone	3102	1007 (2.38-1.02)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1632	 13% (Poor fit), 79% (0-1 outliers), 9% (2 outliers), 11% (3+ outliers or not modelled)
2	B	94	 49% (0-1 outliers), 43% (2 outliers), 6% (3+ outliers or not modelled)
3	C	30	 3% (Poor fit), 47% (0-1 outliers), 47% (2 outliers), 7% (3+ outliers or not modelled)
4	D	9	 78% (0-1 outliers), 22% (2 outliers)

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 15717 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 Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1455	11791	7536	2025	2199	31	0	19	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0Q5Y3
A	-1	SER	-	expression tag	UNP A0Q5Y3
A	0	HIS	-	expression tag	UNP A0Q5Y3
A	995	ALA	ASN	engineered mutation	UNP A0Q5Y3

- Molecule 2 is a RNA chain called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	94	1991	886	350	661	94	0	0	0

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	30	595	285	105	176	29	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*GP*GP*TP*AP*TP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	9	185	89	34	54	8	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0
6	B	2	Total Na 2 2	0	0

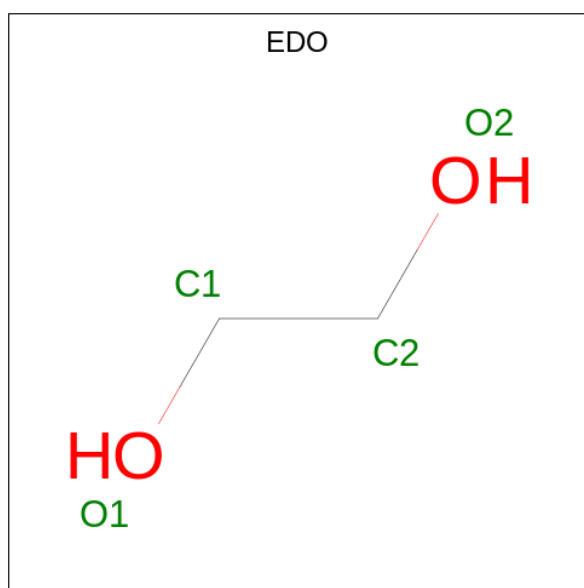
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	10	Total Ca 10 10	0	0
8	B	7	Total Ca 7 7	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



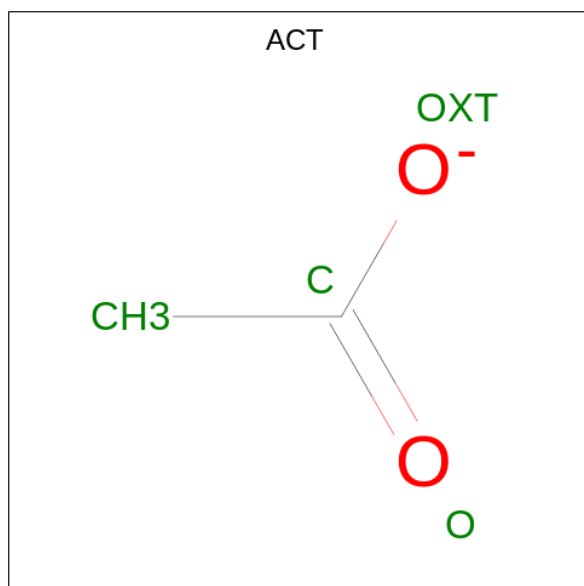
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

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

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

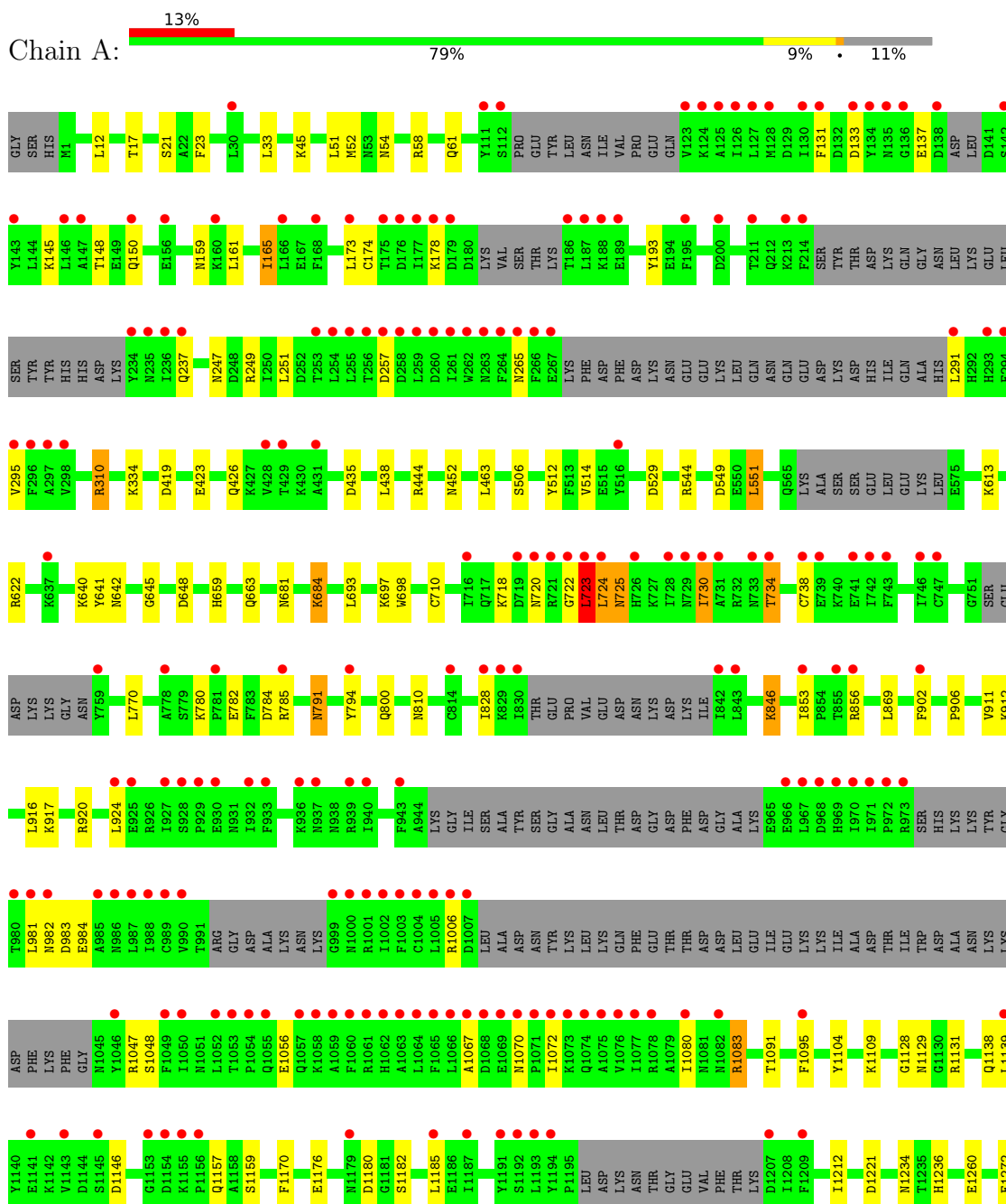
- Molecule 11 is water.

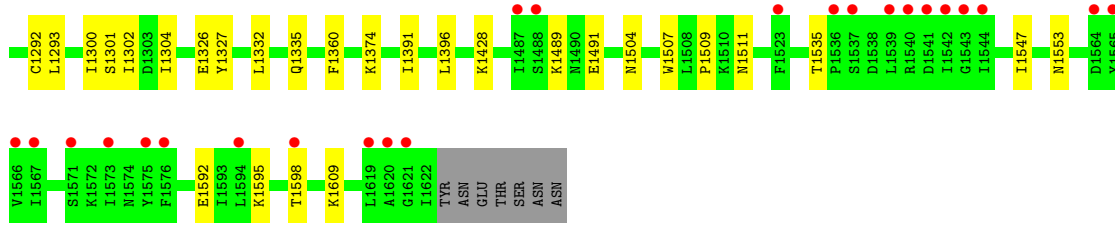
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	618	Total	O	0	0
			618	618		
11	B	334	Total	O	0	0
			334	334		
11	C	71	Total	O	0	0
			71	71		
11	D	8	Total	O	0	0
			8	8		

3 Residue-property plots [i](#)

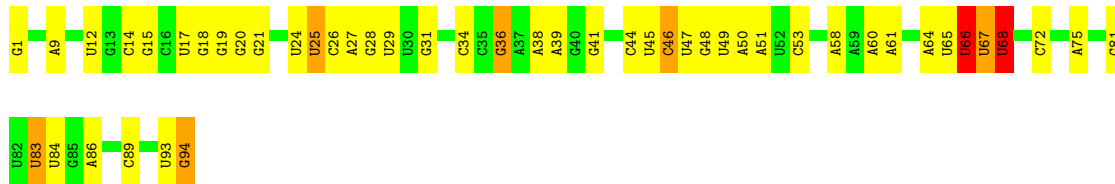
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 Cas9

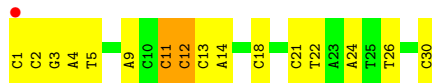




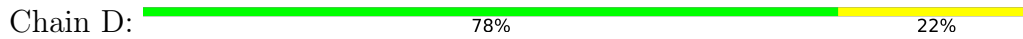
- Molecule 2: Guide RNA



- Molecule 3: Target DNA



- Molecule 4: DNA (5'-D(*TP*GP*GP*TP*AP*TP*CP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.92Å 159.10Å 96.81Å 90.00° 107.04° 90.00°	Depositor
Resolution (Å)	46.28 – 1.70 46.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.28-1.70) 96.1 (46.28-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.184 , 0.207 0.184 , 0.207	Depositor DCC
R_{free} test set	12436 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15717	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: CL, ACT, CA, EDO, ZN, NA

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	0.50	0/12068	0.61	2/16282 (0.0%)
2	B	1.12	5/2224 (0.2%)	1.57	48/3465 (1.4%)
3	C	1.26	3/664 (0.5%)	1.31	8/1018 (0.8%)
4	D	1.02	0/207	1.08	0/319
All	All	0.68	8/15163 (0.1%)	0.89	58/21084 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	G	N7-C5	6.32	1.43	1.39
2	B	21	G	C8-N7	6.14	1.34	1.30
3	C	26	DT	C3'-O3'	-5.87	1.36	1.44
3	C	12	DC	C3'-O3'	-5.36	1.36	1.44
2	B	44	C	C2-O2	5.24	1.29	1.24
2	B	60	A	N3-C4	-5.20	1.31	1.34
3	C	13	DC	C2-N3	-5.10	1.31	1.35
2	B	51	A	C8-N7	5.04	1.35	1.31

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	DC	O5'-P-OP2	-12.03	94.88	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	DC	O5'-P-OP2	-10.69	96.08	105.70
2	B	50	A	N1-C2-N3	-9.66	124.47	129.30
2	B	50	A	C2-N3-C4	8.89	115.05	110.60
3	C	14	DA	O5'-P-OP2	-8.48	98.07	105.70
2	B	66	U	O5'-P-OP1	-7.97	98.53	105.70
2	B	94	G	C8-N9-C4	-7.95	103.22	106.40
2	B	27	A	O5'-P-OP1	-7.92	98.58	105.70
1	A	310	ARG	CG-CD-NE	-7.66	95.70	111.80
2	B	83	U	O5'-P-OP1	-6.95	99.44	105.70
2	B	20	G	C5-C6-N1	6.84	114.92	111.50
2	B	86	A	O4'-C1'-N9	6.64	113.51	108.20
2	B	15	G	C2-N3-C4	6.63	115.22	111.90
2	B	94	G	C2-N3-C4	6.57	115.19	111.90
2	B	46	C	O5'-P-OP2	-6.45	99.90	105.70
2	B	50	A	C8-N9-C4	6.40	108.36	105.80
2	B	49	U	N1-C2-O2	-6.34	118.36	122.80
3	C	9	DA	O4'-C1'-N9	6.11	112.27	108.00
2	B	50	A	N7-C8-N9	-6.05	110.77	113.80
2	B	31	G	C5-C6-O6	-6.00	125.00	128.60
2	B	75	A	C8-N9-C4	5.99	108.20	105.80
2	B	51	A	N1-C2-N3	-5.96	126.32	129.30
2	B	21	G	C8-N9-C4	5.88	108.75	106.40
2	B	94	G	N9-C4-C5	5.88	107.75	105.40
2	B	25	U	C2-N3-C4	-5.88	123.47	127.00
3	C	11	DC	OP1-P-OP2	5.78	128.26	119.60
2	B	19	G	N7-C8-N9	-5.67	110.27	113.10
2	B	24	U	N3-C4-C5	5.60	117.96	114.60
2	B	21	G	C5-C6-N1	5.58	114.29	111.50
2	B	25	U	N3-C4-C5	5.55	117.93	114.60
2	B	72	C	N1-C2-O2	-5.45	115.63	118.90
2	B	14	C	N1-C2-O2	-5.45	115.63	118.90
2	B	41	G	C2-N3-C4	5.41	114.60	111.90
2	B	61	A	C6-N1-C2	5.41	121.84	118.60
2	B	66	U	P-O3'-C3'	5.38	126.15	119.70
1	A	310	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	25	U	C5-C4-O4	-5.33	122.70	125.90
3	C	13	DC	O5'-P-OP2	-5.33	100.90	105.70
2	B	48	G	N3-C4-C5	5.28	131.24	128.60
2	B	12	U	N1-C2-O2	-5.25	119.12	122.80
3	C	13	DC	O4'-C4'-C3'	-5.24	102.40	104.50
2	B	17	U	C5-C6-N1	-5.24	120.08	122.70
2	B	19	G	C5-N7-C8	5.21	106.90	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	75	A	N9-C4-C5	-5.21	103.72	105.80
2	B	66	U	O5'-P-OP2	5.20	116.94	110.70
2	B	61	A	N1-C2-N3	-5.18	126.71	129.30
2	B	36	G	N9-C1'-C2'	-5.18	106.30	112.00
2	B	24	U	N3-C4-O4	-5.17	115.78	119.40
2	B	14	C	N3-C2-O2	5.17	125.52	121.90
2	B	65	U	N3-C2-O2	-5.17	118.58	122.20
3	C	18	DC	O4'-C4'-C3'	-5.15	102.44	104.50
2	B	12	U	C2-N3-C4	-5.14	123.92	127.00
2	B	25	U	C6-N1-C2	5.14	124.09	121.00
2	B	47	U	C2-N3-C4	-5.13	123.92	127.00
2	B	93	U	N3-C2-O2	5.11	125.78	122.20
2	B	68	U	N1-C2-N3	5.10	117.96	114.90
2	B	48	G	N3-C4-N9	-5.08	122.95	126.00
2	B	61	A	C5-C6-N1	-5.02	115.19	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	G	Sidechain

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	11791	0	11524	102	1
2	B	1991	0	997	16	0
3	C	595	0	337	9	0
4	D	185	0	104	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	2	0	0	0	0
8	A	10	0	0	0	0
8	B	7	0	0	0	0
9	A	48	0	72	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	40	0	60	6	0
9	C	4	0	6	0	0
10	A	4	0	3	0	0
10	B	4	0	3	0	0
11	A	618	0	0	12	0
11	B	334	0	0	1	0
11	C	71	0	0	0	0
11	D	8	0	0	0	0
All	All	15717	0	13106	120	1

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 (120) 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:54[B]:ASN:OD1	1:A:58[B]:ARG:NH1	1.99	0.96
1:A:265:ASN:O	1:A:291:LEU:N	2.08	0.87
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.64	0.80
1:A:1335[A]:GLN:NE2	11:A:1801:HOH:O	2.05	0.79
3:C:4:DA:H2''	3:C:5:DT:H5''	1.67	0.76
1:A:734:THR:HG21	1:A:738:CYS:H	1.50	0.75
1:A:648[B]:ASP:OD2	1:A:1104:TYR:OH	2.05	0.74
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.72	0.72
1:A:902:PHE:HA	1:A:924:LEU:HD12	1.71	0.72
1:A:58[A]:ARG:NH2	11:A:1805:HOH:O	2.24	0.70
1:A:782:GLU:OE2	1:A:785:ARG:NH2	2.17	0.70
1:A:1326:GLU:HG3	1:A:1327:TYR:CD2	2.27	0.70
1:A:1335[A]:GLN:OE1	11:A:1802:HOH:O	2.10	0.69
1:A:1236:HIS:HE1	11:A:2043:HOH:O	1.77	0.68
1:A:23:PHE:HB2	9:A:1725:EDO:H22	1.74	0.68
1:A:54[B]:ASN:HD21	1:A:58[B]:ARG:CZ	2.06	0.68
3:C:2:DC:H2'	3:C:3:DG:C8	2.30	0.66
1:A:983:ASP:OD2	1:A:1083:ARG:NH2	2.29	0.66
1:A:463:LEU:HD11	1:A:853:ILE:HG13	1.80	0.63
1:A:1609:LYS:N	3:C:3:DG:OP2	2.27	0.63
1:A:981:LEU:HD12	1:A:1080:ILE:HG21	1.81	0.62
1:A:983:ASP:OD1	1:A:984:GLU:N	2.33	0.62
1:A:828:ILE:HG12	1:A:846:LYS:HG3	1.82	0.62
11:A:2330:HOH:O	9:B:116:EDO:H12	2.02	0.60
1:A:693:LEU:HG	1:A:697:LYS:HE3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:ILE:HG22	1:A:1304:ILE:HG12	1.85	0.58
1:A:734:THR:CG2	1:A:738:CYS:H	2.16	0.58
2:B:94:G:C2	9:B:117:EDO:H11	2.39	0.57
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.38	0.56
1:A:983:ASP:CG	1:A:1083:ARG:HH22	2.09	0.56
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.25	0.55
1:A:1159:SER:OG	1:A:1221:ASP:OD1	2.20	0.55
1:A:791:ASN:H	1:A:791:ASN:HD22	1.55	0.54
1:A:718:LYS:HB2	2:B:9:A:H5'	1.88	0.54
1:A:725:ASN:ND2	1:A:794:TYR:HE2	2.06	0.54
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.72	0.54
3:C:4:DA:C2'	3:C:5:DT:H5''	2.37	0.53
1:A:724:LEU:HD12	1:A:794:TYR:CZ	2.43	0.53
1:A:1489:LYS:HB2	1:A:1491:GLU:HG2	1.90	0.53
2:B:66:U:H4'	2:B:67:U:O5'	2.08	0.53
1:A:174:CYS:HA	1:A:247:ASN:HD21	1.73	0.53
1:A:730:ILE:O	1:A:734:THR:HB	2.09	0.53
3:C:1:DC:O2	4:D:9:DG:N2	2.29	0.52
3:C:24:DA:H5''	3:C:24:DA:H8	1.75	0.52
1:A:1391:ILE:HG12	1:A:1396:LEU:HD11	1.92	0.51
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	1.93	0.51
1:A:698:TRP:CH2	1:A:770:LEU:HD23	2.45	0.51
1:A:1326:GLU:HG3	1:A:1327:TYR:HD2	1.73	0.51
1:A:1070:ASN:OD1	1:A:1072:ILE:HG12	2.12	0.50
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.77	0.50
3:C:11:DC:H2'	3:C:12:DC:C6	2.47	0.50
1:A:869:LEU:HD23	1:A:1095[B]:PHE:CE1	2.47	0.50
1:A:1504:ASN:ND2	11:A:1804:HOH:O	2.14	0.50
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.44	0.50
1:A:659:HIS:HD2	11:B:241:HOH:O	1.94	0.50
1:A:61[A]:GLN:HG3	11:A:2395:HOH:O	2.12	0.48
1:A:1507:TRP:CD1	1:A:1509:PRO:HD2	2.49	0.48
1:A:12:LEU:HD11	1:A:1095[A]:PHE:CE2	2.47	0.48
1:A:52:MET:SD	9:B:116:EDO:H22	2.53	0.48
1:A:145:LYS:O	1:A:148:THR:OG1	2.26	0.48
1:A:710:CYS:HB3	1:A:800:GLN:HB2	1.95	0.48
1:A:641:TYR:CE2	1:A:1109:LYS:HG2	2.49	0.47
2:B:89:C:H4'	9:B:119:EDO:H11	1.96	0.47
2:B:66:U:H1'	2:B:67:U:OP2	2.14	0.47
1:A:1326:GLU:HG2	11:A:1867:HOH:O	2.15	0.47
3:C:21:DC:H2'	3:C:22:DT:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544[B]:ARG:NH1	1:A:551:LEU:HD22	2.30	0.46
2:B:45:U:H2'	2:B:46:C:C6	2.51	0.46
1:A:1293:LEU:HB3	1:A:1300:ILE:HB	1.98	0.45
1:A:983:ASP:HA	1:A:1129:ASN:HD22	1.81	0.45
1:A:1535:THR:HG22	1:A:1547:ILE:HG13	1.98	0.45
1:A:1047:ARG:HD2	2:B:1:G:C6	2.51	0.45
1:A:1592:GLU:O	1:A:1595:LYS:HG2	2.17	0.45
1:A:663[B]:GLN:HG3	2:B:81:G:H5''	1.99	0.45
1:A:920:ARG:O	1:A:924:LEU:HD23	2.17	0.44
2:B:64:A:H1'	9:B:116:EDO:H21	2.00	0.44
1:A:17:THR:HG21	1:A:869:LEU:HD21	2.00	0.44
1:A:173:LEU:HD11	1:A:237:GLN:HG3	1.99	0.44
1:A:423[A]:GLU:CD	1:A:444:ARG:HH22	2.21	0.44
1:A:506:SER:HA	1:A:512:TYR:CZ	2.53	0.44
1:A:1302:ILE:CG2	1:A:1304:ILE:HG12	2.48	0.44
1:A:1131:ARG:NH1	1:A:1176:GLU:OE2	2.51	0.43
1:A:1180:ASP:OD1	1:A:1182:SER:OG	2.25	0.43
1:A:1374:LYS:HE2	11:A:1926:HOH:O	2.17	0.43
1:A:435:ASP:HA	1:A:438:LEU:HD12	2.00	0.43
1:A:51:LEU:HD11	1:A:912:LYS:HA	2.01	0.43
1:A:249:ARG:HG2	1:A:249:ARG:NH1	2.34	0.43
1:A:1292[A]:CYS:SG	1:A:1360:PHE:HE2	2.41	0.43
2:B:38:A:H2'	2:B:39:A:C8	2.54	0.43
1:A:780:LYS:HE3	1:A:784:ASP:OD1	2.19	0.43
1:A:1272:GLU:HG3	11:A:2337:HOH:O	2.19	0.43
1:A:452:ASN:HA	2:B:89:C:N3	2.33	0.43
1:A:1535:THR:HG23	11:A:1817:HOH:O	2.18	0.42
1:A:920:ARG:HA	1:A:920:ARG:HD2	1.65	0.42
1:A:45:LYS:HB3	1:A:911:VAL:HG12	2.01	0.42
1:A:640:LYS:HE3	2:B:68:U:C6	2.54	0.42
1:A:549:ASP:OD1	1:A:551:LEU:HB2	2.19	0.42
1:A:645:GLY:HA2	9:A:1722:EDO:H11	2.01	0.42
1:A:663[A]:GLN:HG3	2:B:81:G:H5''	2.00	0.42
1:A:1091:THR:O	1:A:1095[A]:PHE:HD1	2.01	0.42
2:B:94:G:C4	9:B:117:EDO:H11	2.54	0.42
1:A:33:LEU:HD13	1:A:1185:LEU:HD21	2.02	0.42
1:A:681:ASN:HA	1:A:684:LYS:HG2	2.01	0.42
1:A:174:CYS:HB3	1:A:251:LEU:HB2	2.01	0.42
1:A:178:LYS:HE3	1:A:178:LYS:HB3	1.89	0.42
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.34	0.42
1:A:21:SER:OG	9:A:1725:EDO:H11	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:O	1:A:165:ILE:HG22	2.20	0.42
1:A:1553:ASN:HB2	4:D:2:DG:H3'	2.01	0.42
1:A:419:ASP:O	1:A:423[A]:GLU:HG3	2.19	0.41
1:A:514:VAL:O	1:A:529:ASP:HA	2.19	0.41
1:A:720:ASN:HB3	1:A:723:LEU:HD12	2.02	0.41
1:A:161:LEU:HD13	1:A:295:VAL:HG22	2.02	0.41
1:A:178:LYS:HD3	1:A:251:LEU:HD23	2.02	0.41
1:A:613:LYS:HG2	11:A:2229:HOH:O	2.20	0.41
1:A:1067:ALA:HB3	1:A:1070:ASN:HB2	2.03	0.40
2:B:25:U:H2'	2:B:26:C:C6	2.56	0.40
1:A:1170:PHE:HD2	1:A:1212:ILE:HD13	1.86	0.40
2:B:34:C:H6	2:B:34:C:H5''	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:NH1	1:A:1260:GLU:OE2[2_445]	2.02	0.18

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	1446/1632 (89%)	1405 (97%)	38 (3%)	3 (0%)	47 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	GLY
1	A	723	LEU
1	A	1128	GLY

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	1255/1484 (85%)	1221 (97%)	34 (3%)	44 26

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	PHE
1	A	133	ASP
1	A	137	GLU
1	A	150	GLN
1	A	165	ILE
1	A	257	ASP
1	A	310	ARG
1	A	334	LYS
1	A	426	GLN
1	A	551	LEU
1	A	684	LYS
1	A	723	LEU
1	A	724	LEU
1	A	725	ASN
1	A	730	ILE
1	A	734	THR
1	A	791	ASN
1	A	846	LYS
1	A	856	ARG
1	A	917	LYS
1	A	982	ASN
1	A	1006	ARG
1	A	1048	SER
1	A	1056	GLU
1	A	1083	ARG
1	A	1138	GLN
1	A	1139	LEU
1	A	1146	ASP
1	A	1157	GLN
1	A	1234	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1301	SER
1	A	1428	LYS
1	A	1511	ASN
1	A	1598	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	159	ASN
1	A	247	ASN
1	A	293	HIS
1	A	342	ASN
1	A	426	GLN
1	A	488	GLN
1	A	492	ASN
1	A	604	GLN
1	A	642	ASN
1	A	659	HIS
1	A	677	GLN
1	A	725	ASN
1	A	791	ASN
1	A	938	ASN
1	A	1051	ASN
1	A	1157	GLN
1	A	1234	ASN
1	A	1236	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	92/94 (97%)	8 (8%)	2 (2%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	G
2	B	29	U
2	B	53	C
2	B	58	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	67	U
2	B	68	U
2	B	83	U
2	B	84	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	66	U
2	B	67	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 49 ligands modelled in this entry, 24 are monoatomic - leaving 25 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	$\# Z > 2$
9	EDO	A	1717	-	3,3,3	0.46	0	2,2,2	0.49	0
9	EDO	A	1718	-	3,3,3	0.44	0	2,2,2	0.70	0
9	EDO	A	1725	-	3,3,3	0.47	0	2,2,2	0.17	0
9	EDO	A	1724	-	3,3,3	0.54	0	2,2,2	0.04	0
9	EDO	A	1716	-	3,3,3	0.42	0	2,2,2	0.39	0
9	EDO	B	112	-	3,3,3	0.75	0	2,2,2	0.17	0
10	ACT	B	120	-	3,3,3	0.74	0	3,3,3	1.36	0
9	EDO	B	117	-	3,3,3	0.37	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	115	-	3,3,3	0.50	0	2,2,2	0.11	0
9	EDO	B	113	-	3,3,3	0.82	0	2,2,2	0.18	0
9	EDO	C	101	-	3,3,3	0.59	0	2,2,2	0.22	0
10	ACT	A	1728	-	3,3,3	0.78	0	3,3,3	0.99	0
9	EDO	B	119	-	3,3,3	0.45	0	2,2,2	0.35	0
9	EDO	A	1722	-	3,3,3	0.35	0	2,2,2	0.66	0
9	EDO	B	118	-	3,3,3	0.50	0	2,2,2	0.29	0
9	EDO	A	1727	-	3,3,3	0.38	0	2,2,2	0.60	0
9	EDO	A	1721	-	3,3,3	0.71	0	2,2,2	0.21	0
9	EDO	A	1719	-	3,3,3	0.54	0	2,2,2	0.21	0
9	EDO	A	1726	-	3,3,3	0.52	0	2,2,2	0.12	0
9	EDO	A	1720	-	3,3,3	0.61	0	2,2,2	0.37	0
9	EDO	A	1723	-	3,3,3	0.62	0	2,2,2	0.38	0
9	EDO	B	110	-	3,3,3	0.42	0	2,2,2	0.47	0
9	EDO	B	114	-	3,3,3	0.55	0	2,2,2	0.01	0
9	EDO	B	111	-	3,3,3	0.67	0	2,2,2	0.29	0
9	EDO	B	116	-	3,3,3	0.40	0	2,2,2	0.56	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
9	EDO	A	1717	-	-	0/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	B	117	-	-	0/1/1/1	-
9	EDO	B	115	-	-	1/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	C	101	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	A	1722	-	-	1/1/1/1	-
9	EDO	B	118	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	A	1721	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	A	1726	-	-	1/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	B	114	-	-	1/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-
9	EDO	B	116	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1722	EDO	O1-C1-C2-O2
9	A	1726	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2
9	B	114	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2
9	B	115	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1725	EDO	2	0
9	B	117	EDO	2	0
9	B	119	EDO	1	0
9	A	1722	EDO	1	0
9	B	116	EDO	3	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1455/1632 (89%)	0.57	219 (15%) 2 2	19, 44, 98, 147	0
2	B	93/94 (98%)	-0.33	0 100 100	19, 29, 59, 84	0
3	C	30/30 (100%)	-0.12	1 (3%) 46 51	24, 50, 74, 106	0
4	D	9/9 (100%)	0.20	0 100 100	30, 52, 94, 105	0
All	All	1587/1765 (89%)	0.50	220 (13%) 2 3	19, 43, 97, 147	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1066	LEU	12.7
1	A	723	LEU	10.9
1	A	1071	PRO	10.7
1	A	131	PHE	8.7
1	A	1060	PHE	8.5
1	A	1067	ALA	7.8
1	A	1072	ILE	7.5
1	A	1005	LEU	7.5
1	A	940	ILE	7.4
1	A	981	LEU	7.3
1	A	1049	PHE	7.3
1	A	1050	ILE	7.2
1	A	738	CYS	7.1
1	A	980	THR	7.0
1	A	728	ILE	6.8
1	A	266	PHE	6.5
1	A	1063	ALA	6.5
1	A	1002	ILE	6.3
1	A	1065	PHE	6.3
1	A	973	ARG	6.3
1	A	1059	ALA	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	187	LEU	6.0
1	A	988	ILE	6.0
1	A	261	ILE	5.9
1	A	1046	TYR	5.9
1	A	1052	LEU	5.7
1	A	1053	THR	5.7
1	A	259	LEU	5.6
1	A	1069	GLU	5.6
1	A	967	LEU	5.6
1	A	730	ILE	5.6
1	A	989	CYS	5.5
1	A	264	PHE	5.4
1	A	429	THR	5.4
1	A	742	ILE	5.4
1	A	1003	PHE	5.3
1	A	168	PHE	5.3
1	A	743	PHE	5.3
1	A	134	TYR	5.3
1	A	1619	LEU	5.3
1	A	1156	PRO	5.2
1	A	843	LEU	5.2
1	A	1057	GLN	5.2
1	A	236	ILE	5.1
1	A	1064	LEU	5.1
1	A	943	PHE	5.1
1	A	990	VAL	5.0
1	A	256	THR	4.9
1	A	125	ALA	4.9
1	A	972	PRO	4.9
1	A	1054	PRO	4.9
1	A	720	ASN	4.9
1	A	855	THR	4.9
1	A	1004	CYS	4.8
1	A	175	THR	4.7
1	A	177	ILE	4.7
1	A	724	LEU	4.6
1	A	902	PHE	4.6
1	A	1539	LEU	4.6
1	A	295	VAL	4.6
1	A	969	HIS	4.4
1	A	746	ILE	4.3
1	A	135	ASN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1573	ILE	4.1
1	A	1078	ARG	4.1
1	A	111	TYR	4.1
1	A	1542	ILE	4.1
1	A	1068	ASP	4.1
1	A	257	ASP	4.0
1	A	928	SER	4.0
1	A	143	TYR	3.9
1	A	1575	TYR	3.9
1	A	127	LEU	3.9
1	A	1076	VAL	3.9
1	A	716	ILE	3.9
1	A	186	THR	3.9
1	A	255	LEU	3.8
1	A	130	ILE	3.8
1	A	924	LEU	3.8
1	A	1062	HIS	3.8
1	A	1007	ASP	3.8
1	A	1187	ILE	3.8
1	A	999	GLY	3.8
1	A	778	ALA	3.7
1	A	1006	ARG	3.7
1	A	1055	GLN	3.7
1	A	128	MET	3.7
1	A	842	ILE	3.6
1	A	126	ILE	3.6
1	A	1077	ILE	3.6
1	A	1074	GLN	3.5
1	A	733	ASN	3.5
1	A	1565	TYR	3.5
1	A	298	VAL	3.5
1	A	830	ILE	3.5
1	A	933	PHE	3.4
1	A	721	ARG	3.4
1	A	939	ARG	3.4
1	A	293	HIS	3.4
1	A	1154	ASP	3.3
1	A	1621	GLY	3.3
1	A	987	LEU	3.3
1	A	1061	ARG	3.3
1	A	262	TRP	3.3
1	A	794	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	982	ASN	3.3
1	A	1095[A]	PHE	3.2
1	A	1191	TYR	3.2
1	A	1058	LYS	3.2
1	A	146	LEU	3.2
1	A	254	LEU	3.2
1	A	516	TYR	3.2
1	A	1194	TYR	3.2
1	A	971	ILE	3.2
1	A	739	GLU	3.1
1	A	781	PRO	3.1
1	A	1488	SER	3.1
1	A	123	VAL	3.1
1	A	856	ARG	3.1
1	A	1620	ALA	3.1
1	A	719	ASP	3.1
1	A	133	ASP	3.1
1	A	160	LYS	3.0
1	A	1541	ASP	3.0
1	A	138	ASP	3.0
1	A	178	LYS	3.0
1	A	828	ILE	3.0
1	A	1139	LEU	3.0
1	A	1143	VAL	3.0
1	A	985	ALA	2.9
1	A	1070	ASN	2.9
1	A	211	THR	2.9
1	A	112	SER	2.9
1	A	1523	PHE	2.9
1	A	235	ASN	2.9
1	A	1153	GLY	2.8
1	A	929	PRO	2.8
1	A	291	LEU	2.8
1	A	1487	ILE	2.8
1	A	188	LYS	2.8
1	A	968	ASP	2.7
1	A	1598	THR	2.7
1	A	124	LYS	2.7
1	A	30	LEU	2.7
1	A	173	LEU	2.7
1	A	747	CYS	2.7
1	A	1566	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	966	GLU	2.7
1	A	147	ALA	2.6
1	A	1073	LYS	2.6
1	A	1207	ASP	2.6
1	A	937	ASN	2.6
1	A	294	PHE	2.6
1	A	237	GLN	2.6
1	A	1193	LEU	2.6
1	A	722	GLY	2.5
1	A	1000	ASN	2.5
1	A	1001	ARG	2.5
1	A	1192	SER	2.5
1	A	296	PHE	2.5
1	A	731	ALA	2.5
1	A	1075	ALA	2.5
1	A	263	ASN	2.5
1	A	986	ASN	2.5
1	A	156	GLU	2.5
1	A	428	VAL	2.5
1	A	932	ILE	2.5
1	A	741	GLU	2.5
1	A	637	LYS	2.5
1	A	176	ASP	2.4
1	A	1540	ARG	2.4
1	A	136	GLY	2.4
1	A	1179	ASN	2.4
1	A	1543	GLY	2.4
1	A	1536	PRO	2.4
1	A	1537	SER	2.4
1	A	729	ASN	2.4
1	A	1564	ASP	2.4
1	A	258	ASP	2.4
1	A	1544	ILE	2.4
1	A	785	ARG	2.4
1	A	195	PHE	2.3
1	A	1155	LYS	2.3
1	A	759	TYR	2.3
1	A	853	ILE	2.3
1	A	734	THR	2.3
1	A	234	TYR	2.3
1	A	260	ASP	2.3
1	A	142	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1209	PHE	2.3
1	A	166	LEU	2.2
1	A	297	ALA	2.2
1	A	265	ASN	2.2
3	C	1	DC	2.2
1	A	150	GLN	2.2
1	A	200	ASP	2.2
1	A	431	ALA	2.2
1	A	930	GLU	2.2
1	A	253	THR	2.2
1	A	925	GLU	2.2
1	A	1185	LEU	2.2
1	A	214	PHE	2.1
1	A	189	GLU	2.1
1	A	213	LYS	2.1
1	A	927	ILE	2.1
1	A	970	ILE	2.1
1	A	726	HIS	2.1
1	A	1567	ILE	2.1
1	A	1571	SER	2.1
1	A	267	GLU	2.1
1	A	936	LYS	2.0
1	A	1141	GLU	2.0
1	A	1576	PHE	2.0
1	A	1145	SER	2.0
1	A	1594	LEU	2.0
1	A	829	LYS	2.0
1	A	814	CYS	2.0
1	A	1080	ILE	2.0
1	A	179	ASP	2.0
1	A	1082	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
9	EDO	A	1726	4/4	0.68	0.15	72,74,76,77	0
9	EDO	A	1727	4/4	0.76	0.30	76,76,76,77	0
9	EDO	B	118	4/4	0.82	0.20	44,50,52,53	0
9	EDO	B	119	4/4	0.83	0.18	57,58,58,59	0
6	NA	A	1703	1/1	0.86	0.06	64,64,64,64	0
9	EDO	A	1725	4/4	0.89	0.16	53,57,62,66	0
8	CA	A	1713	1/1	0.90	0.06	87,87,87,87	0
9	EDO	B	115	4/4	0.90	0.17	41,46,52,56	0
9	EDO	B	117	4/4	0.91	0.15	54,56,57,57	0
8	CA	B	106	1/1	0.92	0.09	63,63,63,63	0
9	EDO	A	1717	4/4	0.92	0.12	35,38,39,39	0
9	EDO	B	116	4/4	0.92	0.15	34,43,48,49	0
9	EDO	A	1722	4/4	0.93	0.16	51,52,53,54	0
9	EDO	C	101	4/4	0.93	0.11	42,43,43,43	0
8	CA	B	109	1/1	0.94	0.05	70,70,70,70	0
6	NA	A	1702	1/1	0.94	0.05	45,45,45,45	0
10	ACT	B	120	4/4	0.94	0.15	57,59,60,60	0
9	EDO	A	1721	4/4	0.95	0.08	33,34,35,35	0
8	CA	B	107	1/1	0.95	0.09	63,63,63,63	0
9	EDO	A	1724	4/4	0.95	0.11	42,42,43,43	0
8	CA	A	1710	1/1	0.95	0.05	52,52,52,52	0
9	EDO	A	1716	4/4	0.95	0.10	37,41,43,44	0
8	CA	A	1712	1/1	0.95	0.12	72,72,72,72	0
9	EDO	B	114	4/4	0.95	0.10	40,43,43,46	0
9	EDO	A	1720	4/4	0.96	0.13	31,34,36,37	0
8	CA	B	104	1/1	0.96	0.04	68,68,68,68	0
6	NA	B	102	1/1	0.96	0.12	53,53,53,53	0
8	CA	A	1714	1/1	0.96	0.14	62,62,62,62	0
9	EDO	A	1719	4/4	0.96	0.06	34,36,37,37	0
8	CA	A	1711	1/1	0.97	0.04	66,66,66,66	0
9	EDO	A	1723	4/4	0.97	0.10	30,35,38,42	0
8	CA	B	108	1/1	0.97	0.10	71,71,71,71	0
9	EDO	B	111	4/4	0.97	0.07	29,30,31,33	0
8	CA	A	1715	1/1	0.98	0.05	45,45,45,45	0
8	CA	A	1709	1/1	0.98	0.04	42,42,42,42	0
7	CL	A	1704	1/1	0.98	0.05	42,42,42,42	0
8	CA	A	1706	1/1	0.98	0.05	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	B	110	4/4	0.98	0.07	28,30,32,34	0
9	EDO	A	1718	4/4	0.98	0.07	35,38,41,43	0
9	EDO	B	112	4/4	0.98	0.12	22,23,23,24	0
10	ACT	A	1728	4/4	0.98	0.06	33,35,35,36	0
9	EDO	B	113	4/4	0.98	0.08	27,28,28,29	0
7	CL	A	1705	1/1	0.99	0.04	28,28,28,28	0
8	CA	A	1707	1/1	0.99	0.03	34,34,34,34	0
8	CA	B	105	1/1	0.99	0.03	34,34,34,34	0
8	CA	A	1708	1/1	0.99	0.06	57,57,57,57	0
5	ZN	A	1701	1/1	1.00	0.11	26,26,26,26	0
8	CA	B	103	1/1	1.00	0.04	32,32,32,32	0
6	NA	B	101	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.