



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 02:27 PM EDT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

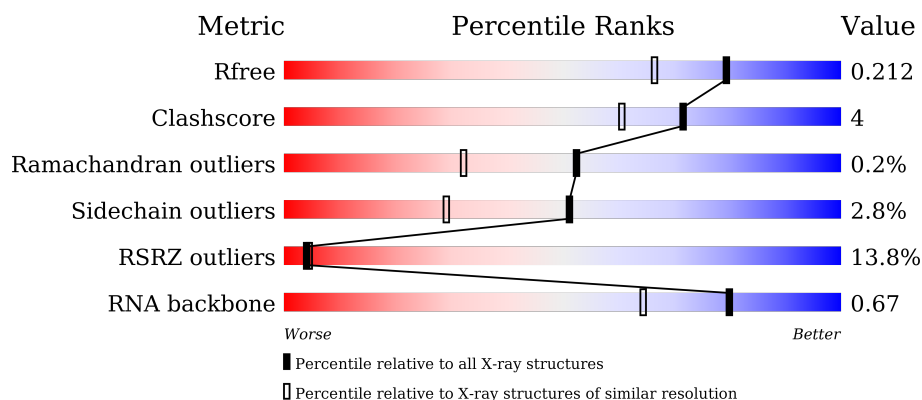
1 Overall quality at a glance

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)
RNA backbone	2183	1045 (2.70-0.88)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>13%</div> <div> <div>79%</div> <div>9%</div> <div>11%</div> </div> </div>
2	B	94	<div> <div>49%</div> <div>43%</div> <div>6%</div> </div>
3	C	30	<div> <div>3%</div> <div>47%</div> <div>47%</div> <div>7%</div> </div>
4	D	9	<div> <div>78%</div> <div>22%</div> </div>

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
10	ACT	B	120	-	-	-	X
9	EDO	A	1717	-	-	-	X
9	EDO	A	1723	-	-	-	X
9	EDO	A	1724	-	-	-	X
9	EDO	A	1725	-	-	-	X
9	EDO	A	1727	-	-	-	X
9	EDO	B	115	-	-	-	X
9	EDO	B	117	-	-	-	X
9	EDO	B	119	-	-	-	X

2 Entry composition

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
1	A	1455	Total	C	N	O	S	0	19	0
			11791	7536	2025	2199	31			

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
2	B	94	Total	C	N	O	P	0	0	0
			1991	886	350	661	94			

- Molecule 3 is a DNA chain called Target DNA.

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

- 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
4	D	9	Total	C	N	O	P	0	0	0
			185	89	34	54	8			

- 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	B	2	Total Na 2 2	0	0
6	A	2	Total Na 2 2	0	0

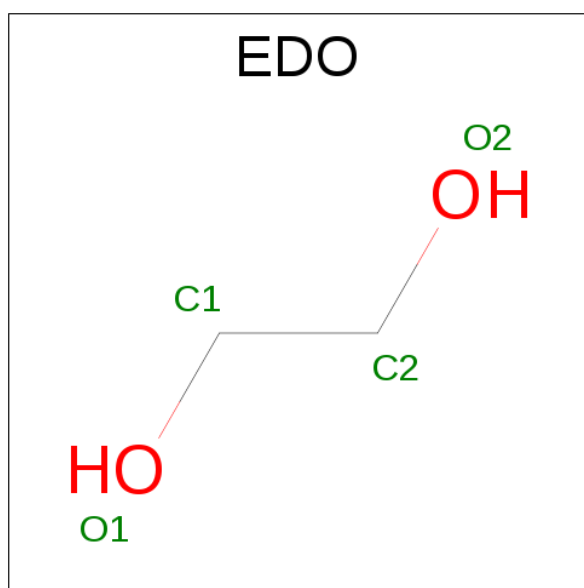
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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	B	7	Total Ca 7 7	0	0
8	A	10	Total Ca 10 10	0	0

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



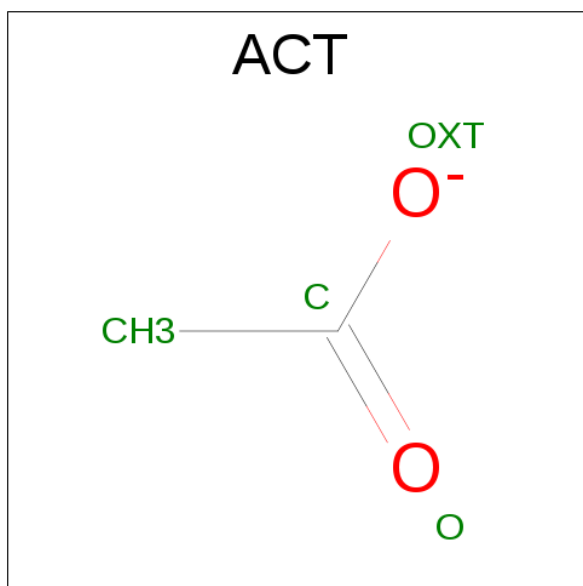
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0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

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

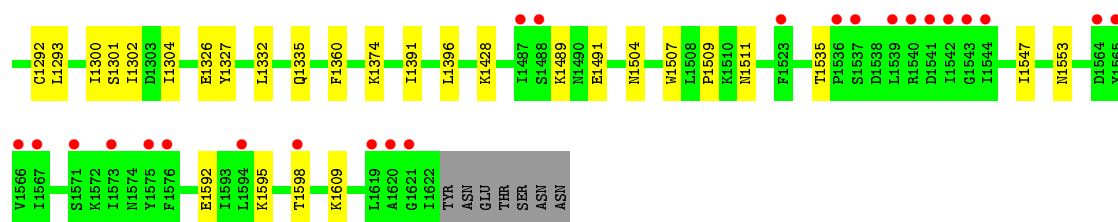
- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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		

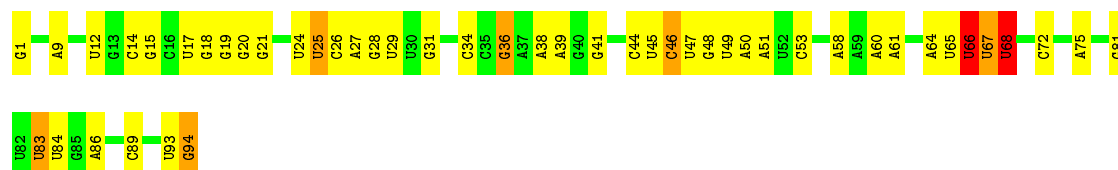
- Molecule 11 is water.

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		



• Molecule 2: Guide RNA

Chain B: 49% 43% 6%



• Molecule 3: Target DNA

Chain C: 3% 47% 47% 7%



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

Chain D: 78% 22%



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)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.207 0.190 , 0.212	Depositor DCC
R_{free} test set	12436 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 249260 reflections	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CL, NA, CA, EDO, ACT

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

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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

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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 ⓘ

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

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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:1326:GLU:HG3	1:A:1327:TYR:CD2	2.27	0.70
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: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

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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:1159:SER:OG	1:A:1221:ASP:OD1	2.20	0.55
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.25	0.55
1:A:791:ASN:HD22	1:A:791:ASN:H	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:H8	3:C:24:DA:H5''	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:1326:GLU:HG3	1:A:1327:TYR:HD2	1.73	0.51
1:A:698:TRP:CH2	1:A:770:LEU:HD23	2.45	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:1504:ASN:ND2	11:A:1804:HOH:O	2.14	0.50
1:A:869:LEU:HD23	1:A:1095[B]:PHE:CE1	2.47	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:1507:TRP:CD1	1:A:1509:PRO:HD2	2.49	0.48
1:A:61[A]:GLN:HG3	11:A:2395:HOH:O	2.12	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

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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:NH1	1:A:249:ARG:HG2	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:1272:GLU:HG3	11:A:2337:HOH:O	2.19	0.43
1:A:780:LYS:HE3	1:A:784:ASP:OD1	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:640:LYS:HE3	2:B:68:U:C6	2.54	0.42
1:A:45:LYS:HB3	1:A:911:VAL:HG12	2.01	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:1091:THR:O	1:A:1095[A]:PHE:HD1	2.01	0.42
1:A:663[A]:GLN:HG3	2:B:81:G:H5''	2.00	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:HB3	1:A:178:LYS:HE3	1.89	0.42
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.34	0.42
1:A:161:LEU:O	1:A:165:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:OG	9:A:1725:EDO:H11	2.19	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

5.3.1 Protein backbone

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%)	52	32

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 ⓘ

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%)	52 31

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

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

Some 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

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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 carbohydrates 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	1716	-	3,3,3	0.41	0	2,2,2	0.46	0
9	EDO	A	1717	-	3,3,3	0.45	0	2,2,2	0.57	0
9	EDO	A	1718	-	3,3,3	0.43	0	2,2,2	0.78	0
9	EDO	A	1719	-	3,3,3	0.53	0	2,2,2	0.17	0
9	EDO	A	1720	-	3,3,3	0.59	0	2,2,2	0.43	0
9	EDO	A	1721	-	3,3,3	0.68	0	2,2,2	0.25	0
9	EDO	A	1722	-	3,3,3	0.34	0	2,2,2	0.74	0
9	EDO	A	1723	-	3,3,3	0.60	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	1724	-	3,3,3	0.52	0	2,2,2	0.05	0
9	EDO	A	1725	-	3,3,3	0.46	0	2,2,2	0.22	0
9	EDO	A	1726	-	3,3,3	0.51	0	2,2,2	0.16	0
9	EDO	A	1727	-	3,3,3	0.37	0	2,2,2	0.68	0
10	ACT	A	1728	-	0,3,3	0.00	-	0,3,3	0.00	-
9	EDO	B	110	-	3,3,3	0.41	0	2,2,2	0.54	0
9	EDO	B	111	-	3,3,3	0.64	0	2,2,2	0.35	0
9	EDO	B	112	-	3,3,3	0.71	0	2,2,2	0.21	0
9	EDO	B	113	-	3,3,3	0.79	0	2,2,2	0.19	0
9	EDO	B	114	-	3,3,3	0.53	0	2,2,2	0.05	0
9	EDO	B	115	-	3,3,3	0.49	0	2,2,2	0.15	0
9	EDO	B	116	-	3,3,3	0.39	0	2,2,2	0.63	0
9	EDO	B	117	-	3,3,3	0.36	0	2,2,2	0.28	0
9	EDO	B	118	-	3,3,3	0.49	0	2,2,2	0.31	0
9	EDO	B	119	-	3,3,3	0.43	0	2,2,2	0.42	0
10	ACT	B	120	-	0,3,3	0.00	-	0,3,3	0.00	-
9	EDO	C	101	-	3,3,3	0.57	0	2,2,2	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1716	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1717	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1718	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1719	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1720	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1721	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1722	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1723	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1724	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1725	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1726	-	-	0/1/1/1	0/0/0/0
9	EDO	A	1727	-	-	0/1/1/1	0/0/0/0
10	ACT	A	1728	-	-	0/0/0/0	0/0/0/0
9	EDO	B	110	-	-	0/1/1/1	0/0/0/0
9	EDO	B	111	-	-	0/1/1/1	0/0/0/0
9	EDO	B	112	-	-	0/1/1/1	0/0/0/0
9	EDO	B	113	-	-	0/1/1/1	0/0/0/0
9	EDO	B	114	-	-	0/1/1/1	0/0/0/0
9	EDO	B	115	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	116	-	-	0/1/1/1	0/0/0/0
9	EDO	B	117	-	-	0/1/1/1	0/0/0/0
9	EDO	B	118	-	-	0/1/1/1	0/0/0/0
9	EDO	B	119	-	-	0/1/1/1	0/0/0/0
10	ACT	B	120	-	-	0/0/0/0	0/0/0/0
9	EDO	C	101	-	-	0/1/1/1	0/0/0/0

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.

5 monomers are involved in 9 short contacts:

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

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	218 (14%) 3 3	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%) 50 54	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	219 (13%) 4 4	19, 43, 97, 147	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1066	LEU	12.7
1	A	723	LEU	11.0
1	A	1071	PRO	10.8
1	A	131	PHE	8.7
1	A	1060	PHE	8.5
1	A	1067	ALA	7.9
1	A	1072	ILE	7.6
1	A	940	ILE	7.4
1	A	1005	LEU	7.4
1	A	981	LEU	7.3
1	A	1049	PHE	7.3
1	A	1050	ILE	7.3
1	A	738	CYS	7.1
1	A	980	THR	7.1
1	A	728	ILE	6.8
1	A	266	PHE	6.6
1	A	1063	ALA	6.5
1	A	973	ARG	6.4
1	A	1059	ALA	6.3
1	A	1002	ILE	6.3
1	A	1065	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	LEU	6.1
1	A	261	ILE	6.0
1	A	988	ILE	6.0
1	A	1046	TYR	5.9
1	A	1052	LEU	5.8
1	A	1053	THR	5.7
1	A	1069	GLU	5.6
1	A	730	ILE	5.6
1	A	259	LEU	5.5
1	A	967	LEU	5.5
1	A	429	THR	5.5
1	A	989	CYS	5.4
1	A	264	PHE	5.4
1	A	1003	PHE	5.3
1	A	742	ILE	5.3
1	A	168	PHE	5.3
1	A	743	PHE	5.3
1	A	1619	LEU	5.3
1	A	134	TYR	5.2
1	A	1156	PRO	5.2
1	A	843	LEU	5.2
1	A	1057	GLN	5.2
1	A	1064	LEU	5.1
1	A	236	ILE	5.0
1	A	256	THR	5.0
1	A	125	ALA	5.0
1	A	943	PHE	5.0
1	A	990	VAL	4.9
1	A	972	PRO	4.9
1	A	720	ASN	4.9
1	A	1054	PRO	4.8
1	A	855	THR	4.8
1	A	1004	CYS	4.8
1	A	175	THR	4.8
1	A	177	ILE	4.7
1	A	724	LEU	4.6
1	A	902	PHE	4.6
1	A	295	VAL	4.6
1	A	1539	LEU	4.5
1	A	969	HIS	4.4
1	A	746	ILE	4.3
1	A	1573	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	ASN	4.1
1	A	1078	ARG	4.1
1	A	111	TYR	4.1
1	A	1068	ASP	4.1
1	A	1542	ILE	4.1
1	A	257	ASP	4.1
1	A	928	SER	4.0
1	A	143	TYR	4.0
1	A	1575	TYR	3.9
1	A	186	THR	3.9
1	A	127	LEU	3.9
1	A	716	ILE	3.8
1	A	924	LEU	3.8
1	A	1062	HIS	3.8
1	A	255	LEU	3.8
1	A	1076	VAL	3.8
1	A	778	ALA	3.8
1	A	1007	ASP	3.8
1	A	130	ILE	3.8
1	A	1055	GLN	3.7
1	A	999	GLY	3.7
1	A	1187	ILE	3.7
1	A	128	MET	3.7
1	A	1006	ARG	3.7
1	A	126	ILE	3.7
1	A	842	ILE	3.6
1	A	830	ILE	3.5
1	A	1074	GLN	3.5
1	A	733	ASN	3.5
1	A	298	VAL	3.5
1	A	1565	TYR	3.5
1	A	1077	ILE	3.5
1	A	933	PHE	3.5
1	A	293	HIS	3.4
1	A	721	ARG	3.4
1	A	1154	ASP	3.4
1	A	939	ARG	3.3
1	A	1621	GLY	3.3
1	A	982	ASN	3.3
1	A	987	LEU	3.3
1	A	794	TYR	3.3
1	A	1061	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	3.3
1	A	1095[A]	PHE	3.2
1	A	1058	LYS	3.2
1	A	1194	TYR	3.2
1	A	146	LEU	3.2
1	A	516	TYR	3.2
1	A	123	VAL	3.2
1	A	254	LEU	3.2
1	A	1191	TYR	3.1
1	A	971	ILE	3.1
1	A	781	PRO	3.1
1	A	856	ARG	3.1
1	A	1620	ALA	3.1
1	A	739	GLU	3.1
1	A	1488	SER	3.1
1	A	133	ASP	3.1
1	A	719	ASP	3.1
1	A	1541	ASP	3.0
1	A	160	LYS	3.0
1	A	1139	LEU	3.0
1	A	1143	VAL	3.0
1	A	138	ASP	3.0
1	A	1070	ASN	3.0
1	A	178	LYS	3.0
1	A	828	ILE	2.9
1	A	1153	GLY	2.9
1	A	1523	PHE	2.9
1	A	112	SER	2.9
1	A	929	PRO	2.9
1	A	985	ALA	2.9
1	A	211	THR	2.8
1	A	291	LEU	2.8
1	A	235	ASN	2.8
1	A	188	LYS	2.8
1	A	1487	ILE	2.7
1	A	124	LYS	2.7
1	A	747	CYS	2.7
1	A	1598	THR	2.7
1	A	968	ASP	2.7
1	A	30	LEU	2.7
1	A	173	LEU	2.7
1	A	1207	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	2.6
1	A	966	GLU	2.6
1	A	1073	LYS	2.6
1	A	1193	LEU	2.6
1	A	1566	VAL	2.6
1	A	937	ASN	2.6
1	A	294	PHE	2.6
1	A	722	GLY	2.6
1	A	237	GLN	2.6
1	A	1000	ASN	2.6
1	A	731	ALA	2.5
1	A	932	ILE	2.5
1	A	1192	SER	2.5
1	A	263	ASN	2.5
1	A	156	GLU	2.5
1	A	1001	ARG	2.5
1	A	1075	ALA	2.5
1	A	986	ASN	2.5
1	A	637	LYS	2.5
1	A	176	ASP	2.5
1	A	296	PHE	2.5
1	A	428	VAL	2.5
1	A	1179	ASN	2.4
1	A	1540	ARG	2.4
1	A	136	GLY	2.4
1	A	741	GLU	2.4
1	A	1564	ASP	2.4
1	A	1544	ILE	2.4
1	A	785	ARG	2.4
1	A	1536	PRO	2.4
1	A	1537	SER	2.4
1	A	729	ASN	2.4
1	A	195	PHE	2.4
1	A	1543	GLY	2.4
1	A	1155	LYS	2.4
1	A	258	ASP	2.3
1	A	759	TYR	2.3
1	A	142	SER	2.3
1	A	853	ILE	2.3
1	A	734	THR	2.3
1	A	234	TYR	2.3
1	A	265	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	200	ASP	2.3
1	A	260	ASP	2.3
1	A	930	GLU	2.2
3	C	1	DC	2.2
1	A	1209	PHE	2.2
1	A	297	ALA	2.2
1	A	431	ALA	2.2
1	A	166	LEU	2.2
1	A	214	PHE	2.2
1	A	150	GLN	2.2
1	A	253	THR	2.2
1	A	925	GLU	2.2
1	A	1571	SER	2.2
1	A	189	GLU	2.2
1	A	726	HIS	2.1
1	A	213	LYS	2.1
1	A	829	LYS	2.1
1	A	267	GLU	2.1
1	A	1185	LEU	2.1
1	A	927	ILE	2.1
1	A	970	ILE	2.1
1	A	1145	SER	2.1
1	A	936	LYS	2.1
1	A	814	CYS	2.1
1	A	1082	ASN	2.1
1	A	1567	ILE	2.1
1	A	1141	GLU	2.0
1	A	179	ASP	2.0
1	A	1576	PHE	2.0
1	A	1594	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	EDO	B	115	4/4	0.89	0.17	12.48	41,46,52,56	0
9	EDO	A	1727	4/4	0.75	0.30	8.31	76,76,76,77	0
10	ACT	B	120	4/4	0.94	0.15	4.65	57,59,60,60	0
9	EDO	A	1725	4/4	0.89	0.16	4.36	53,57,62,66	0
9	EDO	A	1723	4/4	0.97	0.10	3.82	30,35,38,42	0
9	EDO	B	119	4/4	0.83	0.18	2.98	57,58,58,59	0
9	EDO	A	1717	4/4	0.92	0.12	2.54	35,38,39,39	0
9	EDO	A	1724	4/4	0.95	0.11	2.29	42,42,43,43	0
9	EDO	B	117	4/4	0.91	0.15	2.26	54,56,57,57	0
9	EDO	B	116	4/4	0.92	0.15	1.50	34,43,48,49	0
9	EDO	B	111	4/4	0.97	0.07	0.26	29,30,31,33	0
9	EDO	B	114	4/4	0.95	0.10	0.18	40,43,43,46	0
9	EDO	A	1722	4/4	0.93	0.16	0.18	51,52,53,54	0
9	EDO	A	1719	4/4	0.96	0.06	0.13	34,36,37,37	0
5	ZN	A	1701	1/1	1.00	0.11	-0.03	26,26,26,26	0
9	EDO	B	110	4/4	0.98	0.07	-0.25	28,30,32,34	0
9	EDO	B	112	4/4	0.98	0.12	-0.36	22,23,23,24	0
9	EDO	A	1720	4/4	0.96	0.13	-0.53	31,34,36,37	0
9	EDO	C	101	4/4	0.93	0.11	-0.59	42,43,43,43	0
7	CL	A	1704	1/1	0.98	0.05	-0.84	42,42,42,42	0
9	EDO	B	113	4/4	0.98	0.08	-0.86	27,28,28,29	0
9	EDO	A	1721	4/4	0.95	0.08	-1.10	33,34,35,35	0
9	EDO	A	1716	4/4	0.95	0.10	-1.32	37,41,43,44	0
8	CA	A	1706	1/1	0.98	0.05	-1.35	67,67,67,67	0
9	EDO	A	1718	4/4	0.98	0.07	-1.63	35,38,41,43	0
8	CA	A	1715	1/1	0.98	0.05	-1.72	45,45,45,45	0
7	CL	A	1705	1/1	0.99	0.04	-1.73	28,28,28,28	0
6	NA	A	1702	1/1	0.94	0.05	-1.83	45,45,45,45	0
10	ACT	A	1728	4/4	0.98	0.06	-1.90	33,35,35,36	0
8	CA	B	109	1/1	0.94	0.05	-2.21	70,70,70,70	0
8	CA	B	103	1/1	1.00	0.04	-2.56	32,32,32,32	0
6	NA	B	101	1/1	1.00	0.05	-5.83	28,28,28,28	0
8	CA	A	1709	1/1	0.98	0.04	-6.02	42,42,42,42	0
8	CA	B	107	1/1	0.95	0.09	-	63,63,63,63	0
8	CA	A	1714	1/1	0.96	0.14	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NA	A	1703	1/1	0.87	0.06	-	64,64,64,64	0
8	CA	A	1711	1/1	0.97	0.04	-	66,66,66,66	0
6	NA	B	102	1/1	0.96	0.11	-	53,53,53,53	0
8	CA	B	108	1/1	0.96	0.10	-	71,71,71,71	0
9	EDO	B	118	4/4	0.82	0.20	-	44,50,52,53	0
8	CA	B	104	1/1	0.96	0.04	-	68,68,68,68	0
8	CA	B	106	1/1	0.92	0.09	-	63,63,63,63	0
8	CA	A	1710	1/1	0.95	0.05	-	52,52,52,52	0
9	EDO	A	1726	4/4	0.67	0.15	-	72,74,76,77	0
8	CA	A	1713	1/1	0.90	0.06	-	87,87,87,87	0
8	CA	A	1712	1/1	0.95	0.12	-	72,72,72,72	0
8	CA	A	1708	1/1	0.99	0.06	-	57,57,57,57	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

6.5 Other polymers [i](#)

There are no such residues in this entry.