Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:04 PM JST

PDB ID	:	5B2Q
Title	:	Crystal structure of Francisella novicida Cas9 RHA 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:

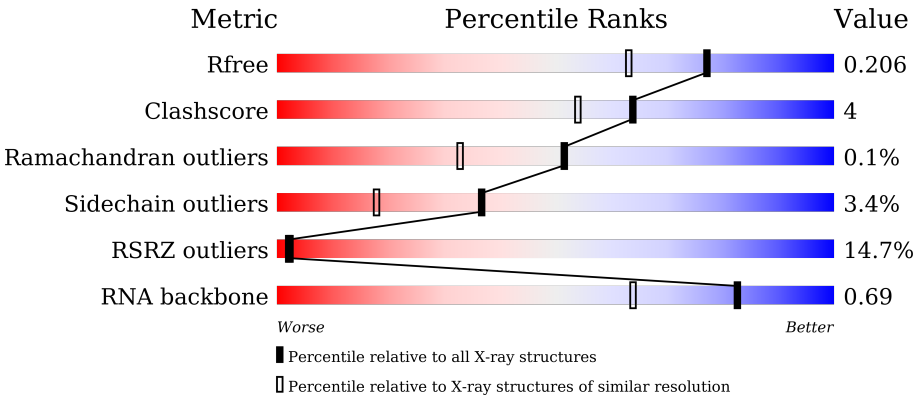
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 <=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	14% 78% 10% · 11%
2	B	94	71% 26% ··
3	C	30	63% 30% 7%
4	D	9	22% 67% 33%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15694 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	11802	7550	2027	2194	31	0	16	0

There are 7 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
A	1369	ARG	GLU	conflict	UNP A0Q5Y3
A	1449	HIS	GLU	conflict	UNP A0Q5Y3
A	1556	ALA	ARG	conflict	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

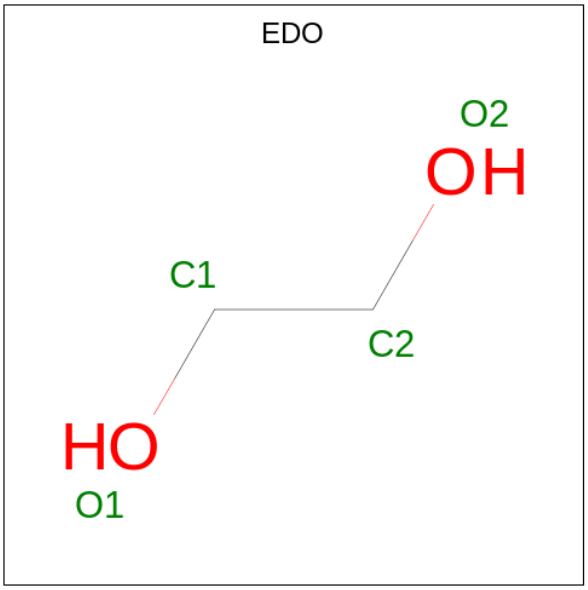
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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: $C_2H_6O_2$).



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

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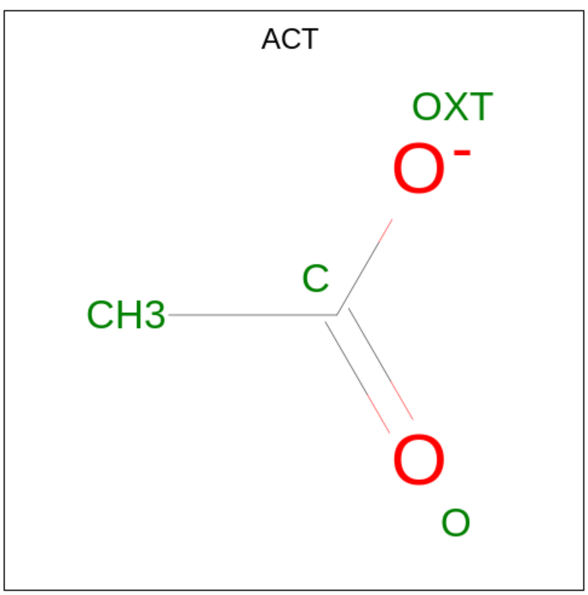
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

- 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 4 2 2	0	0

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

- Molecule 11 is water.

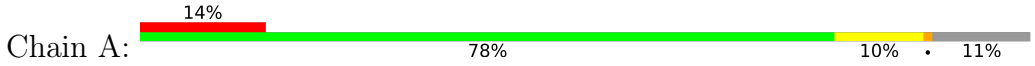
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	588	Total O 588 588	0	0
11	B	334	Total O 334 334	0	0
11	C	64	Total O 64 64	0	0
11	D	7	Total O 7 7	0	0

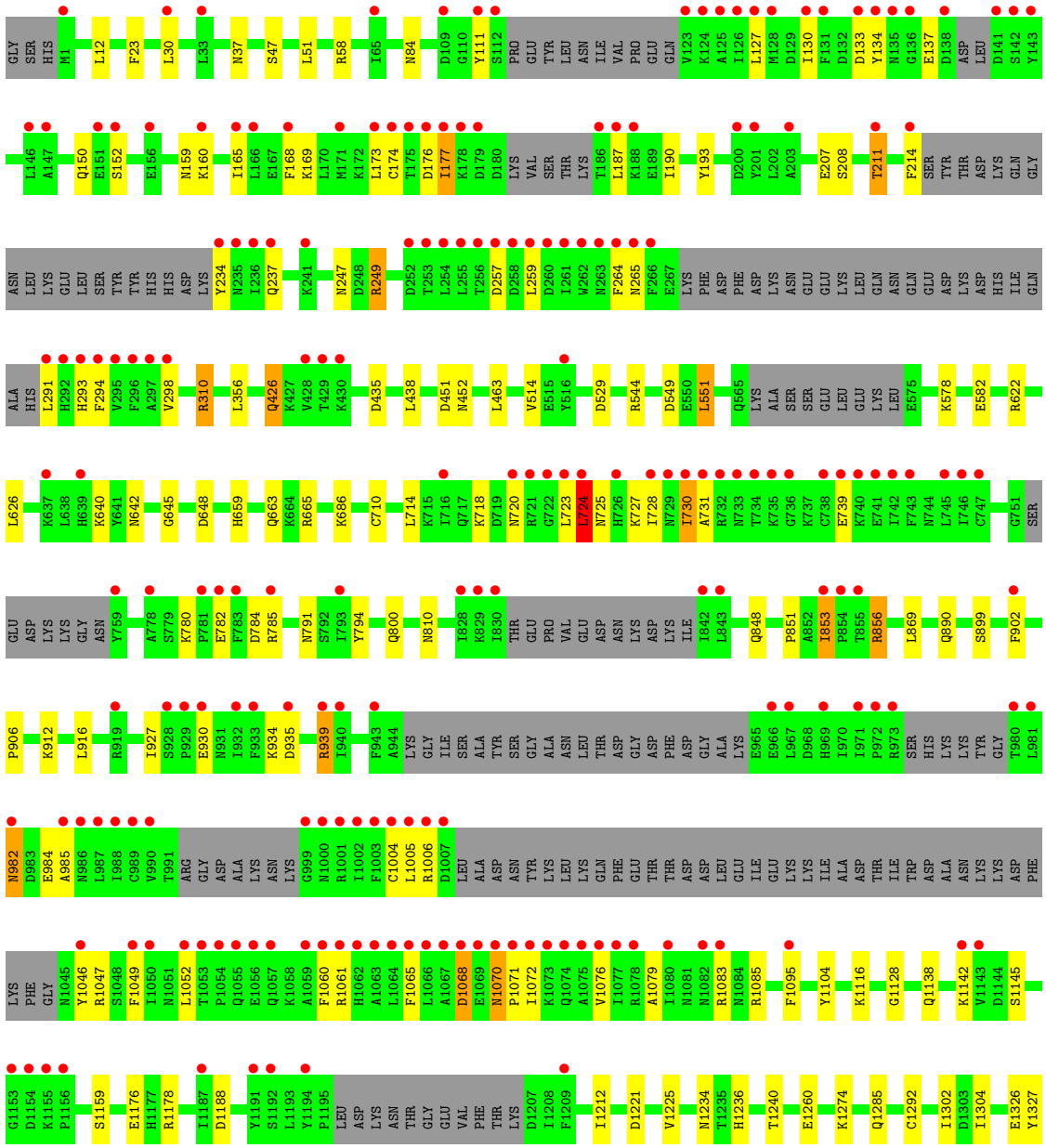
3 Residue-property plots (i)

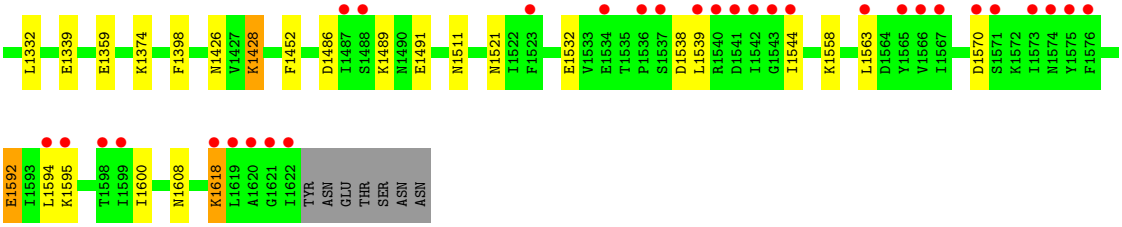
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

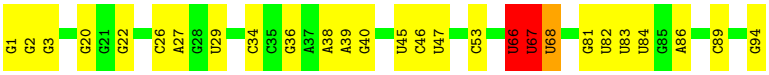






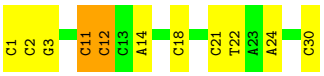
• Molecule 2: Guide RNA

Chain B:



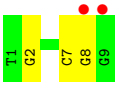
• Molecule 3: Target DNA

Chain C:



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

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	81.56Å 158.98Å 96.74Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	46.29 – 1.70 46.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.29-1.70) 98.9 (46.29-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.183 , 0.206 0.183 , 0.206	Depositor DCC
R_{free} test set	12762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15694	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: ACT, EDO, CA, ZN, NA, CL

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	0.41	0/12077	0.55	2/16290 (0.0%)
2	B	0.88	0/2224	1.31	13/3465 (0.4%)
3	C	1.02	0/664	1.23	6/1018 (0.6%)
4	D	0.82	0/207	1.05	1/319 (0.3%)
All	All	0.55	0/15172	0.78	22/21092 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	27	A	O5'-P-OP2	-13.64	93.43	105.70
3	C	11	DC	O5'-P-OP2	-11.75	95.13	105.70
3	C	12	DC	O5'-P-OP2	-9.99	96.71	105.70
2	B	66	U	O5'-P-OP1	-7.66	98.81	105.70
2	B	47	U	C2-N3-C4	-6.86	122.88	127.00
3	C	11	DC	O4'-C4'-C3'	-6.66	101.84	104.50
3	C	14	DA	O5'-P-OP2	-6.56	99.79	105.70
3	C	11	DC	OP1-P-OP2	6.28	129.02	119.60
3	C	18	DC	O4'-C4'-C3'	-6.28	101.99	104.50
2	B	20	G	C5-C6-N1	6.26	114.63	111.50
1	A	724	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	310	ARG	CG-CD-NE	-6.19	98.80	111.80
2	B	86	A	O4'-C1'-N9	6.11	113.08	108.20
2	B	22	G	C5-C6-O6	-5.98	125.01	128.60
4	D	2	DG	O4'-C1'-N9	-5.93	103.85	108.00
2	B	66	U	P-O3'-C3'	5.76	126.61	119.70
2	B	68	U	C5-C6-N1	-5.61	119.89	122.70
2	B	66	U	O5'-P-OP2	5.33	117.09	110.70
2	B	26	C	N3-C2-O2	5.31	125.62	121.90
2	B	20	G	N1-C6-O6	-5.26	116.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	67	U	N3-C2-O2	-5.18	118.57	122.20
2	B	36	G	N9-C1'-C2'	-5.12	106.37	112.00

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	11802	0	11583	98	1
2	B	1991	0	997	13	0
3	C	595	0	337	11	0
4	D	185	0	104	1	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	4	0
9	B	48	0	72	3	0
10	A	8	0	6	0	0
11	A	588	0	0	9	0
11	B	334	0	0	2	0
11	C	64	0	0	1	0
11	D	7	0	0	0	0
All	All	15694	0	13171	116	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 (116) 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:265:ASN:O	1:A:291:LEU:N	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.59	0.83
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.03	0.76
1:A:578:LYS:NZ	1:A:582:GLU:OE2	2.20	0.75
1:A:169:LYS:HB3	1:A:187:LEU:HD11	1.68	0.74
3:C:22:DT:H5"	3:C:22:DT:H6	1.52	0.72
1:A:1486:ASP:OD1	1:A:1521:ASN:ND2	2.22	0.71
3:C:2:DC:H2'	3:C:3:DG:C8	2.25	0.70
1:A:984:GLU:O	1:A:1061:ARG:NH2	2.26	0.68
1:A:207:GLU:O	1:A:211:THR:OG1	2.13	0.66
1:A:930:GLU:O	1:A:934:LYS:NZ	2.27	0.64
1:A:645:GLY:HA2	9:A:1721:EDO:H11	1.78	0.64
1:A:23:PHE:HB2	9:A:1725:EDO:H22	1.81	0.63
1:A:1326:GLU:HG3	1:A:1327:TYR:CD2	2.34	0.62
3:C:11:DC:OP1	11:C:101:HOH:O	2.16	0.61
1:A:1532:GLU:O	1:A:1618:LYS:NZ	2.31	0.60
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.83	0.60
1:A:1302:ILE:HG22	1:A:1304:ILE:HG12	1.84	0.59
1:A:84:ASN:ND2	11:A:1803:HOH:O	2.21	0.59
1:A:622:ARG:NH2	1:A:848:GLN:OE1	2.36	0.59
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.35	0.59
1:A:782:GLU:OE1	1:A:785:ARG:NH2	2.25	0.58
1:A:1236:HIS:HE1	11:A:1976:HOH:O	1.85	0.58
3:C:1:DC:H6	3:C:1:DC:H5'	1.69	0.58
3:C:24:DA:H5"	3:C:24:DA:H8	1.69	0.58
1:A:1359:GLU:OE2	11:A:1801:HOH:O	2.17	0.57
1:A:174:CYS:HA	1:A:247:ASN:HD21	1.67	0.57
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.70	0.57
2:B:94:G:C2	9:B:120:EDO:H11	2.40	0.57
4:D:7:DC:H2"	4:D:8:DG:C8	2.40	0.56
3:C:22:DT:H5"	3:C:22:DT:C6	2.38	0.55
1:A:1159:SER:OG	1:A:1221:ASP:OD1	2.17	0.55
1:A:725:ASN:HD22	1:A:794:TYR:HE2	1.54	0.55
1:A:1592:GLU:OE2	1:A:1595:LYS:NZ	2.37	0.55
1:A:169:LYS:HB3	1:A:187:LEU:CD1	2.38	0.54
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.40	0.54
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.41	0.53
1:A:1049:PHE:HA	1:A:1052:LEU:HD12	1.90	0.53
1:A:1539:LEU:HB3	1:A:1544:ILE:HD12	1.90	0.53
1:A:168:PHE:HA	1:A:259:LEU:HD13	1.89	0.53
1:A:648[B]:ASP:OD2	1:A:1104:TYR:OH	2.19	0.53
1:A:1070:ASN:ND2	1:A:1072:ILE:HG12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG23	1:A:234:TYR:HB2	1.92	0.51
1:A:58[A]:ARG:NH2	11:A:1828:HOH:O	2.44	0.51
1:A:710:CYS:HB3	1:A:800:GLN:HB2	1.93	0.51
1:A:935:ASP:OD2	1:A:939:ARG:NH2	2.44	0.50
1:A:173:LEU:O	1:A:177:ILE:HG22	2.11	0.50
1:A:30:LEU:HD11	1:A:1212:ILE:HD11	1.93	0.50
1:A:463:LEU:HD11	1:A:853:ILE:HG12	1.93	0.50
1:A:1339:GLU:OE1	11:A:1802:HOH:O	2.20	0.50
1:A:622:ARG:HH22	3:C:30:DC:H4'	1.77	0.49
1:A:899:SER:OG	9:A:1727:EDO:H11	2.12	0.49
1:A:902:PHE:HB2	1:A:927:ILE:HG13	1.93	0.49
2:B:34:C:H6	2:B:34:C:H5"	1.77	0.49
3:C:11:DC:H2'	3:C:12:DC:C6	2.47	0.49
1:A:12:LEU:HD11	1:A:1095[B]:PHE:CE1	2.48	0.49
1:A:659:HIS:HD2	11:B:246:HOH:O	1.95	0.48
1:A:356:LEU:HB2	1:A:438:LEU:HD23	1.94	0.48
2:B:66:U:H1'	2:B:67:U:OP2	2.14	0.48
1:A:47:SER:HB3	1:A:1225:VAL:HA	1.96	0.48
2:B:45:U:H2'	2:B:46:C:C6	2.49	0.47
1:A:1240:THR:HG22	1:A:1452:PHE:HZ	1.80	0.47
1:A:37:ASN:OD1	9:A:1725:EDO:O1	2.29	0.47
1:A:549:ASP:OD1	1:A:551:LEU:HB2	2.15	0.46
1:A:169:LYS:HD3	1:A:187:LEU:HD11	1.97	0.46
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.31	0.46
1:A:1070:ASN:HD22	1:A:1071:PRO:N	2.14	0.46
1:A:663[A]:GLN:HG3	2:B:81:G:H5"	1.96	0.46
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CE1	2.51	0.46
1:A:426:GLN:HE21	1:A:426:GLN:HB3	1.64	0.46
1:A:640:LYS:HE3	2:B:68:U:C6	2.51	0.46
1:A:1138:GLN:O	1:A:1142:LYS:HG2	2.16	0.45
1:A:150:GLN:OE1	1:A:152:SER:N	2.49	0.45
1:A:514:VAL:O	1:A:529:ASP:HA	2.17	0.45
9:B:119:EDO:H12	11:B:310:HOH:O	2.17	0.45
1:A:714:LEU:HG	1:A:718:LYS:HD2	1.98	0.45
3:C:21:DC:H2'	3:C:22:DT:C6	2.52	0.44
1:A:665:ARG:NH1	2:B:82:U:OP1	2.50	0.44
1:A:720:ASN:HD22	1:A:720:ASN:N	2.16	0.44
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	2.00	0.44
1:A:1047:ARG:HD2	2:B:1:G:C6	2.52	0.44
1:A:1326:GLU:HG2	11:A:1893:HOH:O	2.18	0.44
1:A:1608:ASN:HB2	3:C:3:DG:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:LYS:HG3	1:A:1491:GLU:HG2	2.00	0.44
1:A:985:ALA:HA	1:A:1061:ARG:HG2	2.00	0.44
1:A:452:ASN:HA	2:B:89:C:N3	2.33	0.43
1:A:856:ARG:HH21	1:A:856:ARG:HB3	1.84	0.43
1:A:1486:ASP:OD2	1:A:1489:LYS:HG2	2.17	0.43
1:A:1060:PHE:CE1	1:A:1076:VAL:HG22	2.54	0.43
2:B:2:G:H2'	2:B:3:G:C8	2.54	0.43
1:A:1592:GLU:HA	1:A:1595:LYS:HD3	2.00	0.43
1:A:727:LYS:HA	1:A:730:ILE:HG23	2.01	0.43
1:A:890:GLN:HA	1:A:1116:LYS:HB3	1.99	0.43
1:A:294:PHE:O	1:A:298:VAL:HG23	2.18	0.42
2:B:39:A:H2'	2:B:40:G:O4'	2.18	0.42
1:A:851:PRO:HB3	11:A:2130:HOH:O	2.19	0.42
1:A:51:LEU:HD11	1:A:912:LYS:HA	2.02	0.42
1:A:173:LEU:HD11	1:A:237:GLN:HG3	2.01	0.42
1:A:1046:TYR:CB	1:A:1079:ALA:HB1	2.50	0.42
1:A:1538:ASP:OD1	1:A:1538:ASP:N	2.53	0.42
1:A:1274:LYS:O	1:A:1285:GLN:HG2	2.19	0.41
1:A:1004:CYS:HA	1:A:1065:PHE:O	2.20	0.41
1:A:1374:LYS:HE2	11:A:2002:HOH:O	2.20	0.41
2:B:38:A:H2'	2:B:39:A:C8	2.55	0.41
1:A:111:TYR:O	1:A:293:HIS:HE1	2.03	0.41
1:A:780:LYS:HE3	1:A:784:ASP:OD2	2.21	0.41
1:A:724:LEU:HD22	1:A:728:ILE:HG13	2.03	0.41
1:A:731:ALA:HB2	1:A:739:GLU:HB3	2.02	0.41
1:A:1178:ARG:NH1	1:A:1188:ASP:O	2.54	0.41
1:A:1426:ASN:O	1:A:1428:LYS:HE2	2.21	0.40
1:A:451:ASP:OD2	11:A:1804:HOH:O	2.22	0.40
1:A:982:ASN:HD21	1:A:1085:ARG:NH2	2.18	0.40
1:A:1046:TYR:HB2	1:A:1079:ALA:HB1	2.02	0.40
1:A:130:ILE:HG23	1:A:134:TYR:CE2	2.57	0.40
1:A:1563:LEU:HD11	1:A:1600:ILE:HD11	2.03	0.40
2:B:89:C:H4'	9:B:121:EDO:H11	2.04	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:NH2	1:A:1260:GLU:OE2[2_445]	2.11	0.09

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	1444/1632 (88%)	1412 (98%)	30 (2%)	2 (0%)	51 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PHE
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	1260/1483 (85%)	1218 (97%)	42 (3%)	38 19

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	133	ASP
1	A	137	GLU
1	A	160	LYS
1	A	165	ILE
1	A	176	ASP
1	A	177	ILE
1	A	208	SER
1	A	211	THR

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Mol	Chain	Res	Type
1	A	214	PHE
1	A	249	ARG
1	A	257	ASP
1	A	310	ARG
1	A	426	GLN
1	A	435	ASP
1	A	551	LEU
1	A	626	LEU
1	A	686	LYS
1	A	723	LEU
1	A	724	LEU
1	A	730	ILE
1	A	791	ASN
1	A	853	ILE
1	A	856	ARG
1	A	939	ARG
1	A	982	ASN
1	A	1005	LEU
1	A	1006	ARG
1	A	1068	ASP
1	A	1070	ASN
1	A	1083	ARG
1	A	1145	SER
1	A	1176	GLU
1	A	1234	ASN
1	A	1398	PHE
1	A	1428	LYS
1	A	1511	ASN
1	A	1558	LYS
1	A	1570	ASP
1	A	1592	GLU
1	A	1594	LEU
1	A	1618	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	247	ASN
1	A	293	HIS
1	A	342	ASN
1	A	426	GLN

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Mol	Chain	Res	Type
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	720	ASN
1	A	725	ASN
1	A	938	ASN
1	A	982	ASN
1	A	1070	ASN
1	A	1148	GLN
1	A	1234	ASN
1	A	1236	HIS
1	A	1490	ASN
1	A	1578	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	92/94 (97%)	5 (5%)	2 (2%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	29	U
2	B	53	C
2	B	67	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 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 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	1725	-	3,3,3	0.49	0	2,2,2	0.37	0
9	EDO	B	114	-	3,3,3	0.50	0	2,2,2	0.33	0
9	EDO	B	117	-	3,3,3	0.44	0	2,2,2	0.52	0
9	EDO	B	115	-	3,3,3	0.52	0	2,2,2	0.12	0
9	EDO	A	1722	-	3,3,3	0.52	0	2,2,2	0.22	0
9	EDO	A	1726	-	3,3,3	0.50	0	2,2,2	0.15	0
9	EDO	A	1717	-	3,3,3	0.44	0	2,2,2	0.44	0
9	EDO	B	121	-	3,3,3	0.49	0	2,2,2	0.31	0
9	EDO	B	118	-	3,3,3	0.44	0	2,2,2	0.55	0
9	EDO	A	1721	-	3,3,3	0.38	0	2,2,2	0.53	0
9	EDO	A	1718	-	3,3,3	0.49	0	2,2,2	0.09	0
9	EDO	B	120	-	3,3,3	0.37	0	2,2,2	0.31	0
9	EDO	A	1724	-	3,3,3	0.54	0	2,2,2	0.11	0
9	EDO	B	111	-	3,3,3	0.54	0	2,2,2	0.40	0
9	EDO	B	116	-	3,3,3	0.53	0	2,2,2	0.09	0
9	EDO	B	119	-	3,3,3	0.50	0	2,2,2	0.06	0
10	ACT	A	1729	-	3,3,3	0.71	0	3,3,3	1.12	0
9	EDO	B	110	-	3,3,3	0.44	0	2,2,2	0.37	0
9	EDO	A	1716	-	3,3,3	0.40	0	2,2,2	0.40	0
9	EDO	A	1723	-	3,3,3	0.50	0	2,2,2	0.08	0
9	EDO	B	112	-	3,3,3	0.64	0	2,2,2	0.03	0
9	EDO	A	1719	-	3,3,3	0.63	0	2,2,2	0.28	0
10	ACT	A	1728	-	3,3,3	0.73	0	3,3,3	1.39	0
9	EDO	A	1727	-	3,3,3	0.36	0	2,2,2	0.59	0
9	EDO	A	1720	-	3,3,3	0.57	0	2,2,2	0.22	0
9	EDO	B	113	-	3,3,3	0.67	0	2,2,2	0.07	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	1725	-	-	1/1/1/1	-
9	EDO	B	114	-	-	0/1/1/1	-
9	EDO	B	117	-	-	0/1/1/1	-
9	EDO	B	115	-	-	0/1/1/1	-
9	EDO	A	1722	-	-	0/1/1/1	-
9	EDO	A	1726	-	-	1/1/1/1	-
9	EDO	A	1717	-	-	0/1/1/1	-
9	EDO	B	121	-	-	0/1/1/1	-
9	EDO	B	118	-	-	1/1/1/1	-
9	EDO	A	1721	-	-	1/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	B	120	-	-	0/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-
9	EDO	B	116	-	-	1/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	B	113	-	-	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	1726	EDO	O1-C1-C2-O2
9	B	116	EDO	O1-C1-C2-O2
9	A	1721	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2
9	B	118	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1725	EDO	2	0
9	B	121	EDO	1	0
9	A	1721	EDO	1	0
9	B	120	EDO	1	0
9	B	119	EDO	1	0
9	A	1727	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1455/1632 (89%)	0.66	232 (15%) 1 2	18, 45, 101, 143	0
2	B	93/94 (98%)	-0.26	0 100 100	19, 29, 58, 79	0
3	C	30/30 (100%)	-0.12	0 100 100	24, 51, 79, 115	0
4	D	9/9 (100%)	0.51	2 (22%) 0 0	36, 52, 110, 111	0
All	All	1587/1765 (89%)	0.59	234 (14%) 2 2	18, 44, 101, 143	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1066	LEU	12.9
1	A	1059	ALA	10.2
1	A	738	CYS	9.5
1	A	1053	THR	9.2
1	A	723	LEU	8.8
1	A	728	ILE	8.7
1	A	1060	PHE	8.6
1	A	131	PHE	8.2
1	A	981	LEU	8.1
1	A	1050	ILE	8.0
1	A	1071	PRO	7.9
1	A	980	THR	7.9
1	A	1072	ILE	7.6
1	A	261	ILE	7.3
1	A	1077	ILE	7.3
1	A	1052	LEU	7.3
1	A	264	PHE	7.2
1	A	943	PHE	7.1
1	A	1065	PHE	6.8
1	A	1063	ALA	6.8
1	A	1005	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	236	ILE	6.4
1	A	940	ILE	6.3
1	A	127	LEU	6.1
1	A	972	PRO	6.1
1	A	1057	GLN	6.1
1	A	743	PHE	6.1
1	A	1573	ILE	6.0
1	A	1069	GLU	6.0
1	A	429	THR	6.0
1	A	295	VAL	5.9
1	A	259	LEU	5.9
1	A	1002	ILE	5.9
1	A	742	ILE	5.8
1	A	1064	LEU	5.8
1	A	1074	GLN	5.8
1	A	1619	LEU	5.8
1	A	1004	CYS	5.7
1	A	1542	ILE	5.7
1	A	730	ILE	5.7
1	A	175	THR	5.7
1	A	1068	ASP	5.6
1	A	187	LEU	5.6
1	A	967	LEU	5.6
1	A	130	ILE	5.6
1	A	123	VAL	5.5
1	A	256	THR	5.5
1	A	168	PHE	5.5
1	A	177	ILE	5.3
1	A	1049	PHE	5.3
1	A	985	ALA	5.3
1	A	1046	TYR	5.3
1	A	724	LEU	5.2
1	A	988	ILE	5.2
1	A	1622	ILE	5.1
1	A	1054	PRO	5.1
1	A	111	TYR	5.0
1	A	855	THR	5.0
1	A	128	MET	4.9
1	A	266	PHE	4.8
1	A	973	ARG	4.8
1	A	1073	LYS	4.8
1	A	1537	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	747	CYS	4.7
1	A	134	TYR	4.7
1	A	720	ASN	4.7
1	A	136	GLY	4.6
1	A	843	LEU	4.6
1	A	1006	ARG	4.5
1	A	1055	GLN	4.5
1	A	293	HIS	4.4
1	A	186	THR	4.4
1	A	989	CYS	4.4
1	A	258	ASP	4.4
1	A	1539	LEU	4.4
1	A	746	ILE	4.4
1	A	1067	ALA	4.3
1	A	1061	ARG	4.3
1	A	1621	GLY	4.3
1	A	133	ASP	4.3
1	A	135	ASN	4.3
1	A	1488	SER	4.2
1	A	1076	VAL	4.2
1	A	125	ALA	4.1
1	A	126	ILE	4.1
1	A	165	ILE	4.1
1	A	982	ASN	4.1
1	A	1003	PHE	4.1
1	A	1541	ASP	4.1
1	A	146	LEU	4.0
1	A	987	LEU	4.0
1	A	1156	PRO	4.0
1	A	1155	LYS	3.9
1	A	778	ALA	3.8
1	A	1544	ILE	3.8
1	A	257	ASP	3.8
1	A	933	PHE	3.8
1	A	188	LYS	3.8
1	A	1543	GLY	3.7
1	A	1095[A]	PHE	3.7
1	A	729	ASN	3.7
1	A	1082	ASN	3.7
1	A	929	PRO	3.6
1	A	294	PHE	3.6
1	A	291	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	721	ARG	3.6
1	A	1567	ILE	3.6
1	A	731	ALA	3.6
1	A	1575	TYR	3.6
1	A	745	LEU	3.6
1	A	1153	GLY	3.6
1	A	733	ASN	3.5
1	A	932	ILE	3.5
1	A	1062	HIS	3.5
1	A	739	GLU	3.5
1	A	1154	ASP	3.4
1	A	759	TYR	3.4
1	A	1565	TYR	3.4
1	A	716	ILE	3.4
1	A	143	TYR	3.4
1	A	990	VAL	3.4
1	A	986	ASN	3.4
1	A	969	HIS	3.3
1	A	939	ARG	3.3
4	D	9	DG	3.3
1	A	1056	GLU	3.3
1	A	112	SER	3.2
1	A	1571	SER	3.2
1	A	211	THR	3.2
1	A	1078	ARG	3.2
1	A	1191	TYR	3.2
1	A	1070	ASN	3.1
1	A	1000	ASN	3.1
1	A	260	ASP	3.1
1	A	734	THR	3.1
1	A	829	LYS	3.1
1	A	1194	TYR	3.1
1	A	999	GLY	3.1
1	A	174	CYS	3.1
1	A	902	PHE	3.1
1	A	1083	ARG	3.1
1	A	298	VAL	3.1
1	A	296	PHE	3.0
1	A	722	GLY	3.0
1	A	1142	LYS	3.0
1	A	732	ARG	3.0
1	A	254	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1001	ARG	3.0
1	A	1536	PRO	3.0
1	A	1075	ALA	2.9
1	A	1487	ILE	2.9
1	A	928	SER	2.9
1	A	203	ALA	2.9
1	A	151	GLU	2.9
1	A	200	ASP	2.9
1	A	781	PRO	2.9
1	A	785	ARG	2.8
1	A	842	ILE	2.8
1	A	1570	ASP	2.8
1	A	971	ILE	2.8
1	A	30	LEU	2.8
1	A	173	LEU	2.8
1	A	1576	PHE	2.8
1	A	1594	LEU	2.8
1	A	262	TRP	2.8
1	A	171	MET	2.7
1	A	1080	ILE	2.7
1	A	783	PHE	2.7
1	A	235	ASN	2.7
1	A	33	LEU	2.7
1	A	214	PHE	2.7
1	A	735	LYS	2.6
1	A	740	LYS	2.6
1	A	1187	ILE	2.6
1	A	138	ASP	2.6
1	A	241	LYS	2.6
1	A	935	ASP	2.6
1	A	853	ILE	2.6
1	A	178	LYS	2.6
1	A	516	TYR	2.6
1	A	176	ASP	2.6
1	A	1007	ASP	2.6
1	A	830	ILE	2.6
1	A	253	THR	2.6
1	A	124	LYS	2.6
1	A	741	GLU	2.6
1	A	1563	LEU	2.6
1	A	156	GLU	2.5
1	A	1566	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLN	2.5
1	A	930	GLU	2.5
1	A	428	VAL	2.5
1	A	639	HIS	2.5
1	A	166	LEU	2.5
1	A	152	SER	2.4
1	A	265	ASN	2.4
1	A	736	GLY	2.4
1	A	726	HIS	2.4
1	A	1209	PHE	2.4
1	A	255	LEU	2.3
1	A	1523	PHE	2.3
1	A	1540	ARG	2.3
1	A	292	HIS	2.3
1	A	141	ASP	2.3
1	A	252	ASP	2.3
1	A	147	ALA	2.3
1	A	966	GLU	2.3
1	A	263	ASN	2.3
1	A	1599	ILE	2.3
1	A	1574	ASN	2.3
1	A	1192	SER	2.2
1	A	65	ILE	2.2
1	A	637	LYS	2.2
1	A	782	GLU	2.2
1	A	234	TYR	2.2
1	A	1143	VAL	2.2
1	A	1	MET	2.2
1	A	793	ILE	2.2
1	A	109	ASP	2.2
1	A	1618	LYS	2.2
1	A	1595	LYS	2.2
1	A	142	SER	2.1
1	A	179	ASP	2.1
4	D	8	DG	2.1
1	A	160	LYS	2.1
1	A	1620	ALA	2.1
1	A	1598	THR	2.1
1	A	828	ILE	2.1
1	A	201	TYR	2.0
1	A	297	ALA	2.0
1	A	1534	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	854	PRO	2.0
1	A	430	LYS	2.0
1	A	919	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	B	119	4/4	0.49	0.28	63,65,69,70	0
9	EDO	A	1727	4/4	0.77	0.36	81,81,82,83	0
6	NA	A	1703	1/1	0.78	0.10	63,63,63,63	0
9	EDO	A	1726	4/4	0.78	0.17	83,85,85,85	0
9	EDO	B	121	4/4	0.85	0.22	56,59,61,62	0
9	EDO	A	1724	4/4	0.87	0.12	45,47,48,50	0
9	EDO	B	115	4/4	0.89	0.15	47,51,52,56	0
9	EDO	A	1719	4/4	0.90	0.12	30,36,37,38	0
9	EDO	B	120	4/4	0.90	0.11	50,51,55,57	0
9	EDO	A	1720	4/4	0.90	0.13	33,34,36,38	0
9	EDO	A	1725	4/4	0.92	0.12	42,45,51,57	0
9	EDO	A	1721	4/4	0.92	0.11	45,46,47,49	0
9	EDO	B	116	4/4	0.92	0.11	39,43,48,50	0
9	EDO	B	114	4/4	0.94	0.09	34,40,42,44	0
8	CA	A	1712	1/1	0.94	0.11	72,72,72,72	0
9	EDO	B	117	4/4	0.95	0.16	34,46,52,55	0
9	EDO	B	118	4/4	0.95	0.10	45,54,58,58	0
8	CA	B	104	1/1	0.95	0.04	67,67,67,67	0
9	EDO	A	1723	4/4	0.95	0.12	45,45,49,52	0
8	CA	B	108	1/1	0.95	0.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	ACT	A	1728	4/4	0.95	0.15	82,84,84,85	0
8	CA	A	1711	1/1	0.96	0.04	75,75,75,75	0
8	CA	A	1713	1/1	0.96	0.10	82,82,82,82	0
9	EDO	B	111	4/4	0.96	0.10	30,32,32,36	0
9	EDO	A	1716	4/4	0.96	0.12	39,45,45,47	0
10	ACT	A	1729	4/4	0.96	0.07	35,35,36,37	0
8	CA	A	1715	1/1	0.97	0.07	54,54,54,54	0
9	EDO	A	1722	4/4	0.97	0.11	28,34,39,43	0
9	EDO	A	1717	4/4	0.97	0.12	37,42,46,48	0
9	EDO	A	1718	4/4	0.97	0.07	32,37,38,38	0
8	CA	A	1710	1/1	0.97	0.07	47,47,47,47	0
6	NA	A	1702	1/1	0.97	0.04	47,47,47,47	0
8	CA	B	109	1/1	0.98	0.07	70,70,70,70	0
8	CA	A	1714	1/1	0.98	0.14	69,69,69,69	0
7	CL	A	1704	1/1	0.98	0.05	43,43,43,43	0
8	CA	A	1706	1/1	0.98	0.05	67,67,67,67	0
8	CA	B	106	1/1	0.98	0.06	44,44,44,44	0
8	CA	B	107	1/1	0.98	0.08	64,64,64,64	0
9	EDO	B	110	4/4	0.98	0.07	31,32,35,37	0
6	NA	B	102	1/1	0.98	0.15	59,59,59,59	0
9	EDO	B	112	4/4	0.98	0.14	23,24,24,26	0
9	EDO	B	113	4/4	0.98	0.11	29,29,31,33	0
8	CA	A	1709	1/1	0.99	0.05	49,49,49,49	0
7	CL	A	1705	1/1	0.99	0.07	28,28,28,28	0
8	CA	B	103	1/1	0.99	0.04	33,33,33,33	0
6	NA	B	101	1/1	0.99	0.07	28,28,28,28	0
8	CA	B	105	1/1	0.99	0.06	35,35,35,35	0
8	CA	A	1707	1/1	0.99	0.03	36,36,36,36	0
8	CA	A	1708	1/1	0.99	0.04	47,47,47,47	0
5	ZN	A	1701	1/1	1.00	0.11	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.