



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:13 PM UTC

PDB ID : 6JFU / pdb_00006jfu
Title : Crystal structure of Nme2Cas9 in complex with sgRNA and target DNA (AG-GCCC PAM)
Authors : Sun, W.; Yang, J.; Cheng, Z.; Liu, C.; Wang, K.; Huang, X.; Wang, Y.
Deposited on : 2019-02-12
Resolution : 3.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

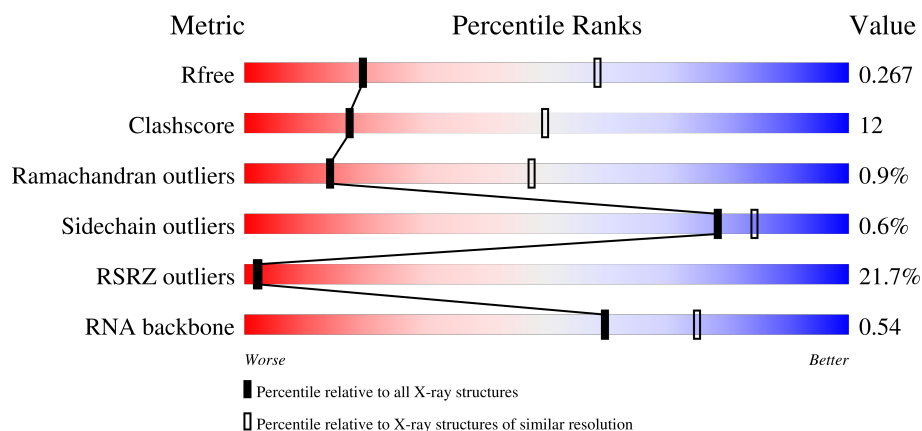
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1083	20% 63% 17% • 18%
2	B	135	2% 30% 41% 7% 22%
3	C	35	49% 51%
4	D	11	45% 55%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9476 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	884	Total	C	N	O	S	0	0	0
			6312	3968	1167	1156	21			

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	P	0	0	0
			2214	990	375	744	105			

- Molecule 3 is a DNA chain called target-strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	P	0	0	0
			720	344	139	203	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			222	107	43	62	10			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

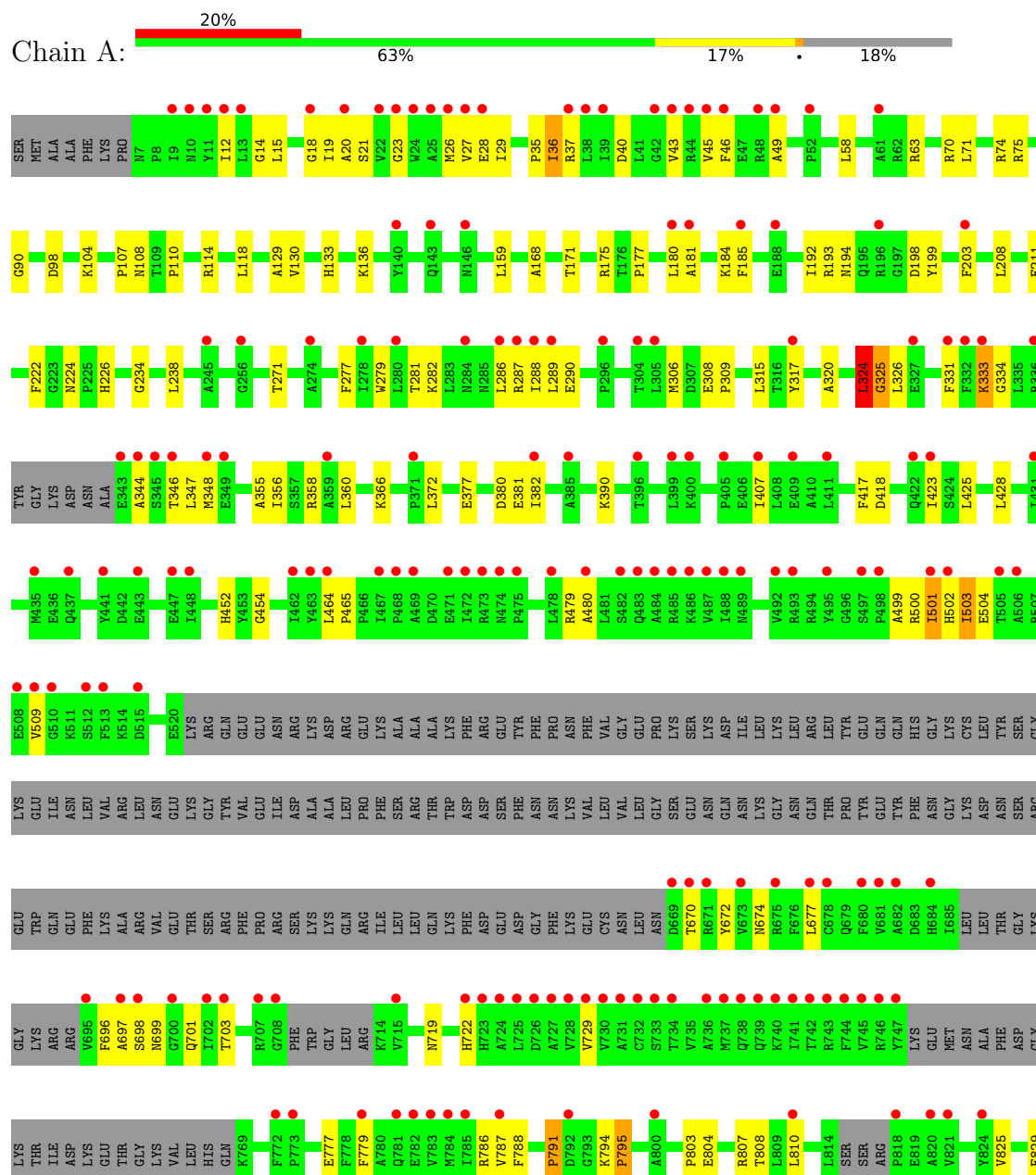


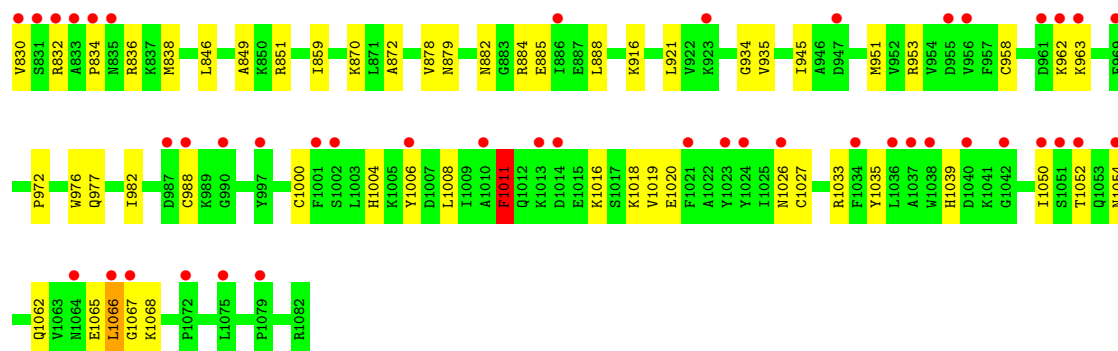
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

3 Residue-property plots

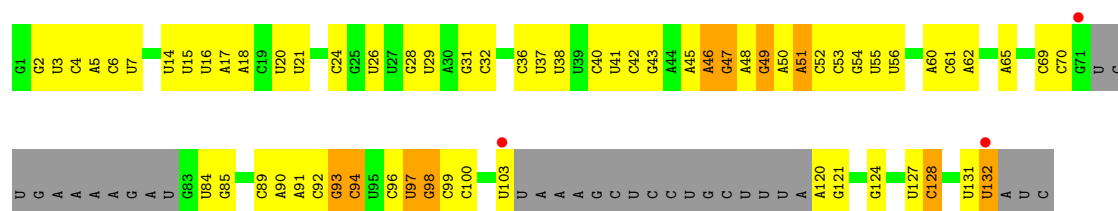
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

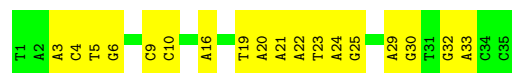




• Molecule 2: sgRNA



• Molecule 3: target-strand DNA



• Molecule 4: non-target strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	153.48Å 166.93Å 179.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 3.20 48.68 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.1 (48.68-3.20) 83.0 (48.68-3.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.254 , 0.271 0.255 , 0.267	Depositor DCC
R_{free} test set	1529 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9476	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/6418	0.52	9/8719 (0.1%)
2	B	0.12	0/2466	0.32	0/3831
3	C	0.20	0/810	0.40	0/1250
4	D	0.19	0/249	0.40	0/383
All	All	0.21	0/9943	0.46	9/14183 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	795	PRO	N-CA-CB	9.31	113.02	103.25
1	A	333	LYS	N-CA-C	8.43	122.73	110.42
1	A	326	LEU	N-CA-C	6.97	115.44	108.75
1	A	791	PRO	N-CA-CB	6.80	110.39	103.25
1	A	1011	PHE	N-CA-C	6.52	119.56	109.07
1	A	794	LYS	CA-C-N	5.96	127.30	119.84
1	A	794	LYS	C-N-CA	5.96	127.30	119.84
1	A	325	GLY	N-CA-C	5.78	126.88	113.18
1	A	324	LEU	N-CA-C	5.55	122.62	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6312	0	5675	156	0
2	B	2214	0	1128	51	0
3	C	720	0	392	23	0
4	D	222	0	122	3	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
All	All	9476	0	7329	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (210) 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:289:LEU:HA	1:A:331:PHE:CB	1.27	1.64
1:A:503:ILE:HG22	1:A:696:PHE:O	1.31	1.23
1:A:289:LEU:CA	1:A:331:PHE:CB	2.21	1.17
1:A:290:GLU:H	1:A:331:PHE:HA	1.12	1.13
1:A:503:ILE:HG21	1:A:697:ALA:CA	1.80	1.10
1:A:503:ILE:HG23	1:A:698:SER:H	1.12	1.08
1:A:503:ILE:CG2	1:A:698:SER:H	1.68	1.06
1:A:503:ILE:CG2	1:A:697:ALA:HA	1.87	1.04
1:A:290:GLU:H	1:A:331:PHE:CA	1.75	0.97
1:A:1011:PHE:HB2	1:A:1020:GLU:O	1.66	0.95
1:A:503:ILE:CG2	1:A:696:PHE:O	2.15	0.95
1:A:1011:PHE:HB3	1:A:1020:GLU:HB2	1.49	0.94
1:A:14:GLY:HA2	1:A:502:HIS:CB	2.00	0.91
1:A:503:ILE:HG21	1:A:697:ALA:HA	0.94	0.90
1:A:290:GLU:N	1:A:331:PHE:HA	1.89	0.87
1:A:15:LEU:H	1:A:502:HIS:CB	1.91	0.84
1:A:958:CYS:N	1:A:1000:CYS:SG	2.54	0.81
1:A:503:ILE:CG2	1:A:698:SER:N	2.43	0.81
1:A:288:ILE:CB	1:A:333:LYS:HB2	2.14	0.77
2:B:99:C:O2	2:B:124:G:N2	2.13	0.75
1:A:804:GLU:HA	1:A:807:ARG:HE	1.54	0.72
2:B:99:C:N3	2:B:124:G:N1	2.33	0.71
1:A:12:ILE:HG13	1:A:27:VAL:HG23	1.73	0.69
1:A:1052:THR:HG21	3:C:4:DC:OP2	1.91	0.69
1:A:15:LEU:N	1:A:502:HIS:CB	2.57	0.67
1:A:503:ILE:HG23	1:A:698:SER:N	1.97	0.67
1:A:12:ILE:HG22	1:A:499:ALA:HB3	1.77	0.66
1:A:878:VAL:O	1:A:882:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:MET:HE1	1:A:1027:CYS:HB3	1.77	0.66
1:A:114:ARG:NH2	1:A:211:GLU:OE1	2.26	0.66
1:A:159:LEU:HG	3:C:16:DA:H5''	1.78	0.65
1:A:672:TYR:HA	3:C:23:DT:H4'	1.77	0.65
1:A:309:PRO:HD3	1:A:315:LEU:HD22	1.77	0.65
1:A:884:ARG:NH2	2:B:53:C:O2	2.29	0.65
1:A:1052:THR:CG2	3:C:4:DC:OP2	2.45	0.65
1:A:14:GLY:CA	1:A:502:HIS:CB	2.74	0.64
1:A:703:THR:O	1:A:729:VAL:HG11	1.97	0.64
1:A:962:LYS:HG3	1:A:963:LYS:H	1.63	0.64
1:A:355:ALA:HA	1:A:358:ARG:HE	1.61	0.63
1:A:838:MET:HE1	1:A:953:ARG:HD3	1.80	0.63
1:A:1011:PHE:CB	1:A:1020:GLU:O	2.45	0.62
1:A:1011:PHE:CB	1:A:1020:GLU:HB2	2.25	0.62
1:A:346:THR:O	1:A:348:MET:N	2.28	0.62
1:A:390:LYS:NZ	1:A:417:PHE:O	2.32	0.62
1:A:870:LYS:HE2	1:A:872:ALA:HB3	1.82	0.61
1:A:701:GLN:OE1	1:A:701:GLN:N	2.33	0.61
1:A:846:LEU:O	2:B:26:U:O2'	2.18	0.61
2:B:51:A:H2'	2:B:52:C:C6	2.36	0.61
1:A:282:LYS:O	1:A:286:LEU:HB2	2.01	0.60
1:A:851:ARG:HD2	1:A:859:ILE:HD11	1.84	0.60
2:B:90:A:H2'	2:B:91:A:C8	2.36	0.60
1:A:118:LEU:HD13	1:A:175:ARG:HD2	1.84	0.60
1:A:503:ILE:HG13	1:A:504:GLU:N	2.15	0.60
1:A:503:ILE:HG23	1:A:503:ILE:O	2.02	0.59
1:A:28:GLU:O	1:A:36:ILE:N	2.36	0.58
1:A:670:THR:HA	3:C:24:DA:H4'	1.86	0.57
1:A:934:GLY:HA3	1:A:945:ILE:HD11	1.86	0.57
4:D:6:DC:H2''	4:D:7:DA:C8	2.39	0.57
1:A:1054:ASN:HD22	3:C:3:DA:H5'	1.68	0.57
1:A:803:PRO:O	1:A:807:ARG:HG3	2.04	0.57
1:A:500:ARG:O	1:A:501:ILE:O	2.22	0.57
1:A:181:ALA:HA	1:A:184:LYS:HG2	1.86	0.56
2:B:96:C:N3	2:B:128:C:O2'	2.36	0.56
1:A:49:ALA:HB2	1:A:479:ARG:HD2	1.88	0.56
2:B:97:U:O2'	2:B:98:G:OP1	2.22	0.56
1:A:63:ARG:NH2	2:B:18:A:OP2	2.32	0.55
1:A:177:PRO:HG2	1:A:208:LEU:HD12	1.89	0.54
3:C:23:DT:H2'	3:C:24:DA:H8	1.70	0.54
2:B:97:U:H2'	2:B:98:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:PRO:HD3	1:A:988:CYS:SG	2.48	0.54
2:B:49:G:H2'	2:B:50:A:H8	1.73	0.54
1:A:333:LYS:O	1:A:334:GLY:C	2.48	0.53
3:C:21:DA:H2'	3:C:22:DA:H8	1.73	0.53
1:A:1066:LEU:O	1:A:1068:LYS:N	2.41	0.53
1:A:1054:ASN:ND2	3:C:3:DA:H5'	2.24	0.53
1:A:360:LEU:HD11	1:A:407:ILE:HG22	1.90	0.53
1:A:884:ARG:NH1	2:B:36:C:O2	2.42	0.53
1:A:346:THR:C	1:A:348:MET:H	2.16	0.53
1:A:37:ARG:HA	1:A:779:PHE:CE2	2.44	0.52
1:A:133:HIS:CD2	2:B:60:A:H5''	2.44	0.52
1:A:324:LEU:CD2	1:A:324:LEU:N	2.73	0.52
1:A:423:ILE:HG23	1:A:428:LEU:HG	1.91	0.52
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.91	0.52
1:A:180:LEU:HD23	1:A:203:PHE:HE1	1.75	0.51
1:A:503:ILE:CG2	1:A:697:ALA:CA	2.64	0.51
1:A:324:LEU:CD2	1:A:324:LEU:H	2.24	0.51
1:A:719:ASN:HA	1:A:722:HIS:HB3	1.91	0.51
2:B:4:C:H2'	2:B:5:A:C8	2.46	0.51
2:B:4:C:H2'	2:B:5:A:H8	1.76	0.51
3:C:22:DA:H2'	3:C:23:DT:C6	2.46	0.51
3:C:5:DT:H2''	3:C:6:DG:C8	2.46	0.51
2:B:93:G:H2'	2:B:94:C:C6	2.46	0.50
1:A:43:VAL:HG23	1:A:830:VAL:HA	1.93	0.50
1:A:1026:ASN:HB2	1:A:1035:TYR:HB2	1.92	0.50
2:B:99:C:H2'	2:B:100:C:C6	2.47	0.50
1:A:962:LYS:HG3	1:A:963:LYS:N	2.26	0.49
2:B:61:C:H2'	2:B:62:A:H8	1.77	0.49
1:A:1050:ILE:O	1:A:1050:ILE:HD12	2.13	0.49
3:C:23:DT:H2'	3:C:24:DA:C8	2.47	0.49
2:B:54:G:H2'	2:B:55:U:O4'	2.12	0.49
1:A:320:ALA:O	1:A:324:LEU:CD2	2.61	0.49
2:B:3:U:H2'	2:B:4:C:C6	2.47	0.49
3:C:21:DA:H2'	3:C:22:DA:C8	2.47	0.49
1:A:308:GLU:N	1:A:309:PRO:HD2	2.28	0.48
1:A:279:TRP:HB2	1:A:348:MET:HE2	1.95	0.48
1:A:418:ASP:OD1	1:A:418:ASP:N	2.45	0.48
1:A:786:ARG:HD2	1:A:825:VAL:HG21	1.95	0.48
1:A:46:PHE:CE2	1:A:480:ALA:HA	2.49	0.48
1:A:98:ASP:HA	1:A:104:LYS:HE2	1.96	0.48
1:A:290:GLU:H	1:A:331:PHE:CB	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLU:O	1:A:808:THR:HG23	2.13	0.48
2:B:31:G:H2'	2:B:32:C:C6	2.49	0.48
2:B:5:A:H2'	2:B:6:C:H6	1.79	0.47
1:A:977:GLN:HG2	1:A:982:ILE:HD11	1.97	0.47
3:C:24:DA:H2'	3:C:25:DG:H8	1.79	0.47
1:A:290:GLU:N	1:A:331:PHE:CA	2.59	0.47
2:B:28:G:H2'	2:B:29:U:C6	2.49	0.47
3:C:22:DA:H2'	3:C:23:DT:H6	1.80	0.47
3:C:32:DG:H2'	3:C:33:DA:C8	2.50	0.47
2:B:60:A:H2'	2:B:61:C:C6	2.50	0.47
1:A:23:GLY:HA3	1:A:43:VAL:HG12	1.96	0.46
1:A:70:ARG:O	1:A:74:ARG:HG3	2.15	0.46
1:A:234:GLY:O	1:A:238:LEU:HD23	2.15	0.46
3:C:9:DC:H2'	3:C:10:DC:C6	2.51	0.46
2:B:6:C:H2'	2:B:7:U:C6	2.50	0.46
4:D:10:DT:H2''	4:D:11:DA:C8	2.51	0.46
2:B:91:A:H2'	2:B:92:C:C6	2.51	0.46
1:A:834:PRO:HA	1:A:1006:TYR:HB2	1.96	0.46
1:A:74:ARG:NH2	2:B:20:U:OP1	2.36	0.46
1:A:193:ARG:HB3	2:B:24:C:OP1	2.17	0.45
1:A:177:PRO:HD2	1:A:211:GLU:HB2	1.97	0.45
1:A:271:THR:HG21	1:A:425:LEU:HD21	1.97	0.45
1:A:699:ASN:O	1:A:703:THR:N	2.50	0.45
1:A:921:LEU:O	2:B:56:U:O2'	2.34	0.45
1:A:286:LEU:O	1:A:288:ILE:N	2.50	0.45
1:A:317:TYR:HB2	1:A:344:ALA:HB1	1.99	0.45
1:A:849:ALA:HB2	1:A:945:ILE:HB	1.98	0.45
1:A:45:VAL:HG22	1:A:832:ARG:HA	1.99	0.45
1:A:888:LEU:HD22	1:A:916:LYS:HE2	1.98	0.45
1:A:935:VAL:HG22	1:A:976:TRP:CE2	2.51	0.45
1:A:1018:LYS:HG2	1:A:1019:VAL:H	1.80	0.45
1:A:324:LEU:HD23	1:A:325:GLY:H	1.82	0.45
1:A:1016:LYS:HA	1:A:1016:LYS:HD3	1.68	0.45
1:A:277:PHE:O	1:A:281:THR:OG1	2.32	0.45
1:A:45:VAL:HG21	1:A:832:ARG:HD2	1.98	0.44
1:A:279:TRP:HE1	1:A:306:MET:HG2	1.82	0.44
1:A:289:LEU:HD23	1:A:331:PHE:CB	2.46	0.44
1:A:829:PHE:HB2	1:A:1039:HIS:HB3	1.99	0.44
1:A:287:ARG:HH22	3:C:29:DA:H4'	1.82	0.44
2:B:97:U:H2'	2:B:98:G:H8	1.82	0.44
2:B:98:G:H2'	2:B:99:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:U:OP2	2:B:132:U:H3'	2.17	0.44
1:A:674:ASN:HB3	1:A:677:LEU:HB3	1.99	0.44
1:A:37:ARG:HA	1:A:779:PHE:HE2	1.81	0.44
1:A:74:ARG:NH1	2:B:21:U:OP2	2.51	0.44
1:A:114:ARG:HG3	1:A:130:VAL:HG22	1.99	0.44
1:A:168:ALA:O	1:A:171:THR:HG22	2.18	0.44
1:A:851:ARG:HH22	1:A:878:VAL:HG13	1.82	0.44
4:D:1:DA:H2'	4:D:2:DG:C8	2.53	0.44
1:A:19:ILE:HB	1:A:509:VAL:HA	2.00	0.44
2:B:6:C:H2'	2:B:7:U:H6	1.81	0.44
1:A:12:ILE:HG13	1:A:27:VAL:CG2	2.43	0.43
1:A:366:LYS:CB	1:A:372:LEU:HD21	2.48	0.43
1:A:879:ASN:ND2	1:A:885:GLU:OE1	2.42	0.43
3:C:23:DT:C2	3:C:24:DA:C8	3.06	0.43
1:A:953:ARG:NH1	2:B:127:U:O4	2.51	0.43
1:A:58:LEU:HD12	1:A:58:LEU:H	1.82	0.43
1:A:777:GLU:HB3	1:A:779:PHE:CE2	2.53	0.43
2:B:16:U:H2'	2:B:17:A:C8	2.54	0.43
2:B:37:U:H2'	2:B:38:U:O4'	2.18	0.43
1:A:787:VAL:HG23	1:A:788:PHE:CD2	2.54	0.43
1:A:198:ASP:OD1	1:A:199:TYR:N	2.48	0.43
1:A:1008:LEU:O	1:A:1062:GLN:CB	2.67	0.43
2:B:131:U:H3'	2:B:132:U:H5'	2.00	0.43
1:A:63:ARG:HD3	2:B:18:A:OP2	2.19	0.43
1:A:290:GLU:N	1:A:331:PHE:CB	2.81	0.42
1:A:185:PHE:CD1	1:A:192:ILE:HG13	2.55	0.42
1:A:377:GLU:O	1:A:381:GLU:HG3	2.19	0.42
1:A:503:ILE:HG21	1:A:697:ALA:C	2.40	0.42
1:A:356:ILE:HD13	1:A:382:ILE:HD11	2.01	0.42
2:B:41:U:H2'	2:B:42:C:C6	2.55	0.42
2:B:46:A:HO2'	2:B:47:G:P	2.43	0.42
1:A:90:GLY:O	1:A:226:HIS:NE2	2.53	0.42
1:A:452:HIS:C	1:A:454:GLY:H	2.28	0.42
1:A:1033:ARG:HD2	3:C:5:DT:H72	2.02	0.42
1:A:271:THR:HG23	1:A:380:ASP:HA	2.02	0.42
2:B:92:C:H2'	2:B:93:G:C8	2.55	0.42
1:A:324:LEU:H	1:A:324:LEU:HD23	1.84	0.42
1:A:836:ARG:HG3	1:A:1004:HIS:CG	2.54	0.42
1:A:107:PRO:HD2	1:A:129:ALA:HB2	2.01	0.42
2:B:41:U:H2'	2:B:42:C:H6	1.85	0.41
1:A:287:ARG:HH12	3:C:30:DG:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:U:H2'	2:B:15:U:C6	2.55	0.41
1:A:194:ASN:HB2	2:B:24:C:O5'	2.21	0.41
2:B:99:C:H2'	2:B:100:C:H6	1.86	0.41
3:C:19:DT:H2'	3:C:20:DA:C8	2.55	0.41
1:A:75:ARG:NH1	1:A:136:LYS:O	2.54	0.41
2:B:40:C:H2'	2:B:41:U:C6	2.56	0.41
1:A:222:PHE:O	1:A:224:ASN:N	2.47	0.41
2:B:92:C:H2'	2:B:93:G:H8	1.85	0.41
1:A:108:ASN:C	1:A:110:PRO:HD3	2.45	0.41
1:A:20:ALA:C	1:A:46:PHE:HB2	2.46	0.41
1:A:26:MET:HB2	1:A:40:ASP:H	1.84	0.41
1:A:810:LEU:HA	1:A:810:LEU:HD23	1.79	0.41
1:A:18:GLY:N	1:A:21:SER:O	2.54	0.40
1:A:29:ILE:HA	1:A:35:PRO:HA	2.03	0.40
2:B:14:U:H2'	2:B:15:U:H6	1.86	0.40
1:A:71:LEU:HD11	2:B:21:U:C5	2.57	0.40
2:B:93:G:HO2'	2:B:94:C:P	2.44	0.40
3:C:32:DG:H2'	3:C:33:DA:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	870/1083 (80%)	771 (89%)	91 (10%)	8 (1%)	14 47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ILE
1	A	795	PRO
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	1065	GLU
1	A	1067	GLY
1	A	791	PRO
1	A	1066	LEU
1	A	36	ILE

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	537/935 (57%)	534 (99%)	3 (1%)	78 84

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

Mol	Chain	Res	Type
1	A	324	LEU
1	A	503	ILE
1	A	1011	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	270	ASN
1	A	452	HIS
1	A	1054	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	103/135 (76%)	20 (19%)	4 (3%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	43	G
2	B	45	A
2	B	47	G
2	B	48	A
2	B	49	G
2	B	51	A
2	B	65	A
2	B	69	C
2	B	70	C
2	B	84	U
2	B	85	G
2	B	89	C
2	B	94	C
2	B	97	U
2	B	98	G
2	B	103	U
2	B	121	G
2	B	128	C
2	B	132	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	46	A
2	B	93	G
2	B	97	U
2	B	120	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
5	EDO	C	101	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	B	201	-	3,3,3	0.43	0	2,2,2	0.38	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
5	EDO	C	101	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	884/1083 (81%)	1.30	222 (25%)  	15, 77, 146, 189	0
2	B	105/135 (77%)	0.32	3 (2%)  	16, 60, 172, 215	0
3	C	35/35 (100%)	0.32	0  	27, 49, 80, 86	0
4	D	11/11 (100%)	0.29	0  	38, 49, 68, 79	0
All	All	1035/1264 (81%)	1.16	225 (21%)  	15, 71, 150, 215	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	LEU	7.1
1	A	669	ASP	6.7
1	A	462	ILE	6.6
1	A	733	SER	6.6
1	A	724	ALA	6.2
1	A	407	ILE	6.2
1	A	726	ASP	5.9
1	A	739	GLN	5.9
1	A	728	VAL	5.6
1	A	27	VAL	5.5
1	A	723	HIS	5.5
1	A	781	GLN	5.4
1	A	488	ILE	5.4
1	A	743	ARG	5.3
1	A	1023	TYR	5.0
1	A	832	ARG	4.8
1	A	24	TRP	4.8
1	A	745	VAL	4.8
1	A	732	CYS	4.6
1	A	18	GLY	4.6
1	A	830	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	670	THR	4.5
1	A	742	THR	4.2
1	A	810	LEU	4.2
1	A	46	PHE	4.2
1	A	833	ALA	4.2
1	A	1013	LYS	4.2
1	A	831	SER	4.1
1	A	1052	THR	4.1
1	A	818	PRO	4.0
1	A	746	ARG	4.0
1	A	1034	PHE	4.0
1	A	463	TYR	4.0
1	A	343	GLU	4.0
1	A	782	GLU	4.0
1	A	10	ASN	3.9
1	A	1064	ASN	3.9
1	A	505	THR	3.9
1	A	684	HIS	3.9
1	A	49	ALA	3.9
1	A	1036	LEU	3.8
1	A	740	LYS	3.8
1	A	772	PHE	3.8
1	A	727	ALA	3.7
1	A	48	ARG	3.7
1	A	747	TYR	3.7
1	A	988	CYS	3.7
1	A	52	PRO	3.6
1	A	487	VAL	3.6
1	A	783	VAL	3.6
1	A	509	VAL	3.6
1	A	44	ARG	3.6
1	A	497	SER	3.6
1	A	317	TYR	3.5
1	A	396	THR	3.4
1	A	702	ILE	3.4
1	A	961	ASP	3.4
1	A	731	ALA	3.4
1	A	196	ARG	3.3
1	A	483	GLN	3.3
1	A	485	ARG	3.3
1	A	675	ARG	3.3
1	A	1054	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	3.3
1	A	1021	PHE	3.3
1	A	471	GLU	3.3
1	A	741	ILE	3.3
1	A	820	ALA	3.3
1	A	331	PHE	3.3
1	A	698	SER	3.2
1	A	26	MET	3.2
1	A	1037	ALA	3.2
1	A	349	GLU	3.2
1	A	140	TYR	3.2
1	A	513	PHE	3.2
1	A	489	ASN	3.2
1	A	435	MET	3.2
1	A	737	MET	3.1
1	A	469	ALA	3.1
1	A	359	ALA	3.1
1	A	682	ALA	3.1
1	A	25	ALA	3.1
1	A	180	LEU	3.1
1	A	286	LEU	3.1
1	A	1072	PRO	3.1
1	A	38	LEU	3.0
1	A	1040	ASP	3.0
1	A	673	VAL	3.0
1	A	188	GLU	3.0
2	B	132	U	3.0
1	A	1014	ASP	3.0
1	A	677	LEU	3.0
1	A	346	THR	3.0
1	A	296	PRO	2.9
1	A	1066	LEU	2.9
1	A	708	GLY	2.9
1	A	515	ASP	2.9
1	A	738	GLN	2.9
1	A	289	LEU	2.9
1	A	474	ASN	2.9
1	A	722	HIS	2.9
1	A	1010	ALA	2.9
1	A	443	GLU	2.9
1	A	473	ARG	2.9
1	A	13	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLN	2.8
1	A	1001	PHE	2.8
1	A	484	ALA	2.8
1	A	43	VAL	2.8
1	A	997	TYR	2.8
2	B	103	U	2.8
1	A	20	ALA	2.8
1	A	11	TYR	2.7
1	A	495	TYR	2.7
1	A	700	GLY	2.7
1	A	990	GLY	2.7
1	A	1067	GLY	2.7
1	A	947	ASP	2.7
1	A	468	PRO	2.7
1	A	9	ILE	2.7
1	A	348	MET	2.7
1	A	678	CYS	2.7
1	A	784	MET	2.7
1	A	1002	SER	2.7
1	A	955	ASP	2.7
1	A	472	ILE	2.7
1	A	834	PRO	2.7
1	A	680	PHE	2.7
1	A	1024	TYR	2.7
1	A	1075	LEU	2.7
1	A	333	LYS	2.6
1	A	512	SER	2.6
1	A	1006	TYR	2.6
1	A	730	VAL	2.6
1	A	824	TYR	2.6
1	A	493	ARG	2.6
1	A	405	PRO	2.6
1	A	203	PHE	2.6
1	A	498	PRO	2.6
1	A	441	TYR	2.6
1	A	510	GLY	2.6
1	A	12	ILE	2.5
1	A	800	ALA	2.5
1	A	423	ILE	2.5
1	A	779	PHE	2.5
1	A	962	LYS	2.5
1	A	385	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	671	ARG	2.5
1	A	508	GLU	2.5
1	A	371	PRO	2.5
1	A	464	LEU	2.5
1	A	785	ILE	2.5
1	A	280	LEU	2.5
1	A	336	ARG	2.5
1	A	23	GLY	2.5
1	A	467	ILE	2.4
1	A	886	ILE	2.4
1	A	478	LEU	2.4
1	A	492	VAL	2.4
1	A	28	GLU	2.4
1	A	502	HIS	2.4
1	A	245	ALA	2.4
1	A	274	ALA	2.4
1	A	400	LYS	2.4
1	A	411	LEU	2.4
1	A	835	ASN	2.4
1	A	1026	ASN	2.4
1	A	39	ILE	2.4
1	A	382	ILE	2.4
1	A	287	ARG	2.4
1	A	501	ILE	2.4
1	A	736	ALA	2.4
1	A	332	PHE	2.4
1	A	1051	SER	2.4
1	A	475	PRO	2.4
1	A	787	VAL	2.3
1	A	345	SER	2.3
1	A	486	LYS	2.3
1	A	278	ILE	2.3
1	A	482	SER	2.3
1	A	1038	TRP	2.3
1	A	987	ASP	2.3
1	A	45	VAL	2.3
1	A	37	ARG	2.3
1	A	1050	ILE	2.3
2	B	71	G	2.3
1	A	821	VAL	2.3
1	A	304	THR	2.3
1	A	703	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	734	THR	2.3
1	A	431	ILE	2.2
1	A	707	ARG	2.2
1	A	422	GLN	2.2
1	A	695	VAL	2.2
1	A	409	GLU	2.2
1	A	792	ASP	2.2
1	A	256	GLY	2.2
1	A	146	ASN	2.2
1	A	447	GLU	2.2
1	A	181	ALA	2.2
1	A	344	ALA	2.2
1	A	506	ALA	2.2
1	A	42	GLY	2.2
1	A	1042	GLY	2.2
1	A	1079	PRO	2.2
1	A	399	LEU	2.1
1	A	963	LYS	2.1
1	A	480	ALA	2.1
1	A	284	ASN	2.1
1	A	729	VAL	2.1
1	A	61	ALA	2.1
1	A	22	VAL	2.1
1	A	681	VAL	2.1
1	A	697	ALA	2.1
1	A	744	PHE	2.1
1	A	437	GLN	2.1
1	A	327	GLU	2.1
1	A	715	VAL	2.0
1	A	923	LYS	2.0
1	A	305	LEU	2.0
1	A	448	ILE	2.0
1	A	185	PHE	2.0
1	A	773	PRO	2.0
1	A	969	PHE	2.0
1	A	956	VAL	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	EDO	C	101	4/4	0.66	0.36	46,46,48,50	0
5	EDO	B	201	4/4	0.67	0.17	23,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.