



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:51 am BST

PDB ID : 5ZQ8
Title : Crystal structure of spRlmCD with U747 stemloop RNA
Authors : Jiang, Y.Y.; Yu, H.L.
Deposited on : 2018-04-17
Resolution : 2.18 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 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

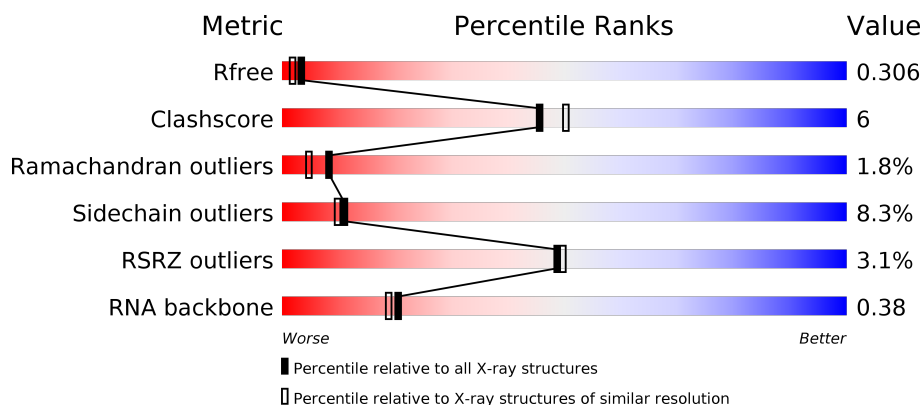
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)
RNA backbone	3102	1052 (2.60-1.76)

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 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	454	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	454	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>•</div> </div> </div>
2	C	12	<div> <div>58%</div> <div>25%</div> <div>17%</div> </div>
2	D	12	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7615 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 Uncharacterized RNA methyltransferase SP_1029.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	454	Total	C	N	O	S	0	0	0
			3536	2257	607	661	11			
1	A	454	Total	C	N	O	S	0	0	0
			3442	2197	593	640	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	443	GLN	GLU	engineered mutation	UNP Q97R12
A	443	GLN	GLU	engineered mutation	UNP Q97R12

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*CP*GP*UP*(MUM)P*GP*AP*AP*AP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			258	117	50	80	11			
2	D	12	Total	C	N	O	P	0	0	0
			258	117	50	80	11			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		
4	A	1	Total	Ni	0	0
			1	1		

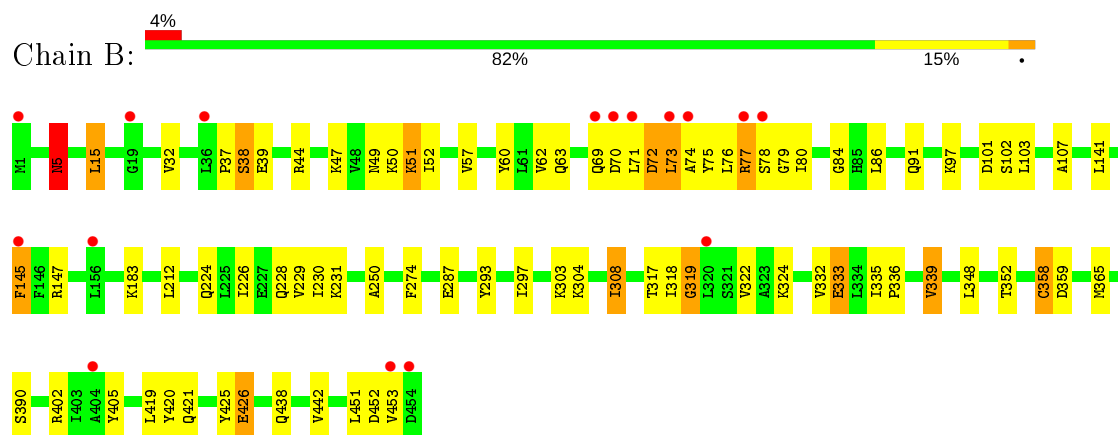
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	31	Total	O	0	0
			31	31		
5	A	28	Total	O	0	0
			28	28		
5	C	5	Total	O	0	0
			5	5		
5	D	3	Total	O	0	0
			3	3		

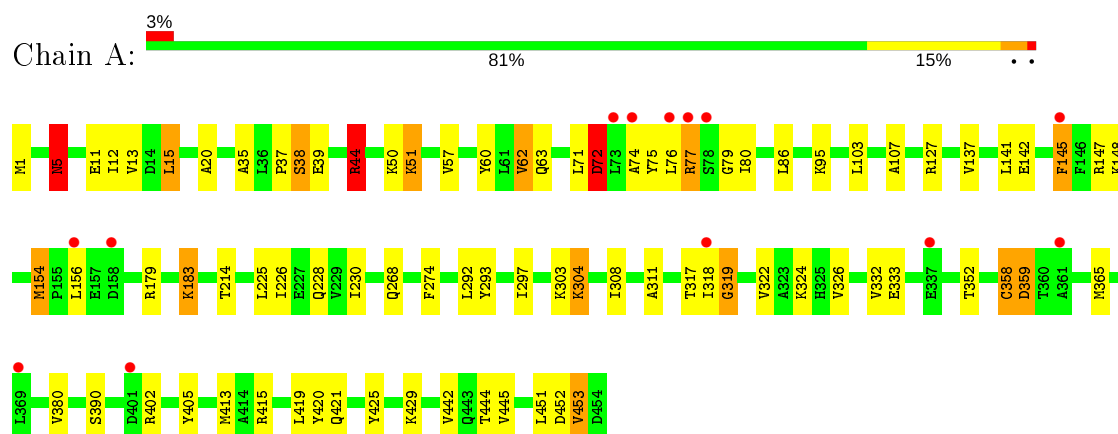
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Uncharacterized RNA methyltransferase SP_1029



- Molecule 1: Uncharacterized RNA methyltransferase SP_1029



- Molecule 2: RNA (5'-R(*CP*CP*GP*UP*(MUM)P*GP*AP*AP*AP*AP*GP*G)-3')



- Molecule 2: RNA (5'-R(*CP*CP*GP*UP*(MUM)P*GP*AP*AP*AP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.23Å 62.26Å 79.82Å 74.58° 85.47° 65.03°	Depositor
Resolution (Å)	56.37 – 2.18 56.37 – 2.18	Depositor EDS
% Data completeness (in resolution range)	87.5 (56.37-2.18) 87.5 (56.37-2.18)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.245 , 0.303 0.248 , 0.306	Depositor DCC
R_{free} test set	2293 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7615	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.68% 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: MUM, NI, SAH

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	0.45	0/3505	0.66	0/4770
1	B	0.45	0/3600	0.66	0/4885
2	C	0.53	0/265	0.99	2/410 (0.5%)
2	D	0.43	0/265	0.84	0/410
All	All	0.45	0/7635	0.68	2/10475 (0.0%)

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
1	A	0	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	751	A	C2'-C3'-O3'	6.09	123.45	113.70
2	C	744	C	C2'-C3'-O3'	5.22	122.05	113.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	ARG	Sidechain
1	A	415	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	44	ARG	Sidechain
1	A	5	ASN	Peptide
1	B	147	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	5	ASN	Peptide

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	3442	0	3337	45	0
1	B	3536	0	3516	48	0
2	C	258	0	122	3	0
2	D	258	0	122	1	0
3	A	26	0	19	1	0
3	B	26	0	19	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	0	4	0
5	B	31	0	0	2	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
All	All	7615	0	7135	94	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 6.

All (94) 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:B:71:LEU:HA	1:B:72:ASP:HB2	1.43	0.99
1:A:147:ARG:NH2	1:A:154:MET:SD	2.39	0.95
1:B:336:PRO:HA	1:B:339:VAL:HG13	1.57	0.84
1:B:5:ASN:HB2	1:B:44:ARG:HH11	1.44	0.83
1:A:451:LEU:O	5:A:601:HOH:O	1.98	0.81
1:B:293:TYR:CE1	1:B:318:ILE:HD11	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:HB2	1:A:44:ARG:HH11	1.53	0.73
1:B:336:PRO:HG3	5:B:630:HOH:O	1.87	0.73
1:B:71:LEU:HA	1:B:72:ASP:CB	2.16	0.72
1:A:293:TYR:OH	3:A:501:SAH:O	2.07	0.70
1:A:183:LYS:HB2	5:A:616:HOH:O	1.92	0.69
1:B:101:ASP:OD1	1:B:102:SER:N	2.25	0.68
1:B:74:ALA:HA	1:B:75:TYR:HB2	1.78	0.66
1:B:69:GLN:HA	1:B:70:ASP:C	2.15	0.66
1:B:50:LYS:O	1:B:51:LYS:CB	2.47	0.62
1:A:50:LYS:O	1:A:51:LYS:CB	2.47	0.61
1:B:336:PRO:CG	5:B:630:HOH:O	2.45	0.61
1:B:72:ASP:O	1:B:73:LEU:C	2.39	0.61
1:B:74:ALA:HB1	1:B:76:LEU:N	2.17	0.60
1:A:95:LYS:HG2	1:A:442:VAL:HG22	1.85	0.59
1:B:421:GLN:HA	1:B:425:TYR:O	2.05	0.57
1:A:421:GLN:HA	1:A:425:TYR:O	2.06	0.55
1:A:292:LEU:CD1	1:A:445:VAL:HG22	2.37	0.54
1:A:141:LEU:C	1:A:141:LEU:HD23	2.29	0.53
1:B:426:GLU:HB2	1:B:451:LEU:HD13	1.91	0.53
1:B:141:LEU:C	1:B:141:LEU:HD23	2.29	0.52
1:B:71:LEU:CA	1:B:72:ASP:HB2	2.28	0.52
1:B:69:GLN:HA	1:B:71:LEU:N	2.24	0.52
1:A:358:CYS:O	1:A:359:ASP:HB2	2.11	0.51
1:B:224:GLN:O	1:B:228:GLN:HG2	2.10	0.51
1:A:292:LEU:HD12	1:A:445:VAL:HG22	1.93	0.51
1:B:145:PHE:CZ	2:C:749:A:C5	2.99	0.51
1:B:71:LEU:CA	1:B:72:ASP:CB	2.89	0.50
1:A:76:LEU:O	1:A:77:ARG:CB	2.59	0.50
1:B:308:ILE:N	1:B:308:ILE:CD1	2.75	0.50
1:B:91:GLN:HE22	1:B:438:GLN:NE2	2.11	0.49
1:A:13:VAL:O	1:A:13:VAL:HG22	2.12	0.49
1:B:333:GLU:O	1:B:359:ASP:O	2.31	0.49
1:B:297:ILE:HG12	1:B:322:VAL:HG12	1.95	0.48
1:A:137:VAL:CG2	1:A:142:GLU:HG3	2.43	0.48
1:B:358:CYS:O	1:B:359:ASP:HB2	2.13	0.48
1:B:57:VAL:HG11	1:B:60:TYR:CZ	2.49	0.48
1:A:333:GLU:O	1:A:359:ASP:O	2.31	0.48
1:A:292:LEU:HD12	1:A:445:VAL:CG2	2.44	0.48
1:B:293:TYR:CD1	1:B:318:ILE:HD11	2.50	0.47
1:A:77:ARG:HA	1:A:156:LEU:HD11	1.95	0.47
1:A:57:VAL:HG11	1:A:60:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TYR:O	1:B:425:TYR:HB2	2.15	0.47
2:C:744:C:H5''	2:C:745:G:H2'	1.97	0.47
1:B:226:ILE:O	1:B:230:ILE:HD13	2.16	0.46
1:B:336:PRO:HA	1:B:339:VAL:CG1	2.37	0.46
1:A:308:ILE:HD11	1:A:326:VAL:HG21	1.97	0.46
1:B:84:GLY:HA2	1:B:438:GLN:HE21	1.80	0.46
1:A:57:VAL:HG11	1:A:60:TYR:CE2	2.50	0.46
1:B:57:VAL:HG11	1:B:60:TYR:CE2	2.50	0.46
1:B:250:ALA:HB2	2:C:745:G:OP1	2.16	0.46
1:A:127:ARG:NH1	5:A:603:HOH:O	2.35	0.46
1:A:318:ILE:O	1:A:319:GLY:C	2.54	0.46
1:B:77:ARG:C	1:B:79:GLY:H	2.20	0.46
1:A:12:ILE:HG13	1:A:35:ALA:HB1	1.97	0.45
1:A:420:TYR:O	1:A:425:TYR:HB2	2.17	0.45
1:A:145:PHE:CZ	2:D:749:A:C5	3.04	0.45
1:B:229:VAL:HG13	1:B:230:ILE:HD12	1.99	0.44
1:B:318:ILE:O	1:B:319:GLY:C	2.56	0.44
1:A:72:ASP:HB3	1:A:76:LEU:CB	2.47	0.44
1:B:37:PRO:O	1:B:38:SER:HB2	2.18	0.44
1:A:39:GLU:HG2	1:A:63:GLN:HA	2.00	0.44
1:A:103:LEU:O	1:A:107:ALA:HB3	2.17	0.44
1:B:39:GLU:HG2	1:B:63:GLN:HA	1.99	0.44
1:B:74:ALA:HB1	1:B:75:TYR:C	2.38	0.44
1:A:413:MET:SD	1:A:444:THR:OG1	2.72	0.44
1:B:76:LEU:O	1:B:78:SER:N	2.51	0.43
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.89	0.43
1:B:49:ASN:ND2	1:B:52:ILE:HG13	2.34	0.43
1:B:103:LEU:O	1:B:107:ALA:HB3	2.18	0.43
1:A:304:LYS:HD3	1:A:304:LYS:O	2.19	0.43
1:B:308:ILE:HD12	1:B:308:ILE:N	2.33	0.43
1:A:226:ILE:O	1:A:230:ILE:HG23	2.19	0.42
1:B:339:VAL:HG11	1:B:358:CYS:SG	2.60	0.42
1:A:74:ALA:HA	1:A:75:TYR:C	2.40	0.42
1:A:37:PRO:O	1:A:38:SER:HB2	2.18	0.42
1:A:5:ASN:HB2	1:A:44:ARG:NH1	2.30	0.41
1:A:274:PHE:CE2	1:A:317:THR:HA	2.55	0.41
1:A:297:ILE:HG12	1:A:322:VAL:HG12	2.01	0.41
1:B:91:GLN:HE22	1:B:438:GLN:HE22	1.68	0.41
1:A:15:LEU:HD12	1:A:20:ALA:O	2.21	0.41
1:A:453:VAL:CG2	5:A:601:HOH:O	2.68	0.41
1:B:15:LEU:HA	1:B:15:LEU:HD12	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG23	1:A:142:GLU:HG3	2.03	0.40
1:A:77:ARG:CB	1:A:80:ILE:CB	2.99	0.40
1:B:274:PHE:CE2	1:B:317:THR:HA	2.56	0.40
1:A:39:GLU:HA	1:A:62:VAL:O	2.21	0.40
1:A:225:LEU:HD23	1:A:225:LEU:O	2.21	0.40
1:A:311:ALA:HB3	1:A:380:VAL:HG12	2.03	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	452/454 (100%)	419 (93%)	25 (6%)	8 (2%)	8	5
1	B	452/454 (100%)	424 (94%)	20 (4%)	8 (2%)	8	5
All	All	904/908 (100%)	843 (93%)	45 (5%)	16 (2%)	8	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	LYS
1	B	72	ASP
1	A	51	LYS
1	B	73	LEU
1	B	77	ARG
1	A	72	ASP
1	A	77	ARG
1	B	5	ASN
1	B	38	SER
1	B	319	GLY
1	A	5	ASN
1	A	38	SER

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Mol	Chain	Res	Type
1	A	319	GLY
1	A	79	GLY
1	A	359	ASP
1	B	80	ILE

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	351/398 (88%)	321 (92%)	30 (8%)	10	9
1	B	376/398 (94%)	346 (92%)	30 (8%)	12	11
All	All	727/796 (91%)	667 (92%)	60 (8%)	11	10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	LEU
1	B	32	VAL
1	B	47	LYS
1	B	62	VAL
1	B	86	LEU
1	B	97	LYS
1	B	145	PHE
1	B	183	LYS
1	B	212	LEU
1	B	231	LYS
1	B	287	GLU
1	B	303	LYS
1	B	304	LYS
1	B	308	ILE
1	B	324	LYS
1	B	332	VAL
1	B	333	GLU
1	B	335	ILE
1	B	339	VAL

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Mol	Chain	Res	Type
1	B	348	LEU
1	B	352	THR
1	B	358	CYS
1	B	365	MET
1	B	390	SER
1	B	405	TYR
1	B	419	LEU
1	B	426	GLU
1	B	442	VAL
1	B	452	ASP
1	B	453	VAL
1	A	1	MET
1	A	5	ASN
1	A	11	GLU
1	A	15	LEU
1	A	44	ARG
1	A	62	VAL
1	A	71	LEU
1	A	72	ASP
1	A	86	LEU
1	A	145	PHE
1	A	148	LYS
1	A	154	MET
1	A	179	ARG
1	A	183	LYS
1	A	214	THR
1	A	228	GLN
1	A	268	GLN
1	A	303	LYS
1	A	304	LYS
1	A	324	LYS
1	A	332	VAL
1	A	352	THR
1	A	358	CYS
1	A	365	MET
1	A	390	SER
1	A	405	TYR
1	A	419	LEU
1	A	429	LYS
1	A	452	ASP
1	A	453	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	363	ASN
1	B	438	GLN
1	A	203	HIS
1	A	343	GLN
1	A	363	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/12 (83%)	2 (20%)	0
2	D	10/12 (83%)	3 (30%)	0
All	All	20/24 (83%)	5 (25%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	748	G
2	C	751	A
2	D	746	U
2	D	748	G
2	D	751	A

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	MUM	C	747	1,2	19,22,22	1.26	3 (15%)	20,32,32	1.45	4 (20%)
2	MUM	D	747	1,2	19,22,22	1.21	3 (15%)	20,32,32	1.58	6 (30%)

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
2	MUM	C	747	1,2	-	3/7/41/41	0/2/2/2
2	MUM	D	747	1,2	-	3/7/41/41	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	747	MUM	C4-N3	-3.29	1.31	1.37
2	C	747	MUM	C4-N3	-2.81	1.32	1.37
2	C	747	MUM	C2-N1	-2.63	1.31	1.35
2	C	747	MUM	C2-N3	-2.36	1.33	1.38
2	D	747	MUM	C2-N1	-2.11	1.32	1.35
2	D	747	MUM	C2-N3	-2.01	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	747	MUM	C4-N3-C2	-4.11	121.83	126.86
2	C	747	MUM	C4-N3-C2	-3.88	122.11	126.86
2	D	747	MUM	N3-C2-N1	2.66	119.47	116.65
2	C	747	MUM	O2-C2-N1	-2.58	119.87	123.11
2	D	747	MUM	O4'-C1'-N1	2.46	112.66	109.30
2	D	747	MUM	O3'-C3'-C2'	2.23	119.02	111.82
2	C	747	MUM	C5-C6-N1	-2.18	106.82	111.11
2	D	747	MUM	O2-C2-N1	-2.14	120.42	123.11
2	C	747	MUM	N3-C2-N1	2.03	118.80	116.65
2	D	747	MUM	C5-C6-N1	-2.02	107.13	111.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	747	MUM	O4'-C1'-N1-C6
2	D	747	MUM	O4'-C1'-N1-C6
2	C	747	MUM	O4'-C1'-N1-C2
2	C	747	MUM	C2'-C1'-N1-C2
2	D	747	MUM	O4'-C1'-N1-C2
2	D	747	MUM	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	SAH	A	501	-	21,28,28	1.20	2 (9%)	20,40,40	1.53	2 (10%)
3	SAH	B	501	-	21,28,28	1.17	2 (9%)	20,40,40	1.38	2 (10%)

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
3	SAH	A	501	-	-	2/7/31/31	0/3/3/3
3	SAH	B	501	-	-	4/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	SAH	C2-N3	2.75	1.36	1.32
3	B	501	SAH	C2-N3	2.63	1.36	1.32
3	B	501	SAH	C5-C4	2.52	1.47	1.40
3	A	501	SAH	C5-C4	2.19	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	SAH	N3-C2-N1	-3.66	122.96	128.68
3	B	501	SAH	N3-C2-N1	-3.18	123.71	128.68
3	A	501	SAH	N6-C6-N1	2.87	124.52	118.57
3	B	501	SAH	N6-C6-N1	2.53	123.82	118.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

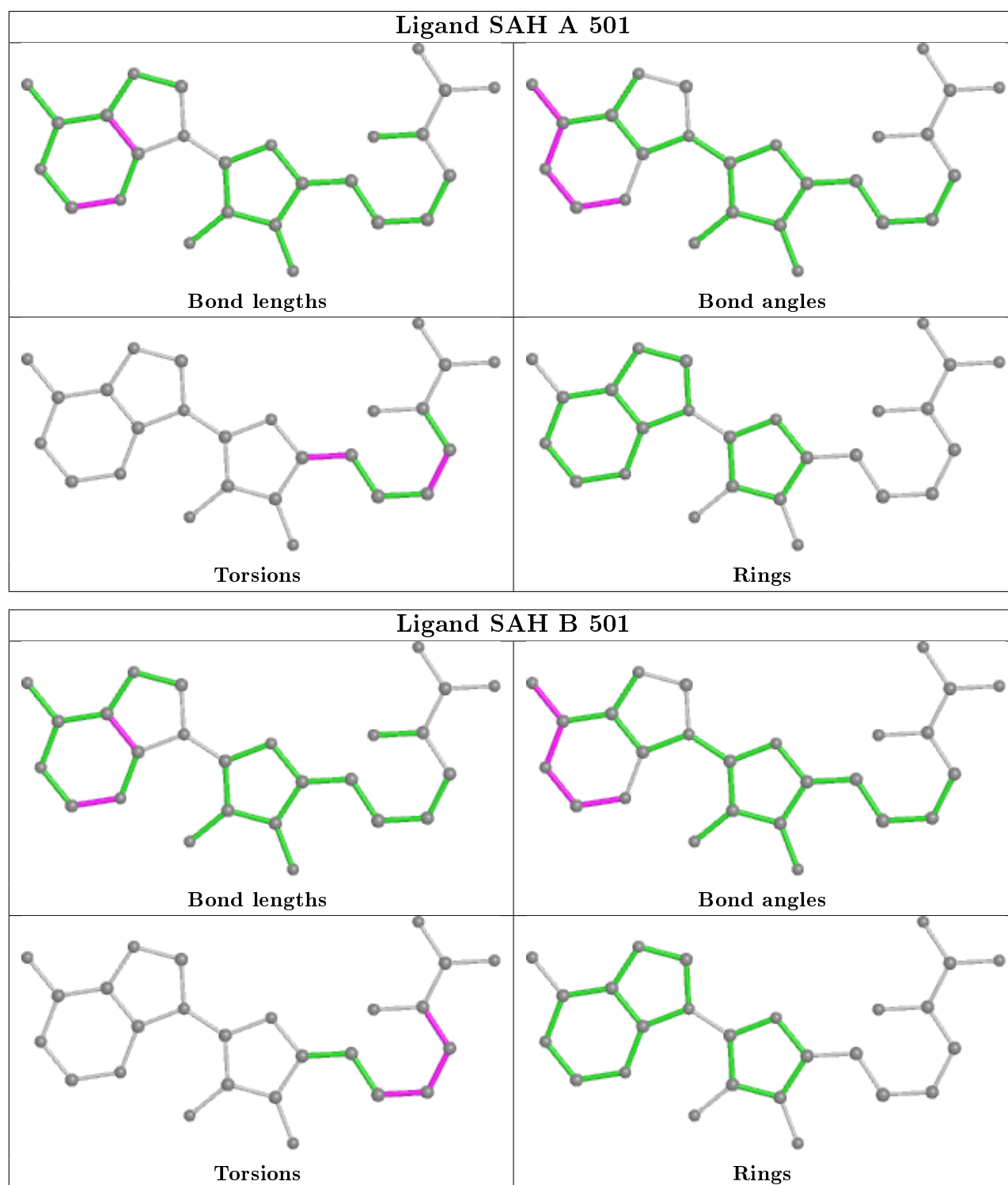
Mol	Chain	Res	Type	Atoms
3	A	501	SAH	CA-CB-CG-SD
3	B	501	SAH	N-CA-CB-CG
3	B	501	SAH	C-CA-CB-CG
3	B	501	SAH	CA-CB-CG-SD
3	B	501	SAH	CB-CG-SD-C5'
3	A	501	SAH	O4'-C4'-C5'-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	454/454 (100%)	0.28	13 (2%)	51	52	19, 41, 70, 108	0
1	B	454/454 (100%)	0.33	16 (3%)	44	44	20, 41, 67, 109	0
2	C	11/12 (91%)	-0.97	0	100	100	24, 32, 37, 38	0
2	D	11/12 (91%)	-0.95	0	100	100	26, 33, 35, 38	0
All	All	930/932 (99%)	0.27	29 (3%)	49	50	19, 40, 68, 109	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	8.3
1	A	78	SER	5.5
1	A	77	ARG	4.5
1	B	73	LEU	4.5
1	A	76	LEU	4.0
1	B	78	SER	3.7
1	A	74	ALA	3.6
1	A	369	LEU	3.2
1	A	145	PHE	3.0
1	B	70	ASP	2.6
1	A	361	ALA	2.6
1	B	74	ALA	2.5
1	B	36	LEU	2.5
1	B	69	GLN	2.4
1	B	1	MET	2.4
1	A	337	GLU	2.3
1	A	318	ILE	2.3
1	B	71	LEU	2.3
1	B	156	LEU	2.2
1	B	145	PHE	2.2
1	B	453	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	156	LEU	2.2
1	B	454	ASP	2.2
1	B	320	LEU	2.1
1	B	19	GLY	2.1
1	B	404	ALA	2.1
1	B	77	ARG	2.1
1	A	401	ASP	2.0
1	A	158	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MUM	C	747	21/21	0.95	0.11	23,25,31,34	0
2	MUM	D	747	21/21	0.95	0.11	18,24,32,36	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

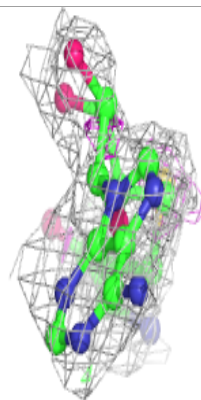
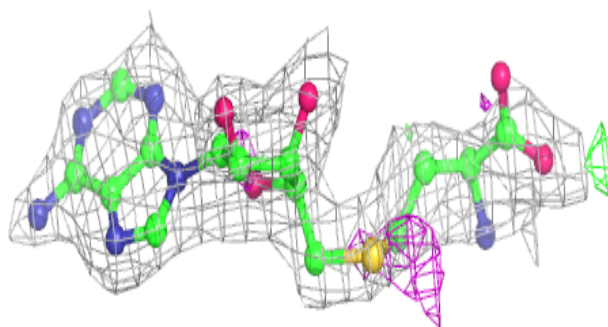
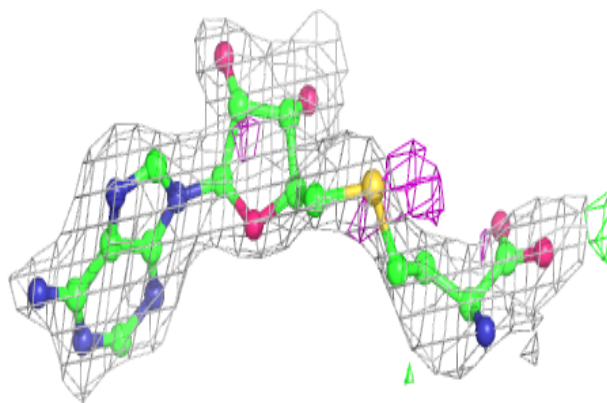
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SAH	B	501	26/26	0.83	0.23	46,54,69,73	0
3	SAH	A	501	26/26	0.87	0.21	44,54,68,74	0
4	NI	A	502	1/1	0.98	0.05	50,50,50,50	0
4	NI	B	502	1/1	0.99	0.05	50,50,50,50	0

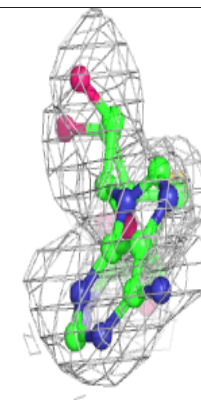
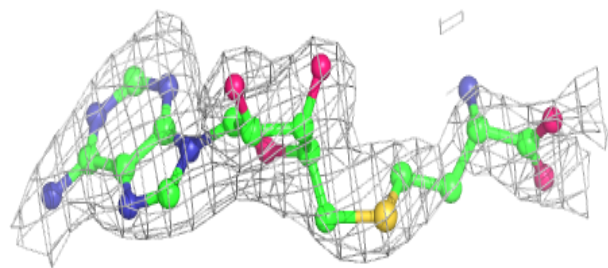
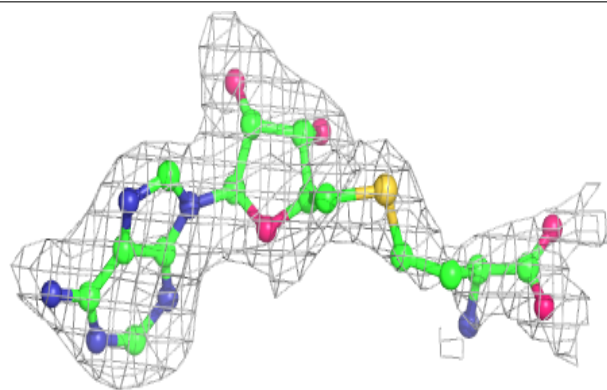
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAH A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.