



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 9FZ6 / pdb_00009fz6
Title : A 2.58Å crystal structure of S. aureus DNA gyrase and DNA with metals identified through anomalous scattering
Authors : Morgan, H.; Duman, R.; Bax, B.D.; Warren, A.J.
Deposited on : 2024-07-04
Resolution : 2.58 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

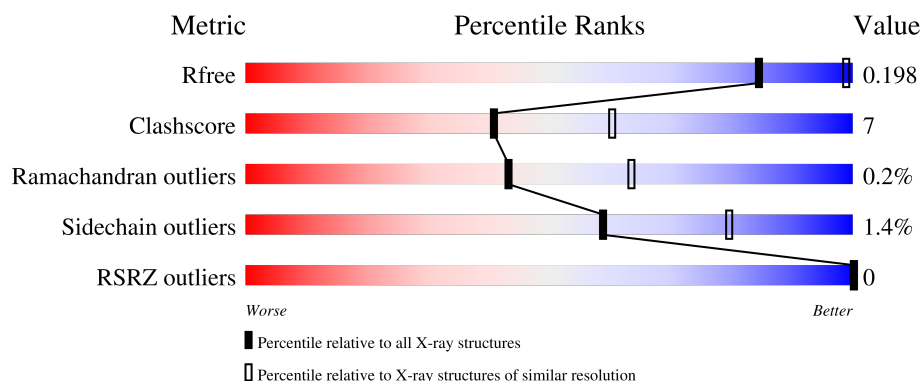
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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.



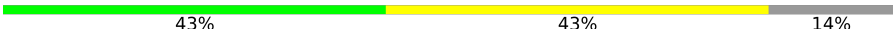
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	483	81% 18%
1	C	483	83% 17%
2	B	190	89% 11%
2	D	190	77% 21% ..
3	E	8	62% 38%

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Mol	Chain	Length	Quality of chain
3	F	8	 88%12%
4	G	14	 43%43%14%
4	H	14	 57%29%14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11963 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	4	0
			3870	2405	708	741	16			
1	C	481	Total	C	N	O	S	0	8	0
			3891	2417	713	744	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	TYR	engineered mutation	UNP P20831
A	457	THR	ALA	conflict	UNP P20831
C	123	PHE	TYR	engineered mutation	UNP P20831
C	457	THR	ALA	conflict	UNP P20831

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	0	0
			1486	933	256	288	9			
2	D	189	Total	C	N	O	S	0	2	0
			1492	935	257	291	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	-	linker	UNP P0A0K8
B	545	GLY	-	linker	UNP P0A0K8
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8

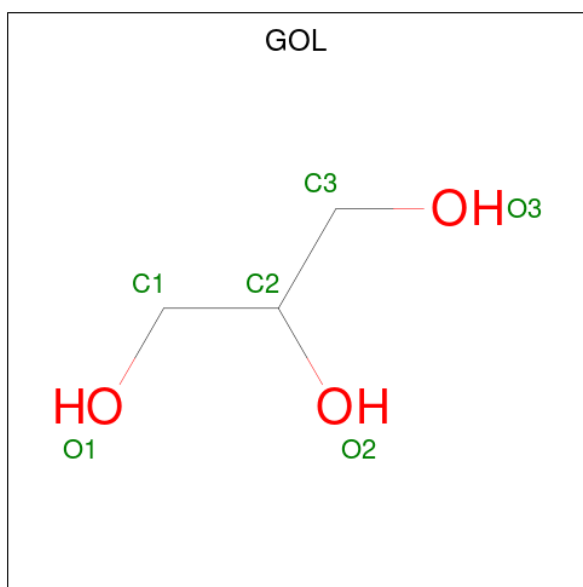
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
3	F	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	12	Total	C	N	O	P	0	1	0
			266	126	48	79	13			
4	H	12	Total	C	N	O	P	0	0	0
			219	101	37	69	12			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

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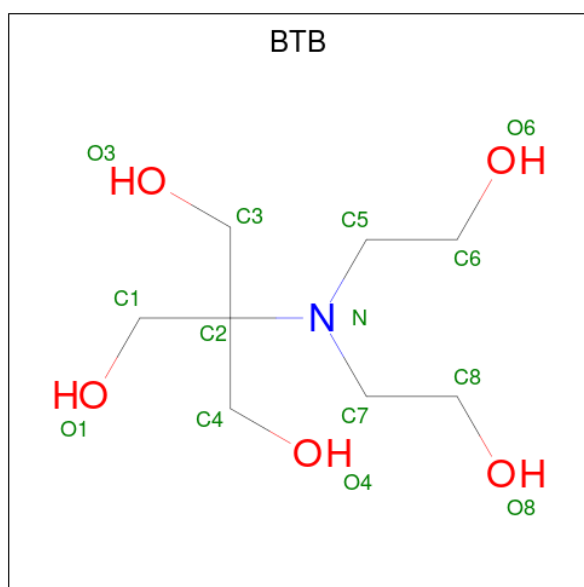
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mn	0	0
			1	1		
6	C	1	Total	Mn	0	1
			1	1		
6	D	1	Total	Mn	0	0
			1	1		
6	G	1	Total	Mn	0	0
			1	1		
6	H	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	1
			28	16	2	10		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	107	Total 107	O 107	0	0
8	B	27	Total 27	O 27	0	0
8	C	137	Total 137	O 137	0	0
8	D	29	Total 29	O 29	0	0
8	E	6	Total 6	O 6	0	0
8	F	9	Total 9	O 9	0	0
8	G	11	Total 12	O 12	0	1
8	H	11	Total 11	O 11	0	0

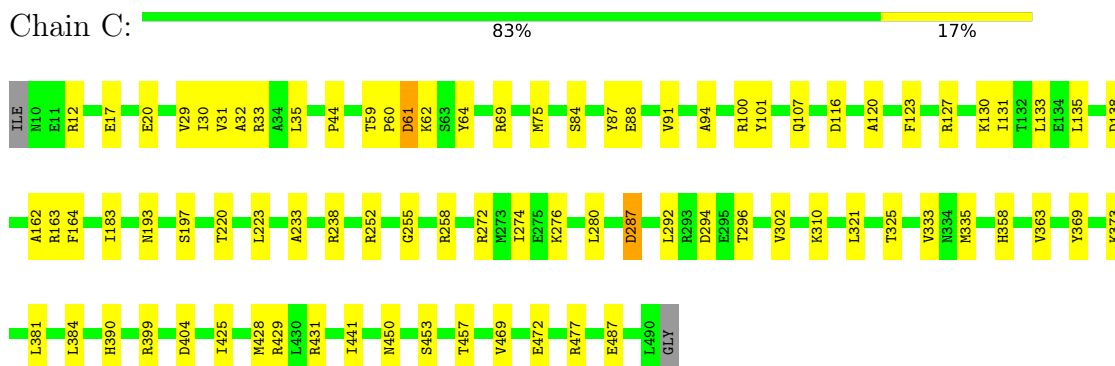
3 Residue-property plots

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.

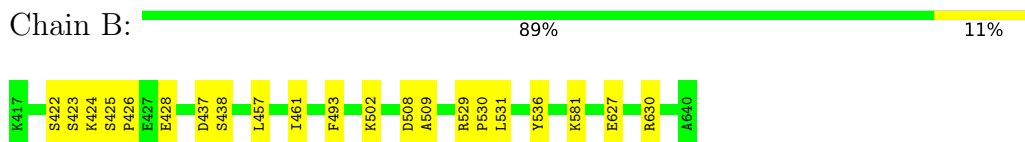
• Molecule 1: DNA gyrase subunit A



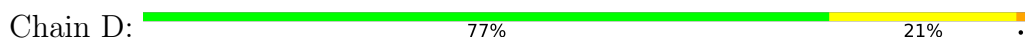
• Molecule 1: DNA gyrase subunit A

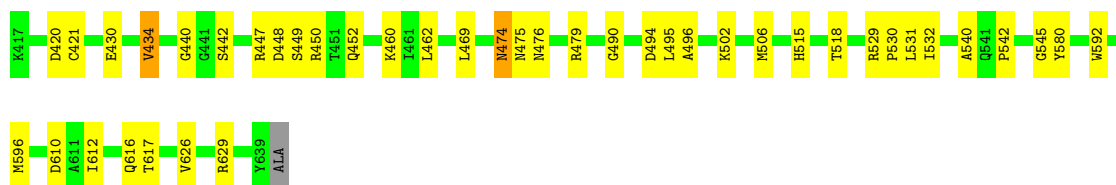


• Molecule 2: DNA gyrase subunit B



• Molecule 2: DNA gyrase subunit B

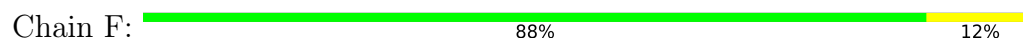




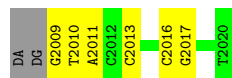
- Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3')



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



- Molecule 4: DNA (5'-D(*AP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



- Molecule 4: DNA (5'-D(*AP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.63Å 93.63Å 410.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.72 – 2.58 57.72 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.72-2.58) 99.8 (57.72-2.58)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???), REFMAC 5.8.0425	Depositor
R, R_{free}	0.140 , 0.200 0.133 , 0.198	Depositor DCC
R_{free} test set	3166 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11963	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: MN, BTB, GOL

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	0.52	0/3918	0.85	0/5274
1	C	0.51	0/3940	0.82	0/5304
2	B	0.49	0/1510	0.86	0/2037
2	D	0.48	0/1515	0.79	0/2045
3	E	0.39	0/183	0.92	1/281 (0.4%)
3	F	0.40	0/183	0.83	0/281
4	G	0.36	0/297	0.83	0/456
4	H	0.39	0/243	0.87	0/373
All	All	0.50	0/11789	0.83	1/16051 (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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	DG	O3'-P-O5'	-5.77	95.34	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364	ARG	Sidechain
1	C	429	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3870	0	3927	55	0
1	C	3891	0	3941	51	0
2	B	1486	0	1460	13	0
2	D	1492	0	1451	22	0
3	E	163	0	91	2	0
3	F	163	0	91	1	0
4	G	266	0	147	7	0
4	H	219	0	119	4	0
5	A	12	0	16	0	0
5	C	24	0	32	0	0
5	E	6	0	8	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	C	28	0	34	2	0
8	A	107	0	0	5	0
8	B	27	0	0	3	0
8	C	137	0	0	8	0
8	D	29	0	0	1	0
8	E	6	0	0	0	0
8	F	9	0	0	0	0
8	G	12	0	0	2	0
8	H	11	0	0	0	0
All	All	11963	0	11317	148	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 7.

All (148) 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)
2:D:460:LYS:NZ	8:D:801:HOH:O	2.02	0.92
1:C:94:ALA:O	8:C:1001:HOH:O	2.05	0.74
1:C:358:HIS:HD2	8:C:1087:HOH:O	1.71	0.74
1:C:62:LYS:O	1:C:127:ARG:NH1	2.24	0.70
2:D:447:ARG:NH1	2:D:452:GLN:O	2.24	0.70
1:A:431:ARG:NH1	1:C:404:ASP:OD2	2.25	0.68
1:A:48:ARG:HH11	1:A:79:HIS:HD2	1.42	0.67
1:C:116:ASP:OD2	8:C:1002:HOH:O	2.11	0.67
2:D:434:VAL:HG21	2:D:440:GLY:HA2	1.77	0.66
1:C:12:ARG:NH2	1:C:20:GLU:OE1	2.31	0.64
1:A:66:LYS:NZ	1:A:125:GLU:OE2	2.26	0.64
2:D:592:TRP:HA	2:D:596:MET:HB2	1.81	0.63
1:C:384:LEU:HD22	1:C:428:MET:HE2	1.82	0.62
2:B:423:SER:OG	2:B:428:GLU:OE2	2.16	0.61
1:A:321:LEU:O	1:A:325:THR:OG1	2.12	0.61
1:A:392:ASP:OD1	8:A:601:HOH:O	2.16	0.60
2:D:545:GLY:O	2:D:580:TYR:N	2.36	0.59
1:C:138:ASP:N	8:C:1003:HOH:O	2.22	0.57
1:C:390[A]:HIS:HE1	7:C:902[A]:BTB:O6	1.86	0.57
1:A:192:ILE:HG21	1:A:477:ARG:HB2	1.87	0.56
2:D:420:ASP:OD1	2:D:421:CYS:N	2.38	0.56
1:A:60:PRO:HA	1:A:127:ARG:HD2	1.88	0.56
1:A:280:LEU:HD22	1:A:285:LYS:HB2	1.88	0.56
1:C:163:ARG:NH2	1:C:472:GLU:OE1	2.34	0.55
1:C:453:SER:O	1:C:457:THR:HG23	2.06	0.55
1:C:193:ASN:OD1	1:C:477:ARG:NH1	2.38	0.55
1:A:397:THR:O	1:A:401:SER:OG	2.23	0.55
2:D:462:LEU:HB2	2:D:475:ASN:ND2	2.21	0.55
1:C:294:ASP:OD1	1:C:296:THR:OG1	2.20	0.54
1:A:430:LEU:HD12	1:C:425:ILE:O	2.08	0.54
2:D:476[B]:ASN:OD1	2:D:479:ARG:NH2	2.41	0.53
2:B:493:PHE:CE2	2:B:530:PRO:HB2	2.44	0.53
1:C:381:LEU:HD23	1:C:384:LEU:HD12	1.90	0.52
1:A:298:LEU:HB2	1:A:299:ARG:HD3	1.91	0.52
1:C:381:LEU:HD22	1:C:441:ILE:HG23	1.92	0.51
2:B:581:LYS:HE2	8:B:811:HOH:O	2.10	0.51
2:B:627:GLU:OE2	2:B:630:ARG:NH2	2.43	0.51
1:C:135:LEU:HD23	1:C:162:ALA:HA	1.92	0.51
4:H:2012:DC:H4'	4:H:2013:DC:OP1	2.10	0.51
1:C:223:LEU:HD13	1:C:487:GLU:HB3	1.93	0.51
2:B:508:ASP:O	2:B:509:ALA:HB3	2.10	0.50
4:G:2016:DC:H2''	4:G:2017:DG:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2010:DT:H2''	4:G:2011:DA:H5''	1.93	0.50
1:A:65:LYS:HD3	1:A:70:ILE:HG12	1.94	0.50
2:B:502:LYS:HG3	8:B:804:HOH:O	2.12	0.49
4:H:2011:DA:H3'	4:H:2012:DC:H5''	1.95	0.49
1:C:120:ALA:HB3	1:C:123:PHE:CD2	2.48	0.49
2:B:457:LEU:HB3	2:B:461:ILE:HD11	1.93	0.48
1:C:321:LEU:O	1:C:325:THR:OG1	2.22	0.48
1:A:10:ASN:ND2	8:A:612:HOH:O	2.46	0.48
2:D:474:ASN:N	2:D:474:ASN:OD1	2.46	0.48
1:C:296:THR:HG23	1:C:302:VAL:HA	1.95	0.48
7:C:902[A]:BTB:H32	7:C:902[A]:BTB:H51	1.67	0.48
1:C:252:ARG:HD3	1:C:258:ARG:HB3	1.95	0.48
4:G:2011:DA:N1	4:H:2010:DT:H2'	2.29	0.48
1:A:423:GLN:HE22	1:C:431:ARG:HH22	1.62	0.48
1:A:100:ARG:HA	1:A:219:PRO:HB3	1.94	0.48
1:C:272:ARG:NH1	8:C:1016:HOH:O	2.47	0.47
1:A:461:ASP:OD1	1:A:462:GLU:N	2.46	0.47
1:C:363:VAL:HG21	1:C:469:VAL:HG22	1.97	0.47
1:A:135:LEU:HD23	1:A:162:ALA:HA	1.96	0.47
2:D:515:HIS:O	2:D:518:THR:OG1	2.29	0.47
1:A:391:ILE:O	1:A:395:ILE:HG12	2.15	0.47
1:C:12:ARG:NE	1:C:17:GLU:OE1	2.47	0.47
1:A:224:ILE:HG21	1:A:230:ILE:HD11	1.97	0.47
2:D:430:GLU:HG2	2:D:502:LYS:HB2	1.97	0.47
1:A:432:ARG:NH1	1:A:437:GLU:OE2	2.47	0.46
2:B:502:LYS:NZ	8:B:804:HOH:O	2.48	0.46
1:A:377:ARG:HB3	1:A:448:LEU:HD21	1.96	0.46
1:A:113:MET:HE2	1:A:264:ILE:HD11	1.96	0.46
2:B:422:SER:O	2:B:424:LYS:HE2	2.15	0.46
1:C:274:ILE:HG23	1:C:292:LEU:HD21	1.97	0.46
2:D:540:ALA:O	2:D:542:PRO:HD3	2.15	0.46
1:A:233:ALA:HB1	1:A:333:VAL:HG11	1.98	0.46
1:A:234:TYR:O	1:A:347:ASN:HB2	2.15	0.46
2:D:469:LEU:O	2:D:469:LEU:HG	2.16	0.46
1:A:378:ALA:HB2	1:A:448:LEU:HD23	1.97	0.45
1:A:54:ASN:HB2	1:A:136:LEU:HD13	1.98	0.45
1:A:274:ILE:HG23	1:A:292:LEU:HD21	1.98	0.45
1:A:384:LEU:HD22	1:A:428:MET:HE2	1.98	0.45
1:C:30:ILE:HG23	1:C:35:LEU:HD12	1.97	0.45
3:F:1:DA:N3	3:F:1:DA:H2'	2.32	0.45
1:A:272:ARG:HA	1:A:275:GLU:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:NZ	1:A:173:SER:O	2.46	0.45
2:B:425:SER:HB3	2:B:428:GLU:HG2	1.98	0.45
2:B:424:LYS:O	2:B:426:PRO:HD3	2.17	0.45
2:D:626:VAL:HG22	2:D:629:ARG:HH21	1.82	0.45
1:C:84:SER:O	1:C:88:GLU:HG2	2.16	0.45
1:C:233:ALA:HB1	1:C:333:VAL:HG11	1.98	0.45
4:G:2016:DC:H2''	4:G:2017:DG:C5'	2.47	0.45
1:C:130:LYS:O	1:C:133:LEU:HB2	2.16	0.45
2:D:448:ASP:C	2:D:450:ARG:H	2.25	0.44
1:C:64:TYR:CD2	1:C:127:ARG:HG2	2.52	0.44
1:C:238:ARG:HA	1:C:333:VAL:O	2.18	0.44
1:A:439:ASP:HB2	8:A:652:HOH:O	2.16	0.44
3:E:4:DC:H5''	5:E:101:GOL:O1	2.17	0.44
1:C:32:ALA:HA	1:C:44:PRO:HG2	1.98	0.44
2:D:529:ARG:N	2:D:530:PRO:CD	2.81	0.44
1:A:291:ASP:OD1	1:A:292:LEU:N	2.50	0.44
1:C:29:VAL:HA	1:C:33:ARG:HB3	1.99	0.44
1:C:131:ILE:N	8:C:1011:HOH:O	2.42	0.44
1:A:130:LYS:O	1:A:133:LEU:HB2	2.18	0.43
1:C:255:GLY:HA3	1:C:310:LYS:HE3	2.00	0.43
1:C:369:TYR:CE1	1:C:373[B]:LYS:HD2	2.53	0.43
4:G:2013:DC:N4	8:G:2202:HOH:O	2.51	0.43
1:A:192:ILE:O	1:A:196:LEU:HG	2.18	0.43
1:A:367:THR:HG23	1:A:455:LEU:HD22	2.00	0.43
1:C:272:ARG:HH11	1:C:272:ARG:HG3	1.84	0.43
1:A:183:ILE:HG12	1:A:335:MET:HG2	2.01	0.43
4:G:2009[B]:DG:N7	8:G:2201:HOH:O	2.45	0.43
1:C:183:ILE:HG12	1:C:335:MET:HG2	2.01	0.42
2:D:447:ARG:HG3	2:D:449:SER:N	2.34	0.42
1:A:273:MET:HE2	1:A:273:MET:HB3	1.88	0.42
1:C:87:TYR:O	1:C:91:VAL:HG23	2.19	0.42
1:A:364:ARG:NE	8:A:609:HOH:O	2.40	0.42
2:D:494:ASP:OD1	2:D:496:ALA:N	2.51	0.42
1:A:175:ILE:HD12	3:E:5:DG:C2	2.54	0.42
1:C:276:LYS:O	1:C:280:LEU:HG	2.19	0.42
1:C:399:ARG:HG3	1:C:399:ARG:HH11	1.85	0.42
2:D:612:ILE:O	2:D:616:GLN:HG3	2.19	0.42
1:A:18:MET:HE3	1:A:18:MET:HB3	1.82	0.42
1:A:139:ILE:HD12	1:A:161:PRO:HD3	2.01	0.42
1:A:48:ARG:HH11	1:A:79:HIS:CD2	2.30	0.42
1:A:149:ASN:ND2	1:A:151:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:SER:OG	1:A:265:PRO:HD3	2.19	0.42
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.88	0.42
2:D:434:VAL:HG12	2:D:506:MET:HE3	2.02	0.42
2:D:495:LEU:HD12	2:D:531:LEU:HD23	2.01	0.42
1:A:37:ASP:HB3	1:A:40:ASP:OD1	2.20	0.42
1:A:109:ASN:HB2	2:D:442:SER:OG	2.20	0.42
1:C:100:ARG:HG3	1:C:101:TYR:CE2	2.56	0.41
2:B:531:LEU:HD23	2:B:536:TYR:HD2	1.85	0.41
1:C:60:PRO:HA	1:C:127:ARG:HD2	2.02	0.41
1:A:76:GLY:HA3	1:C:69:ARG:HD2	2.02	0.41
1:A:407:ALA:O	1:A:411:LEU:HG	2.20	0.41
1:C:135:LEU:HG	1:C:164:PHE:CE2	2.56	0.41
1:C:163:ARG:O	8:C:1004:HOH:O	2.22	0.41
1:A:394:ILE:O	1:A:398:ILE:HG13	2.21	0.41
1:A:368:GLN:O	1:A:372:ARG:HG3	2.21	0.41
1:C:59:THR:OG1	1:C:61:ASP:OD1	2.35	0.41
1:A:454:GLU:O	1:A:458:ILE:HD13	2.21	0.41
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.92	0.41
2:B:529:ARG:N	2:B:530:PRO:CD	2.84	0.40
1:A:46:HIS:ND1	8:A:608:HOH:O	2.37	0.40
1:A:138:ASP:HA	1:A:141:LYS:HD3	2.03	0.40
1:C:287[A]:ASP:HA	8:C:1056:HOH:O	2.20	0.40
1:A:210:MET:HE2	1:A:210:MET:HB3	1.95	0.40
4:G:2011:DA:C6	4:H:2010:DT:H2'	2.57	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	485/483 (100%)	460 (95%)	25 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	487/483 (101%)	465 (96%)	22 (4%)	0	100	100
2	B	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
2	D	187/190 (98%)	170 (91%)	15 (8%)	2 (1%)	11	24
All	All	1347/1346 (100%)	1277 (95%)	68 (5%)	2 (0%)	43	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	490	GLY
2	D	610	ASP

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	420/417 (101%)	418 (100%)	2 (0%)	81	91
1	C	423/417 (101%)	413 (98%)	10 (2%)	43	68
2	B	156/158 (99%)	154 (99%)	2 (1%)	61	81
2	D	157/158 (99%)	153 (98%)	4 (2%)	42	67
All	All	1156/1150 (100%)	1138 (98%)	18 (2%)	59	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	GLN
1	A	457	THR
2	B	437	ASP
2	B	438	SER
1	C	31	VAL
1	C	61	ASP
1	C	75	MET
1	C	107	GLN
1	C	197	SER

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Mol	Chain	Res	Type
1	C	220	THR
1	C	287[A]	ASP
1	C	287[B]	ASP
1	C	450[A]	ASN
1	C	450[B]	ASN
2	D	434	VAL
2	D	474	ASN
2	D	532	ILE
2	D	617	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	590	GLN
1	C	56	GLN
1	C	81	HIS
1	C	107	GLN
1	C	340	ASN
1	C	412	GLN
1	C	446	ASN
2	D	463	ASN
2	D	475	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\# Z > 2$
7	BTB	C	902[B]	-	13,13,13	0.92	0	7,16,16	0.36	0
7	BTB	C	902[A]	6	13,13,13	0.87	0	7,16,16	0.40	0
5	GOL	A	501	-	5,5,5	0.12	0	5,5,5	0.37	0
5	GOL	C	903	-	5,5,5	0.12	0	5,5,5	0.37	0
5	GOL	E	101	-	5,5,5	0.06	0	5,5,5	0.18	0
5	GOL	C	904	-	5,5,5	0.13	0	5,5,5	0.37	0
5	GOL	C	905	-	5,5,5	0.17	0	5,5,5	0.40	0
5	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.23	0
5	GOL	C	906	-	5,5,5	0.09	0	5,5,5	0.22	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
7	BTB	C	902[B]	-	-	2/21/21/21	-
7	BTB	C	902[A]	6	-	4/21/21/21	-
5	GOL	A	501	-	-	2/4/4/4	-
5	GOL	C	903	-	-	1/4/4/4	-
5	GOL	E	101	-	-	0/4/4/4	-
5	GOL	C	904	-	-	2/4/4/4	-
5	GOL	C	905	-	-	2/4/4/4	-
5	GOL	A	502	-	-	0/4/4/4	-
5	GOL	C	906	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

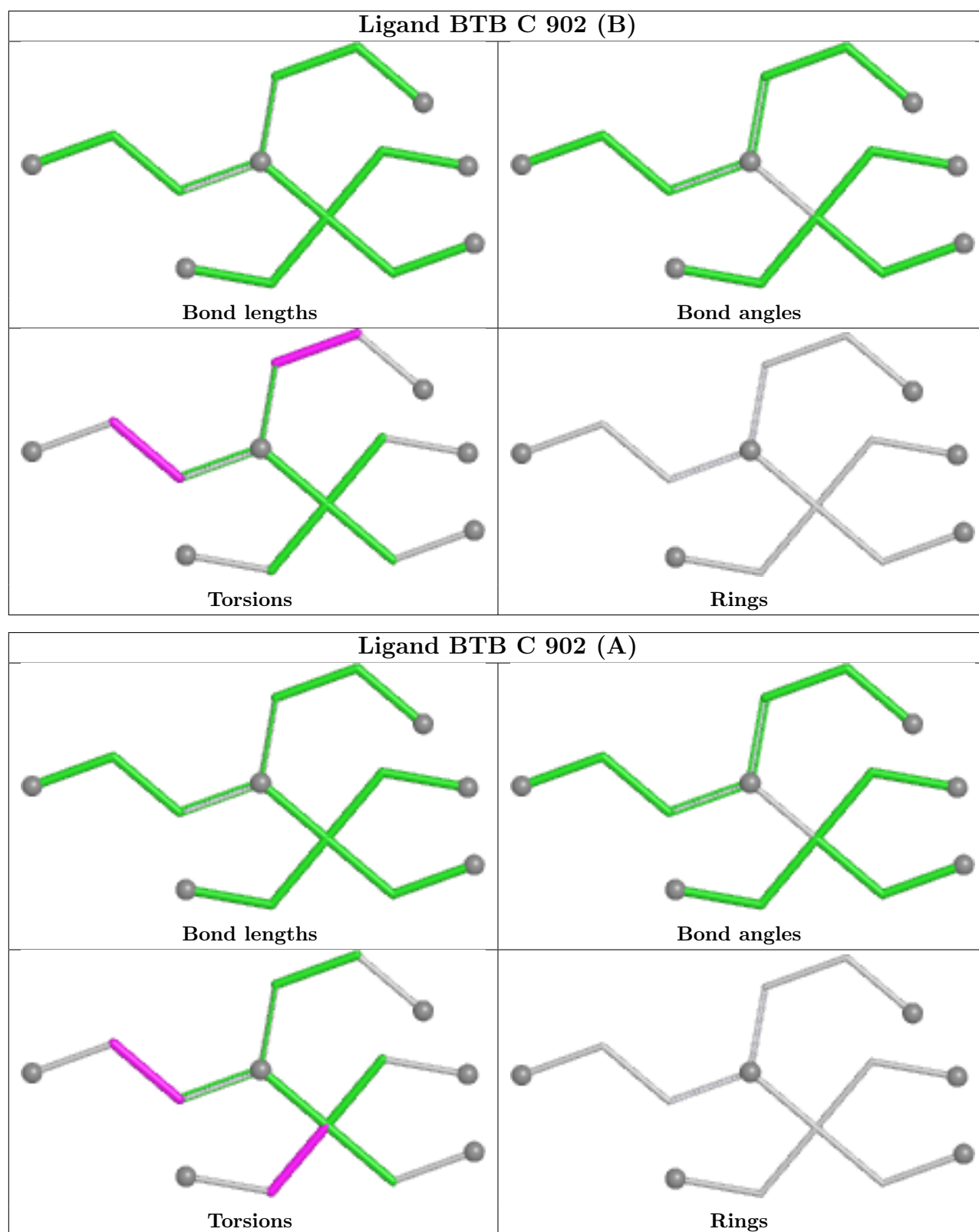
Mol	Chain	Res	Type	Atoms
5	A	501	GOL	O1-C1-C2-C3
5	C	904	GOL	C1-C2-C3-O3
7	C	902[A]	BTB	O1-C1-C2-C3
7	C	902[A]	BTB	O1-C1-C2-C4
7	C	902[A]	BTB	O1-C1-C2-N
7	C	902[B]	BTB	N-C5-C6-O6
7	C	902[A]	BTB	N-C7-C8-O8
5	C	905	GOL	C1-C2-C3-O3
5	A	501	GOL	O1-C1-C2-O2
5	C	905	GOL	O2-C2-C3-O3
5	C	904	GOL	O2-C2-C3-O3
7	C	902[B]	BTB	N-C7-C8-O8
5	C	903	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	902[A]	BTB	2	0
5	E	101	GOL	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	545:GLY	C	580:TYR	N	3.31

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	483/483 (100%)	-1.50	0 100 100	25, 59, 82, 106	4 (0%)
1	C	481/483 (99%)	-1.50	0 100 100	24, 60, 81, 97	8 (1%)
2	B	190/190 (100%)	-1.45	0 100 100	47, 68, 91, 123	0
2	D	189/190 (99%)	-1.29	0 100 100	52, 83, 116, 155	2 (1%)
3	E	8/8 (100%)	-1.87	0 100 100	54, 60, 62, 67	0
3	F	8/8 (100%)	-1.93	0 100 100	54, 62, 73, 76	0
4	G	12/14 (85%)	-1.73	0 100 100	49, 60, 109, 127	1 (8%)
4	H	12/14 (85%)	-1.70	0 100 100	41, 66, 131, 132	0
All	All	1383/1390 (99%)	-1.47	0 100 100	24, 63, 93, 155	15 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

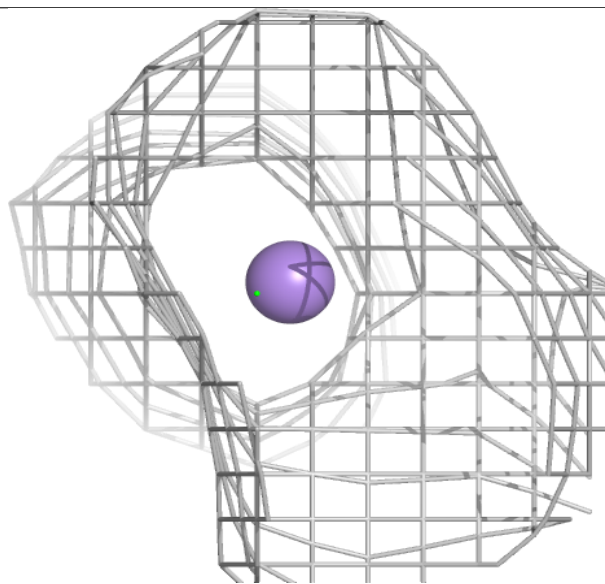
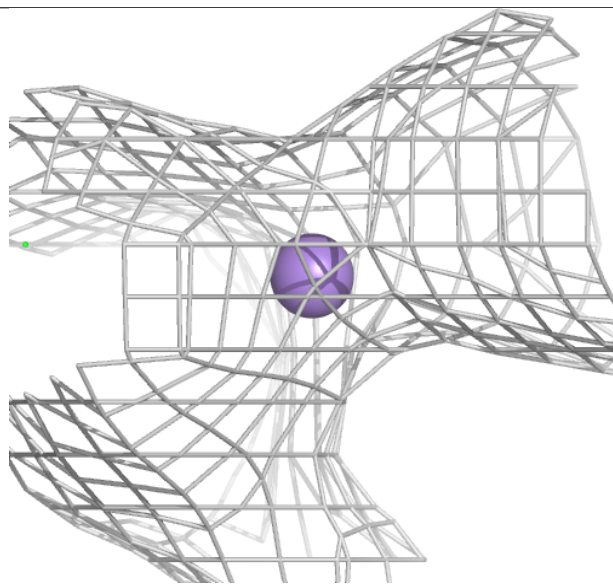
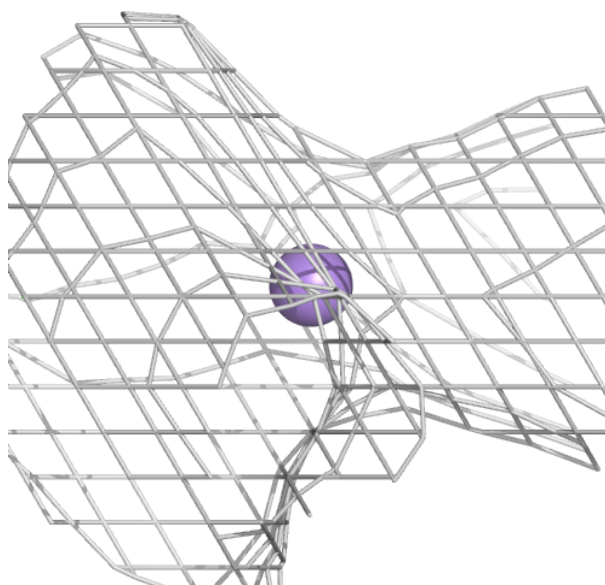
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	GOL	C	906	6/6	0.96	0.05	104,110,121,126	0
5	GOL	C	905	6/6	0.98	0.06	62,69,78,80	0
5	GOL	C	903	6/6	0.99	0.06	76,84,92,98	0
5	GOL	C	904	6/6	0.99	0.05	117,122,126,129	0
5	GOL	A	501	6/6	0.99	0.03	68,84,85,90	0
5	GOL	A	502	6/6	0.99	0.07	68,74,82,89	0
5	GOL	E	101	6/6	0.99	0.06	94,99,105,109	0
6	MN	C	901[A]	1/1	0.99	0.05	60,60,60,60	1
6	MN	G	2101	1/1	0.99	0.03	89,89,89,89	1
7	BTB	C	902[A]	14/14	0.99	0.07	57,59,61,63	14
7	BTB	C	902[B]	14/14	0.99	0.07	160,182,187,190	14
6	MN	H	2101	1/1	1.00	0.02	98,98,98,98	1
6	MN	D	701	1/1	1.00	0.01	59,59,59,59	0
6	MN	B	701	1/1	1.00	0.03	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.

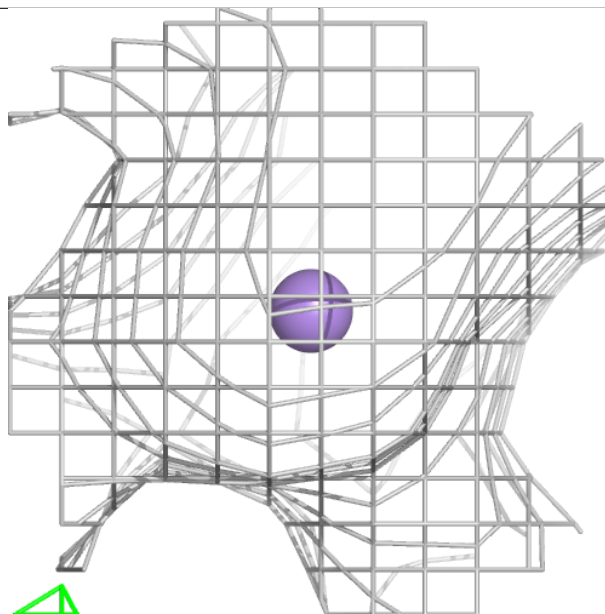
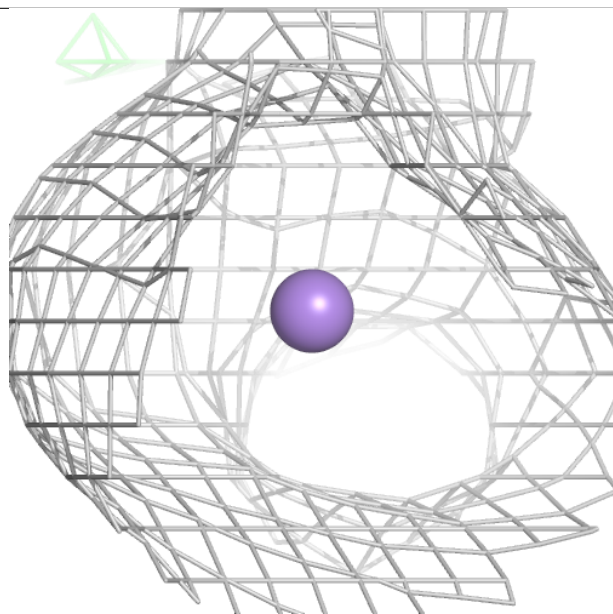
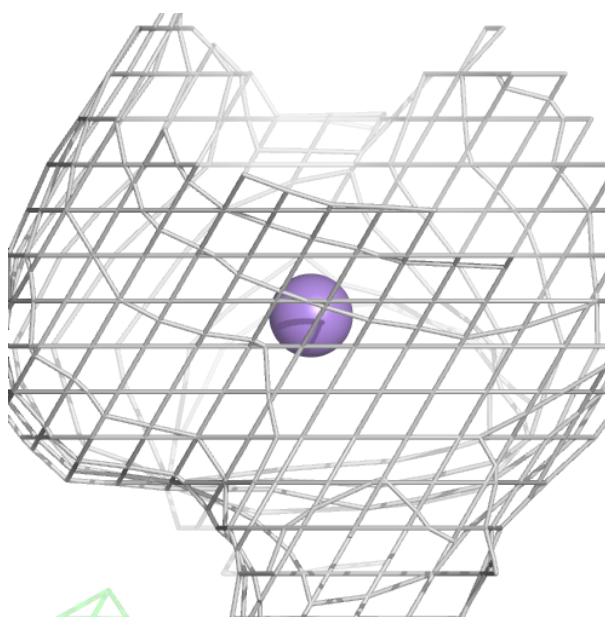
Electron density around MN C 901 (A):

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



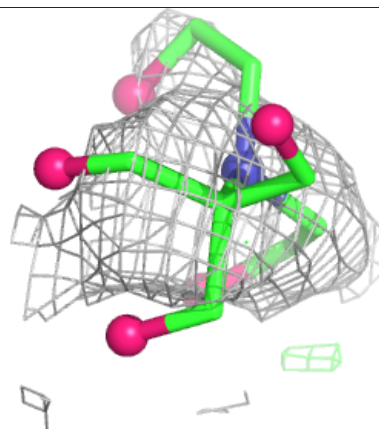
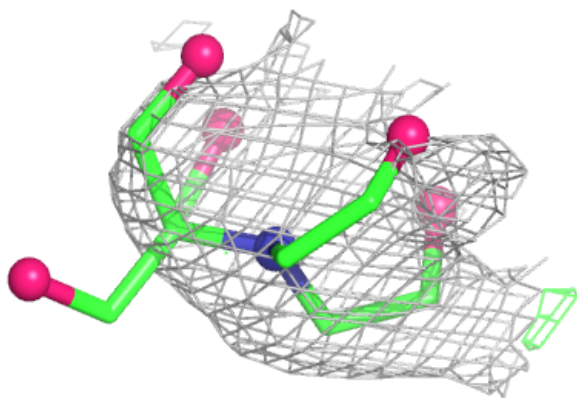
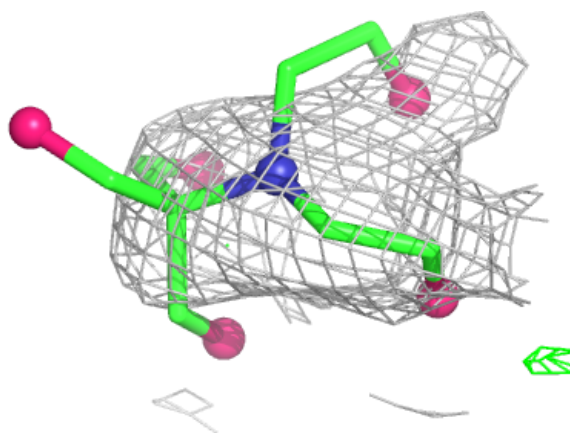
Electron density around MN G 2101:

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



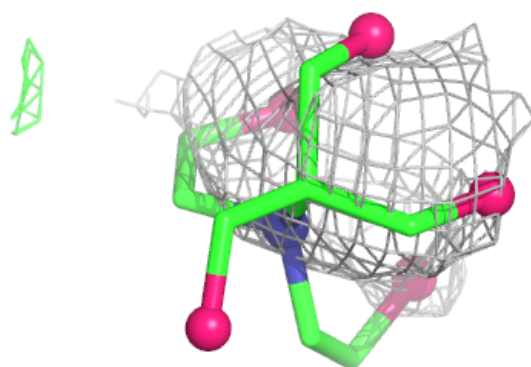
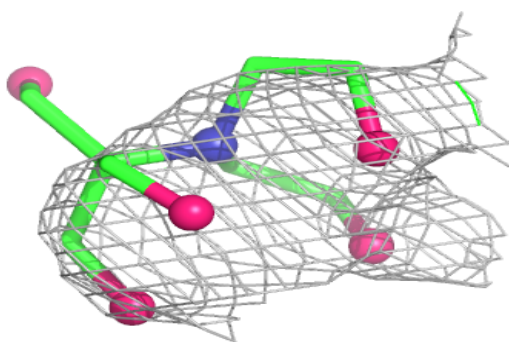
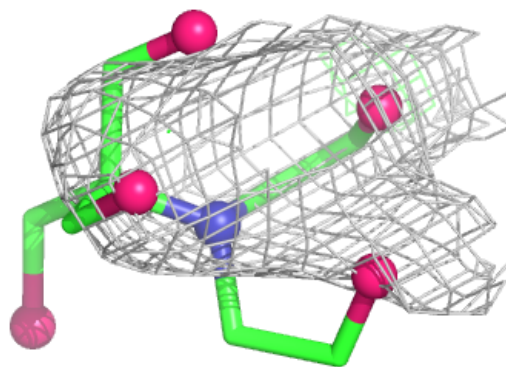
Electron density around BTB C 902 (A):

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



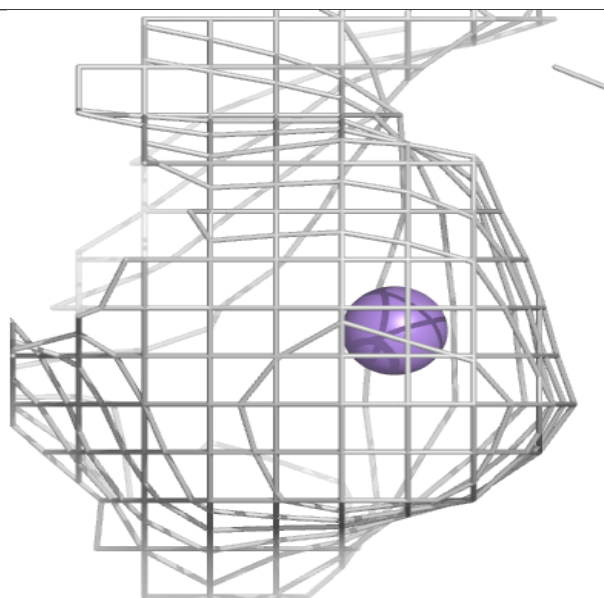
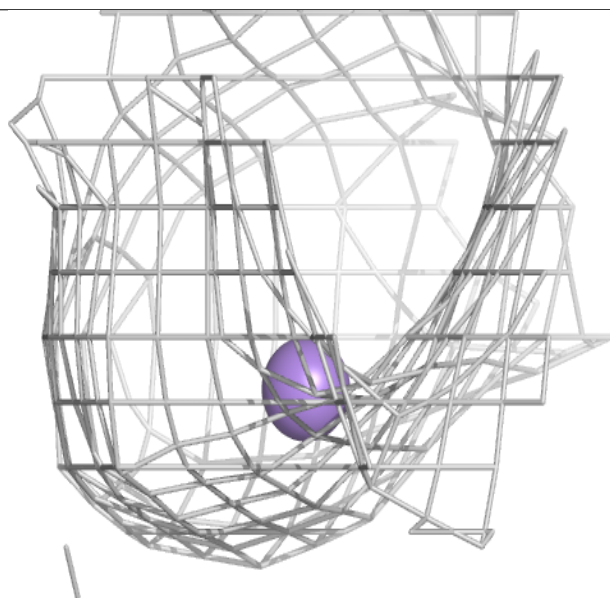
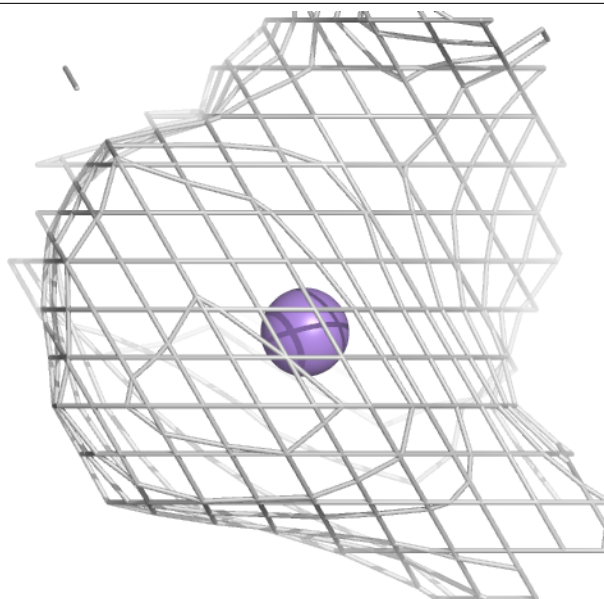
Electron density around BTB C 902 (B):

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



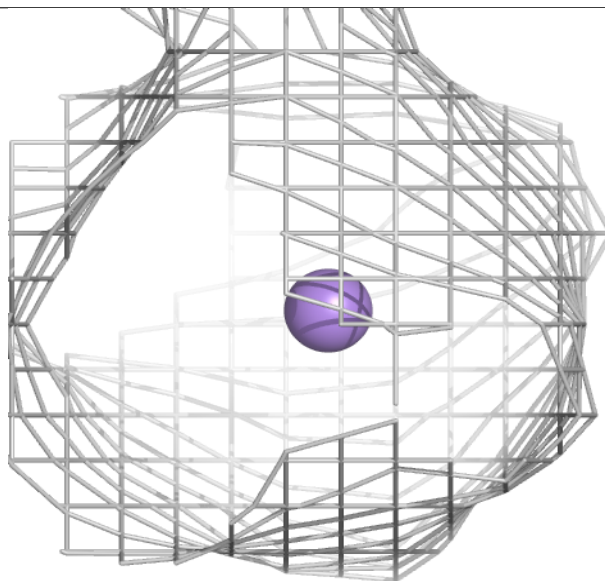
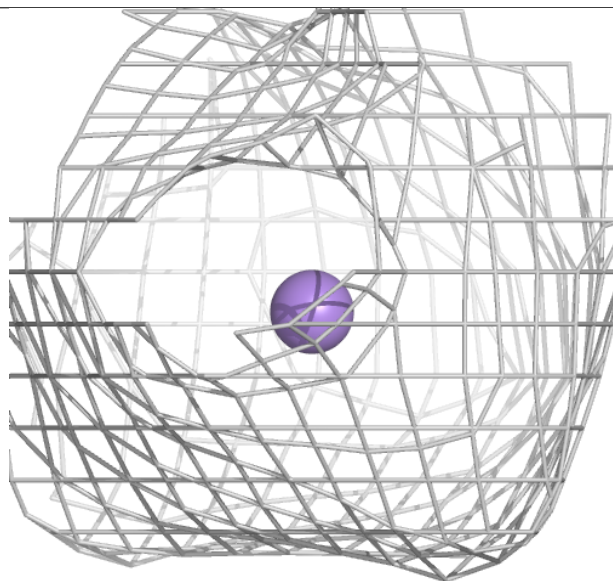
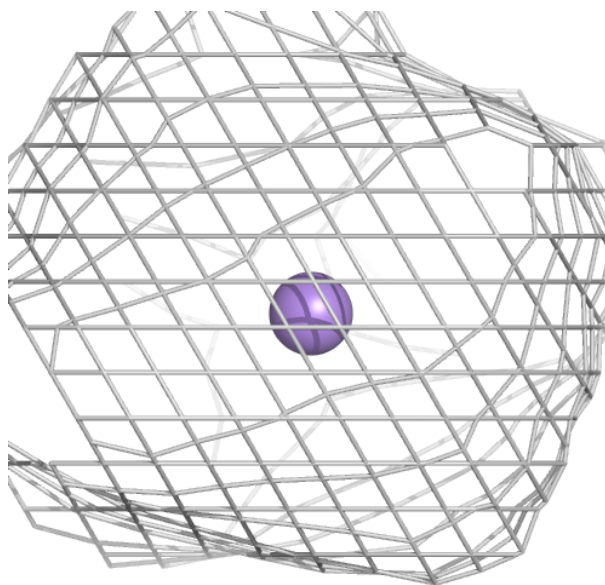
Electron density around MN H 2101:

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



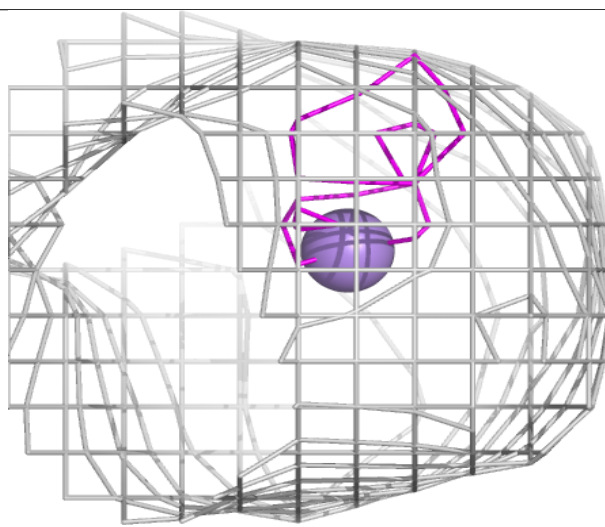
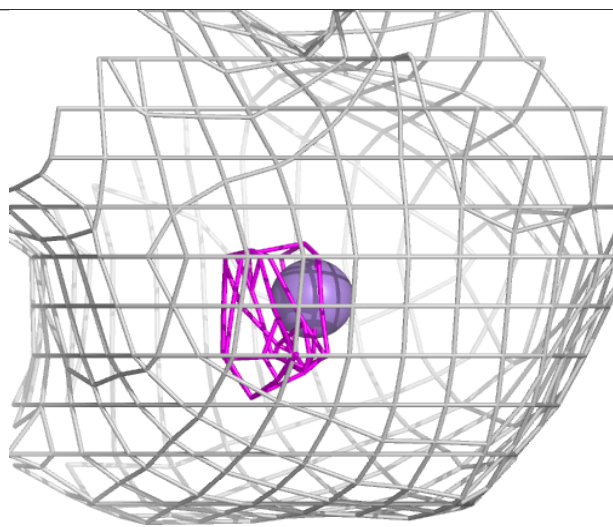
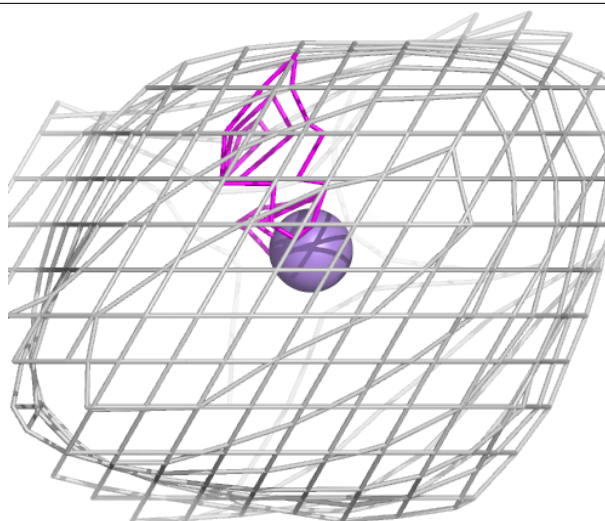
Electron density around MN D 701:

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



Electron density around MN B 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.