wwPDB X-ray Structure Validation Summary Report (i)

Jul 14, 2022 – 01:18 pm BST

PDB ID	:	7Z5O
Title	:	W-formate dehydrogenase from Desulfovibrio vulgaris - Dithionite reduced form
Authors	:	Mota, C.; Oliveira, A.R.; Klymanska, K.; Pereira, I.C.; Romao, M.J.
Deposited on	:	2022-03-09
Resolution	:	1.53 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

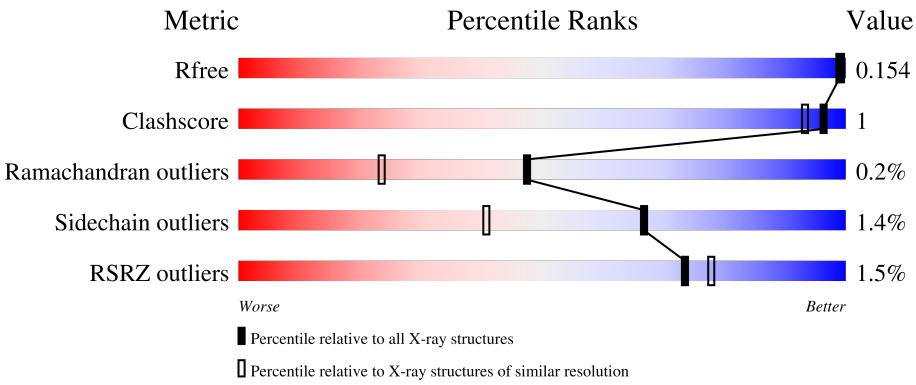
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

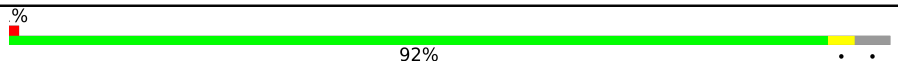
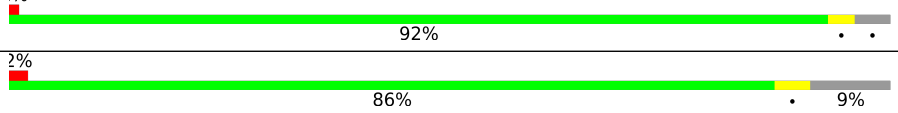
The reported resolution of this entry is 1.53 Å.

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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	AAA	1009	
2	BBB	236	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10136 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 Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	AAA	964	7547	4811	1315	1379	41	1	0	0	0

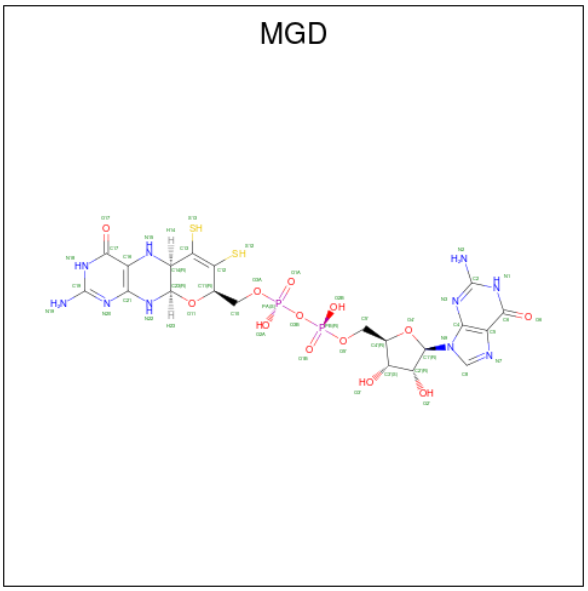
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1006	TRP	-	expression tag	UNP Q72EJ1
AAA	1007	SER	-	expression tag	UNP Q72EJ1
AAA	1008	HIS	-	expression tag	UNP Q72EJ1
AAA	1009	PRO	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

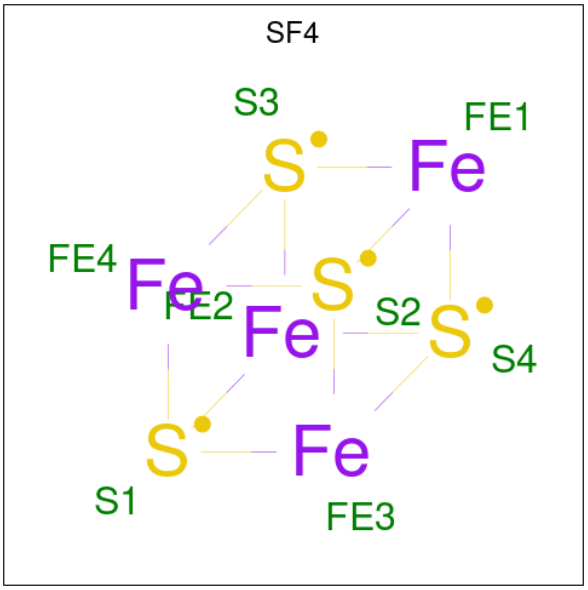
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	214	1664	1041	291	316	16	0	0	0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	AAA	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
3	AAA	1	47	20	10	13	2	2	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	AAA	1	8	4	4	0	0
			Total	Fe	S		
4	BBB	1	8	4	4	0	0

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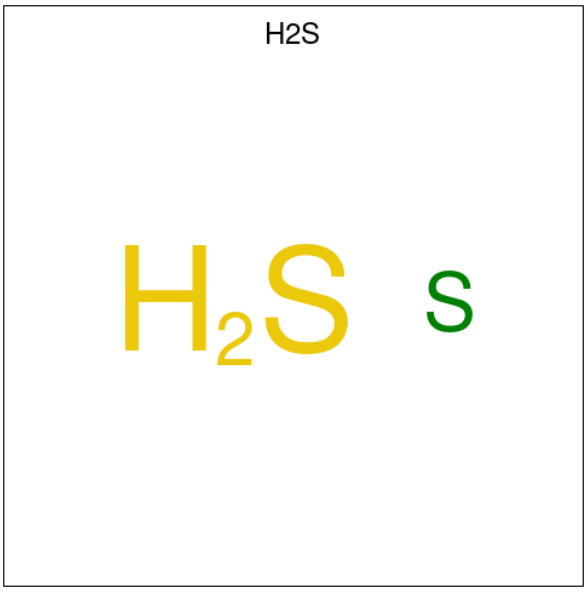
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	BBB	1	8	4	4	0	0
			Total	Fe	S		
4	BBB	1	8	4	4	0	0

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).

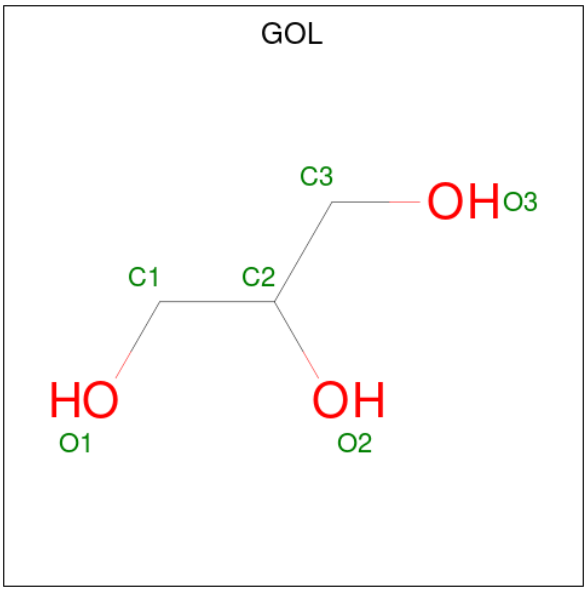


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	S		
5	AAA	1	1	1	0	0

- Molecule 6 is TUNGSTEN ION (three-letter code: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

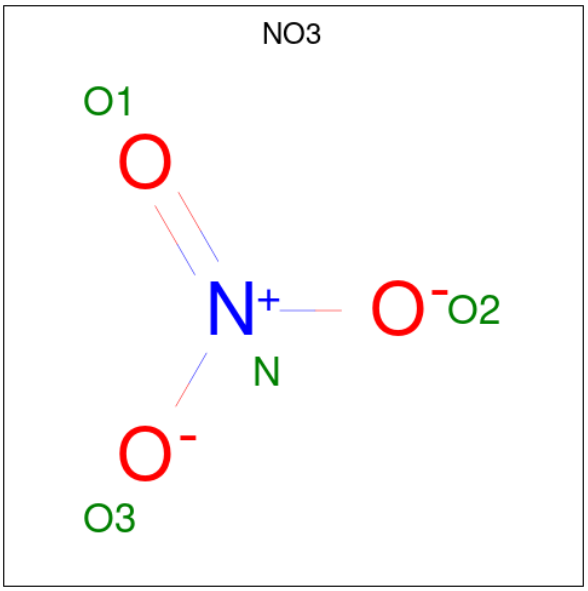
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	W		
6	AAA	1	1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



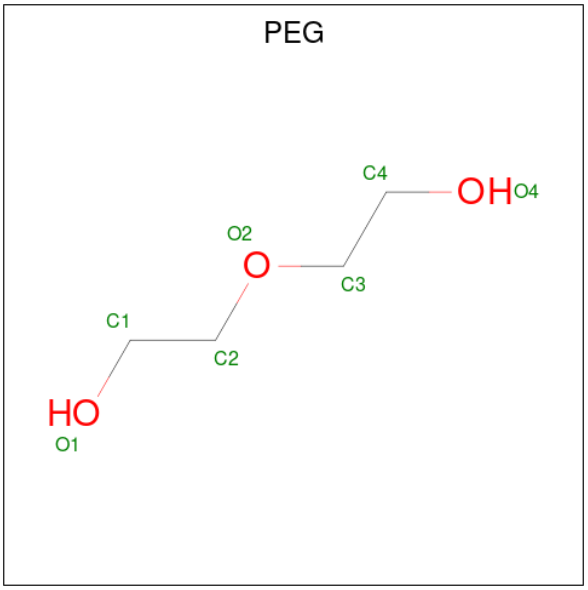
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0
			Total	C	O		
7	AAA	1	6	3	3	0	0

- Molecule 8 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
8	AAA	1	4	1	3	0	0
			Total	N	O		
8	AAA	1	4	1	3	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	AAA	1	7	4	3	0	0

- Molecule 10 is water.

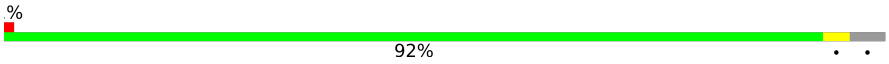
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	AAA	582	591	591	0	8
			Total	O		
10	BBB	140	143	143	0	3

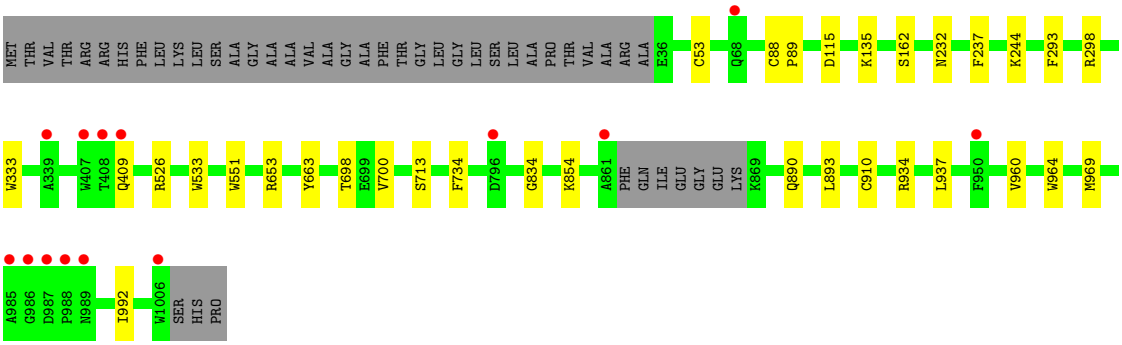
3 Residue-property plots (i)

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: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain AAA:





• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain BBB:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.81Å 124.15Å 149.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.74 – 1.53 95.55 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.74-1.53) 99.6 (95.55-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.119 , 0.153 0.120 , 0.154	Depositor DCC
R_{free} test set	9121 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: H2S, W, GOL, SEC, NO3, PEG, MGD, SF4

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	AAA	0.63	0/7749	0.72	0/10513
2	BBB	0.61	0/1699	0.70	0/2302
All	All	0.63	0/9448	0.72	0/12815

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	7547	0	7376	14	0
2	BBB	1664	0	1633	5	0
3	AAA	94	0	44	1	0
4	AAA	8	0	0	0	0
4	BBB	24	0	0	0	0
5	AAA	1	0	0	0	0
6	AAA	1	0	0	0	0
7	AAA	48	0	64	1	0
8	AAA	8	0	0	0	0
9	AAA	7	0	10	0	0
10	AAA	591	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BBB	143	0	0	0	0
All	All	10136	0	9127	19	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 1.

The worst 5 of 19 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:BBB:146:GLN:HE21	2:BBB:146:GLN:HA	1.70	0.55
1:AAA:910:CYS:SG	1:AAA:960:VAL:HG13	2.48	0.54
1:AAA:88:CYS:HB2	1:AAA:89:PRO:HD2	1.92	0.50
1:AAA:890:GLN:HA	1:AAA:964:TRP:CH2	2.49	0.48
1:AAA:526:ARG:NH2	10:AAA:1207:HOH:O	2.46	0.48

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)
10:AAA:1669:HOH:O	10:AAA:1707:HOH:O[3_455]	1.97	0.23

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	AAA	959/1009 (95%)	938 (98%)	19 (2%)	2 (0%)	47 23
2	BBB	212/236 (90%)	204 (96%)	8 (4%)	0	100 100
All	All	1171/1245 (94%)	1142 (98%)	27 (2%)	2 (0%)	47 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	533	TRP
1	AAA	663	TYR

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	AAA	783/815 (96%)	773 (99%)	10 (1%)	69	43
2	BBB	185/204 (91%)	181 (98%)	4 (2%)	52	21
All	All	968/1019 (95%)	954 (99%)	14 (1%)	67	41

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	854	LYS
1	AAA	934	ARG
2	BBB	168	GLN
2	BBB	98	GLU
2	BBB	146	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 17 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	GOL	AAA	1114	-	5,5,5	0.08	0	5,5,5	0.32	0
7	GOL	AAA	1111	-	5,5,5	0.12	0	5,5,5	0.35	0
7	GOL	AAA	1106	-	5,5,5	0.16	0	5,5,5	0.39	0
7	GOL	AAA	1109	-	5,5,5	0.10	0	5,5,5	0.31	0
7	GOL	AAA	1110	-	5,5,5	0.16	0	5,5,5	0.37	0
7	GOL	AAA	1108	-	5,5,5	0.15	0	5,5,5	0.39	0
8	NO3	AAA	1116	-	1,3,3	0.12	0	0,3,3	-	-
7	GOL	AAA	1107	-	5,5,5	0.17	0	5,5,5	0.40	0
4	SF4	BBB	303	2	0,12,12	-	-	-		
7	GOL	AAA	1112	-	5,5,5	0.11	0	5,5,5	0.30	0
4	SF4	BBB	301	2	0,12,12	-	-	-		
4	SF4	AAA	1103	1	0,12,12	-	-	-		
4	SF4	BBB	302	2	0,12,12	-	-	-		
3	MGD	AAA	1101	6	41,52,52	0.87	2 (4%)	40,81,81	1.05	2 (5%)
3	MGD	AAA	1102	6	41,52,52	0.81	1 (2%)	40,81,81	1.17	4 (10%)
8	NO3	AAA	1113	-	1,3,3	0.07	0	0,3,3	-	-
9	PEG	AAA	1115	-	6,6,6	0.21	0	5,5,5	0.12	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	GOL	AAA	1114	-	-	4/4/4/4	-
7	GOL	AAA	1111	-	-	0/4/4/4	-
7	GOL	AAA	1106	-	-	0/4/4/4	-
7	GOL	AAA	1109	-	-	3/4/4/4	-
7	GOL	AAA	1110	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	AAA	1108	-	-	0/4/4/4	-
7	GOL	AAA	1107	-	-	0/4/4/4	-
4	SF4	BBB	303	2	-	-	0/6/5/5
7	GOL	AAA	1112	-	-	3/4/4/4	-
3	MGD	AAA	1101	6	-	1/18/66/66	0/6/6/6
4	SF4	AAA	1103	1	-	-	0/6/5/5
4	SF4	BBB	301	2	-	-	0/6/5/5
4	SF4	BBB	302	2	-	-	0/6/5/5
3	MGD	AAA	1102	6	-	4/18/66/66	0/6/6/6
9	PEG	AAA	1115	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	1101	MGD	C5-C6	-2.66	1.42	1.47
3	AAA	1102	MGD	C5-C6	-2.44	1.42	1.47
3	AAA	1101	MGD	C8-N7	-2.03	1.31	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	1102	MGD	O11-C23-C14	3.23	111.12	108.96
3	AAA	1102	MGD	C19-N20-C21	3.06	118.96	113.43
3	AAA	1101	MGD	C19-N20-C21	2.56	118.05	113.43
3	AAA	1102	MGD	O6-C6-C5	2.53	129.31	124.37
3	AAA	1101	MGD	O6-C6-C5	2.32	128.91	124.37

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1102	MGD	C4'-C5'-O5'-PB
7	AAA	1110	GOL	C1-C2-C3-O3
7	AAA	1112	GOL	C1-C2-C3-O3
3	AAA	1102	MGD	O4'-C4'-C5'-O5'
3	AAA	1102	MGD	C3'-C4'-C5'-O5'

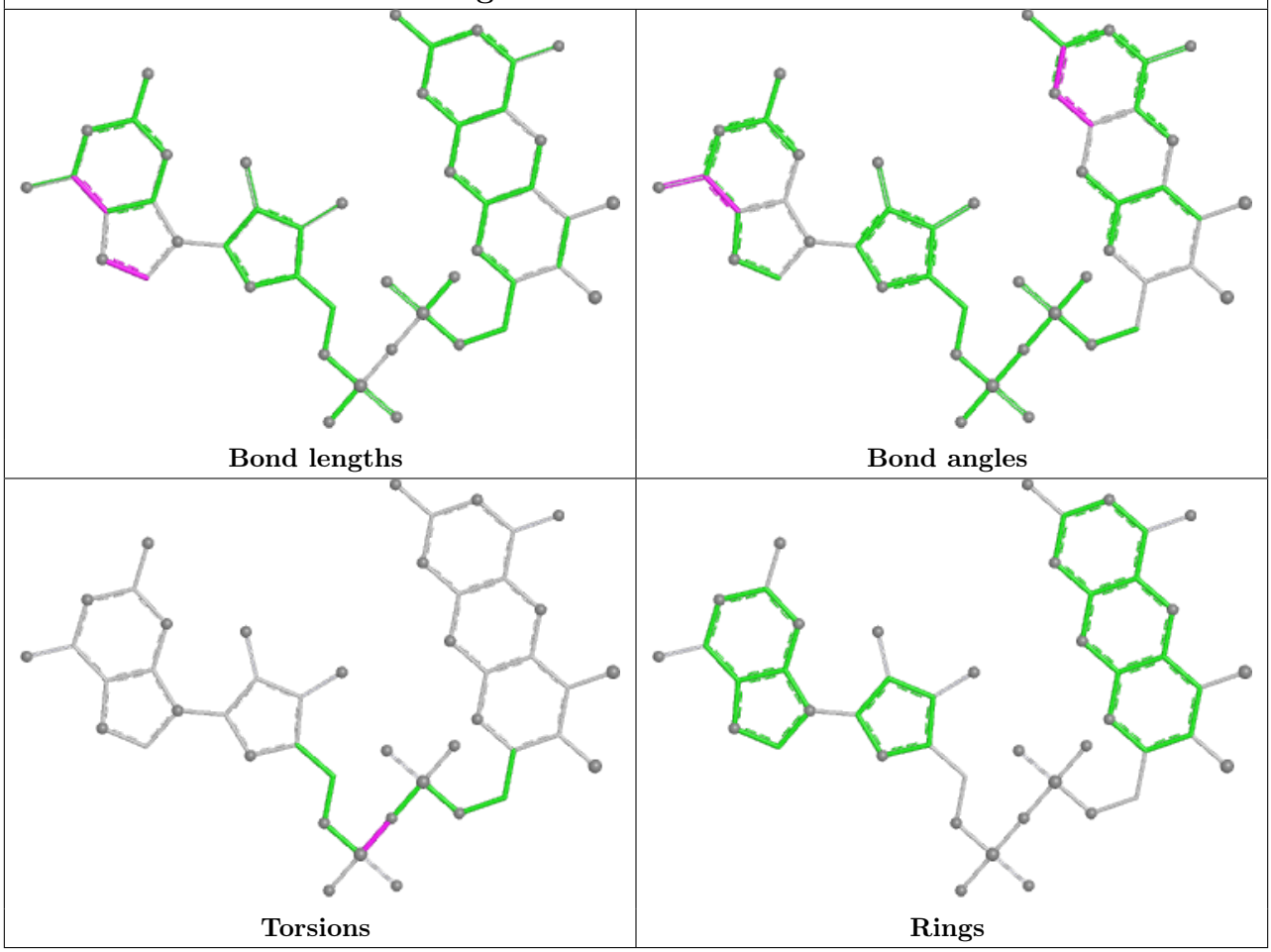
There are no ring outliers.

2 monomers are involved in 2 short contacts:

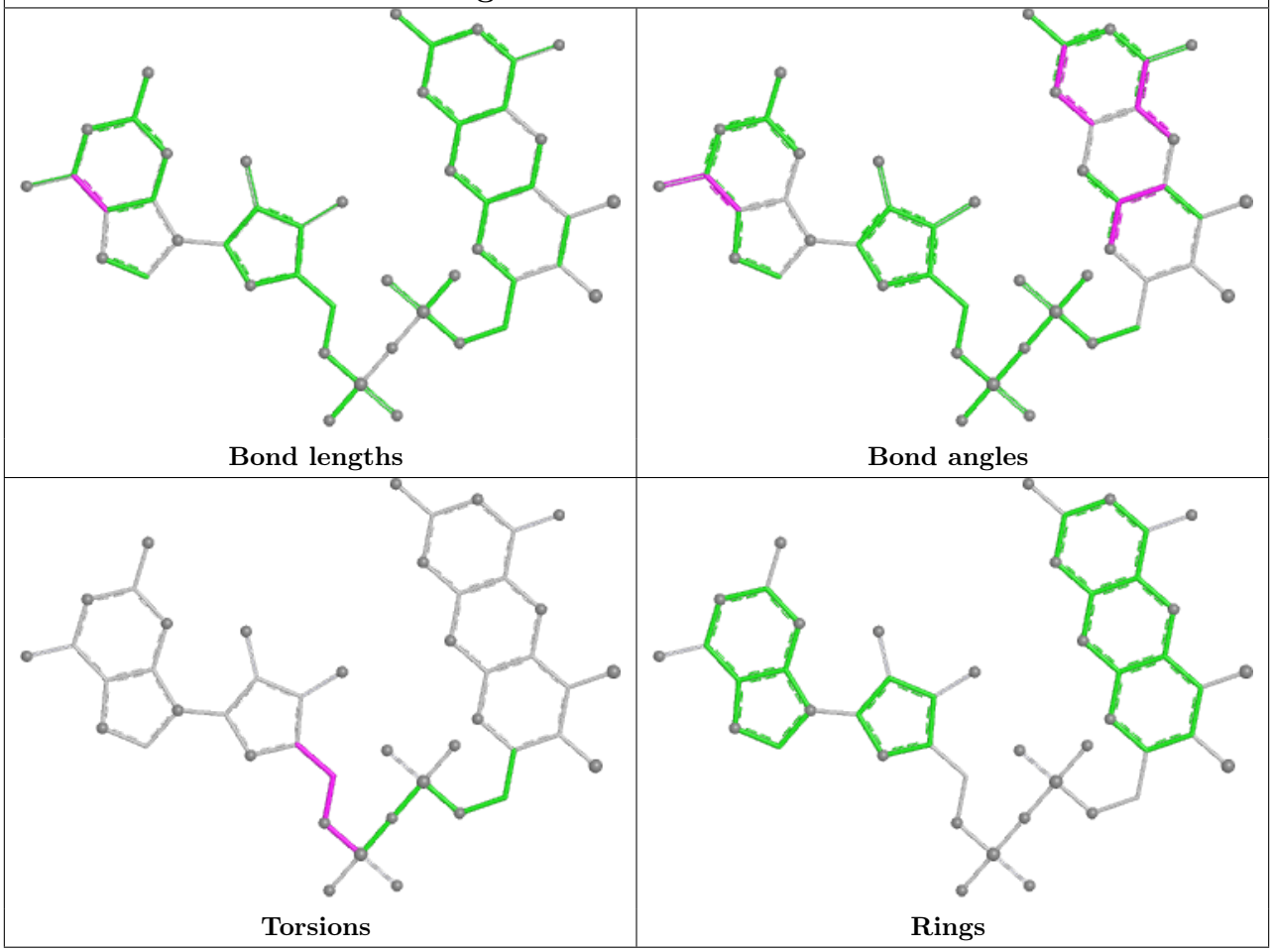
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	1114	GOL	1	0
3	AAA	1101	MGD	1	0

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 then 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.

Ligand MGD AAA 1101



Ligand MGD AAA 1102



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 (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	AAA	963/1009 (95%)	-0.07	14 (1%)	73	78	12, 22, 42, 83	0
2	BBB	214/236 (90%)	0.00	4 (1%)	66	71	13, 24, 48, 64	0
All	All	1177/1245 (94%)	-0.06	18 (1%)	73	78	12, 22, 45, 83	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1006	TRP	8.9
1	AAA	988	PRO	7.5
1	AAA	339	ALA	4.4
1	AAA	985	ALA	4.2
1	AAA	407	TRP	3.5

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)

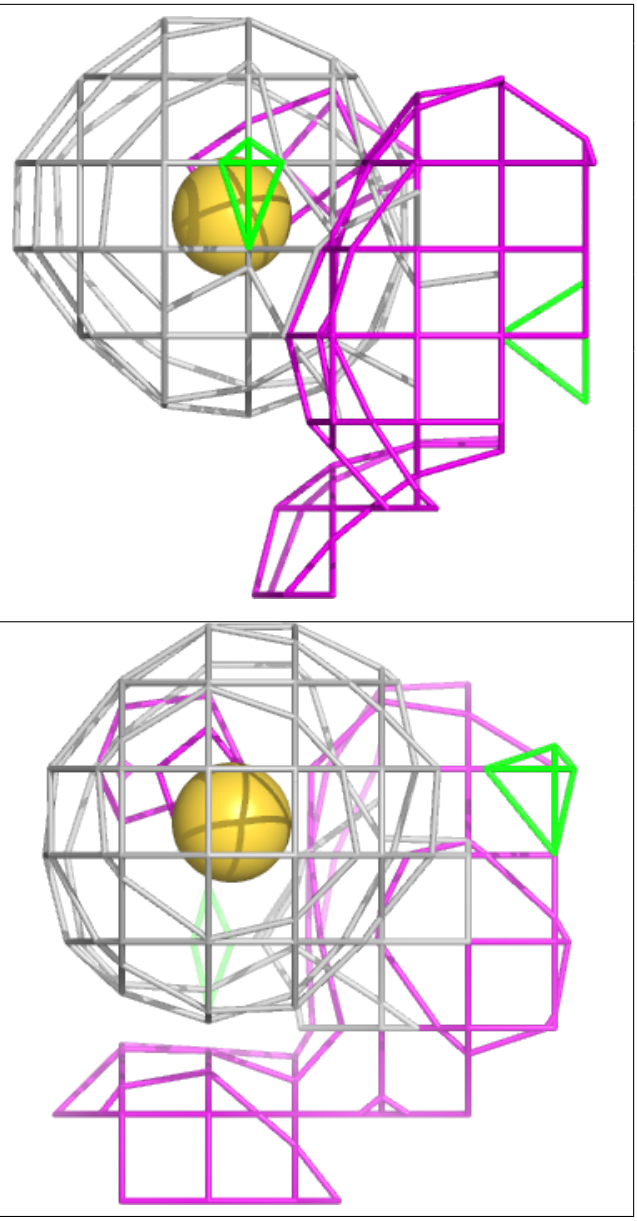
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	AAA	1110	6/6	0.69	0.29	36,36,38,38	0
8	NO3	AAA	1113	4/4	0.70	0.14	45,49,59,62	0
7	GOL	AAA	1112	6/6	0.83	0.22	45,50,55,70	0
7	GOL	AAA	1114	6/6	0.88	0.11	52,58,62,63	0
7	GOL	AAA	1109	6/6	0.91	0.18	27,30,32,34	0
7	GOL	AAA	1111	6/6	0.93	0.14	35,49,52,64	0
8	NO3	AAA	1116	4/4	0.93	0.09	63,66,73,77	0
9	PEG	AAA	1115	7/7	0.94	0.09	37,58,63,65	0
7	GOL	AAA	1108	6/6	0.95	0.06	27,28,31,36	0
7	GOL	AAA	1106	6/6	0.96	0.08	15,18,18,21	0
5	H2S	AAA	1104	1/1	0.97	0.08	17,17,17,17	0
3	MGD	AAA	1101	47/47	0.97	0.08	11,13,16,18	0
7	GOL	AAA	1107	6/6	0.97	0.09	20,24,26,29	0
3	MGD	AAA	1102	47/47	0.97	0.07	14,17,20,24	0
4	SF4	BBB	302	8/8	0.98	0.08	22,24,25,25	0
4	SF4	BBB	301	8/8	0.99	0.11	13,13,13,14	0
4	SF4	AAA	1103	8/8	0.99	0.11	11,12,12,12	0
4	SF4	BBB	303	8/8	0.99	0.09	16,17,18,18	0
6	W	AAA	1105	1/1	1.00	0.06	14,14,14,14	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.

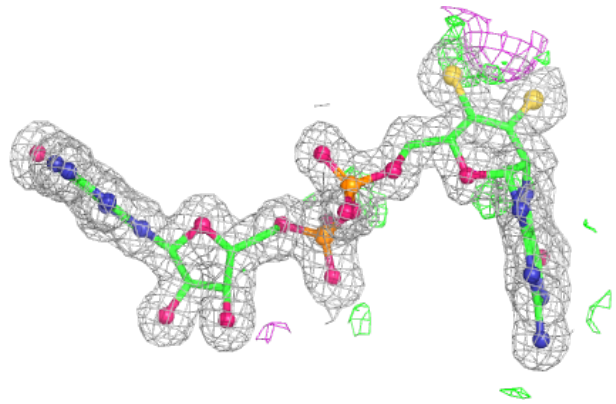
Electron density around H2S AAA 1104:

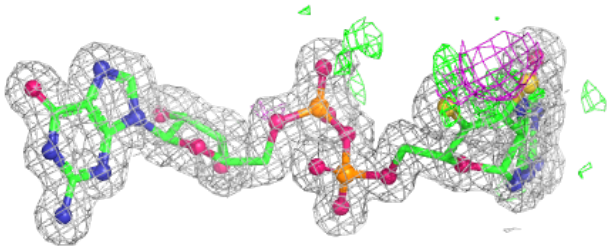
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

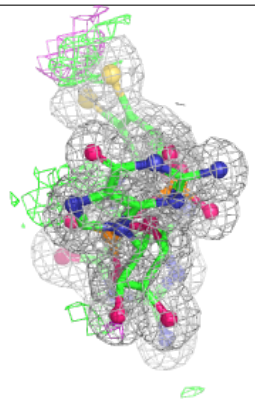


Electron density around MGD AAA 1101:

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

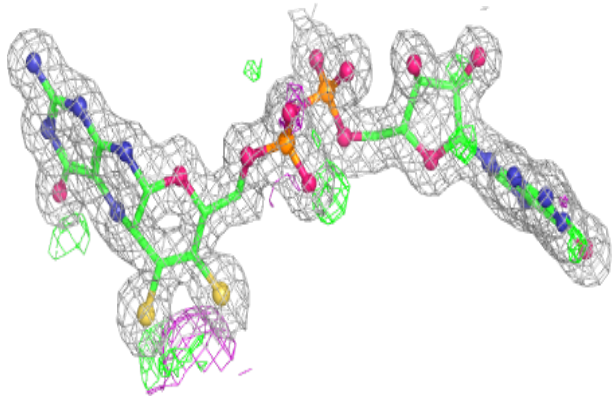


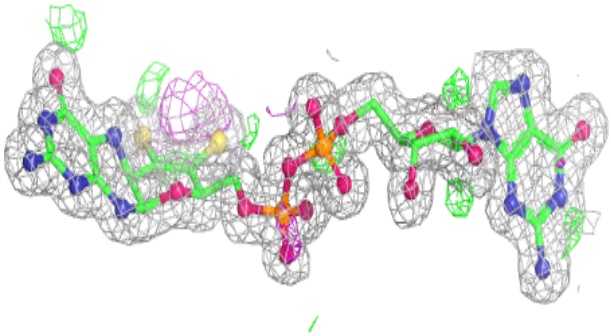


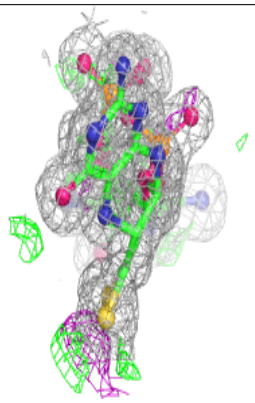


Electron density around MGD AAA 1102:

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







Electron density around W AAA 1105:

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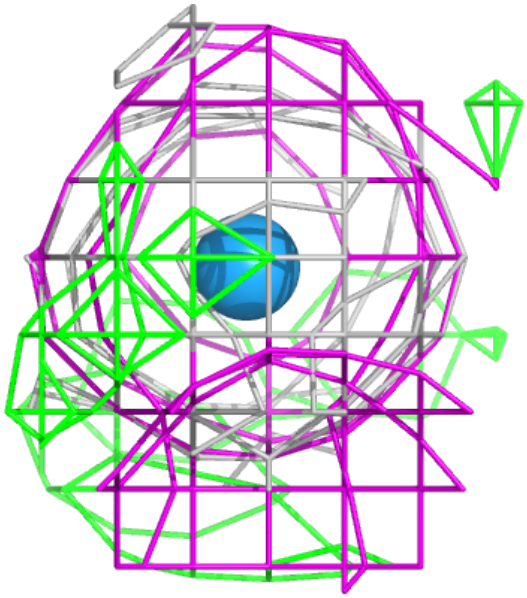
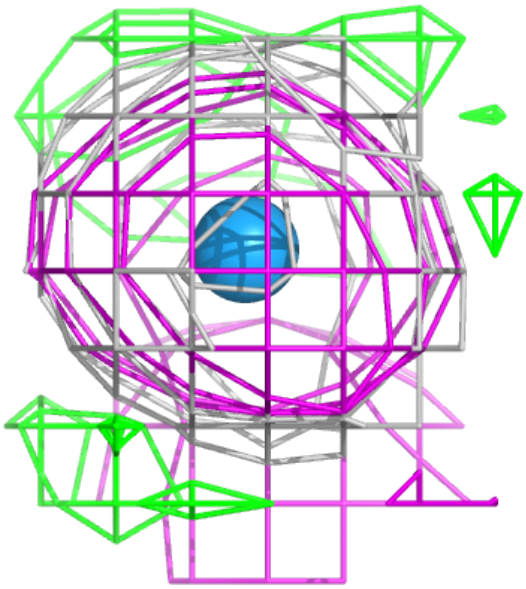
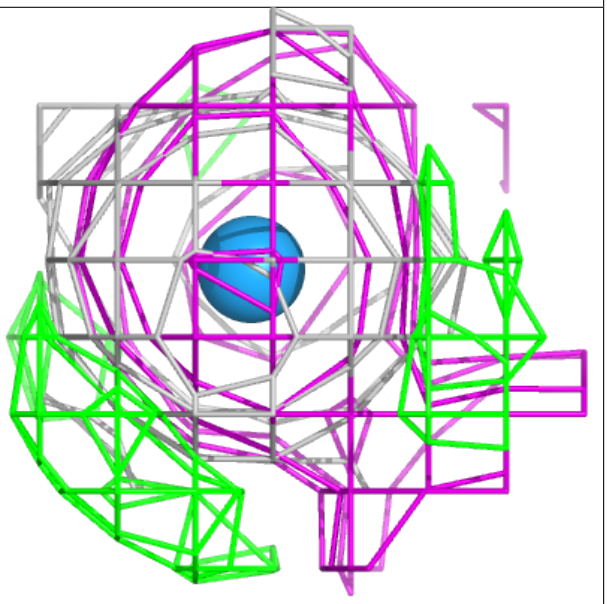
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.