Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 04:15 pm GMT

PDB ID	:	6SDR
Title	:	W-formate dehydrogenase from Desulfovibrio vulgaris - Oxidized form
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Deposited on	:	2019-07-29
Resolution	:	2.10 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 (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:

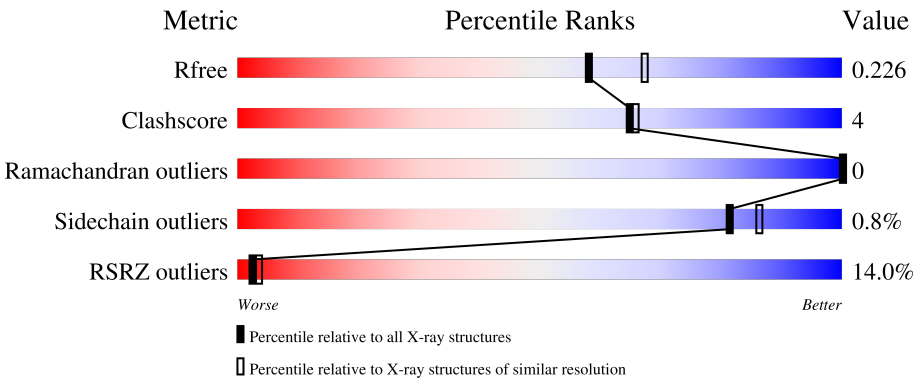
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1005	13% 87% 9% .
2	B	236	17% 81% 9% 9%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9959 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.

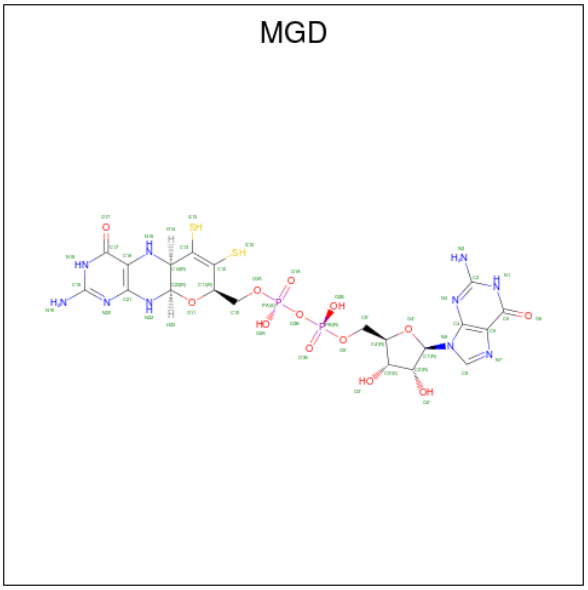
- Molecule 1 is a protein called Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	963	7533	4800	1313	1378	41	1	0	0	0

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

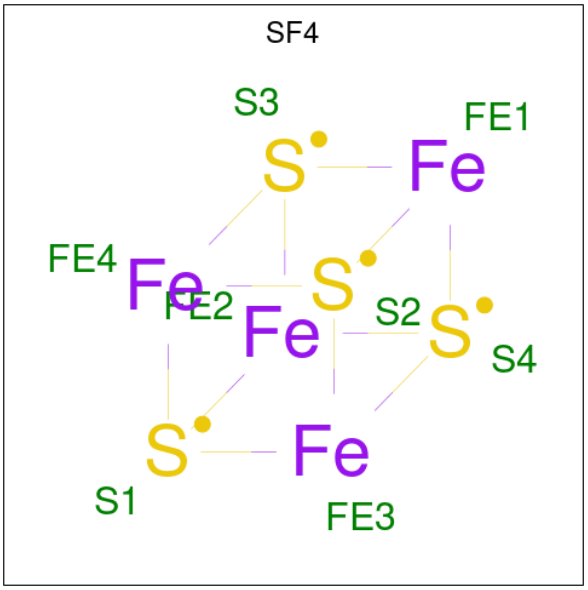
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1679	1050	294	319	16	0	2	0

- 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).



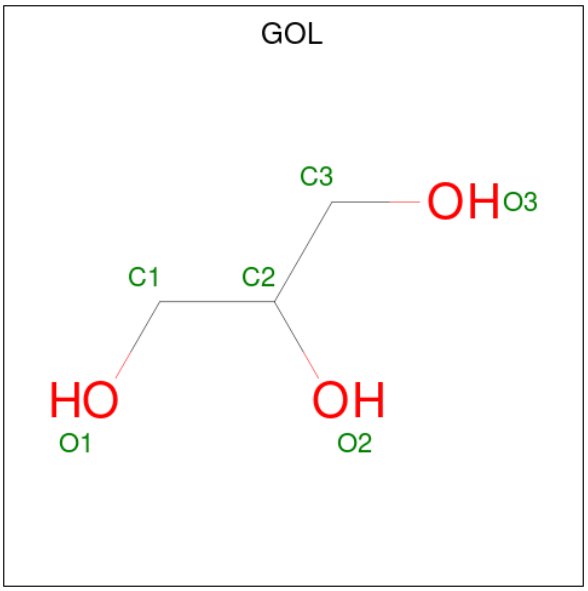
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
3	A	1	47	20	10	13	2	2	0	0

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



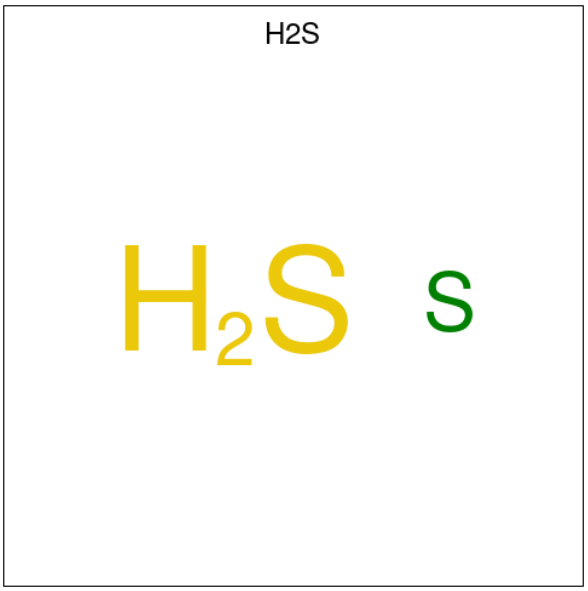
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total S 1 1	0	0

- Molecule 7 is TUNGSTEN ION (three-letter code: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total W 1 1	0	0

- Molecule 8 is water.

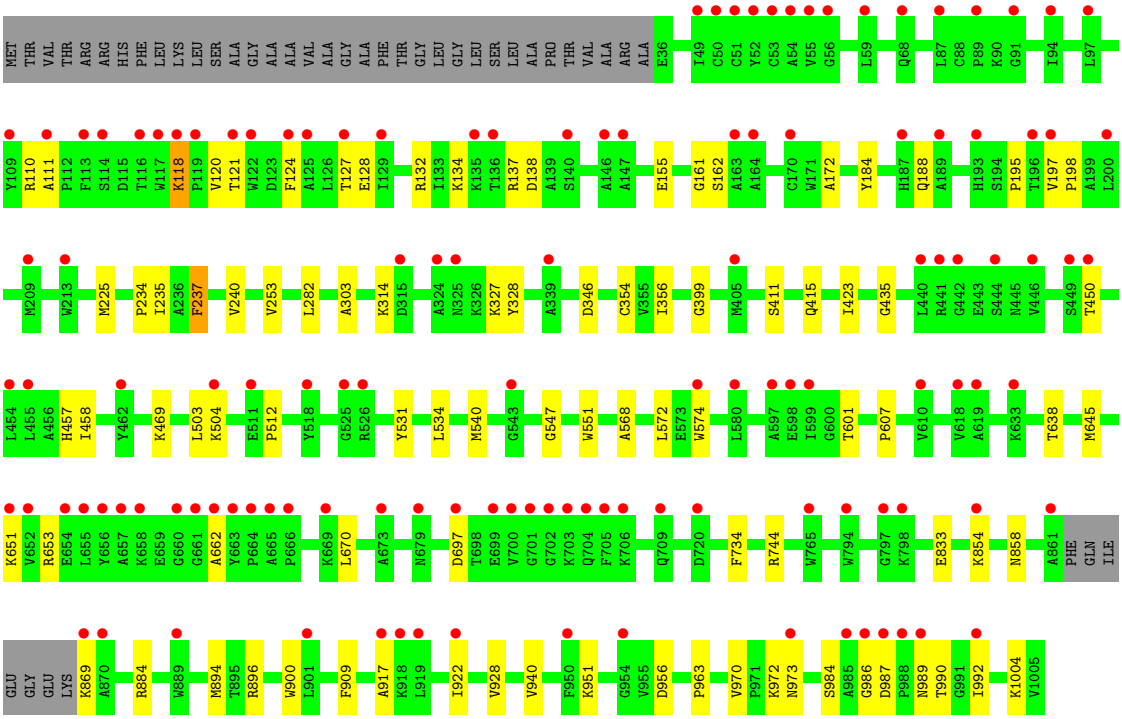
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	479	Total O 481 481	0	2
8	B	107	Total O 108 108	0	1

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.

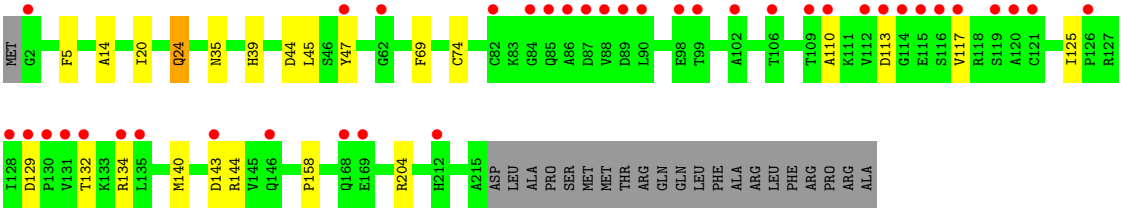
• Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain A:



• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.59Å 127.64Å 148.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.10 48.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.36-2.10) 99.0 (48.36-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.226 0.186 , 0.226	Depositor DCC
R_{free} test set	3585 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9959	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, MGD, SEC, GOL, 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	A	0.29	0/7733	0.47	0/10490
2	B	0.30	0/1717	0.47	0/2326
All	All	0.29	0/9450	0.47	0/12816

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	A	7533	0	7366	62	0
2	B	1679	0	1648	17	0
3	A	94	0	44	3	0
4	A	8	0	0	1	0
4	B	24	0	0	0	0
5	A	30	0	40	5	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	481	0	0	3	0
8	B	108	0	0	1	0
All	All	9959	0	9098	75	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 4.

All (75) 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:951:LYS:HE3	1:A:956:ASP:OD1	1.56	1.05
1:A:951:LYS:CE	1:A:956:ASP:OD1	2.23	0.86
1:A:195:PRO:HG3	1:A:992:ILE:HD13	1.70	0.73
2:B:204:ARG:NH2	8:B:500[B]:HOH:O	2.20	0.73
1:A:990:THR:HB	1:A:992:ILE:HD12	1.76	0.67
1:A:197:VAL:HG21	5:A:1107:GOL:H12	1.78	0.65
1:A:411:SER:HB2	1:A:858:ASN:HD22	1.60	0.65
1:A:303:ALA:HB1	1:A:356:ILE:HB	1.79	0.65
1:A:540:MET:HE1	1:A:572:LEU:HD11	1.80	0.64
1:A:940:VAL:HG11	2:B:35:ASN:HB3	1.81	0.62
1:A:121:THR:HG23	1:A:124:PHE:H	1.64	0.62
1:A:172:ALA:HB3	1:A:645:MET:HE1	1.84	0.59
1:A:469:LYS:NZ	8:A:1202:HOH:O	2.32	0.58
2:B:110:ALA:HB2	2:B:134:ARG:HG3	1.87	0.56
1:A:540:MET:HG2	1:A:568:ALA:HB1	1.89	0.55
2:B:132:THR:OG1	2:B:134:ARG:HD3	2.07	0.55
2:B:113:ASP:O	2:B:117:VAL:HG23	2.08	0.54
1:A:155:GLU:HG2	1:A:184:TYR:CE2	2.44	0.52
1:A:744:ARG:NH1	8:A:1214:HOH:O	2.43	0.52
1:A:195:PRO:HG3	1:A:992:ILE:CD1	2.39	0.52
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.50	0.51
1:A:235:ILE:HG13	2:B:158:PRO:HB3	1.93	0.51
2:B:47:TYR:CG	2:B:129:ASP:HB2	2.46	0.50
2:B:74:CYS:HB2	2:B:125:ILE:HG21	1.93	0.50
1:A:127:THR:HG23	1:A:651:LYS:HE3	1.93	0.50
1:A:162:SER:HB2	1:A:551:TRP:O	2.12	0.50
1:A:111:ALA:H	1:A:118:LYS:NZ	2.10	0.49
1:A:896:ARG:HD2	1:A:970:VAL:O	2.12	0.49
1:A:110:ARG:NH1	1:A:601:THR:O	2.45	0.49
1:A:922:ILE:HD13	1:A:928:VAL:HG12	1.93	0.49
5:A:1104:GOL:H31	2:B:39:HIS:CE1	2.48	0.49
1:A:450:THR:HG21	5:A:1107:GOL:H11	1.94	0.49
2:B:5:PHE:HE1	2:B:140:MET:HG3	1.78	0.48
1:A:237:PHE:HA	1:A:240:VAL:HB	1.95	0.48
1:A:120:VAL:HG21	1:A:124:PHE:CD1	2.48	0.48
1:A:884:ARG:HH22	3:A:1102:MGD:H15	1.62	0.48
5:A:1104:GOL:H31	2:B:39:HIS:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LYS:HE3	1:A:512:PRO:HG3	1.96	0.47
1:A:137:ARG:NH1	1:A:662:ALA:O	2.43	0.47
1:A:984:SER:OG	8:A:1201:HOH:O	2.20	0.47
1:A:346:ASP:HB3	1:A:354:CYS:SG	2.55	0.46
1:A:234:PRO:HD2	4:A:1103:SF4:S3	2.55	0.46
1:A:653:ARG:NH1	1:A:670:LEU:O	2.46	0.46
1:A:990:THR:CB	1:A:992:ILE:HD12	2.44	0.46
1:A:607:PRO:HB2	1:A:638:THR:HG22	1.97	0.45
1:A:225:MET:HE2	1:A:253:VAL:HG21	1.99	0.45
1:A:917:ALA:HB1	1:A:922:ILE:O	2.15	0.45
1:A:534:LEU:CD2	1:A:986:GLY:HA3	2.47	0.45
1:A:399:GLY:O	1:A:435:GLY:HA2	2.17	0.45
1:A:128:GLU:O	1:A:132:ARG:HG2	2.16	0.45
1:A:184:TYR:CE1	1:A:531:TYR:HA	2.52	0.45
1:A:450:THR:HG21	5:A:1106:GOL:H32	1.99	0.45
1:A:161:GLY:HA2	1:A:162:SER:HA	1.81	0.44
1:A:987:ASP:OD1	1:A:989:ASN:HB2	2.18	0.44
1:A:282:LEU:HD23	1:A:423:ILE:HD13	2.00	0.44
2:B:129:ASP:OD2	2:B:132:THR:HG22	2.18	0.44
1:A:951:LYS:HE2	1:A:956:ASP:OD1	2.13	0.43
1:A:547:GLY:HA3	1:A:574:TRP:CZ2	2.53	0.43
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.53	0.43
1:A:972:LYS:NZ	1:A:973:ASN:HD21	2.16	0.43
1:A:909:PHE:CE2	1:A:963:PRO:HG3	2.53	0.43
1:A:327:LYS:HG2	1:A:328:TYR:N	2.34	0.43
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.53	0.42
1:A:457:HIS:CD2	1:A:458:ILE:HG23	2.55	0.42
2:B:44:ASP:OD1	2:B:45:LEU:N	2.53	0.42
1:A:503:LEU:C	1:A:504:LYS:HE2	2.40	0.41
1:A:197:VAL:HG22	1:A:198:PRO:HD3	2.02	0.41
1:A:922:ILE:HD13	1:A:928:VAL:CG1	2.51	0.41
1:A:900:TRP:HB3	2:B:20:ILE:HG13	2.02	0.41
1:A:188:GLN:HB3	3:A:1102:MGD:S12	2.60	0.41
1:A:411:SER:HB2	1:A:858:ASN:ND2	2.31	0.41
1:A:415:GLN:HE21	1:A:833:GLU:HB2	1.86	0.41
1:A:134:LYS:NZ	1:A:138:ASP:OD2	2.31	0.40
1:A:922:ILE:HG12	1:A:1004:LYS:HB2	2.04	0.40
2:B:143:ASP:OD1	2:B:144:ARG:N	2.53	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	958/1005 (95%)	930 (97%)	28 (3%)	0	100	100
2	B	214/236 (91%)	209 (98%)	5 (2%)	0	100	100
All	All	1172/1241 (94%)	1139 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	782/811 (96%)	775 (99%)	7 (1%)	78	84
2	B	187/204 (92%)	186 (100%)	1 (0%)	88	92
All	All	969/1015 (96%)	961 (99%)	8 (1%)	81	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	237	PHE
1	A	314	LYS
1	A	697	ASP
1	A	734	PHE
1	A	854	LYS
1	A	869	LYS
2	B	24	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	679	ASN
1	A	973	ASN
1	A	989	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 11 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	MGD	A	1102	7	41,52,52	1.30	4 (9%)	40,81,81	1.95	11 (27%)
4	SF4	A	1103	1	0,12,12	-	-	-		
3	MGD	A	1101	7	41,52,52	1.24	6 (14%)	40,81,81	2.15	11 (27%)
5	GOL	A	1106	-	5,5,5	0.99	0	5,5,5	0.86	0
5	GOL	A	1108	-	5,5,5	0.84	0	5,5,5	1.07	0
5	GOL	A	1104	-	5,5,5	1.05	0	5,5,5	0.85	0
5	GOL	A	1107	-	5,5,5	0.89	0	5,5,5	1.07	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	B	302	2	0,12,12	-	-	-		
4	SF4	B	301	2	0,12,12	-	-	-		
5	GOL	A	1105	-	5,5,5	0.89	0	5,5,5	0.95	0
4	SF4	B	303	2	0,12,12	-	-	-		

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	MGD	A	1102	7	-	6/18/66/66	0/6/6/6
4	SF4	A	1103	1	-	-	0/6/5/5
3	MGD	A	1101	7	-	3/18/66/66	0/6/6/6
5	GOL	A	1106	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	0/4/4/4	-
5	GOL	A	1104	-	-	4/4/4/4	-
5	GOL	A	1107	-	-	0/4/4/4	-
4	SF4	B	302	2	-	-	0/6/5/5
4	SF4	B	301	2	-	-	0/6/5/5
5	GOL	A	1105	-	-	0/4/4/4	-
4	SF4	B	303	2	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	MGD	C21-N22	3.61	1.39	1.35
3	A	1101	MGD	C5-C6	-2.83	1.41	1.47
3	A	1101	MGD	C21-N22	2.77	1.38	1.35
3	A	1102	MGD	O4'-C1'	2.68	1.44	1.41
3	A	1102	MGD	C8-N7	-2.65	1.30	1.35
3	A	1101	MGD	C8-N7	-2.64	1.30	1.35
3	A	1102	MGD	C5-C6	-2.61	1.42	1.47
3	A	1101	MGD	O4'-C1'	2.59	1.44	1.41
3	A	1101	MGD	C10-C11	2.14	1.54	1.52
3	A	1101	MGD	C17-N18	-2.01	1.35	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	MGD	O11-C23-N22	-8.86	99.46	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	MGD	O11-C23-N22	4.99	113.69	108.57
3	A	1102	MGD	PA-O3B-PB	-4.86	116.16	132.83
3	A	1102	MGD	C19-N20-C21	4.17	120.95	113.43
3	A	1102	MGD	O4'-C1'-C2'	-3.85	101.30	106.93
3	A	1101	MGD	C19-N20-C21	3.70	120.12	113.43
3	A	1101	MGD	PA-O3B-PB	-3.47	120.93	132.83
3	A	1102	MGD	C8-N7-C5	3.40	109.47	102.99
3	A	1101	MGD	C8-N7-C5	3.32	109.32	102.99
3	A	1101	MGD	O4'-C1'-C2'	-3.09	102.41	106.93
3	A	1101	MGD	O11-C23-C14	-2.98	106.98	108.96
3	A	1102	MGD	C19-N18-C17	-2.78	120.03	125.10
3	A	1101	MGD	C5-C6-N1	2.55	118.45	113.95
3	A	1102	MGD	C5-C6-N1	2.51	118.39	113.95
3	A	1102	MGD	O17-C17-C16	-2.50	121.50	127.24
3	A	1102	MGD	C2-N1-C6	-2.42	120.64	125.10
3	A	1101	MGD	C2-N1-C6	-2.40	120.68	125.10
3	A	1102	MGD	O11-C23-C14	2.22	110.44	108.96
3	A	1101	MGD	O6-C6-C5	-2.06	120.36	124.37
3	A	1101	MGD	C17-C16-N15	2.05	122.28	116.76
3	A	1101	MGD	C19-N18-C17	-2.05	121.36	125.10
5	A	1107	GOL	C3-C2-C1	-2.03	103.81	111.70
3	A	1102	MGD	C16-C17-N18	2.03	118.35	112.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	GOL	O1-C1-C2-C3
5	A	1106	GOL	C1-C2-C3-O3
3	A	1102	MGD	O4'-C4'-C5'-O5'
3	A	1102	MGD	C3'-C4'-C5'-O5'
5	A	1104	GOL	C1-C2-C3-O3
5	A	1104	GOL	O1-C1-C2-O2
5	A	1106	GOL	O2-C2-C3-O3
3	A	1102	MGD	PA-O3B-PB-O1B
3	A	1102	MGD	C4'-C5'-O5'-PB
5	A	1104	GOL	O2-C2-C3-O3
3	A	1101	MGD	PA-O3B-PB-O5'
3	A	1102	MGD	C5'-O5'-PB-O3B
3	A	1101	MGD	PA-O3B-PB-O1B
3	A	1101	MGD	PA-O3B-PB-O2B
3	A	1102	MGD	C5'-O5'-PB-O1B

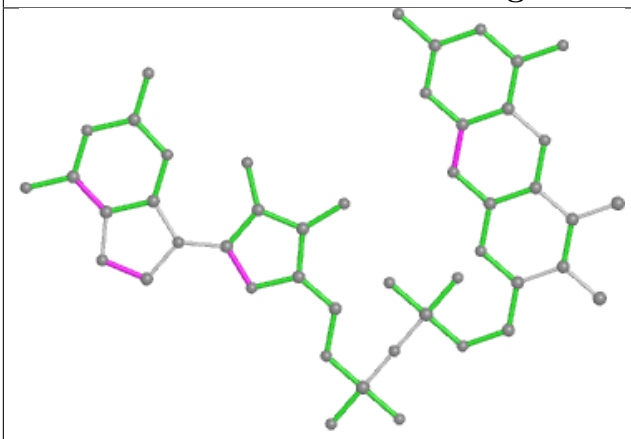
There are no ring outliers.

5 monomers are involved in 9 short contacts:

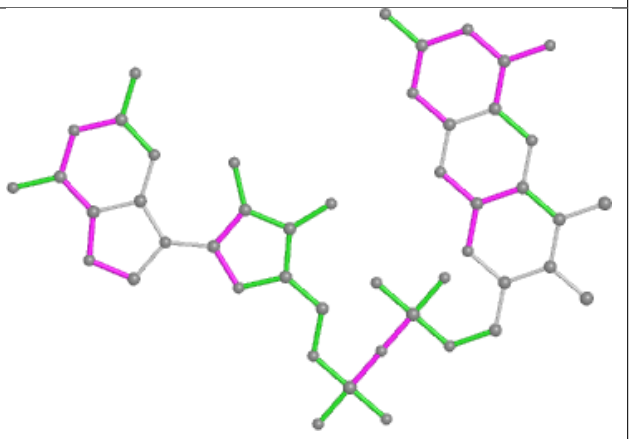
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	MGD	3	0
4	A	1103	SF4	1	0
5	A	1106	GOL	1	0
5	A	1104	GOL	2	0
5	A	1107	GOL	2	0

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.

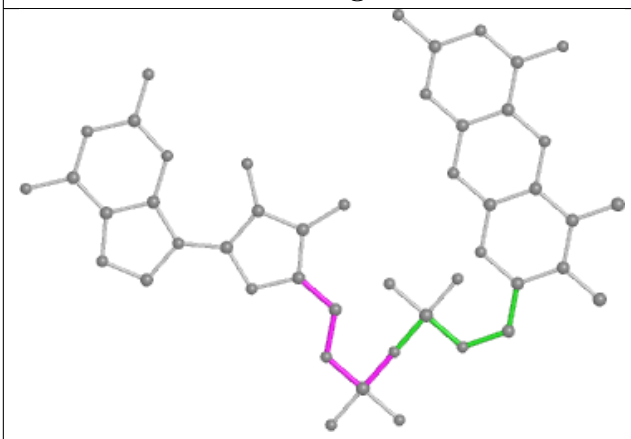
Ligand MGD A 1102



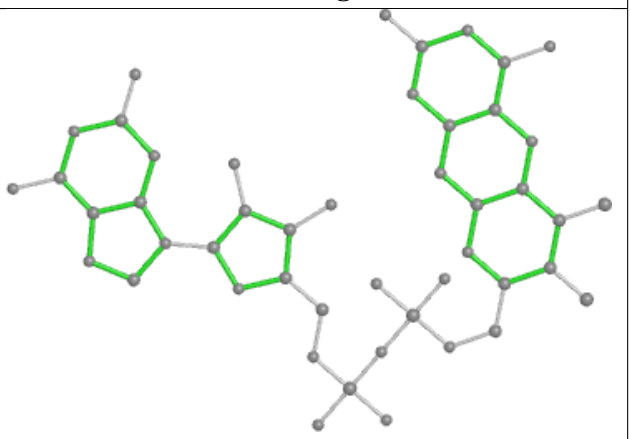
Bond lengths



Bond angles

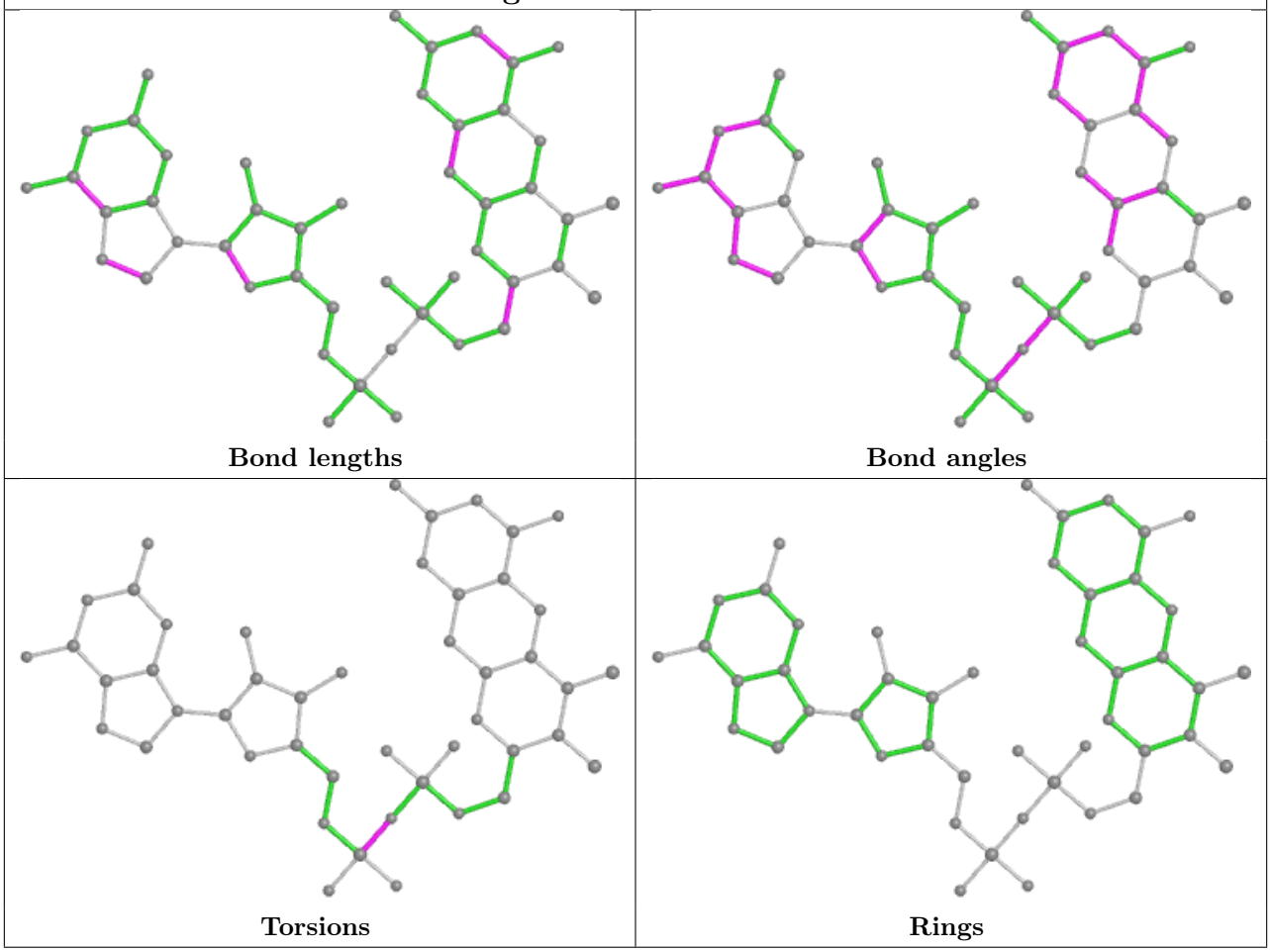


Torsions



Rings

Ligand MGD A 1101



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	A	962/1005 (95%)	0.94	126 (13%) 3 4	15, 36, 66, 92	0
2	B	214/236 (90%)	1.03	39 (18%) 1 1	20, 39, 69, 78	0
All	All	1176/1241 (94%)	0.95	165 (14%) 2 3	15, 37, 66, 92	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	ALA	7.8
1	A	660	GLY	7.1
1	A	702	GLY	6.1
1	A	146	ALA	6.0
2	B	88	VAL	5.4
1	A	988	PRO	5.4
1	A	661	GLY	5.2
1	A	109	TYR	4.8
2	B	112	VAL	4.8
1	A	339	ALA	4.7
1	A	658	LYS	4.2
2	B	131	VAL	4.1
2	B	120	ALA	4.1
2	B	86	ALA	4.1
2	B	98	GLU	4.1
1	A	446	VAL	4.1
2	B	130	PRO	4.0
1	A	147	ALA	4.0
1	A	324	ALA	4.0
1	A	706	LYS	4.0
1	A	664	PRO	3.9
1	A	861	ALA	3.9
1	A	986	GLY	3.9
2	B	128	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	705	PHE	3.9
1	A	985	ALA	3.8
1	A	140	SER	3.8
1	A	111	ALA	3.8
1	A	440	LEU	3.8
1	A	197	VAL	3.8
2	B	62	GLY	3.7
1	A	113	PHE	3.7
1	A	699	GLU	3.6
1	A	504	LYS	3.6
2	B	99	THR	3.5
1	A	136	THR	3.5
1	A	196	THR	3.5
1	A	656	TYR	3.4
1	A	55	VAL	3.4
2	B	134	ARG	3.4
1	A	657	ALA	3.4
1	A	122	TRP	3.3
1	A	987	ASP	3.3
2	B	143	ASP	3.2
1	A	679	ASN	3.2
2	B	82	CYS	3.2
1	A	989	ASN	3.2
1	A	163	ALA	3.2
1	A	700	VAL	3.2
1	A	703	LYS	3.2
1	A	164	ALA	3.1
1	A	950	PHE	3.1
1	A	124	PHE	3.1
2	B	114	GLY	3.1
2	B	146[A]	GLN	3.1
1	A	54	ALA	3.0
2	B	132	THR	3.0
1	A	598	GLU	3.0
1	A	922	ILE	3.0
1	A	662	ALA	3.0
1	A	992	ILE	3.0
1	A	917	ALA	3.0
1	A	129	ILE	2.9
1	A	673	ALA	2.9
1	A	442	GLY	2.9
1	A	525	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	121	THR	2.9
1	A	189	ALA	2.9
2	B	135	LEU	2.9
1	A	652	VAL	2.9
1	A	118	LYS	2.9
1	A	119	PRO	2.9
1	A	619	ALA	2.8
1	A	53	CYS	2.8
1	A	574	TRP	2.8
1	A	697	ASP	2.8
1	A	462	TYR	2.8
1	A	213	TRP	2.8
2	B	90	LEU	2.8
1	A	654	GLU	2.8
2	B	117	VAL	2.8
1	A	454	LEU	2.8
1	A	889	TRP	2.7
2	B	113	ASP	2.7
1	A	455	LEU	2.7
1	A	618	VAL	2.7
2	B	102	ALA	2.7
2	B	168[A]	GLN	2.7
1	A	325	ASN	2.7
1	A	901	LEU	2.7
1	A	798	LYS	2.6
1	A	450	THR	2.6
1	A	543	GLY	2.6
1	A	526	ARG	2.6
2	B	106	THR	2.6
1	A	117	TRP	2.6
1	A	794	TRP	2.6
1	A	116	THR	2.6
1	A	669	LYS	2.6
1	A	89	PRO	2.6
1	A	127	THR	2.6
1	A	441	ARG	2.5
1	A	135	LYS	2.5
1	A	633	LYS	2.5
1	A	869	LYS	2.5
1	A	125	ALA	2.5
1	A	52	TYR	2.5
1	A	444	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	116	SER	2.5
1	A	870	ALA	2.5
1	A	87	LEU	2.4
1	A	511	GLU	2.4
1	A	50	CYS	2.4
2	B	129	ASP	2.4
1	A	97	LEU	2.4
1	A	663	TYR	2.4
1	A	518	TYR	2.4
1	A	580	LEU	2.4
1	A	919	LEU	2.4
1	A	405	MET	2.3
1	A	610	VAL	2.3
2	B	121	CYS	2.3
1	A	720	ASP	2.3
2	B	87	ASP	2.3
1	A	187	HIS	2.3
1	A	315	ASP	2.2
1	A	51	CYS	2.2
1	A	49	ILE	2.2
1	A	68	GLN	2.2
1	A	704	GLN	2.2
1	A	666	PRO	2.2
1	A	701	GLY	2.2
2	B	126	PRO	2.2
2	B	47	TYR	2.2
2	B	84	GLY	2.2
1	A	209	MET	2.2
1	A	449	SER	2.2
2	B	115	GLU	2.2
2	B	169	GLU	2.2
1	A	91	GLY	2.2
1	A	797	GLY	2.2
1	A	954	GLY	2.2
1	A	200	LEU	2.1
1	A	765	TRP	2.1
2	B	89	ASP	2.1
1	A	193	HIS	2.1
1	A	94	ILE	2.1
1	A	709	GLN	2.1
2	B	85	GLN	2.1
2	B	110	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	854	LYS	2.1
2	B	212	HIS	2.1
1	A	973	ASN	2.1
1	A	651	LYS	2.1
1	A	59	LEU	2.1
2	B	109	THR	2.1
1	A	599	ILE	2.0
1	A	665	ALA	2.0
1	A	114	SER	2.0
1	A	918	LYS	2.0
2	B	119	SER	2.0
1	A	655	LEU	2.0
1	A	170	CYS	2.0
1	A	56	GLY	2.0
2	B	2	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	GOL	A	1107	6/6	0.70	0.39	39,44,47,53	0
5	GOL	A	1106	6/6	0.80	0.47	42,45,53,59	0
5	GOL	A	1105	6/6	0.91	0.13	28,36,38,38	0
5	GOL	A	1108	6/6	0.91	0.37	33,38,39,40	0
5	GOL	A	1104	6/6	0.93	0.25	20,31,35,37	0
4	SF4	B	302	8/8	0.94	0.09	37,40,41,45	0
3	MGD	A	1102	47/47	0.94	0.17	19,28,34,38	0
4	SF4	B	303	8/8	0.95	0.09	26,28,33,33	0

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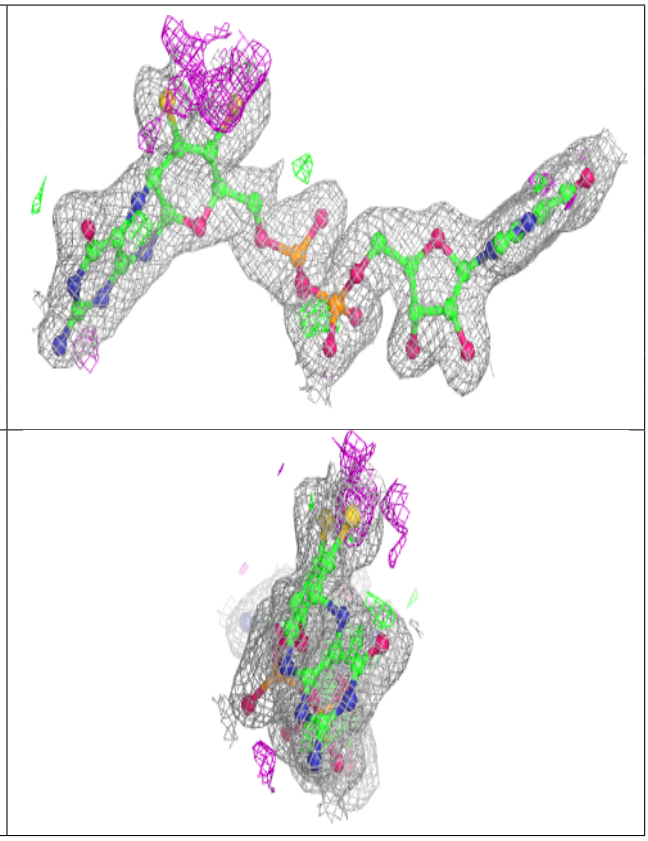
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MGD	A	1101	47/47	0.95	0.17	14,19,25,29	0
6	H2S	A	1109	1/1	0.95	0.14	27,27,27,27	0
4	SF4	B	301	8/8	0.96	0.08	18,22,24,24	0
4	SF4	A	1103	8/8	0.97	0.09	14,17,18,20	0
7	W	A	1110	1/1	1.00	0.06	26,26,26,26	0

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.

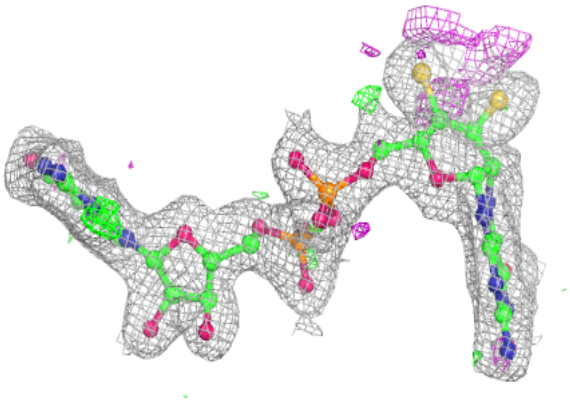
Electron density around MGD A 1102:

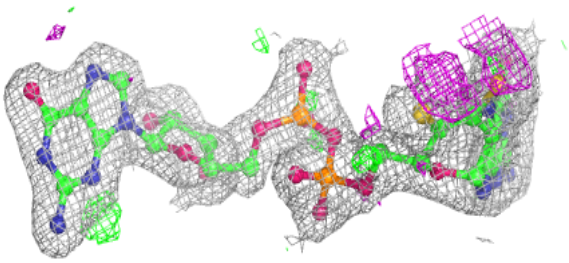
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

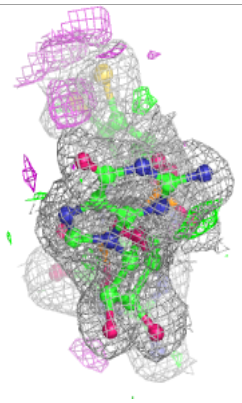


Electron density around MGD A 1101:

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







Electron density around H2S A 1109:

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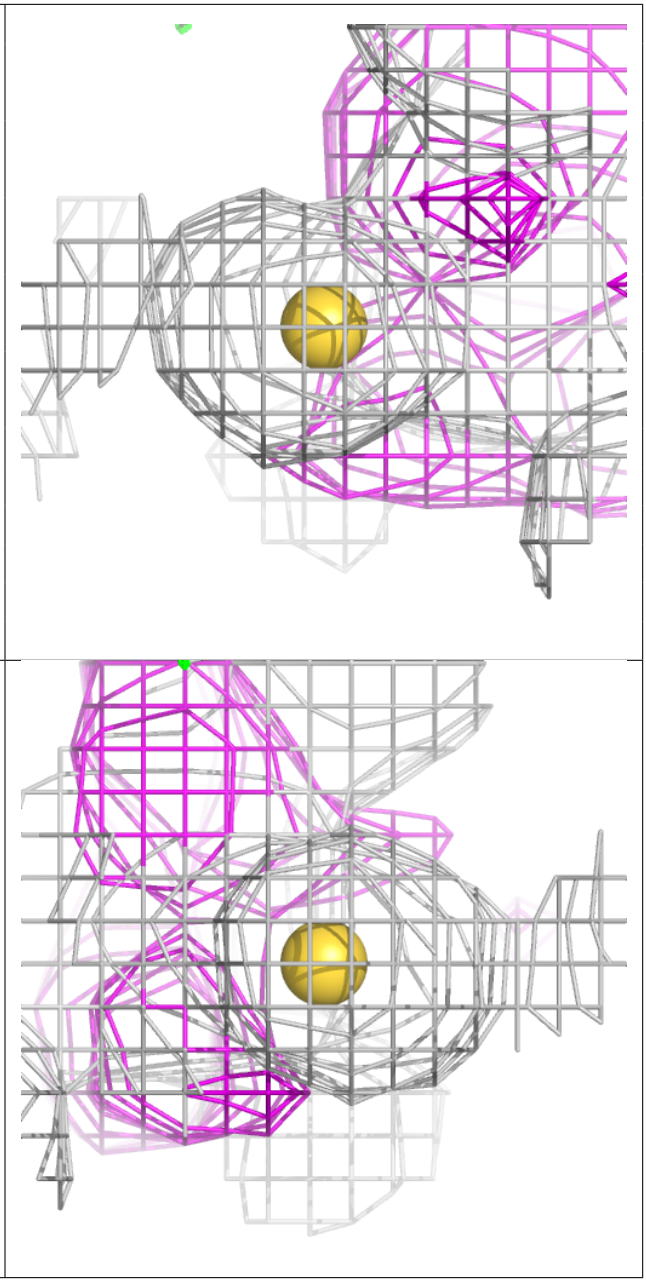
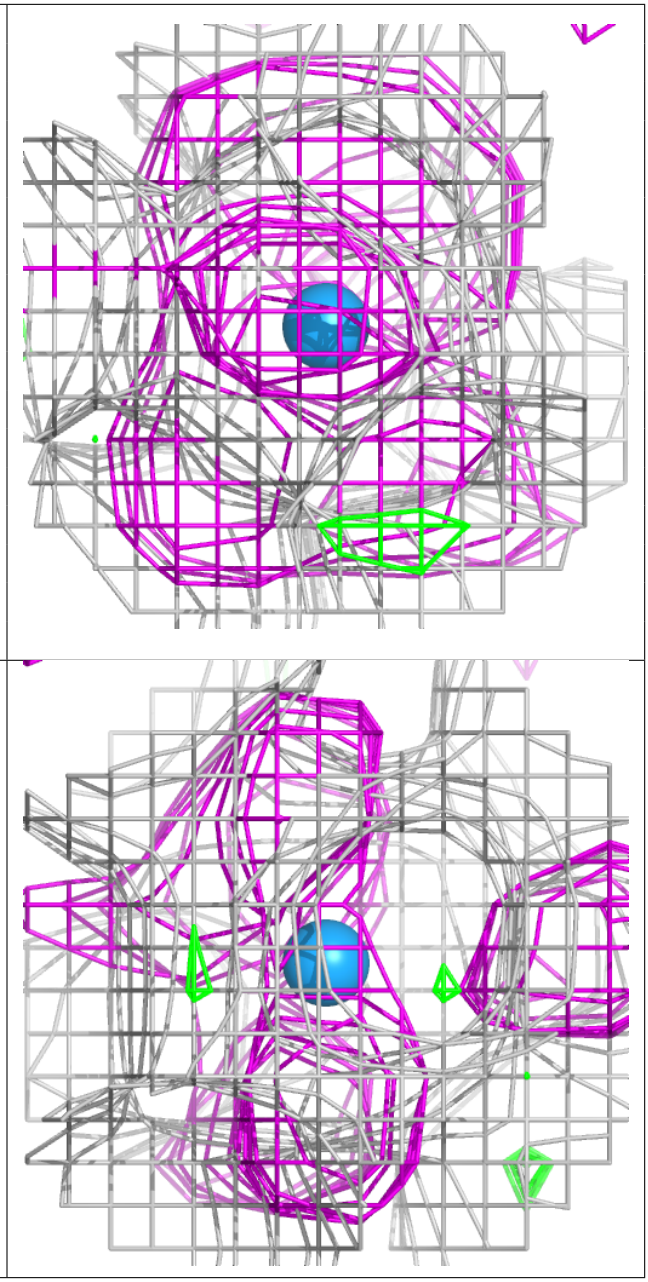
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W A 1110:

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.