



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:18 PM BST

PDB ID : 6SDV
Title : W-formate dehydrogenase from Desulfovibrio vulgaris - Formate reduced form
Authors : Oliveira, A.R.; Mota, C.; Mourato, C.; Domingos, R.M.; Santos, M.F.A.;
Gesto, D.; Guigliarelli, B.; Santos-Silva, T.; Romao, M.J.; Pereira, I.C.
Deposited on : 2019-07-29
Resolution : 1.90 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 : 2.13.1
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) : 2.13.1

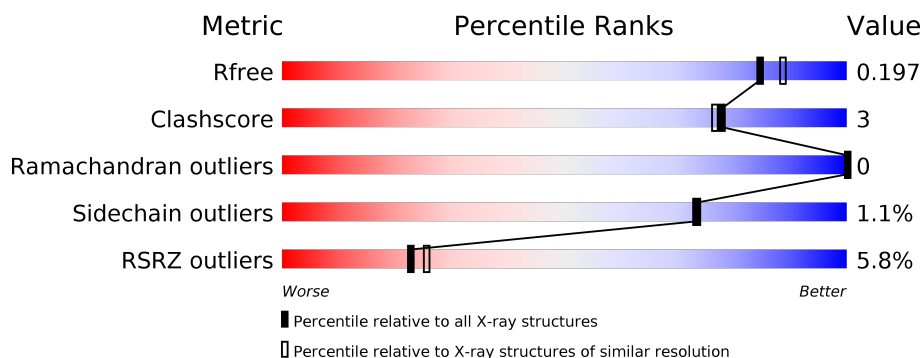
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1009	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> <div></div> </div>
2	B	236	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> <div></div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10205 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.

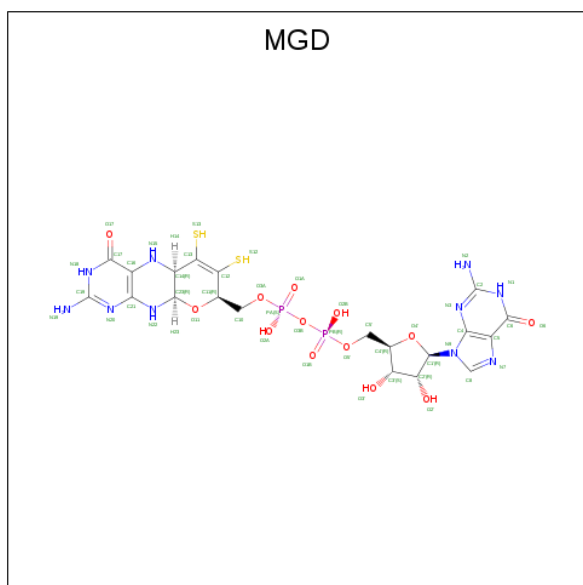
- Molecule 1 is a protein called Formate dehydrogenase, alpha subunit, selenocysteine-containing, Formate dehydrogenase, alpha subunit, selenocysteine-containing, W-formate dehydrogenase - alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	967	Total	C	N	O	S	Se	0	0	0
			7570	4825	1320	1383	41	1			

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

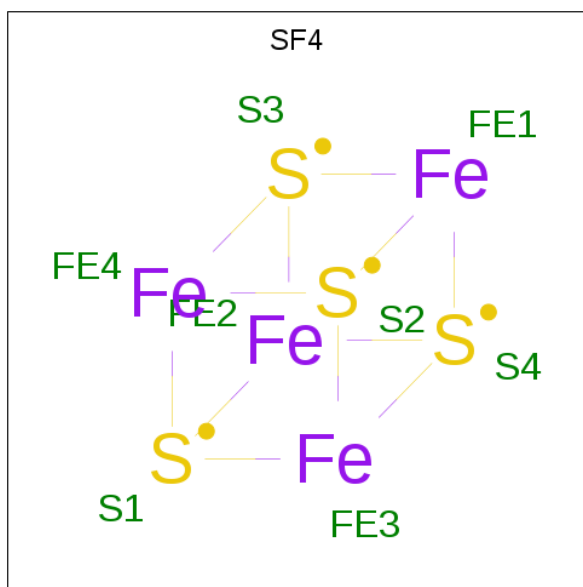
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			

- 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 author).



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

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

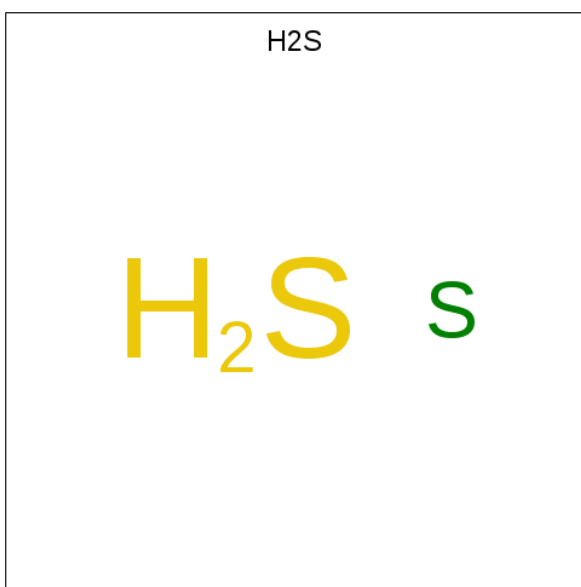


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe S		
			8 4 4		0	0
4	B	1	Total	Fe S		
			8 4 4		0	0
4	B	1	Total	Fe S		
			8 4 4		0	0
4	B	1	Total	Fe S		
			8 4 4		0	0

- Molecule 5 is TUNGSTEN ION (three-letter code: W) (formula: W) (labeled as "Ligand of Interest" by author).

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

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



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



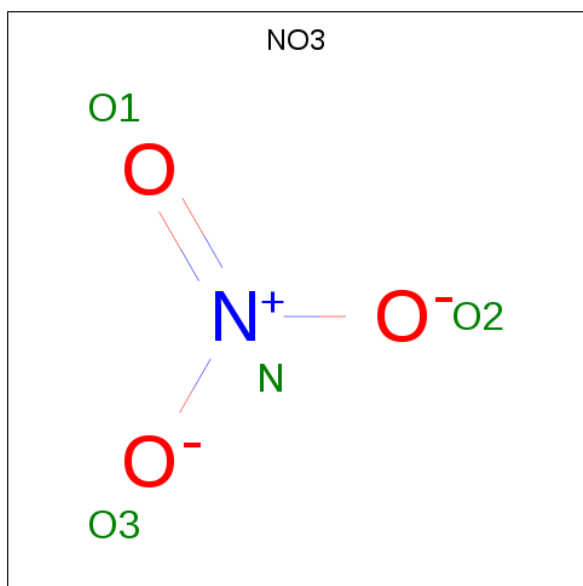
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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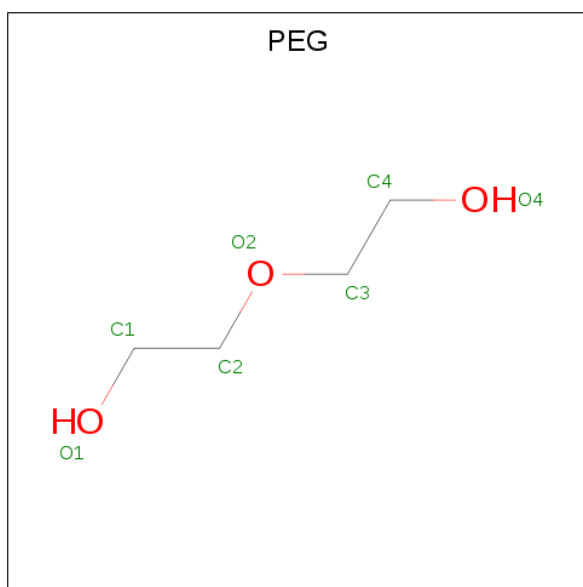
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

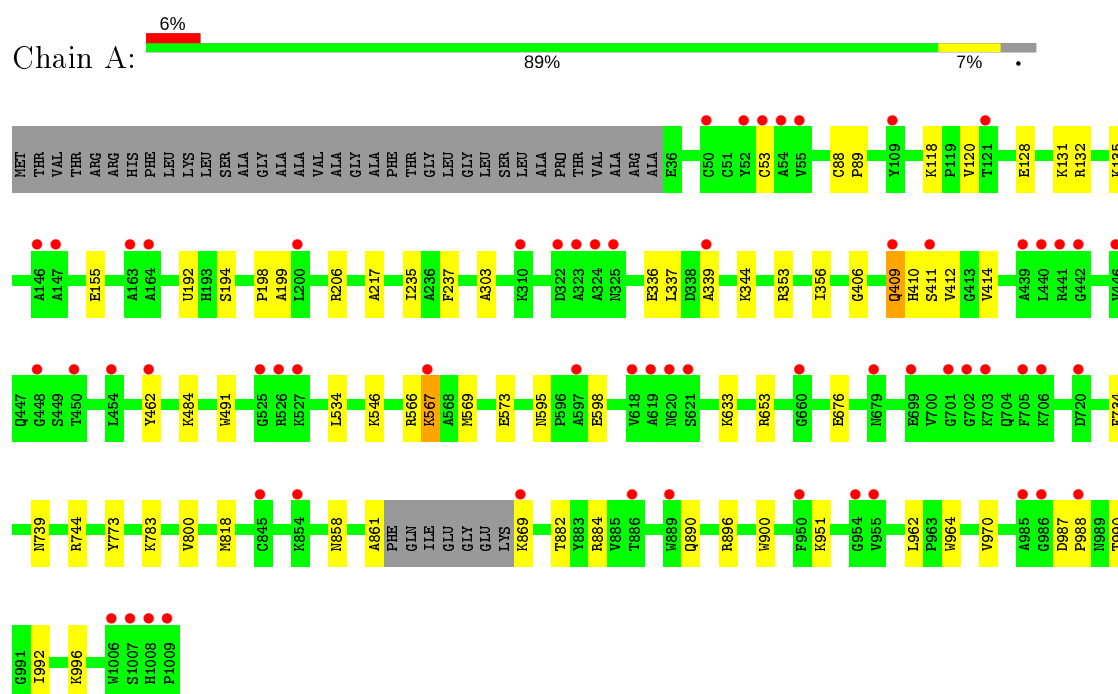
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	582	Total	O	0	0
			582	582		
10	B	186	Total	O	0	0
			186	186		

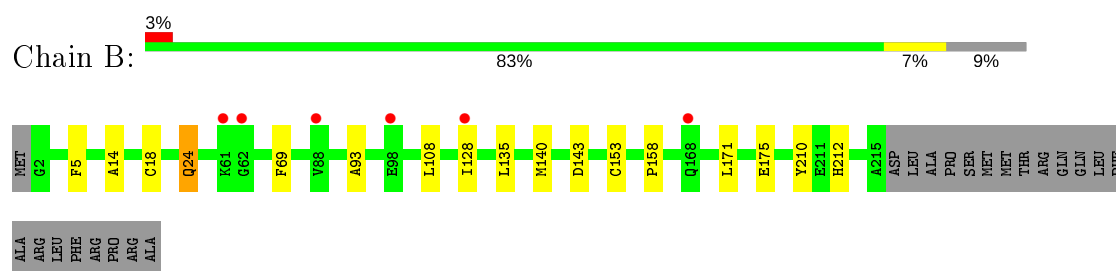
3 Residue-property plots

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: Formate dehydrogenase, alpha subunit, selenocysteine-containing, Formate dehydrogenase, alpha subunit, selenocysteine-containing, W-formate dehydrogenase - alpha subunit



- Molecule 2: Formate dehydrogenase, beta subunit, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.89Å 128.56Å 149.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 1.90 48.76 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.76-1.90) 99.6 (48.76-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.159 , 0.197 0.159 , 0.197	Depositor DCC
R_{free} test set	4896 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10205	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MGD, SF4, H2S, SEC, W, PEG, NO3

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	0.47	0/7774	0.60	0/10548
2	B	0.48	0/1699	0.59	1/2302 (0.0%)
All	All	0.47	0/9473	0.60	1/12850 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ASP	CB-CG-OD1	6.43	124.09	118.30

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	7570	0	7395	46	0
2	B	1664	0	1633	11	0
3	A	94	0	44	2	0
4	A	8	0	0	0	0
4	B	24	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	60	0	78	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	8	0	0	0	0
9	A	7	0	10	3	0
10	A	582	0	0	6	0
10	B	186	0	0	0	0
All	All	10205	0	9160	54	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 3.

All (54) 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:217:ALA:HB3	7:A:1115:GOL:H12	1.61	0.81
1:A:783:LYS:NZ	10:A:1201:HOH:O	2.14	0.79
1:A:411:SER:HB3	1:A:858:ASN:HD22	1.50	0.77
1:A:800:VAL:HA	7:A:1114:GOL:H31	1.77	0.66
1:A:120:VAL:HG12	9:A:1118:PEG:H32	1.83	0.60
1:A:118:LYS:HZ1	9:A:1118:PEG:H22	1.69	0.58
1:A:131:LYS:HG2	7:A:1113:GOL:H31	1.87	0.56
1:A:336:GLU:OE2	1:A:353:ARG:NH2	2.40	0.55
1:A:595:ASN:HB3	1:A:598:GLU:HG3	1.87	0.55
1:A:410:HIS:HD2	1:A:412:VAL:H	1.54	0.55
1:A:566:ARG:HA	1:A:569:MET:HE3	1.89	0.55
2:B:128:ILE:HG12	2:B:135:LEU:CD2	2.38	0.53
1:A:135:LYS:HB2	7:A:1113:GOL:H12	1.91	0.52
1:A:409:GLN:HB3	1:A:992:ILE:HG21	1.92	0.51
1:A:118:LYS:NZ	9:A:1118:PEG:H22	2.26	0.50
2:B:5:PHE:HE1	2:B:140:MET:HG3	1.76	0.50
1:A:411:SER:HA	1:A:987:ASP:OD1	2.12	0.49
1:A:567:LYS:HD3	1:A:567:LYS:N	2.29	0.47
1:A:135:LYS:NZ	10:A:1211:HOH:O	2.47	0.47
1:A:739:ASN:HD22	7:A:1111:GOL:H12	1.80	0.46
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.50	0.46
1:A:633:LYS:NZ	10:A:1212:HOH:O	2.48	0.46
1:A:987:ASP:HB3	1:A:990:THR:OG1	2.15	0.46
1:A:194:SER:O	1:A:198:PRO:HD2	2.16	0.45
1:A:128:GLU:O	1:A:132:ARG:HG2	2.16	0.45
2:B:93:ALA:HA	2:B:108:LEU:HB2	1.97	0.45
1:A:462:TYR:CZ	7:A:1106:GOL:H11	2.52	0.45
1:A:546:LYS:HD2	1:A:573:GLU:HG3	2.00	0.44
1:A:339:ALA:N	10:A:1206:HOH:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ALA:HB2	1:A:414:VAL:HG13	1.97	0.44
1:A:896:ARG:HD2	1:A:970:VAL:O	2.18	0.44
1:A:303:ALA:HB1	1:A:356:ILE:HB	2.00	0.44
1:A:861:ALA:C	1:A:988:PRO:HG2	2.39	0.43
2:B:18:CYS:HB2	2:B:153:CYS:HB2	2.00	0.43
2:B:171:LEU:O	2:B:175:GLU:HG3	2.19	0.43
1:A:192:SEC:CB	3:A:1101:MGD:S12	3.06	0.43
1:A:337:LEU:O	1:A:344:LYS:HE3	2.18	0.43
1:A:88:CYS:HB2	1:A:89:PRO:HD2	2.00	0.42
1:A:884:ARG:HE	3:A:1101:MGD:H15	1.68	0.42
1:A:882:THR:HA	1:A:962:LEU:O	2.18	0.42
1:A:566:ARG:HA	1:A:569:MET:CE	2.50	0.42
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.55	0.42
1:A:235:ILE:HD12	2:B:158:PRO:HB3	2.02	0.42
1:A:155:GLU:HG3	10:A:1467:HOH:O	2.19	0.41
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.56	0.41
1:A:235:ILE:CD1	2:B:158:PRO:HB3	2.49	0.41
1:A:744:ARG:NH1	10:A:1223:HOH:O	2.53	0.41
2:B:128:ILE:HG12	2:B:135:LEU:HD23	2.02	0.41
1:A:406:GLY:O	1:A:996:LYS:HE2	2.21	0.41
1:A:206:ARG:HB2	1:A:773:TYR:OH	2.21	0.41
1:A:491:TRP:HB3	1:A:818:MET:SD	2.61	0.40
1:A:534:LEU:HA	1:A:534:LEU:HD12	1.74	0.40
1:A:546:LYS:HD3	1:A:546:LYS:HA	1.90	0.40
2:B:210:TYR:CE2	2:B:212:HIS:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	962/1009 (95%)	937 (97%)	25 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	212/236 (90%)	203 (96%)	9 (4%)	0	100	100
All	All	1174/1245 (94%)	1140 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	786/815 (96%)	776 (99%)	10 (1%)	69	68
2	B	185/204 (91%)	184 (100%)	1 (0%)	88	89
All	All	971/1019 (95%)	960 (99%)	11 (1%)	73	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	237	PHE
1	A	409	GLN
1	A	484	LYS
1	A	567	LYS
1	A	653	ARG
1	A	676	GLU
1	A	734	PHE
1	A	869	LYS
1	A	951	LYS
2	B	24	GLN

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

5.3.3 RNA ⓘ

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 21 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 19 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	$\# Z > 2$
4	SF4	A	1103	1	0,12,12	0.00	-	-		
7	GOL	A	1111	-	5,5,5	0.88	0	5,5,5	0.98	0
7	GOL	A	1110	-	5,5,5	0.92	0	5,5,5	1.02	0
8	NO3	A	1117	-	1,3,3	0.78	0	0,3,3	0.00	-
7	GOL	A	1112	-	5,5,5	1.00	0	5,5,5	0.88	0
7	GOL	A	1108	-	5,5,5	1.05	0	5,5,5	1.05	0
8	NO3	A	1116	-	1,3,3	0.63	0	0,3,3	0.00	-
7	GOL	A	1106	-	5,5,5	0.79	0	5,5,5	1.19	0
4	SF4	B	301	2	0,12,12	0.00	-	-		
7	GOL	A	1115	-	5,5,5	1.34	1 (20%)	5,5,5	1.00	1 (20%)
7	GOL	A	1109	-	5,5,5	1.17	1 (20%)	5,5,5	0.81	0
7	GOL	A	1114	-	5,5,5	0.83	0	5,5,5	1.02	0
3	MGD	A	1101	5	41,52,52	1.25	5 (12%)	43,81,81	2.57	19 (44%)
7	GOL	A	1113	-	5,5,5	0.77	0	5,5,5	1.09	0
7	GOL	A	1107	-	5,5,5	1.49	1 (20%)	5,5,5	0.89	0
4	SF4	B	302	2	0,12,12	0.00	-	-		
9	PEG	A	1118	-	6,6,6	0.50	0	5,5,5	0.46	0
3	MGD	A	1102	5	41,52,52	1.26	6 (14%)	43,81,81	2.28	14 (32%)
4	SF4	B	303	2	0,12,12	0.00	-	-		

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
4	SF4	A	1103	1	-	-	0/6/5/5
7	GOL	A	1111	-	-	4/4/4/4	-
7	GOL	A	1110	-	-	4/4/4/4	-
4	SF4	B	303	2	-	-	0/6/5/5
7	GOL	A	1112	-	-	0/4/4/4	-
7	GOL	A	1108	-	-	0/4/4/4	-
7	GOL	A	1106	-	-	2/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
7	GOL	A	1115	-	-	2/4/4/4	-
7	GOL	A	1109	-	-	0/4/4/4	-
3	MGD	A	1101	5	-	3/18/66/66	0/6/6/6
7	GOL	A	1113	-	-	4/4/4/4	-
7	GOL	A	1107	-	-	0/4/4/4	-
4	SF4	B	302	2	-	-	0/6/5/5
9	PEG	A	1118	-	-	1/4/4/4	-
3	MGD	A	1102	5	-	3/18/66/66	0/6/6/6
7	GOL	A	1114	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MGD	C14-N15	3.36	1.50	1.45
3	A	1102	MGD	O4'-C1'	3.03	1.45	1.41
3	A	1101	MGD	O4'-C1'	2.70	1.44	1.41
3	A	1101	MGD	C16-N15	2.48	1.43	1.38
7	A	1107	GOL	C3-C2	2.47	1.61	1.51
3	A	1101	MGD	C17-N18	2.46	1.37	1.33
7	A	1115	GOL	O2-C2	-2.34	1.36	1.43
3	A	1102	MGD	C10-C11	2.30	1.55	1.52
3	A	1102	MGD	C2-N2	2.19	1.38	1.33
3	A	1102	MGD	C8-N7	-2.18	1.30	1.34
3	A	1102	MGD	C16-N15	2.12	1.42	1.38
3	A	1101	MGD	C19-N20	-2.10	1.31	1.35
3	A	1102	MGD	C14-N15	2.02	1.48	1.45
7	A	1109	GOL	C3-C2	2.00	1.60	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	O11-C23-N22	-8.70	99.63	108.57
3	A	1102	MGD	C17-C16-C21	4.88	118.90	114.57
3	A	1102	MGD	N3-C2-N1	-4.85	120.75	127.22
3	A	1102	MGD	C17-C16-N15	4.42	122.83	119.12
3	A	1102	MGD	C2-N3-C4	4.24	120.20	115.36
3	A	1102	MGD	PA-O3B-PB	-4.09	118.79	132.83
3	A	1101	MGD	C17-C16-C21	4.08	118.19	114.57
3	A	1101	MGD	C5-C6-N1	-4.00	117.96	123.43
3	A	1101	MGD	C16-C21-N22	3.89	121.69	118.13
3	A	1101	MGD	C17-C16-N15	3.86	122.36	119.12
3	A	1101	MGD	N3-C2-N1	-3.84	122.10	127.22
3	A	1102	MGD	C6-N1-C2	3.76	121.90	115.93
3	A	1102	MGD	C5-C6-N1	-3.72	118.35	123.43
3	A	1101	MGD	C6-N1-C2	3.63	121.70	115.93
3	A	1101	MGD	O11-C23-C14	-3.63	106.55	108.96
3	A	1102	MGD	C6-C5-C4	-3.62	117.34	120.80
3	A	1101	MGD	C6-C5-C4	-3.51	117.45	120.80
3	A	1101	MGD	C2-N3-C4	3.51	119.36	115.36
3	A	1101	MGD	C17-N18-C19	3.46	121.43	115.93
3	A	1102	MGD	C16-C21-N22	3.23	121.09	118.13
3	A	1102	MGD	C19-N20-C21	3.11	121.51	114.54
3	A	1101	MGD	O4'-C1'-C2'	-2.95	102.62	106.93
3	A	1102	MGD	C17-N18-C19	2.86	120.47	115.93
3	A	1101	MGD	C19-N20-C21	2.75	120.71	114.54
3	A	1102	MGD	N18-C19-N20	-2.74	121.12	125.42
3	A	1101	MGD	N18-C19-N20	-2.54	121.44	125.42
3	A	1101	MGD	C4-C5-N7	-2.49	106.81	109.40
3	A	1101	MGD	C16-C17-N18	-2.31	117.45	124.01
3	A	1101	MGD	N19-C19-N18	2.29	120.81	117.25
3	A	1102	MGD	C3'-C2'-C1'	-2.27	97.56	100.98
3	A	1101	MGD	C1'-N9-C4	-2.12	122.91	126.64
3	A	1102	MGD	C1'-N9-C4	-2.10	122.95	126.64
7	A	1115	GOL	C3-C2-C1	-2.03	103.80	111.70
3	A	1101	MGD	PB-O5'-C5'	-2.02	109.83	121.68

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1111	GOL	O1-C1-C2-O2
7	A	1111	GOL	C1-C2-C3-O3
7	A	1110	GOL	C1-C2-C3-O3
7	A	1113	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	O4'-C4'-C5'-O5'
3	A	1102	MGD	C3'-C4'-C5'-O5'
7	A	1110	GOL	O2-C2-C3-O3
7	A	1113	GOL	O2-C2-C3-O3
7	A	1111	GOL	O1-C1-C2-C3
7	A	1106	GOL	O1-C1-C2-C3
7	A	1115	GOL	O1-C1-C2-C3
7	A	1113	GOL	O1-C1-C2-C3
7	A	1111	GOL	O2-C2-C3-O3
7	A	1115	GOL	O1-C1-C2-O2
7	A	1106	GOL	O1-C1-C2-O2
3	A	1102	MGD	C4'-C5'-O5'-PB
3	A	1101	MGD	PA-O3B-PB-O5'
7	A	1114	GOL	O1-C1-C2-O2
7	A	1110	GOL	O1-C1-C2-C3
7	A	1113	GOL	O1-C1-C2-O2
7	A	1110	GOL	O1-C1-C2-O2
3	A	1101	MGD	PA-O3B-PB-O1B
3	A	1101	MGD	PA-O3B-PB-O2B
7	A	1114	GOL	O1-C1-C2-C3
9	A	1118	PEG	O1-C1-C2-O2

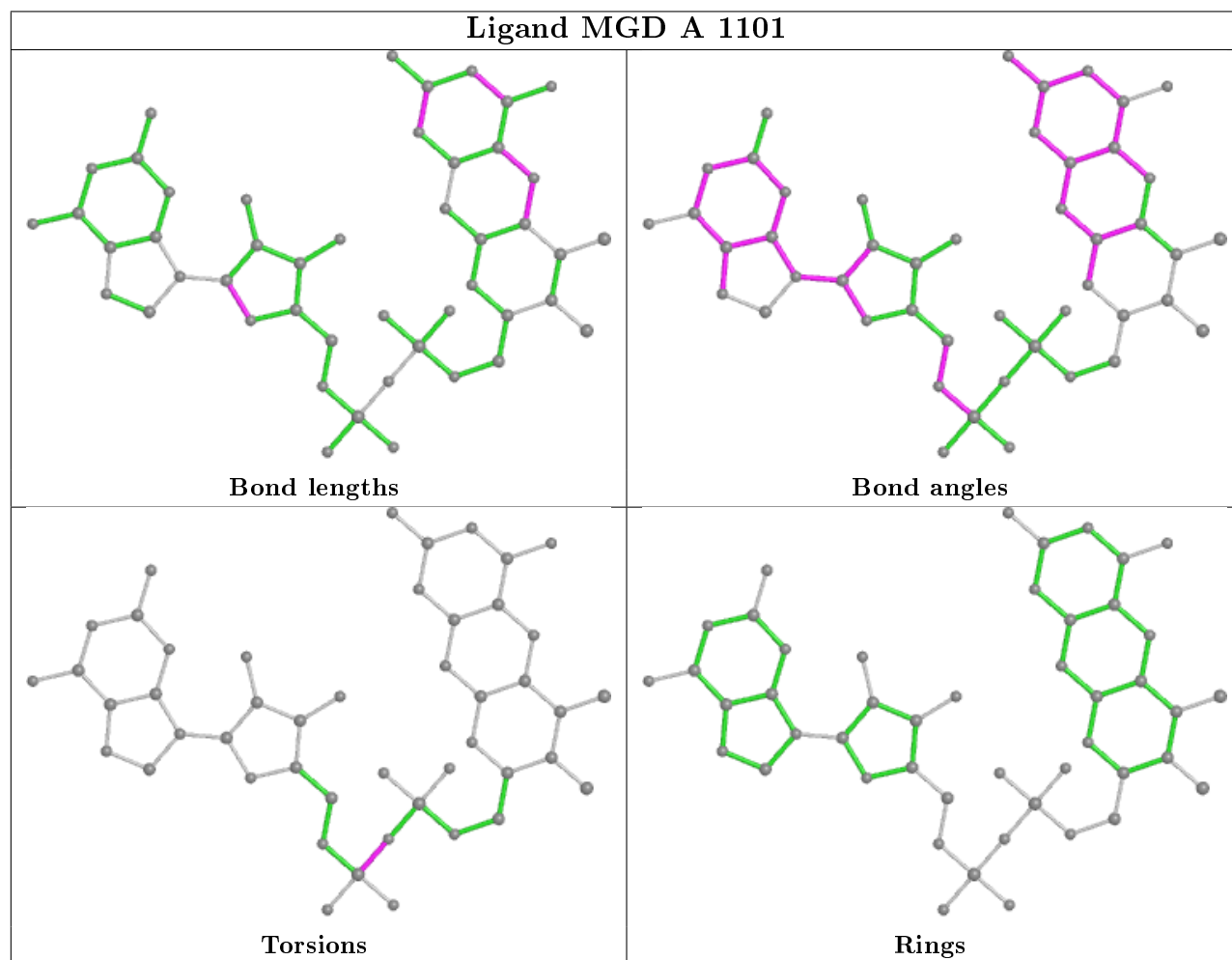
There are no ring outliers.

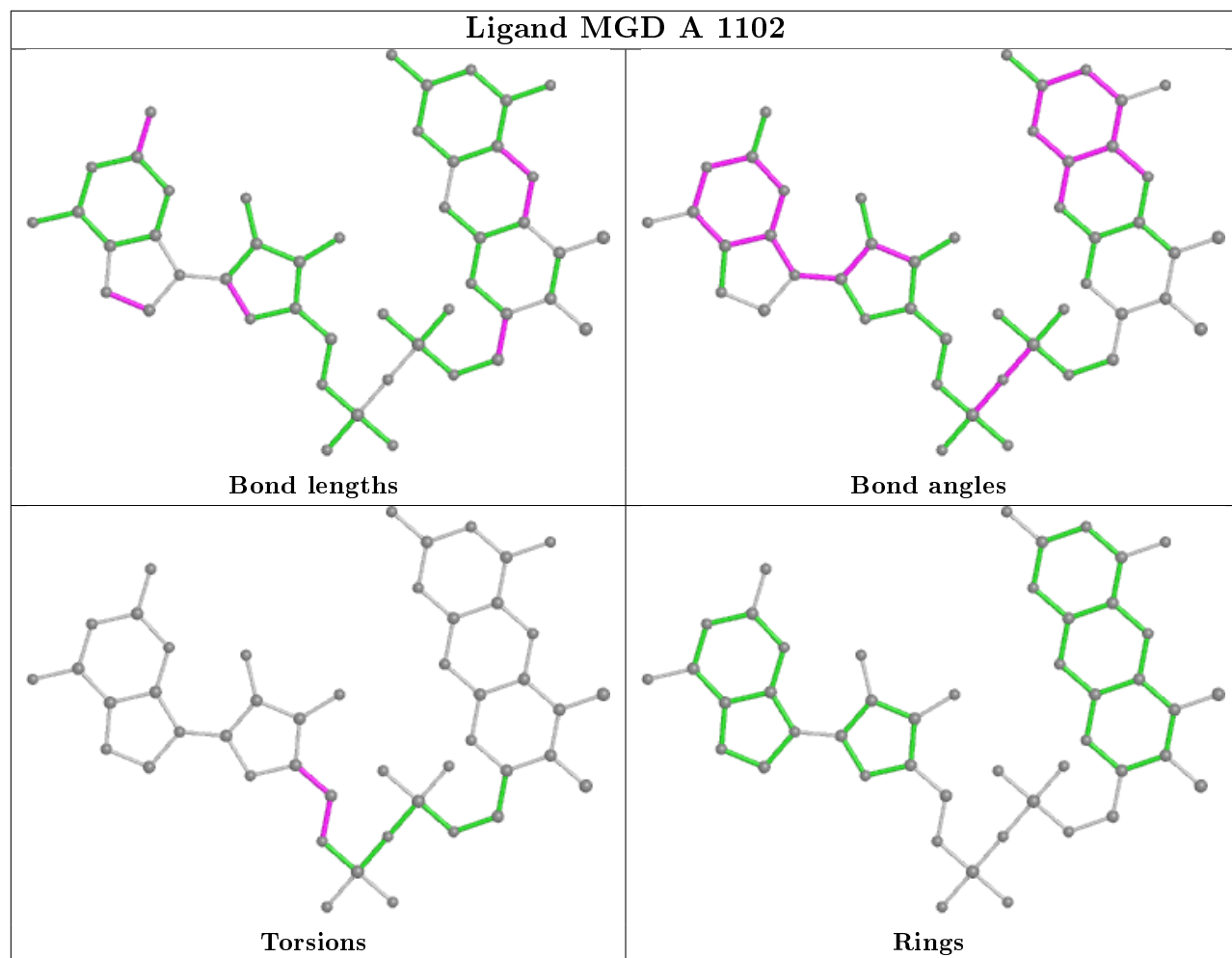
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1111	GOL	1	0
7	A	1106	GOL	1	0
7	A	1115	GOL	1	0
7	A	1114	GOL	1	0
3	A	1101	MGD	2	0
7	A	1113	GOL	2	0
9	A	1118	PEG	3	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	966/1009 (95%)	0.39	62 (6%)	19 22	12, 26, 48, 83	0
2	B	214/236 (90%)	0.16	6 (2%)	53 56	13, 25, 43, 55	0
All	All	1180/1245 (94%)	0.35	68 (5%)	23 25	12, 26, 48, 83	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1006	TRP	6.7
1	A	146	ALA	5.6
1	A	702	GLY	5.6
1	A	988	PRO	5.5
1	A	339	ALA	4.9
1	A	954	GLY	4.6
1	A	440	LEU	4.2
1	A	985	ALA	4.0
1	A	163	ALA	3.9
1	A	409	GLN	3.8
1	A	950	PHE	3.8
1	A	619	ALA	3.7
2	B	62	GLY	3.7
1	A	986	GLY	3.7
1	A	526	ARG	3.7
1	A	525	GLY	3.6
1	A	618	VAL	3.5
1	A	1009	PRO	3.5
1	A	1007	SER	3.4
1	A	446	VAL	3.4
1	A	325	ASN	3.4
1	A	164	ALA	3.3
1	A	955	VAL	3.2
1	A	54	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	168	GLN	3.1
1	A	324	ALA	3.1
1	A	706	LYS	3.1
1	A	703	LYS	3.0
2	B	88	VAL	3.0
1	A	147	ALA	3.0
1	A	55	VAL	2.9
1	A	869	LYS	2.9
1	A	1008	HIS	2.8
1	A	854	LYS	2.8
1	A	597	ALA	2.8
1	A	323	ALA	2.7
1	A	442	GLY	2.7
1	A	889	TRP	2.7
1	A	53	CYS	2.7
1	A	454	LEU	2.6
2	B	98	GLU	2.6
1	A	660	GLY	2.6
1	A	462	TYR	2.5
1	A	845	CYS	2.3
1	A	441	ARG	2.3
1	A	527	LYS	2.3
1	A	109	TYR	2.3
1	A	322	ASP	2.3
1	A	52	TYR	2.2
1	A	720	ASP	2.2
1	A	701	GLY	2.2
1	A	200	LEU	2.2
1	A	621	SER	2.2
1	A	699	GLU	2.2
1	A	50	CYS	2.2
2	B	128	ILE	2.1
1	A	411	SER	2.1
1	A	448	GLY	2.1
1	A	439	ALA	2.1
1	A	567	LYS	2.1
1	A	705	PHE	2.1
1	A	679	ASN	2.1
1	A	450	THR	2.0
1	A	310	LYS	2.0
1	A	121	THR	2.0
1	A	886	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	61	LYS	2.0
1	A	620	ASN	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](#)

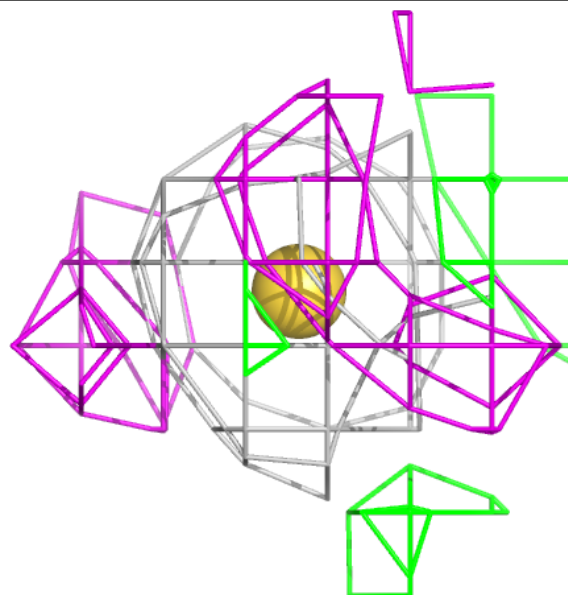
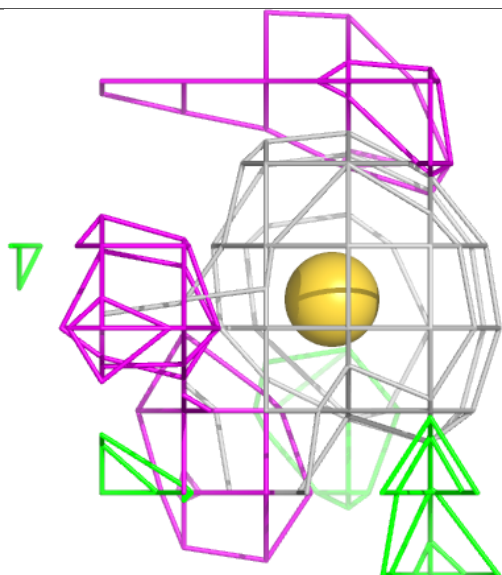
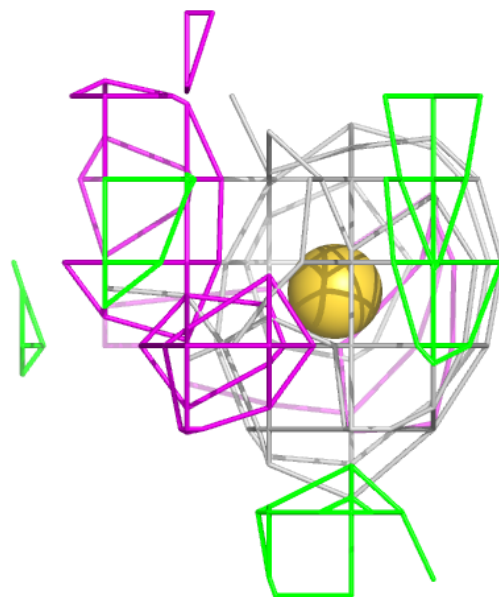
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	A	1112	6/6	0.78	0.22	54,61,66,67	0
7	GOL	A	1113	6/6	0.80	0.27	56,65,67,68	0
8	NO3	A	1116	4/4	0.82	0.20	51,57,58,61	0
7	GOL	A	1114	6/6	0.83	0.21	51,54,60,63	0
6	H2S	A	1105	1/1	0.86	0.17	22,22,22,22	0
8	NO3	A	1117	4/4	0.86	0.21	51,56,61,64	0
7	GOL	A	1109	6/6	0.87	0.20	25,35,45,46	0
7	GOL	A	1111	6/6	0.90	0.18	43,46,50,60	0
7	GOL	A	1115	6/6	0.90	0.23	37,41,51,60	0
9	PEG	A	1118	7/7	0.91	0.26	34,58,64,65	0
7	GOL	A	1110	6/6	0.92	0.18	47,50,54,55	0
7	GOL	A	1106	6/6	0.95	0.30	32,35,39,40	0
7	GOL	A	1107	6/6	0.96	0.17	20,22,22,24	0
3	MGD	A	1101	47/47	0.96	0.13	11,17,24,25	0
3	MGD	A	1102	47/47	0.96	0.14	17,22,27,28	0
4	SF4	B	303	8/8	0.97	0.08	17,18,19,20	0
7	GOL	A	1108	6/6	0.98	0.10	20,26,31,32	0
4	SF4	B	301	8/8	0.98	0.09	13,16,17,17	0
4	SF4	B	302	8/8	0.98	0.07	21,23,23,24	0
4	SF4	A	1103	8/8	0.99	0.11	13,14,14,15	0
5	W	A	1104	1/1	1.00	0.07	22,22,22,22	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.

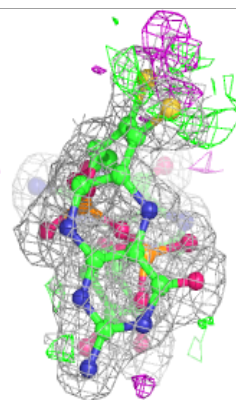
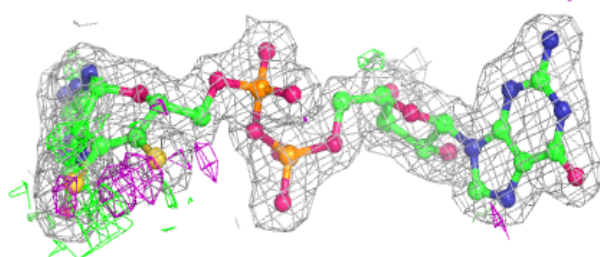
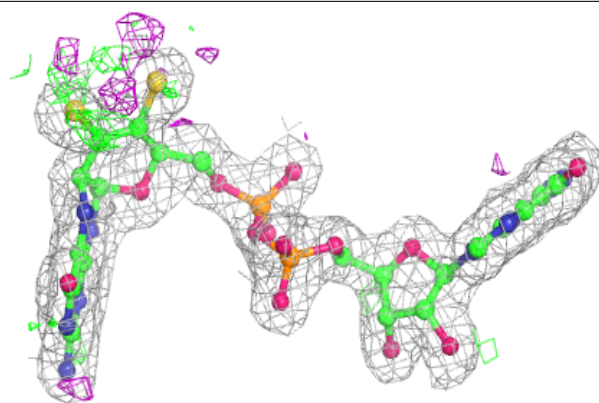
Electron density around H2S A 1105:

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

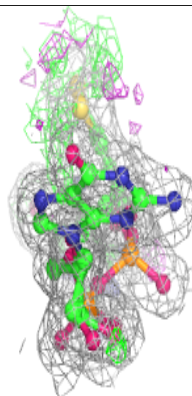
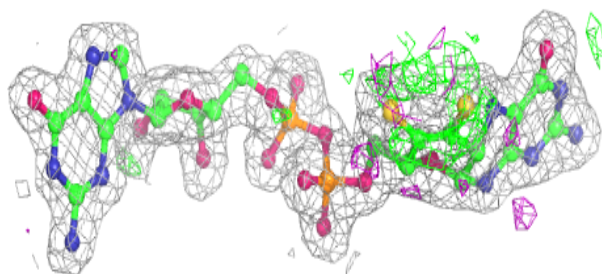
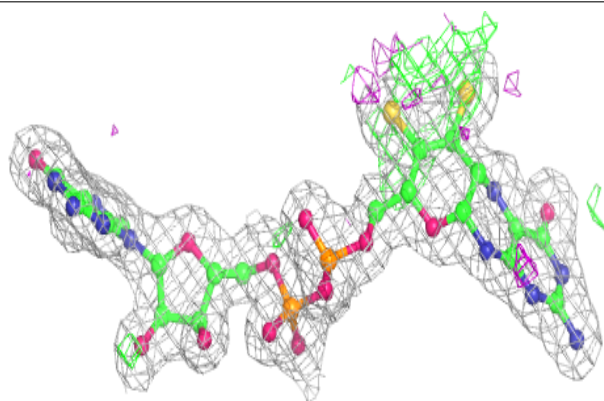


Electron density around MGD A 1101:

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

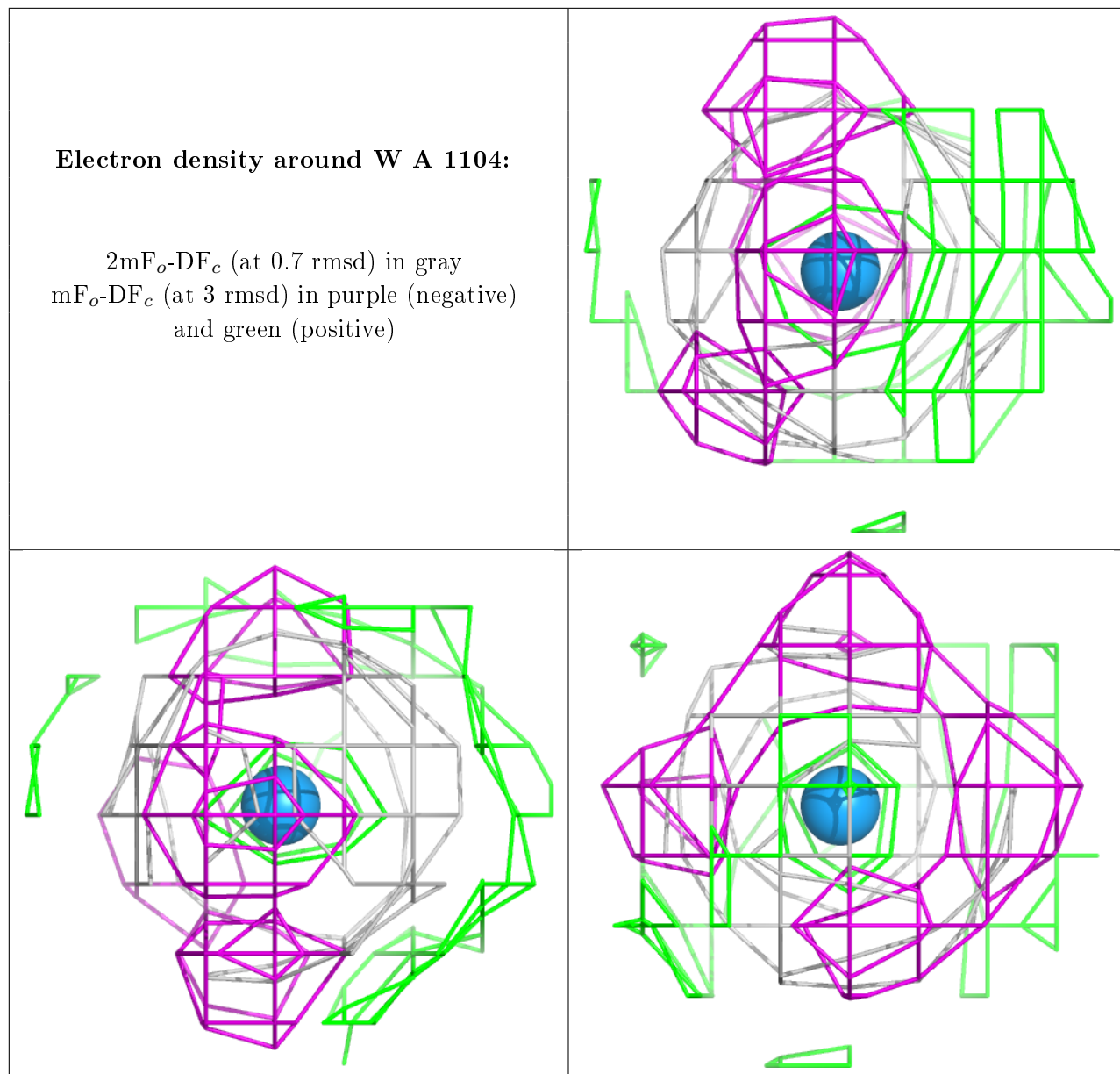
**Electron density around MGD A 1102:**

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



Electron density around W A 1104:

$2mF_o-DF_c$ (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.