

wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2023 – 12:27 pm GMT

PDB ID		•
1 Itie	:	W-formate dehydrogenase from Desulfovibrio vulgaris - Soaking with Formate 3 min
Authors	:	Vilela-Alves, G.; Mota, C.; Oliveira, A.R.; Manuel, R.R.; Pereira, I.C.; Romao, M.J.
Deposited on Resolution		2022-11-21 2.36 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:

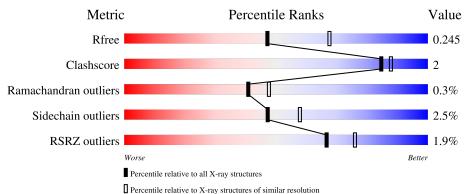
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.36 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$1164 \ (2.36-2.36)$
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	А	1013	2% 88 %	7% 5%
2	В	236	3% 84%	6% 9%



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9442 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-contai ning.

Mol	Chain	Residues			Atom	.S			ZeroOcc	AltConf	Trace
1	А	963	Total 7543	C 4806	N 1316	O 1379	S 41	Se 1	0	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP Q72EJ1
А	2	THR	-	expression tag	UNP Q72EJ1
А	3	VAL	-	expression tag	UNP Q72EJ1
А	4	THR	-	expression tag	UNP Q72EJ1
А	5	ARG	-	expression tag	UNP Q72EJ1
А	6	ARG	-	expression tag	UNP Q72EJ1
А	7	HIS	-	expression tag	UNP Q72EJ1
А	8	PHE	-	expression tag	UNP Q72EJ1
А	9	LEU	-	expression tag	UNP Q72EJ1
А	10	LYS	-	expression tag	UNP Q72EJ1
А	11	LEU	-	expression tag	UNP Q72EJ1
А	12	SER	-	expression tag	UNP Q72EJ1
А	13	ALA	-	expression tag	UNP Q72EJ1
А	14	GLY	-	expression tag	UNP Q72EJ1
А	15	ALA	-	expression tag	UNP Q72EJ1
А	16	ALA	-	expression tag	UNP Q72EJ1
А	17	VAL	-	expression tag	UNP Q72EJ1
А	18	ALA	-	expression tag	UNP Q72EJ1
А	19	GLY	-	expression tag	UNP Q72EJ1
А	20	ALA	-	expression tag	UNP Q72EJ1
А	21	PHE	-	expression tag	UNP Q72EJ1
А	22	THR	-	expression tag	UNP Q72EJ1
А	23	GLY	-	expression tag	UNP Q72EJ1
А	24	LEU	-	expression tag	UNP Q72EJ1
А	25	GLY	-	expression tag	UNP Q72EJ1
А	26	LEU	-	expression tag	UNP Q72EJ1

There are 43 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	27	SER	-	expression tag	UNP Q72EJ1
А	28	LEU	-	expression tag	UNP Q72EJ1
A	29	ALA	-	expression tag	UNP Q72EJ1
А	30	PRO	-	expression tag	UNP Q72EJ1
A	31	THR	-	expression tag	UNP Q72EJ1
А	32	VAL	-	expression tag	UNP Q72EJ1
А	33	ALA	-	expression tag	UNP Q72EJ1
A	34	ARG	-	expression tag	UNP Q72EJ1
А	35	ALA	-	expression tag	UNP Q72EJ1
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
А	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
А	1012	GLU	-	expression tag	UNP Q72EJ1
А	1013	LYS	-	expression tag	UNP Q72EJ1

Continued from previous page...

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	214	Total 1664	C 1041	N 291	0 316	S 16	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

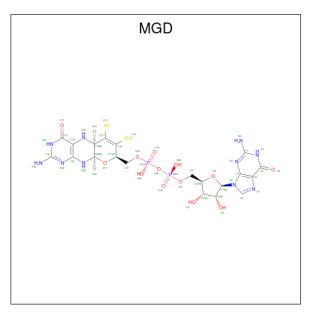
Chain	Residue	Modelled	Actual	Comment	Reference
В	1	MET	-	initiating methionine	UNP Q72EJ0
В	216	ASP	-	expression tag	UNP Q72EJ0
В	217	LEU	-	expression tag	UNP Q72EJ0
В	218	ALA	-	expression tag	UNP Q72EJ0
В	219	PRO	-	expression tag	UNP Q72EJ0
В	220	SER	-	expression tag	UNP Q72EJ0
В	221	MET	-	expression tag	UNP Q72EJ0
В	222	MET	-	expression tag	UNP Q72EJ0
В	223	THR	-	expression tag	UNP Q72EJ0
В	224	ARG	-	expression tag	UNP Q72EJ0
В	225	GLN	-	expression tag	UNP Q72EJ0
В	226	GLN	-	expression tag	UNP Q72EJ0
В	227	LEU	-	expression tag	UNP Q72EJ0
В	228	PHE	-	expression tag	UNP Q72EJ0
В	229	ALA	-	expression tag	UNP Q72EJ0



Chain	Residue	Modelled	Actual	Comment	Reference
В	230	ARG	-	expression tag	UNP Q72EJ0
В	231	LEU	-	expression tag	UNP Q72EJ0
В	232	PHE	-	expression tag	UNP Q72EJ0
В	233	ARG	-	expression tag	UNP Q72EJ0
В	234	PRO	-	expression tag	UNP Q72EJ0
В	235	ARG	-	expression tag	UNP Q72EJ0
В	236	ALA	-	expression tag	UNP Q72EJ0

Continued from previous page...

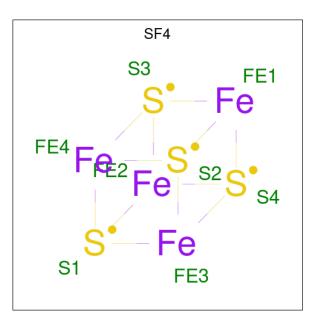
• Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Δ	1	Total	С	Ν	Ο	Р	S	0	0
0	A	1	47	20	10	13	2	2	0	0
2	Λ	1	Total	С	Ν	Ο	Р	S	0	0
0	A	1	47	20	10	13	2	2	0	0

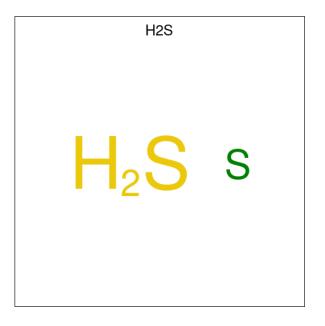
• Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	TotalFeS844	0	0
4	В	1	TotalFeS844	0	0
4	В	1	TotalFeS844	0	0
4	В	1	TotalFeS844	0	0

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



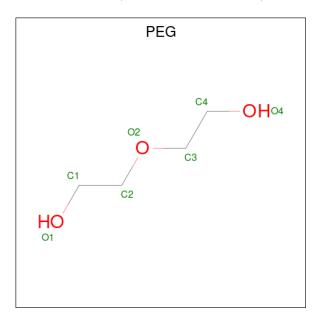


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total S 1 1	0	0

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

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

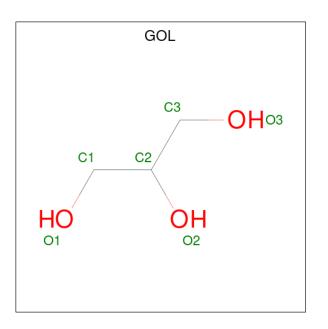
• Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



N	Aol	Chain	Residues	Atoms	ZeroOcc	AltConf
	7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
	7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

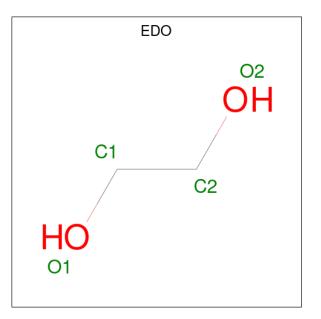
• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 10 is water.

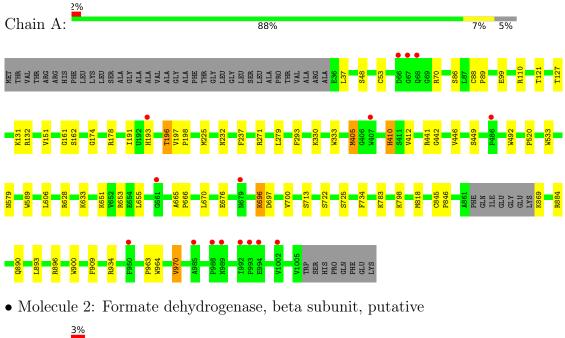
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
10	В	13	Total O 13 13	0	0

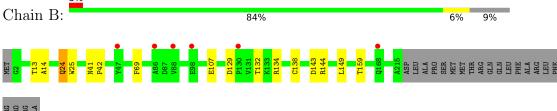


3 Residue-property plots (i)

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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	64.99Å 123.75Å 150.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.73 - 2.36	Depositor
Resolution (A)	95.55 - 2.36	EDS
% Data completeness	98.0 (95.73-2.36)	Depositor
(in resolution range)	98.0 (95.55 - 2.36)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.04 (at 2.34 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.213 , 0.248	Depositor
R, R_{free}	0.219 , 0.245	DCC
R_{free} test set	2409 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 31.1	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PEG, EDO, SF4, W, MGD, GOL, H2S, SEC

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	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.63	0/7744	0.74	0/10505
2	В	0.64	0/1699	0.74	0/2302
All	All	0.64	0/9443	0.74	0/12807

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	А	7543	0	7372	36	0
2	В	1664	0	1633	8	0
3	А	94	0	44	4	0
4	А	8	0	0	0	0
4	В	24	0	0	0	0
5	А	1	0	0	0	0
6	А	1	0	0	0	0
7	А	14	0	20	0	0
8	А	12	0	16	0	0
9	А	12	0	18	0	0
9	В	4	0	6	0	0



Mol	3	Non-H	1 0	H(added)	Clashes	Symm-Clashes
10	А	52	0	0	0	0
10	В	13	0	0	0	0
All	All	9442	0	9109	42	0

Continued from previous page...

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 2.

The worst 5 of 42 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:70:ARG:NH2	1:A:633:LYS:O	2.18	0.76
1:A:405:MET:HE1	1:A:884:ARG:NH1	2.06	0.69
1:A:70:ARG:HD3	1:A:99:GLU:OE1	1.99	0.63
1:A:653:ARG:NH2	1:A:670:LEU:O	2.35	0.59
1:A:405:MET:HE1	1:A:884:ARG:HH12	1.67	0.58

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	Perce	entiles
1	А	959/1013~(95%)	916 (96%)	39~(4%)	4 (0%)	34	38
2	В	212/236~(90%)	194 (92%)	18 (8%)	0	100	100
All	All	1171/1249~(94%)	1110 (95%)	57~(5%)	4 (0%)	41	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	196	THR
1	А	410	HIS



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	А	533	TRP
1	А	725	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	783/819~(96%)	762~(97%)	21 (3%)	44 55
2	В	185/204 (91%)	182 (98%)	3 (2%)	62 75
All	All	968/1023~(95%)	944~(98%)	24 (2%)	47 58

5 of 24 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	713	SER
1	А	798	LYS
1	А	783	LYS
1	А	869	LYS
1	А	293	PHE

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 16 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 14 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).

Mal	T a	Chain	Dec	T : 1-	Bo	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MGD	А	1102	6	$41,\!52,\!52$	0.91	3 (7%)	40,81,81	1.22	5 (12%)
9	EDO	А	1110	-	3,3,3	0.08	0	2,2,2	0.15	0
7	PEG	А	1109	-	$6,\!6,\!6$	0.19	0	$5,\!5,\!5$	0.12	0
4	SF4	В	301	2	0,12,12	-	-	-		
3	MGD	А	1101	6	$41,\!52,\!52$	0.80	2 (4%)	40,81,81	1.14	4 (10%)
8	GOL	А	1108	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.26	0
9	EDO	А	1112	-	3,3,3	0.11	0	2,2,2	0.20	0
9	EDO	В	304	-	3,3,3	0.20	0	2,2,2	0.41	0
9	EDO	А	1111	-	3,3,3	0.07	0	2,2,2	0.17	0
4	SF4	А	1103	1	0,12,12	-	-	-		
4	SF4	В	303	2	0,12,12	-	-	-		
4	SF4	В	302	2	0,12,12	-	-	-		
7	PEG	А	1106	-	$6,\!6,\!6$	0.16	0	$5,\!5,\!5$	0.23	0
8	GOL	А	1107	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.23	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
3	MGD	А	1102	6	-	5/18/66/66	0/6/6/6
9	EDO	А	1110	-	-	1/1/1/1	-
7	PEG	А	1109	-	-	2/4/4/4	-
4	SF4	В	301	2	-	-	0/6/5/5
3	MGD	А	1101	6	-	3/18/66/66	0/6/6/6
8	GOL	А	1108	-	-	0/4/4/4	-
9	EDO	А	1112	-	-	1/1/1/1	-
9	EDO	В	304	-	-	1/1/1/1	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	А	1111	-	-	0/1/1/1	-
4	SF4	А	1103	1	-	-	0/6/5/5
4	SF4	В	303	2	-	-	0/6/5/5
4	SF4	В	302	2	-	-	0/6/5/5
7	PEG	А	1106	-	-	2/4/4/4	-
8	GOL	А	1107	-	-	2/4/4/4	-

Continued from previous page...

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	1102	MGD	C23-C14	3.10	1.56	1.53
3	А	1101	MGD	C5-C6	-2.46	1.42	1.47
3	А	1102	MGD	C5-C6	-2.45	1.42	1.47
3	А	1101	MGD	C8-N7	-2.12	1.31	1.35
3	А	1102	MGD	C8-N7	-2.05	1.31	1.35

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	1102	MGD	O11-C23-C14	3.64	111.39	108.96
3	А	1101	MGD	C19-N20-C21	3.15	119.11	113.43
3	А	1102	MGD	C19-N20-C21	2.93	118.71	113.43
3	А	1101	MGD	O11-C23-C14	2.62	110.71	108.96
3	А	1101	MGD	O4'-C1'-C2'	-2.26	103.63	106.93

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1101	MGD	PA-O3B-PB-O5'
3	А	1102	MGD	O4'-C4'-C5'-O5'
3	А	1102	MGD	C4'-C5'-O5'-PB
7	А	1106	PEG	O1-C1-C2-O2
7	А	1106	PEG	O2-C3-C4-O4

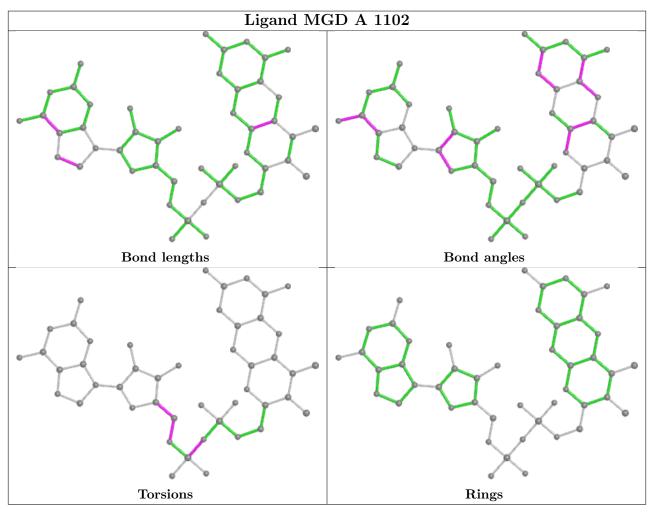
There are no ring outliers.

2 monomers are involved in 4 short contacts:

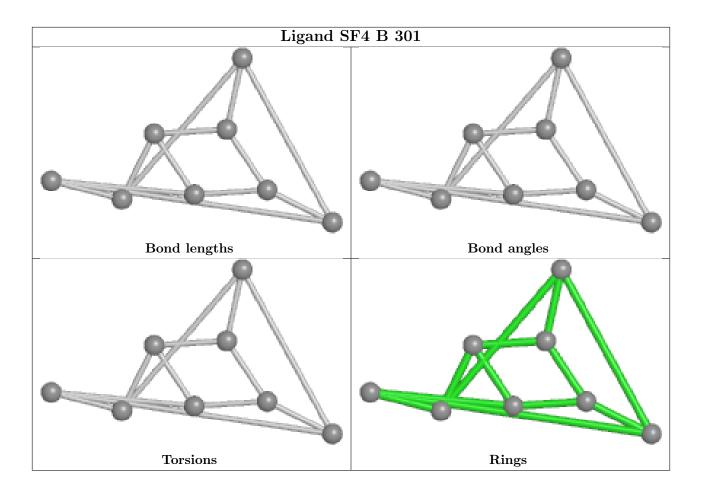
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1102	MGD	2	0
3	А	1101	MGD	2	0



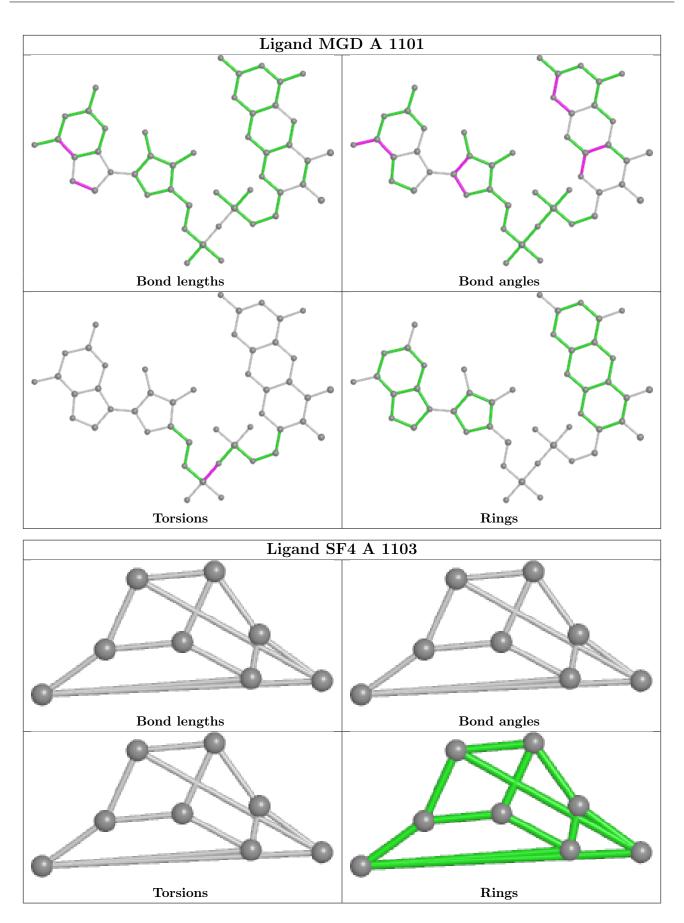
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



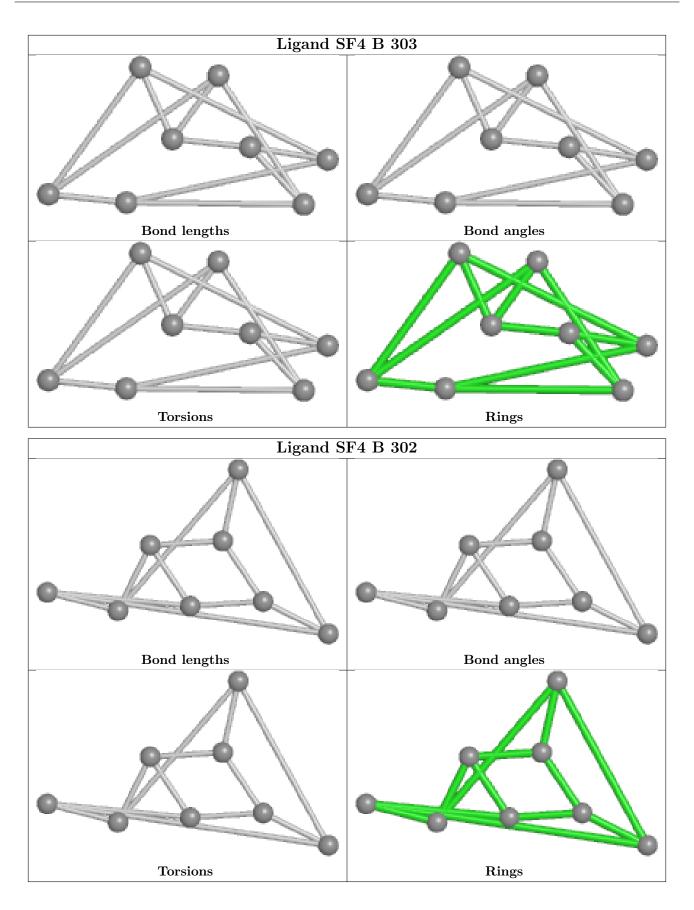














5.7 Other polymers (i)

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 (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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	962/1013~(94%)	0.26	16 (1%) 70 78	28, 45, 67, 104	0
2	В	214/236~(90%)	0.37	6 (2%) 53 64	31, 48, 70, 77	0
All	All	1176/1249~(94%)	0.28	22 (1%) 66 76	28, 46, 68, 104	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	68	GLN	5.0
1	А	988	PRO	4.0
1	А	985	ALA	3.7
1	А	193[A]	HIS	3.5
1	А	992	ILE	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)

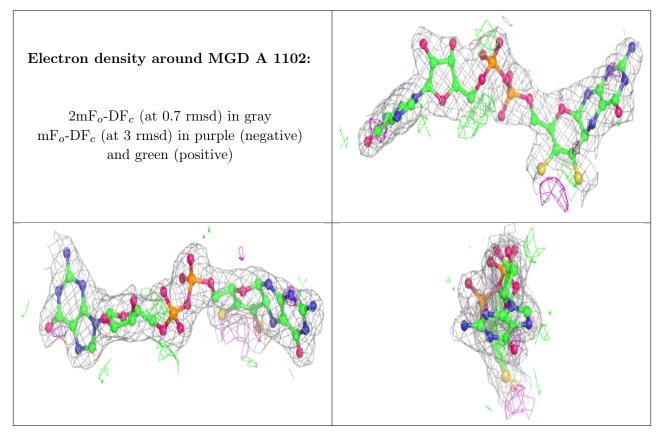
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



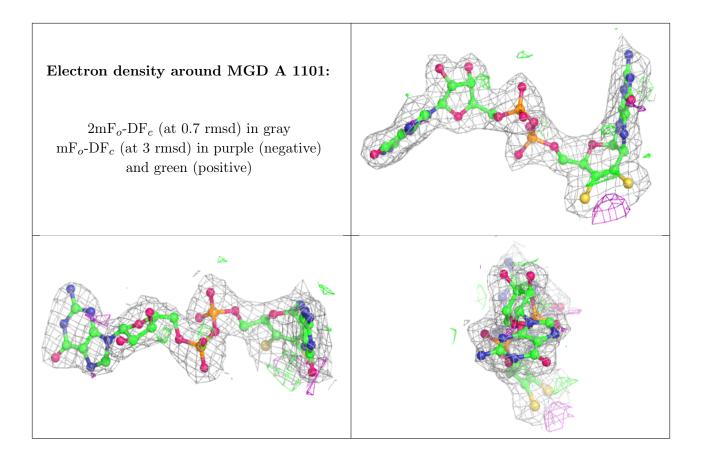
8BQI

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PEG	А	1109	7/7	0.75	0.19	$50,\!55,\!58,\!59$	0
7	PEG	А	1106	7/7	0.79	0.23	$56,\!57,\!59,\!59$	0
9	EDO	А	1111	4/4	0.84	0.19	50,52,53,57	0
9	EDO	В	304	4/4	0.86	0.18	36,44,44,48	0
9	EDO	А	1112	4/4	0.94	0.22	49,51,51,56	0
9	EDO	А	1110	4/4	0.94	0.14	46,47,47,48	0
3	MGD	А	1102	47/47	0.95	0.15	32,39,46,50	0
8	GOL	А	1107	6/6	0.95	0.14	38,40,43,43	0
8	GOL	А	1108	6/6	0.96	0.15	35,37,39,40	0
3	MGD	А	1101	47/47	0.97	0.14	29,34,39,40	0
4	SF4	В	302	8/8	0.97	0.09	46,49,51,52	0
4	SF4	В	301	8/8	0.98	0.11	32,34,35,36	0
5	H2S	А	1104	1/1	0.99	0.09	37,37,37,37	0
4	SF4	А	1103	8/8	0.99	0.10	31,32,34,34	0
4	SF4	В	303	8/8	0.99	0.09	36,40,41,44	0
6	W	А	1105	1/1	1.00	0.14	37,37,37,37	0

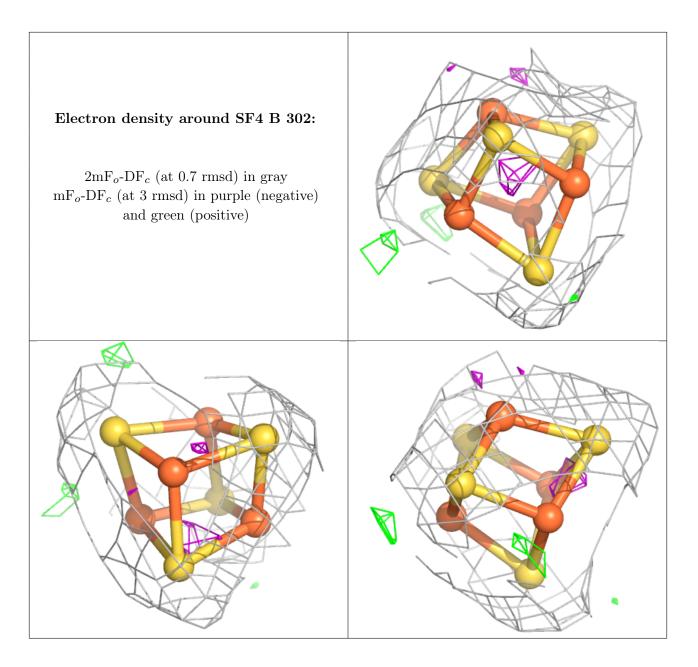
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



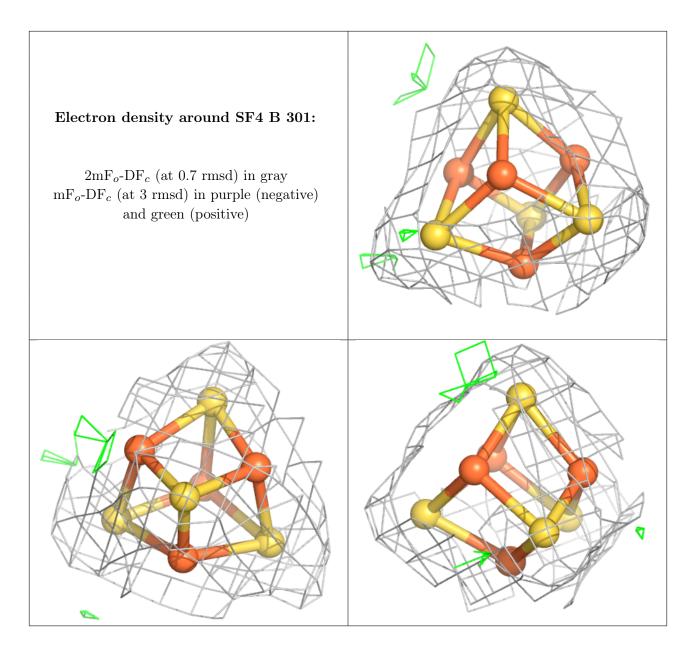




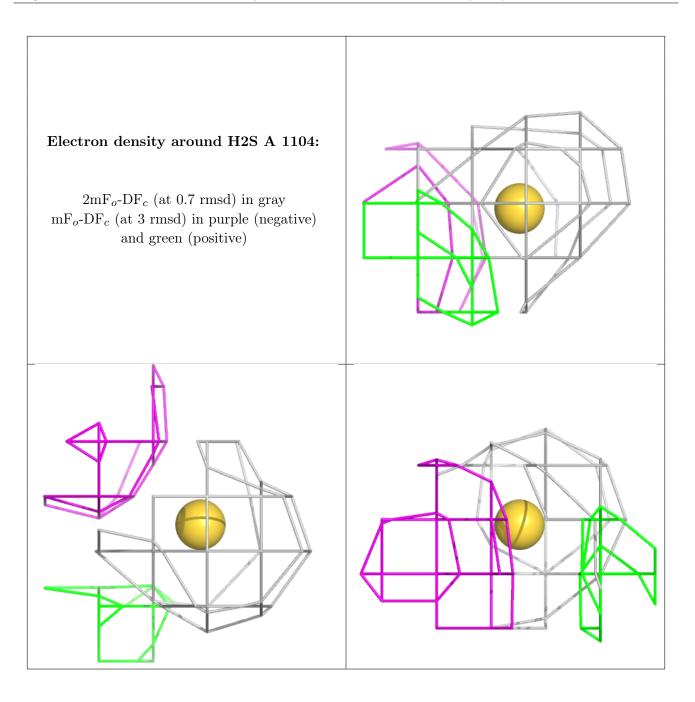




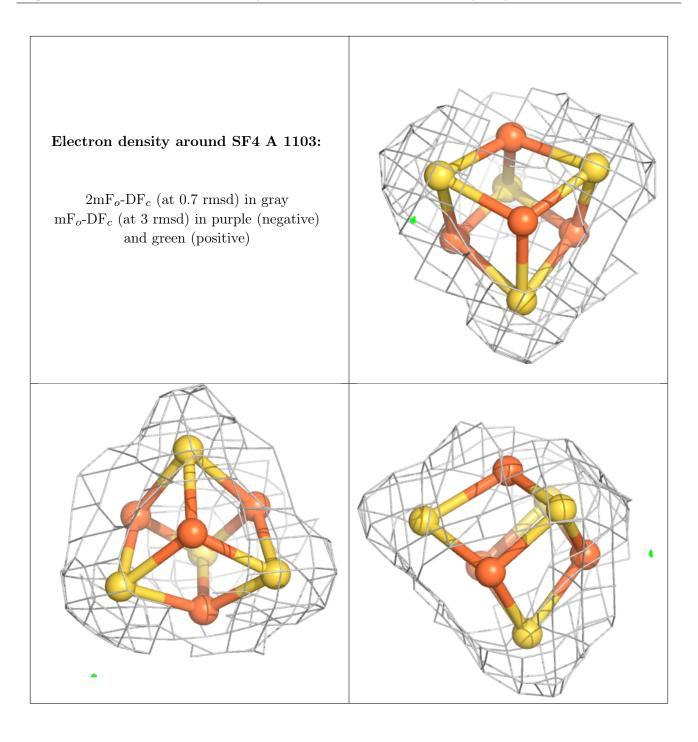




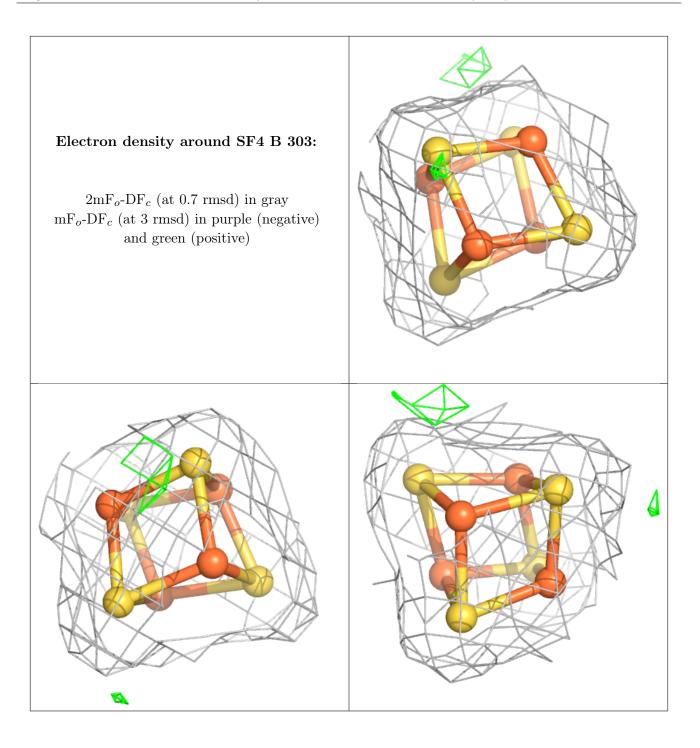




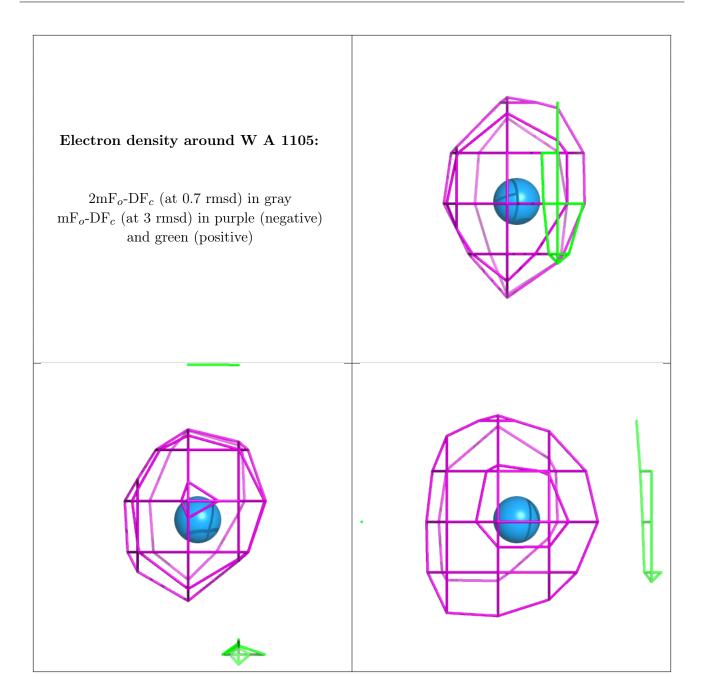












6.5 Other polymers (i)

There are no such residues in this entry.

