



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 02:32 pm GMT

PDB ID : 9I5A
Title : Crystal structure of wild type perlecan region 3 construct I876-V1272 construct including one laminin IV-like and four laminin EGF-like domains.
Authors : Sohail, A.A.; Koski, M.K.; Ruddock, L.R.
Deposited on : 2025-01-27
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

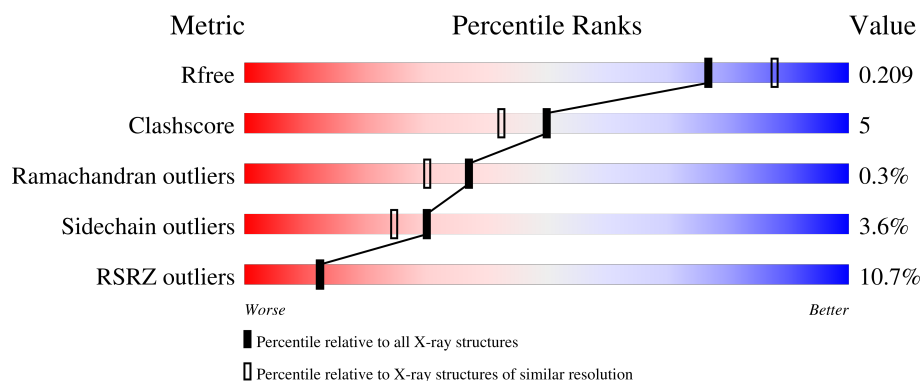
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	397	<div> <div>8%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	397	<div> <div>12%</div> <div>78%</div> <div>11%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1304	-	-	X	-
3	GOL	B	1305	-	-	X	-

2 Entry composition [i](#)

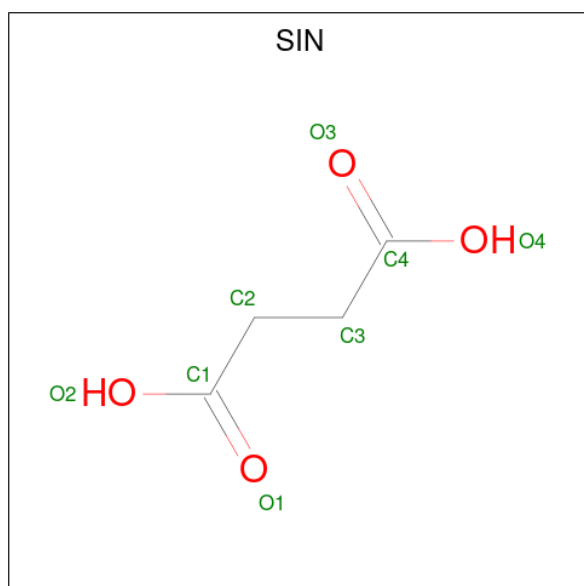
There are 4 unique types of molecules in this entry. The entry contains 11466 atoms, of which 5293 are hydrogens and 0 are deuteriums.

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 Basement membrane-specific heparan sulfate proteoglycan core protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	H	N	O	S	110	3	0
			5689	1789	2726	546	594	34			
1	B	356	Total	C	H	N	O	S	98	3	0
			5205	1635	2503	493	542	32			

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			12	4	4	4		
2	B	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		

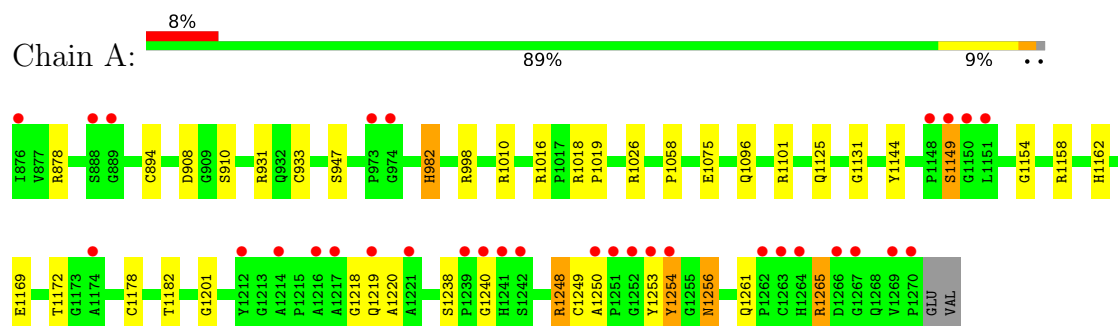
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	183	Total	O	0	0
			183	183		

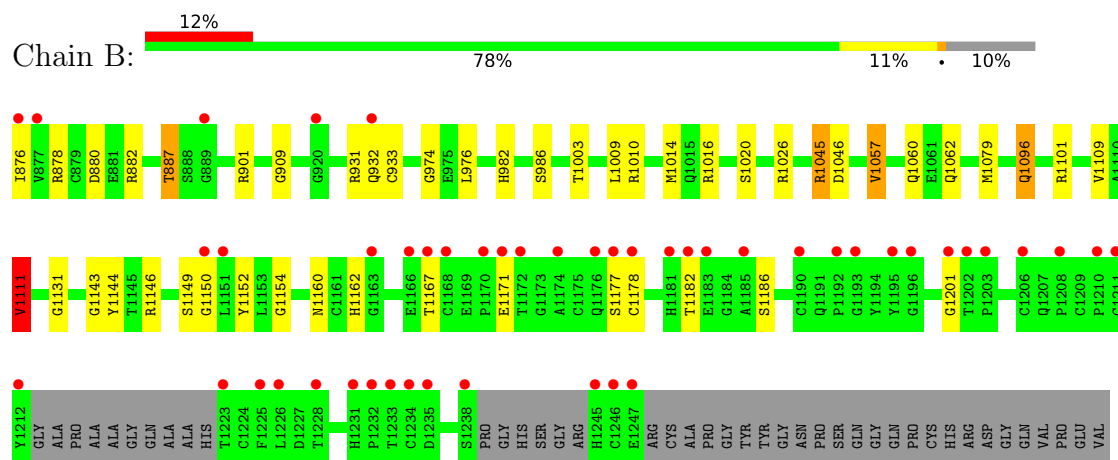
3 Residue-property plots

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: Basement membrane-specific heparan sulfate proteoglycan core protein



- Molecule 1: Basement membrane-specific heparan sulfate proteoglycan core protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.64Å 74.61Å 78.77Å 74.38° 74.08° 79.73°	Depositor
Resolution (Å)	46.24 – 2.04 46.24 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.24-2.04) 98.3 (46.24-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.178 , 0.209 0.178 , 0.209	Depositor DCC
R_{free} test set	2043 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 61.2	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	11466	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SIN

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	0.51	0/3049	0.84	5/4145 (0.1%)
1	B	0.52	0/2775	0.86	5/3766 (0.1%)
All	All	0.51	0/5824	0.85	10/7911 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1016	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	A	908	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	A	998	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	1111	VAL	N-CA-CB	-6.08	98.12	111.50
1	A	1075	GLU	CG-CD-OE1	5.90	130.09	118.30
1	A	1016	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	1075	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	B	1014	MET	CG-SD-CE	5.42	108.87	100.20
1	B	1010[A]	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	1010[B]	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1010	ARG	Sidechain
1	A	1018	ARG	Sidechain
1	A	1101	ARG	Sidechain
1	A	1149	SER	Peptide
1	A	931	ARG	Sidechain
1	B	1101	ARG	Sidechain
1	B	1146	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2963	2726	2702	22	0
1	B	2702	2503	2485	35	0
2	A	8	4	4	1	0
2	B	8	4	4	0	0
3	A	18	24	24	0	0
3	B	24	32	32	12	0
4	A	267	0	0	4	0
4	B	183	0	0	7	0
All	All	6173	5293	5251	57	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 5.

All (57) 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:B:1003:THR:HG23	3:B:1305:GOL:H11	1.43	1.00
1:B:1160:ASN:O	1:B:1186:SER:HB2	1.86	0.74
1:B:1003:THR:CG2	3:B:1305:GOL:H11	2.17	0.74
1:B:1060[A]:GLN:OE1	1:B:1062:GLN:HB2	1.92	0.70
1:B:974:GLY:HA2	3:B:1304:GOL:H11	1.75	0.69
1:A:947[A]:SER:OG	4:A:1401:HOH:O	2.10	0.68
1:B:1009:LEU:HB3	1:B:1057:VAL:HG13	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:THR:HG23	3:B:1305:GOL:C1	2.24	0.66
1:B:1060[A]:GLN:NE2	1:B:1062:GLN:OE1	2.24	0.60
1:B:1109:VAL:HG11	3:B:1302:GOL:H12	1.84	0.59
1:B:1143:GLY:HA2	1:B:1171:GLU:O	2.03	0.59
1:A:1250:ALA:O	1:A:1253:TYR:HB2	2.03	0.59
1:A:982:HIS:CD2	1:A:982:HIS:H	2.21	0.58
1:A:1125:GLN:NE2	4:A:1410:HOH:O	2.36	0.58
1:B:878:ARG:N	1:B:878:ARG:HD2	2.20	0.57
1:B:1003:THR:CG2	3:B:1305:GOL:C1	2.83	0.55
1:B:1045:ARG:HD2	4:B:1444:HOH:O	2.06	0.55
1:B:974:GLY:CA	3:B:1304:GOL:H11	2.37	0.55
1:B:1149:SER:HB2	1:B:1154:GLY:HA2	1.89	0.54
1:A:1240:GLY:O	1:A:1250:ALA:N	2.33	0.54
1:B:880:ASP:OD1	1:B:882:ARG:HD3	2.08	0.54
1:B:1096:GLN:NE2	4:B:1409:HOH:O	2.40	0.54
1:A:1254:TYR:C	1:A:1254:TYR:CD1	2.85	0.50
1:B:1026:ARG:HD3	4:B:1454:HOH:O	2.12	0.50
1:B:976:LEU:HD21	3:B:1304:GOL:H31	1.93	0.49
1:A:1158:ARG:HH11	1:A:1158:ARG:HG3	1.77	0.49
1:B:876:ILE:O	1:B:878:ARG:NH1	2.46	0.48
1:B:1111:VAL:HG22	4:B:1501:HOH:O	2.13	0.48
3:B:1302:GOL:O2	4:B:1401:HOH:O	2.12	0.48
1:B:878:ARG:N	1:B:878:ARG:CD	2.77	0.48
1:A:1240:GLY:O	1:A:1249:CYS:HA	2.13	0.48
1:B:887:THR:OG1	4:B:1402:HOH:O	2.20	0.47
1:A:1220:ALA:HB1	1:B:1177:SER:O	2.14	0.47
1:A:1026:ARG:NH1	4:A:1409:HOH:O	2.35	0.47
1:A:1131:GLY:HA2	1:A:1144:TYR:CD1	2.50	0.47
1:A:1169:GLU:OE1	1:A:1172:THR:HG23	2.15	0.47
1:B:909:GLY:HA2	1:B:931:ARG:O	2.15	0.47
1:A:1254:TYR:CD1	1:A:1254:TYR:O	2.69	0.46
1:B:974:GLY:H	3:B:1304:GOL:H11	1.80	0.46
1:B:1131:GLY:HA2	1:B:1144:TYR:CD1	2.50	0.46
1:A:910:SER:O	4:A:1402:HOH:O	2.20	0.45
1:B:901[A]:ARG:HG2	1:B:901[A]:ARG:HH11	1.82	0.44
1:A:894:CYS:HB2	2:A:1301:SIN:H31	1.99	0.44
1:B:1178:CYS:HB3	1:B:1182:THR:OG1	2.18	0.44
1:B:1162:HIS:O	1:B:1201:GLY:HA2	2.19	0.43
1:B:1079:MET:CE	1:B:1152:TYR:HA	2.49	0.43
1:A:1149:SER:O	1:A:1154:GLY:HA2	2.18	0.42
1:A:1162:HIS:O	1:A:1201:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:ARG:HG3	1:A:1158:ARG:NH1	2.35	0.42
1:A:1256:ASN:H	1:A:1261:GLN:HB2	1.85	0.42
1:B:974:GLY:N	3:B:1304:GOL:H11	2.36	0.41
1:A:1178:CYS:HB3	1:A:1182:THR:OG1	2.21	0.41
1:B:974:GLY:H	3:B:1304:GOL:C1	2.34	0.41
1:B:932:GLN:NE2	4:B:1412:HOH:O	2.49	0.41
1:A:1248:ARG:CZ	1:A:1248:ARG:HB3	2.50	0.41
1:A:1253:TYR:CE1	1:A:1265:ARG:HD3	2.56	0.41
1:B:880:ASP:OD2	1:B:882:ARG:NH1	2.54	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	396/397 (100%)	382 (96%)	13 (3%)	1 (0%)	37	30
1	B	353/397 (89%)	337 (96%)	15 (4%)	1 (0%)	37	30
All	All	749/794 (94%)	719 (96%)	28 (4%)	2 (0%)	37	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	GLY
1	A	1218	GLY

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	332/331 (100%)	320 (96%)	12 (4%)	30	25
1	B	307/331 (93%)	296 (96%)	11 (4%)	30	25
All	All	639/662 (96%)	616 (96%)	23 (4%)	30	25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	878	ARG
1	A	933	CYS
1	A	982	HIS
1	A	1019	PRO
1	A	1058	PRO
1	A	1096	GLN
1	A	1219	GLN
1	A	1238	SER
1	A	1248	ARG
1	A	1254	TYR
1	A	1256	ASN
1	A	1265	ARG
1	B	887	THR
1	B	933	CYS
1	B	982	HIS
1	B	986	SER
1	B	1020	SER
1	B	1045	ARG
1	B	1046	ASP
1	B	1057	VAL
1	B	1096	GLN
1	B	1111	VAL
1	B	1167	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	982	HIS
1	A	1219	GLN
1	A	1256	ASN
1	B	896	ASN
1	B	1027	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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	GOL	A	1302	-	5,5,5	0.11	0	5,5,5	0.32	0
3	GOL	B	1304	-	5,5,5	0.27	0	5,5,5	0.62	0
2	SIN	B	1301	-	7,7,7	1.12	0	8,8,8	1.67	2 (25%)
3	GOL	B	1303	-	5,5,5	0.31	0	5,5,5	0.54	0
3	GOL	A	1303	-	5,5,5	0.15	0	5,5,5	0.47	0
2	SIN	A	1301	-	7,7,7	1.25	0	8,8,8	0.97	0
3	GOL	A	1304	-	5,5,5	0.10	0	5,5,5	0.25	0
3	GOL	B	1302	-	5,5,5	0.10	0	5,5,5	0.37	0
3	GOL	B	1305	-	5,5,5	0.14	0	5,5,5	0.46	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	GOL	A	1302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1304	-	-	4/4/4/4	-
2	SIN	B	1301	-	-	3/5/5/5	-
3	GOL	B	1303	-	-	2/4/4/4	-
3	GOL	A	1303	-	-	3/4/4/4	-
2	SIN	A	1301	-	-	5/5/5/5	-
3	GOL	A	1304	-	-	2/4/4/4	-
3	GOL	B	1302	-	-	2/4/4/4	-
3	GOL	B	1305	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	SIN	C2-C3-C4	3.07	120.22	113.60
2	B	1301	SIN	C3-C2-C1	2.33	118.62	113.60

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	GOL	O1-C1-C2-O2
3	A	1302	GOL	O1-C1-C2-C3
3	A	1304	GOL	O1-C1-C2-C3
3	B	1302	GOL	O1-C1-C2-C3
3	B	1303	GOL	O1-C1-C2-C3
3	B	1304	GOL	C1-C2-C3-O3
3	B	1305	GOL	C1-C2-C3-O3
2	B	1301	SIN	C1-C2-C3-C4
3	A	1303	GOL	C1-C2-C3-O3
3	B	1304	GOL	O1-C1-C2-C3
3	B	1305	GOL	O1-C1-C2-C3
3	B	1302	GOL	O1-C1-C2-O2
3	B	1304	GOL	O2-C2-C3-O3
3	B	1305	GOL	O1-C1-C2-O2
3	A	1303	GOL	O2-C2-C3-O3
3	A	1304	GOL	O1-C1-C2-O2
3	B	1305	GOL	O2-C2-C3-O3
2	A	1301	SIN	C1-C2-C3-C4
3	B	1304	GOL	O1-C1-C2-O2

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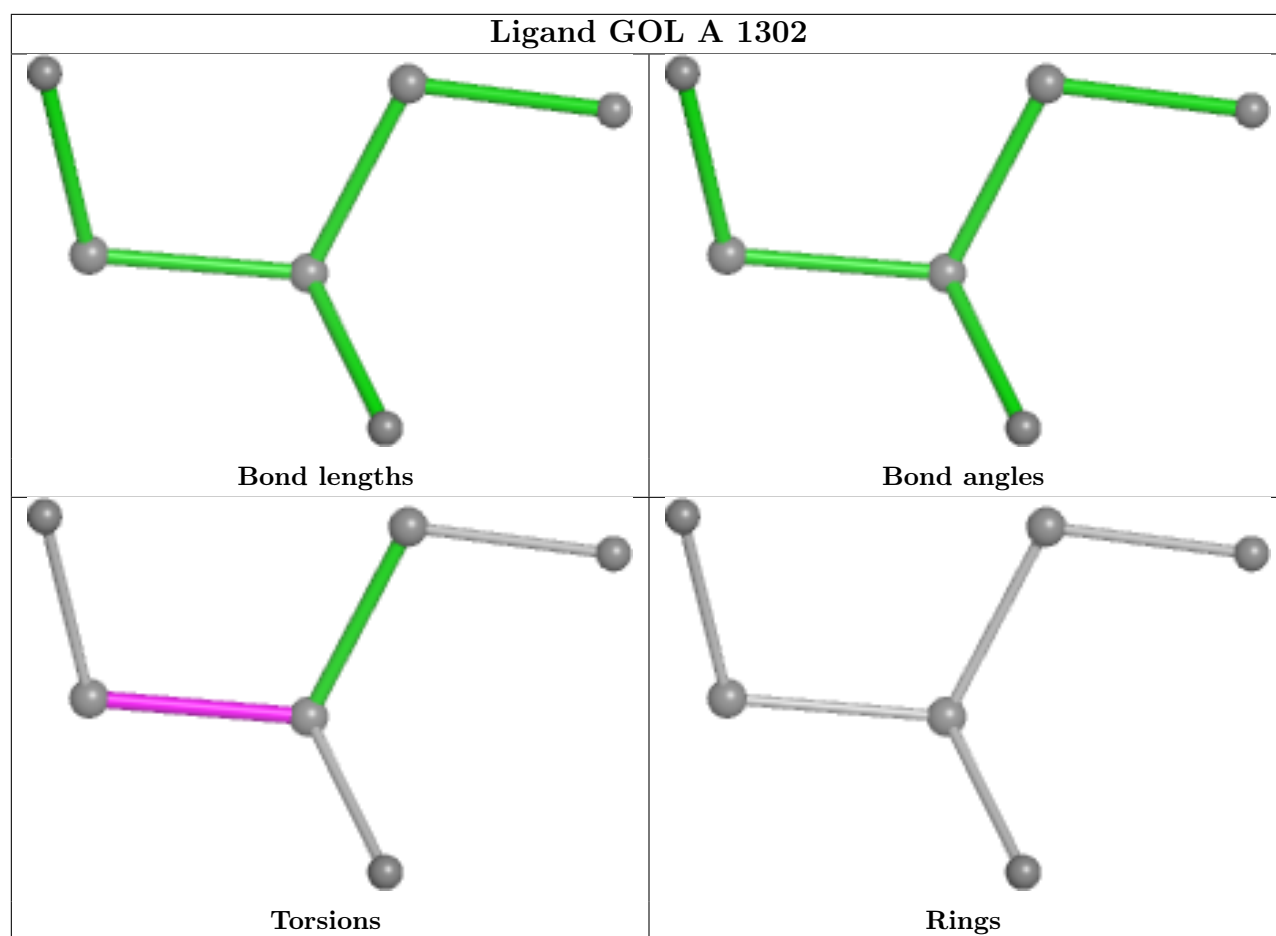
Mol	Chain	Res	Type	Atoms
3	A	1303	GOL	O1-C1-C2-O2
2	A	1301	SIN	C2-C3-C4-O3
2	A	1301	SIN	C2-C3-C4-O4
2	B	1301	SIN	O1-C1-C2-C3
2	B	1301	SIN	O2-C1-C2-C3
2	A	1301	SIN	O1-C1-C2-C3
3	B	1303	GOL	O1-C1-C2-O2
2	A	1301	SIN	O2-C1-C2-C3

There are no ring outliers.

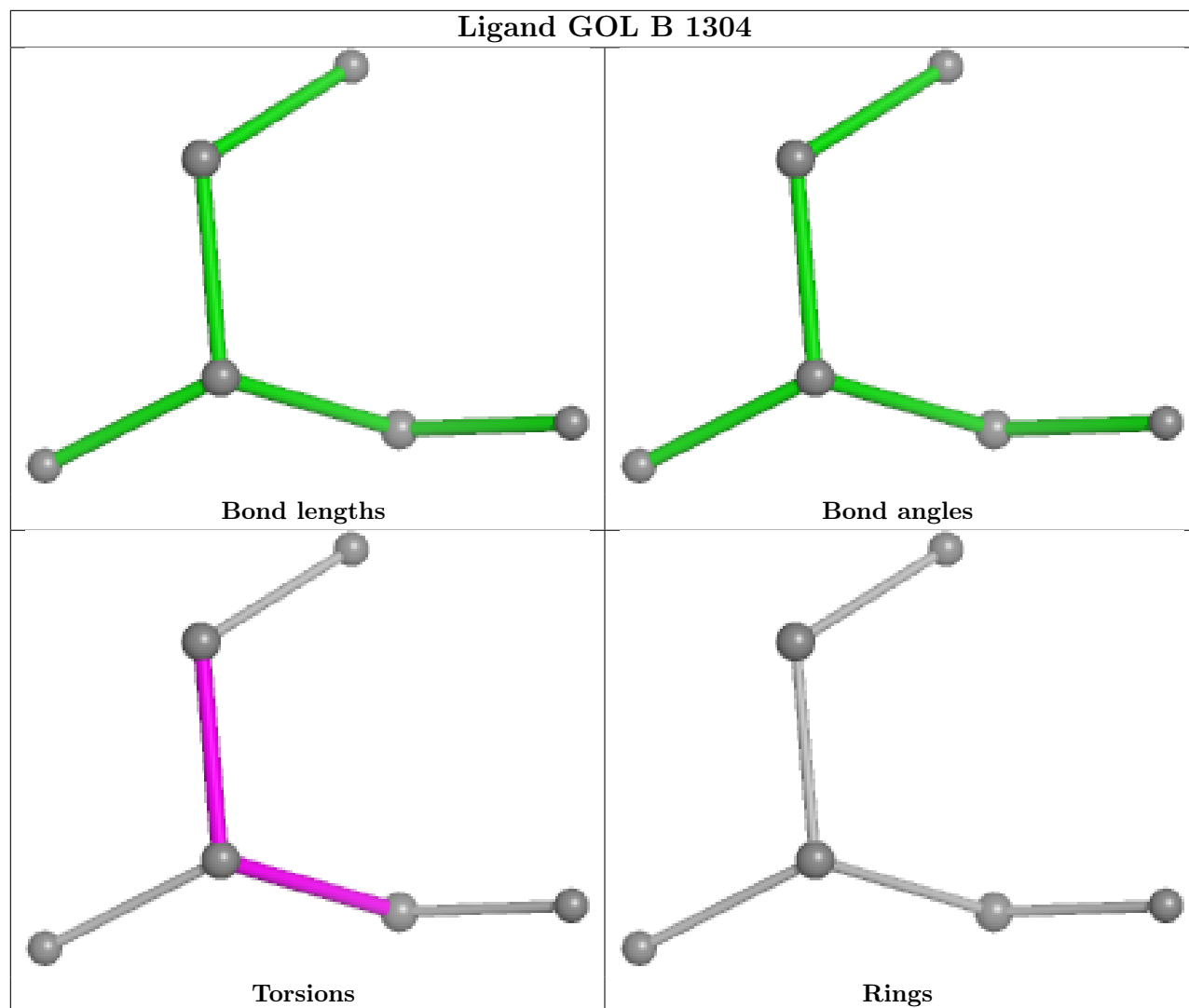
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1304	GOL	6	0
2	A	1301	SIN	1	0
3	B	1302	GOL	2	0
3	B	1305	GOL	4	0

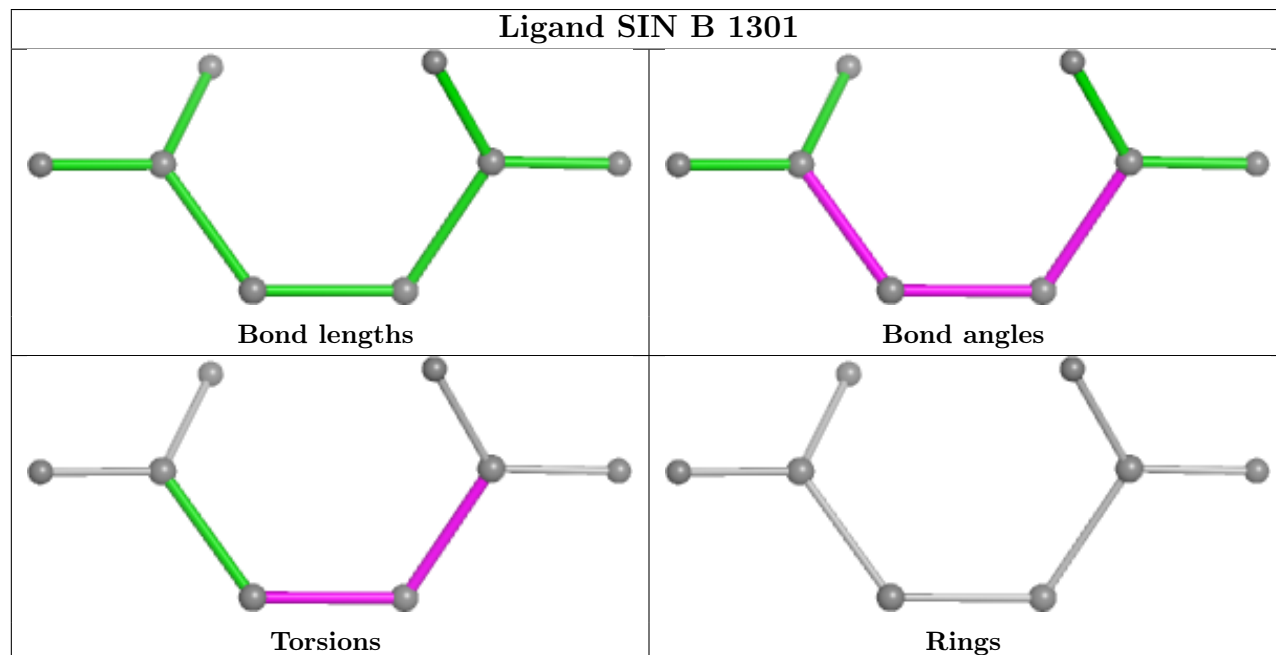
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

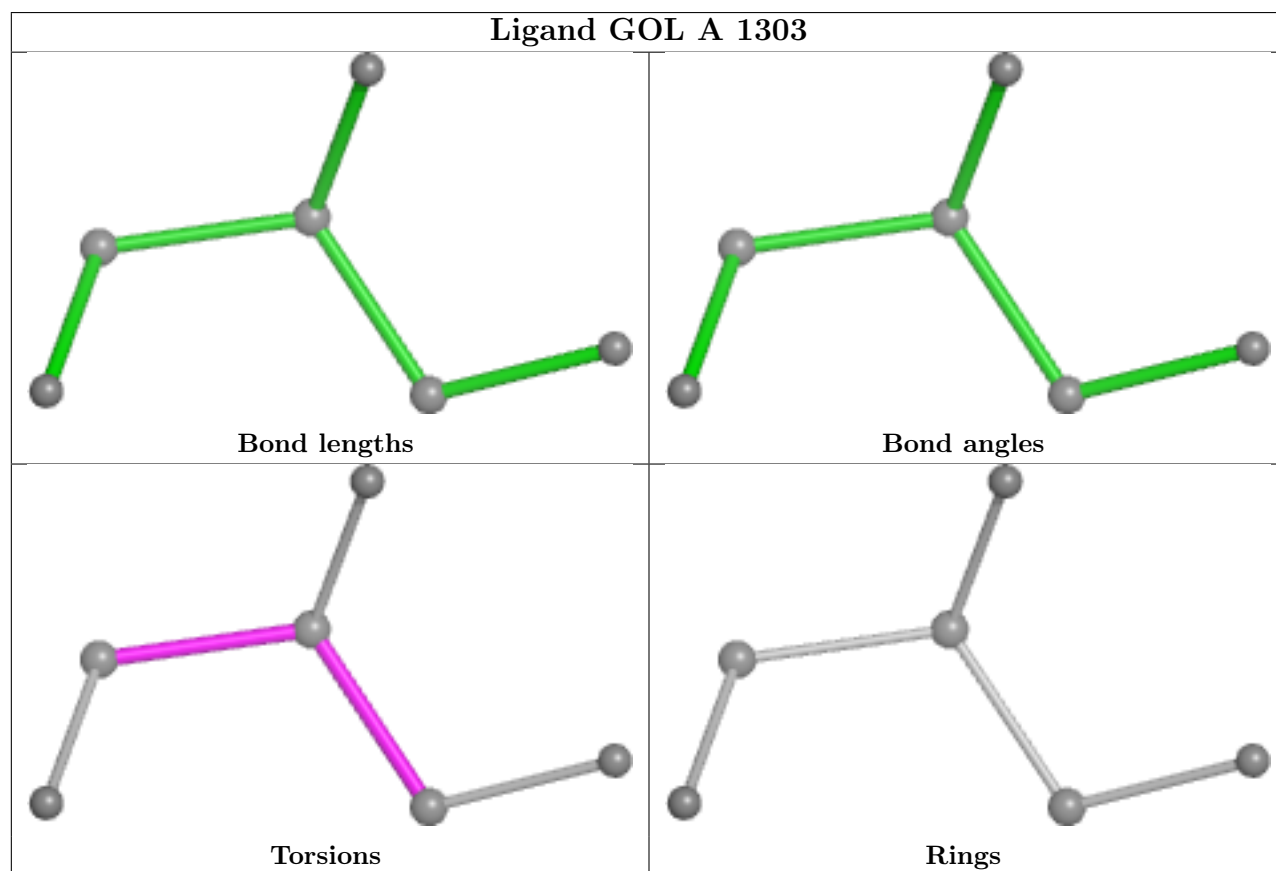
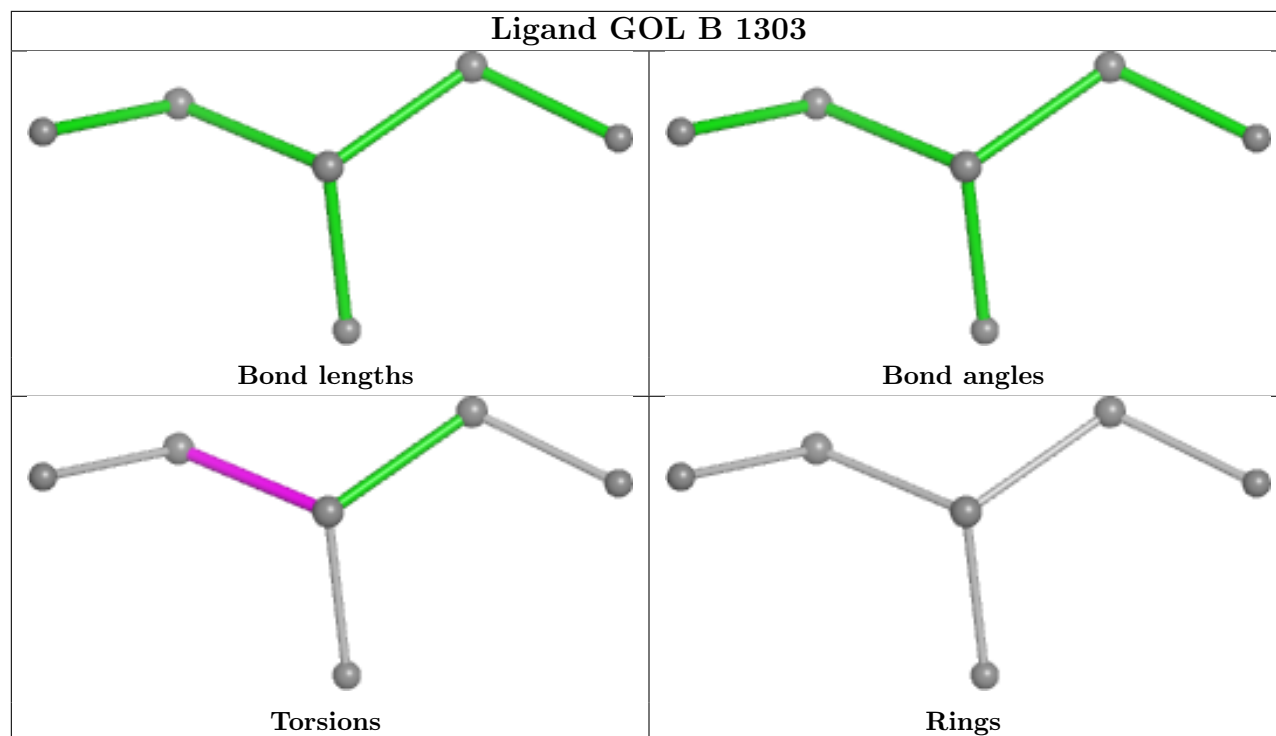


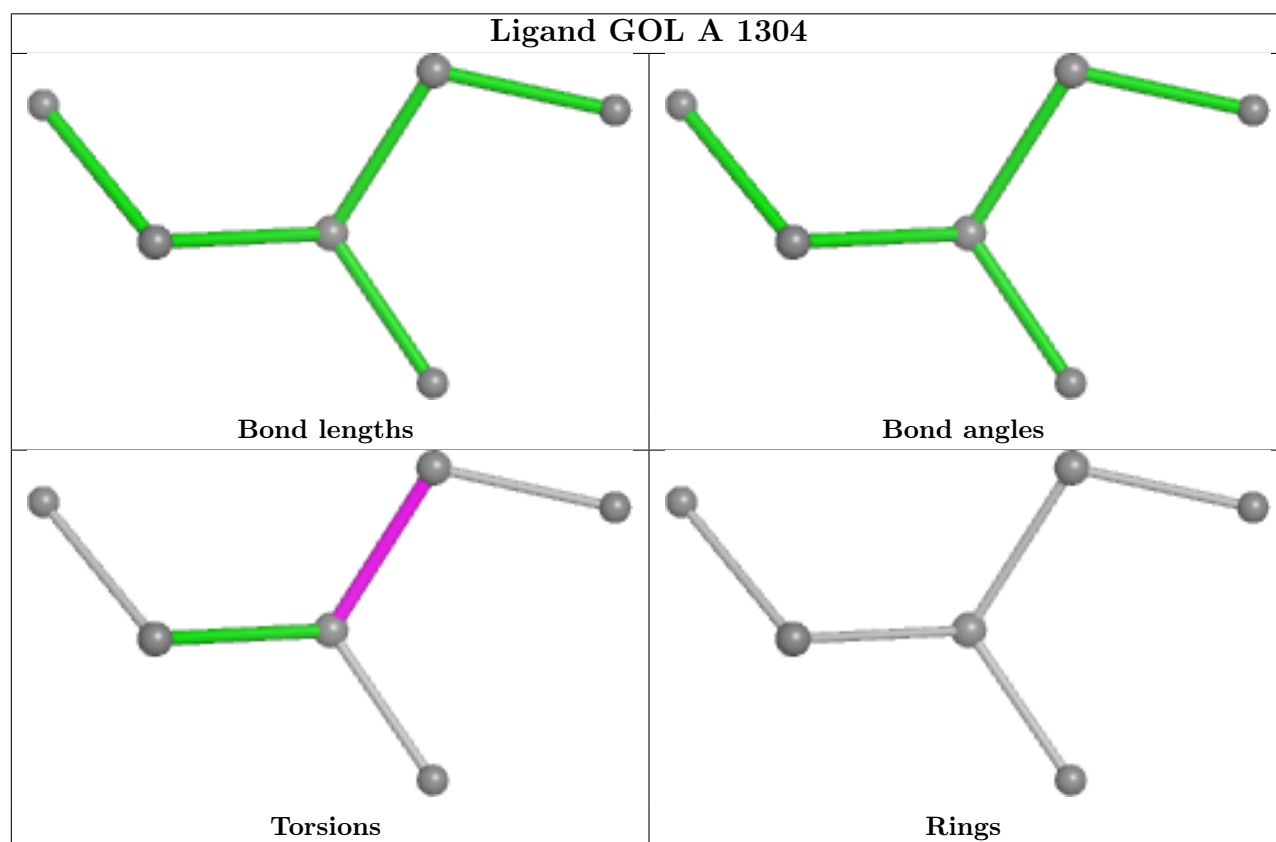
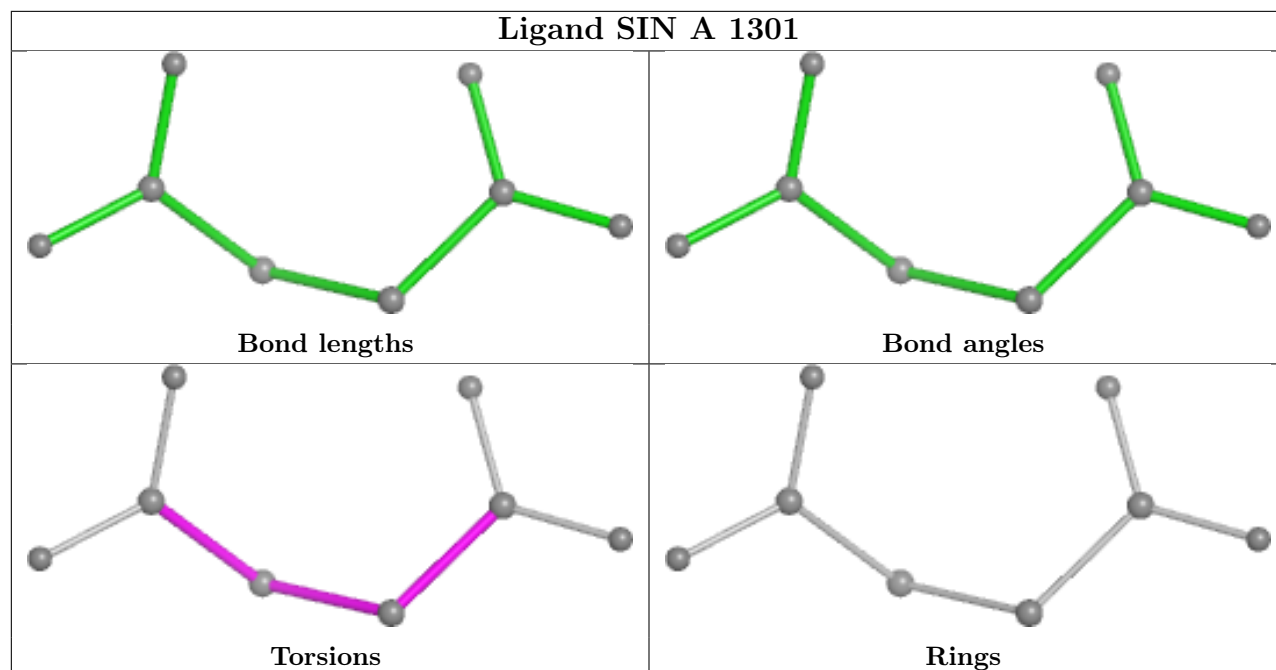
Ligand GOL B 1304

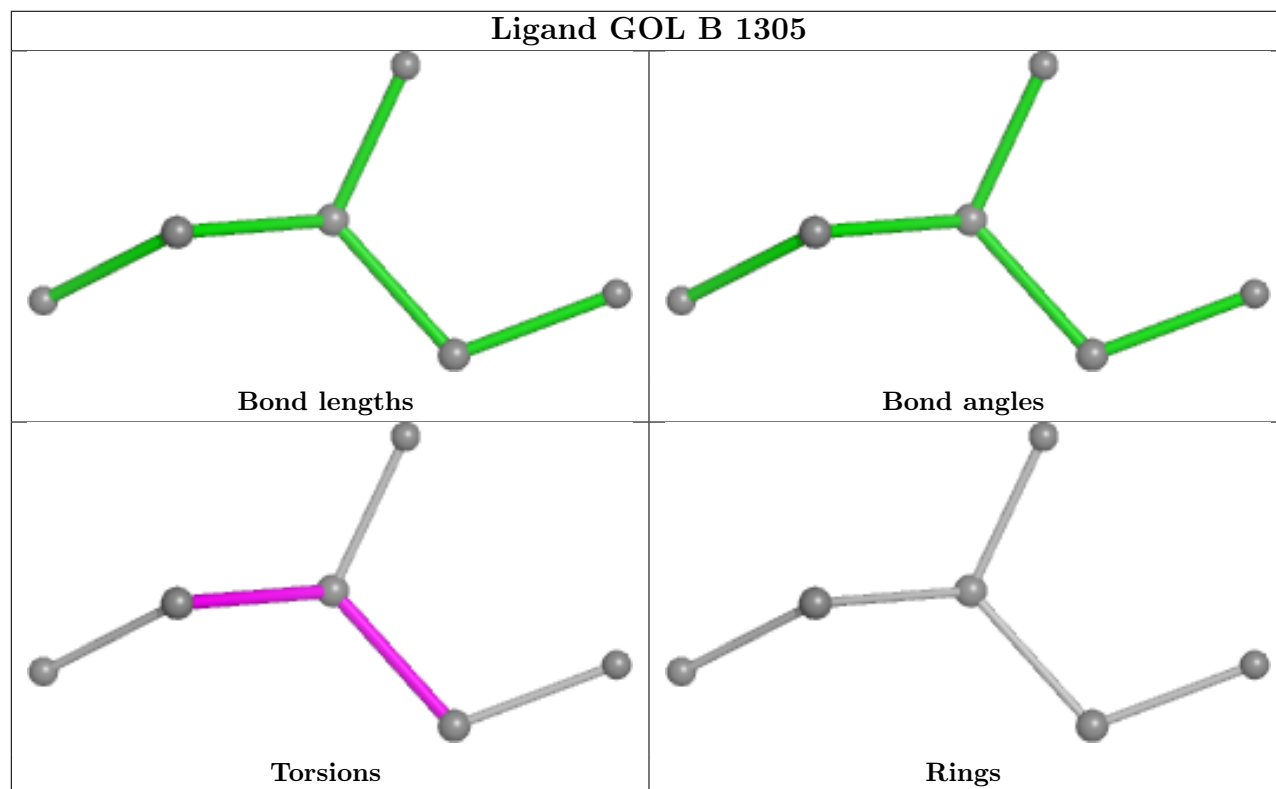
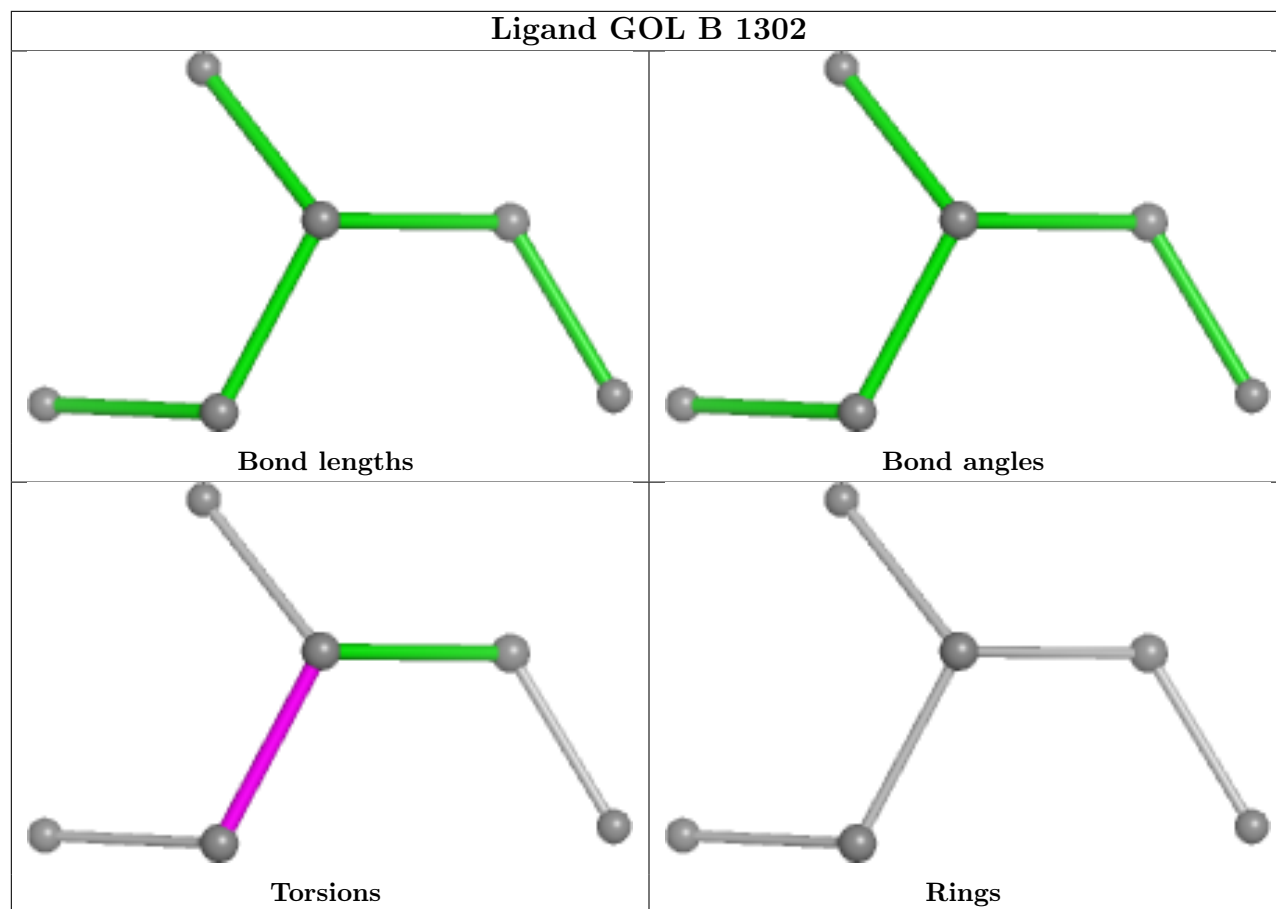


Ligand SIN B 1301









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	395/397 (99%)	0.22	32 (8%) 19 21	24, 46, 105, 142	2 (0%)
1	B	356/397 (89%)	0.47	48 (13%) 8 8	21, 49, 182, 217	3 (0%)
All	All	751/794 (94%)	0.34	80 (10%) 12 12	21, 48, 157, 217	5 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1270	PRO	7.6
1	B	1212	TYR	7.3
1	A	1217	ALA	5.6
1	A	974	GLY	4.6
1	B	1208	PRO	4.4
1	B	1177	SER	4.3
1	A	1254	TYR	4.3
1	A	1151	LEU	4.2
1	B	1245	HIS	4.1
1	B	876	ILE	4.1
1	B	1170	PRO	4.1
1	B	1163	GLY	4.1
1	A	876	ILE	4.1
1	A	1269	VAL	4.0
1	B	1167	THR	3.9
1	A	1264	HIS	3.9
1	A	1267	GLY	3.8
1	A	1262	PRO	3.7
1	A	1148	PRO	3.4
1	B	1203	PRO	3.4
1	B	1181	HIS	3.3
1	B	1223	THR	3.3
1	B	1201	GLY	3.2
1	B	1206	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1192	PRO	3.2
1	B	1174	ALA	3.2
1	A	1251	PRO	3.1
1	B	1210	PRO	3.0
1	B	1182	THR	3.0
1	B	1226	LEU	3.0
1	A	1240	GLY	2.9
1	A	1214	ALA	2.9
1	B	1185	ALA	2.9
1	B	1228	THR	2.9
1	A	1266	ASP	2.9
1	B	1168	CYS	2.9
1	B	1190	CYS	2.9
1	B	1232	PRO	2.8
1	B	1172	THR	2.8
1	A	1253	TYR	2.8
1	B	1183	GLU	2.8
1	B	1247	GLU	2.8
1	B	1238	SER	2.8
1	A	1263	CYS	2.7
1	B	1196	GLY	2.7
1	A	1242	SER	2.7
1	B	1225	PHE	2.7
1	B	1178	CYS	2.7
1	B	1151	LEU	2.6
1	B	1202	THR	2.6
1	B	1176	GLN	2.6
1	B	1231	HIS	2.6
1	A	1149	SER	2.6
1	A	889	GLY	2.5
1	B	1195	TYR	2.5
1	B	932	GLN	2.5
1	A	1219	GLN	2.5
1	B	1211	CYS	2.5
1	B	1150	GLY	2.5
1	B	1234	CYS	2.5
1	A	1174	ALA	2.5
1	A	973	PRO	2.4
1	A	888	SER	2.3
1	B	877	VAL	2.3
1	A	1150	GLY	2.3
1	A	1212	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1233	THR	2.3
1	A	1241	HIS	2.2
1	B	1235	ASP	2.2
1	A	1239	PRO	2.2
1	A	1252	GLY	2.2
1	B	920	GLY	2.2
1	B	1193	GLY	2.1
1	A	1221	ALA	2.1
1	A	1250	ALA	2.1
1	B	1166	GLU	2.1
1	B	1246	CYS	2.1
1	B	889	GLY	2.0
1	B	1171	GLU	2.0
1	A	1216	ALA	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](#)

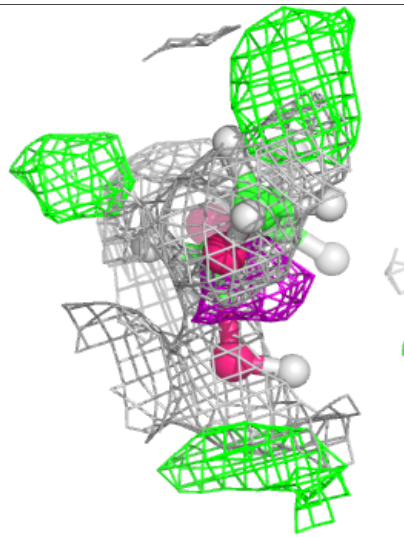
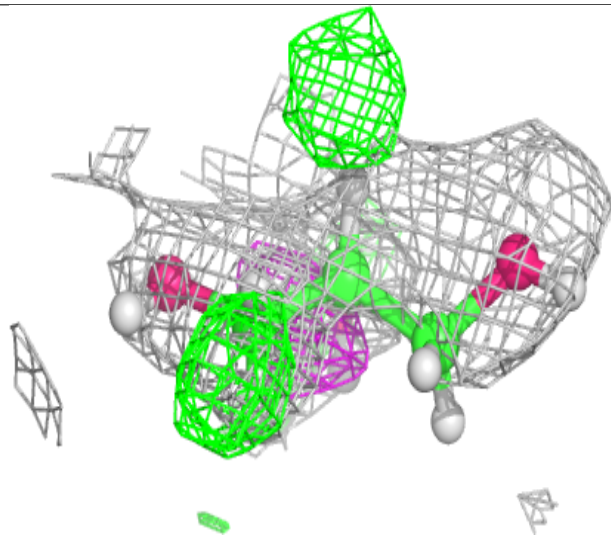
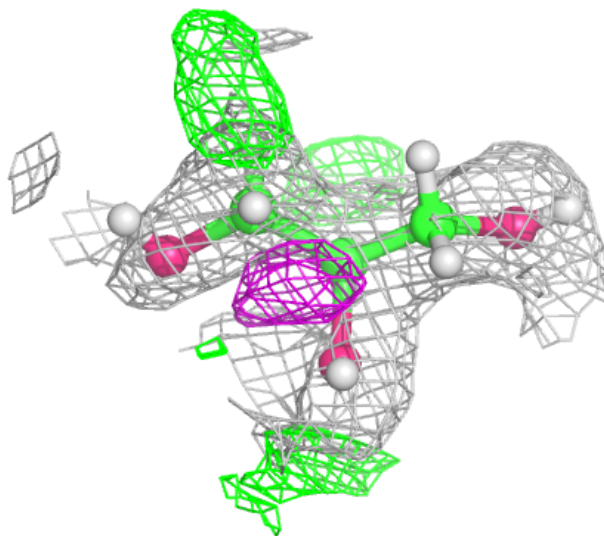
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	1303	6/6	0.72	0.21	30,82,98,98	3
3	GOL	B	1304	6/6	0.83	0.18	30,78,81,82	3
3	GOL	A	1302	6/6	0.88	0.15	30,66,82,84	3
3	GOL	A	1303	6/6	0.90	0.16	30,73,85,87	3
3	GOL	A	1304	6/6	0.91	0.17	30,96,98,99	3
2	SIN	A	1301	8/8	0.92	0.16	62,70,76,100	0
3	GOL	B	1302	6/6	0.92	0.15	30,67,80,82	3
3	GOL	B	1305	6/6	0.92	0.12	30,68,74,75	3
2	SIN	B	1301	8/8	0.95	0.11	55,65,75,76	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.

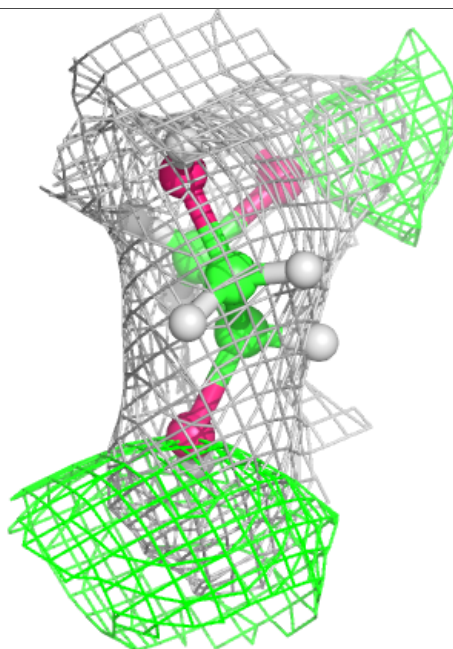
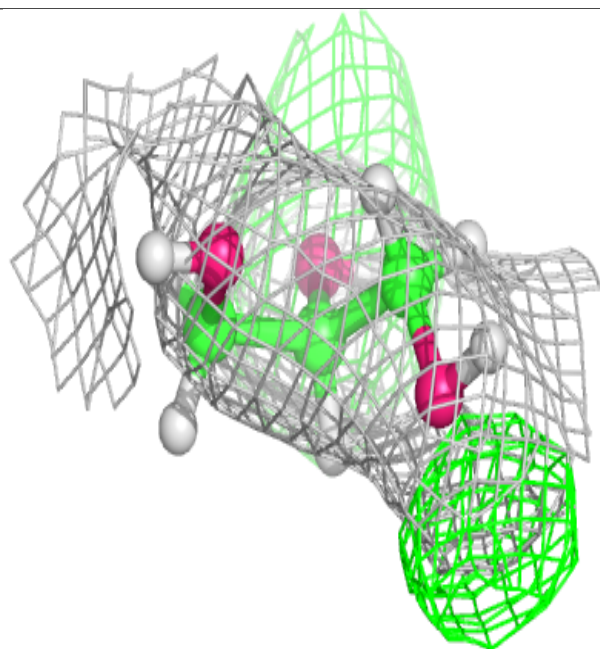
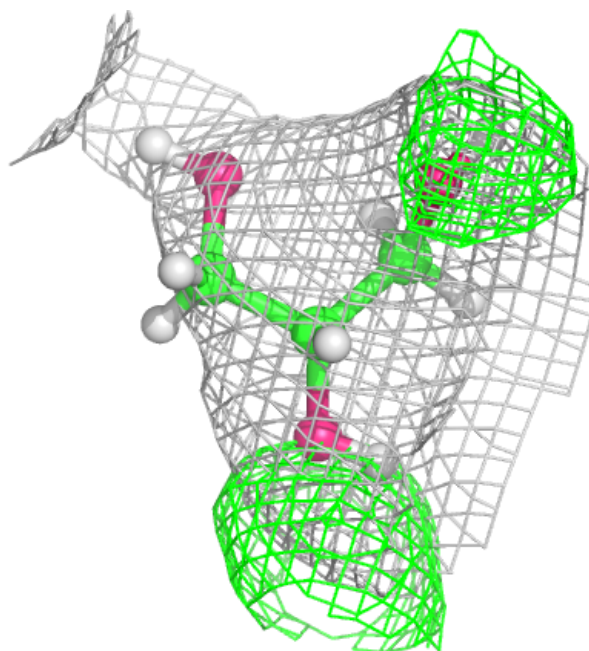
Electron density around GOL B 1303:

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



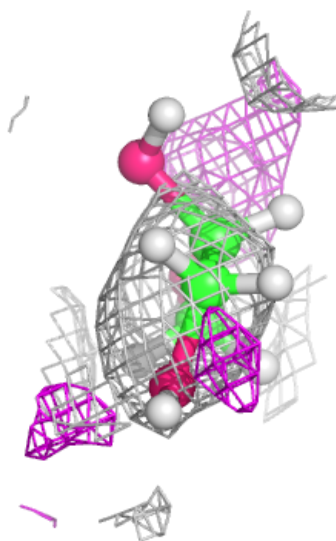
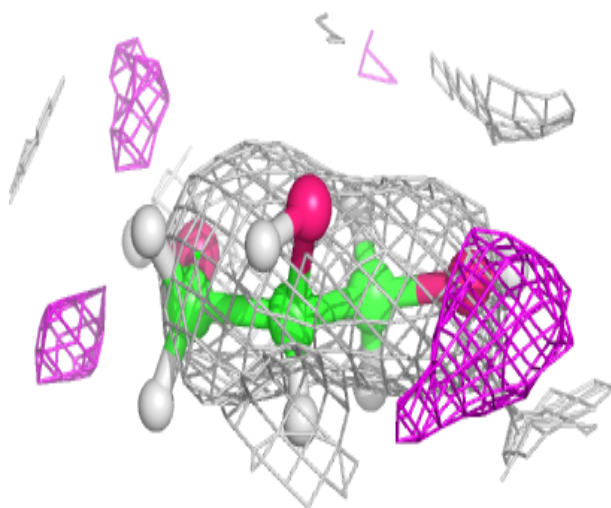
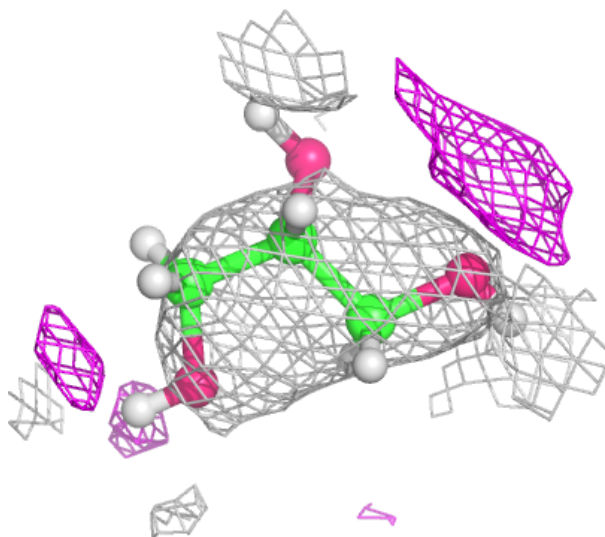
Electron density around GOL B 1304:

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



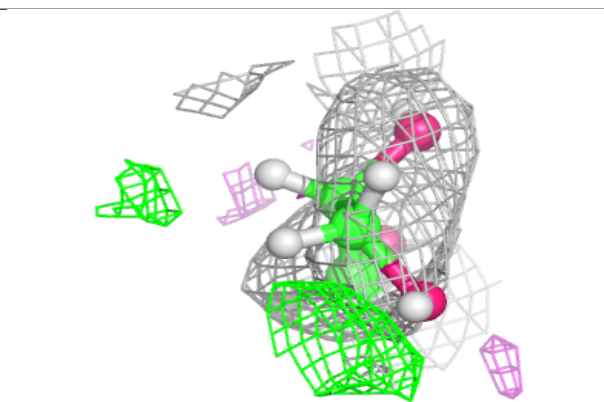
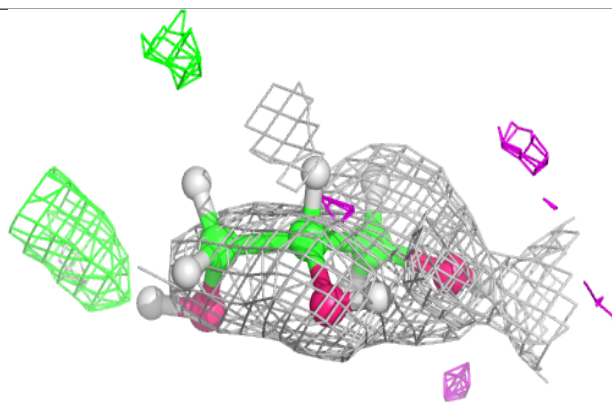
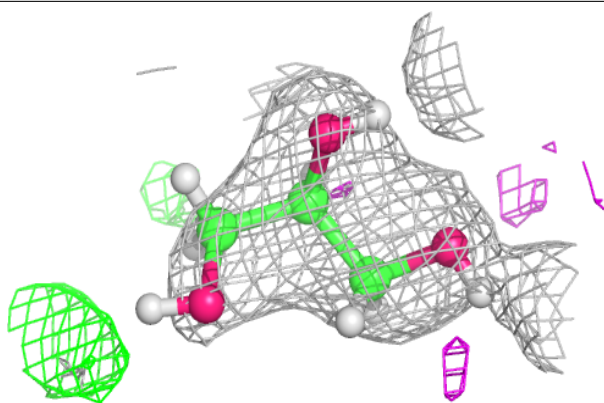
Electron density around GOL A 1302:

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

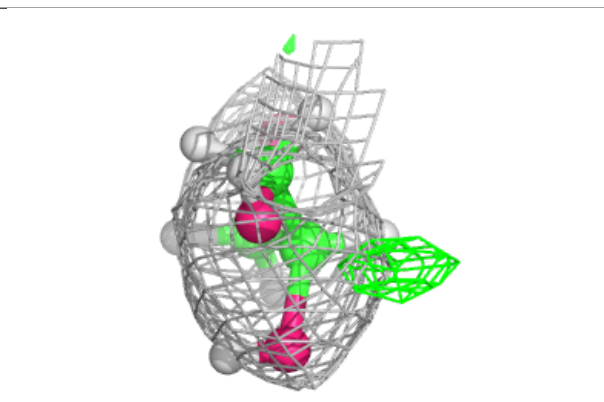
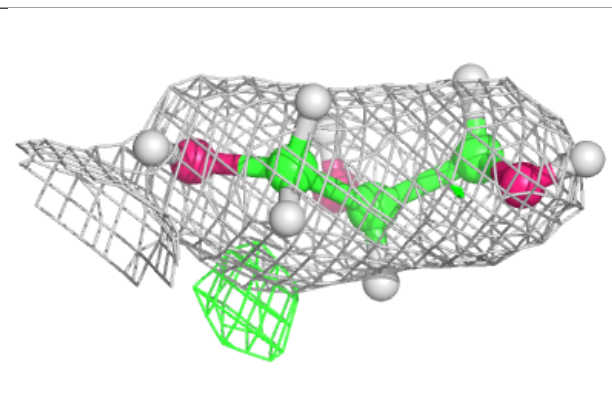
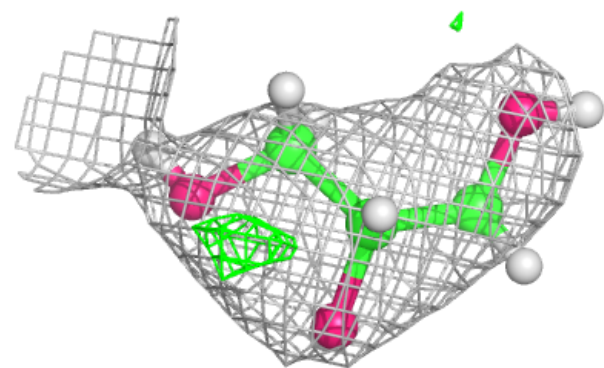


Electron density around GOL A 1303:

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

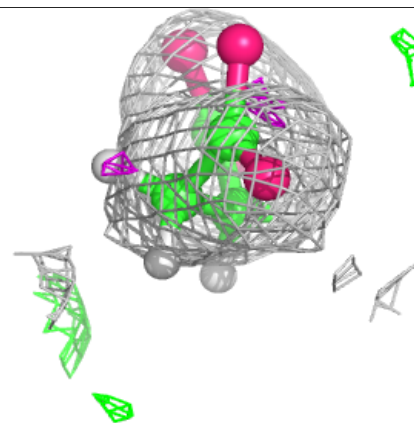
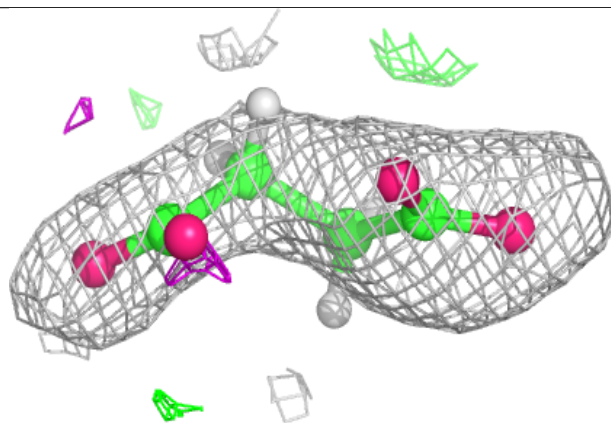
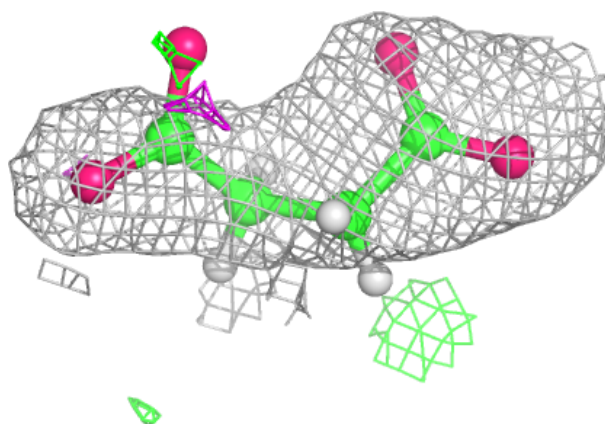
**Electron density around GOL A 1304:**

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



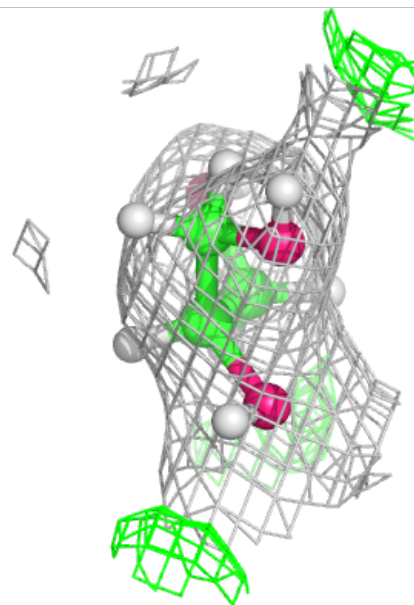
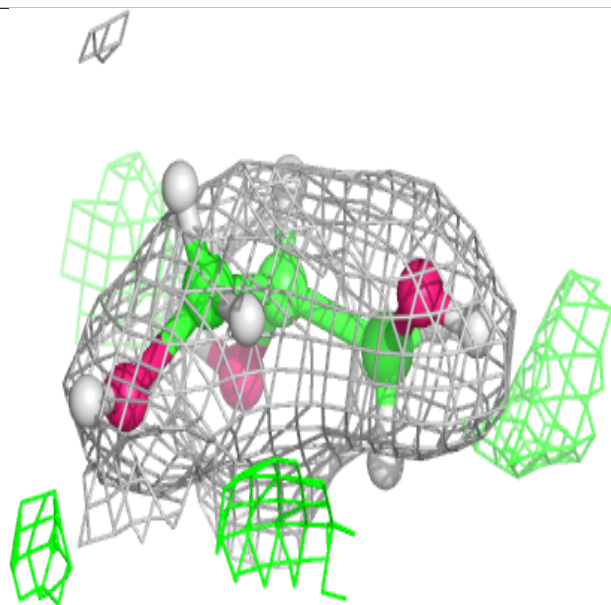
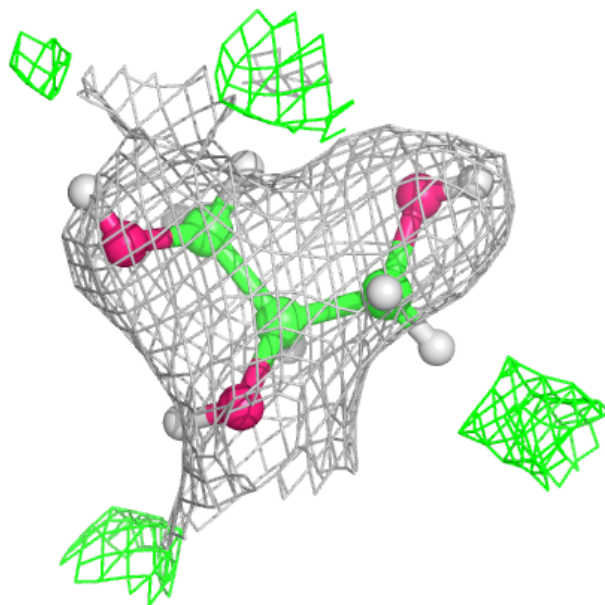
Electron density around SIN A 1301:

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



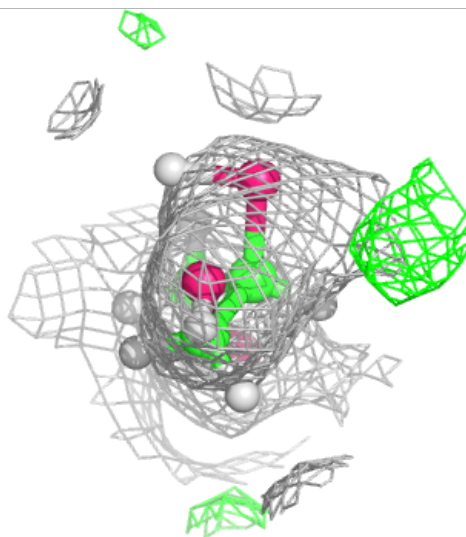
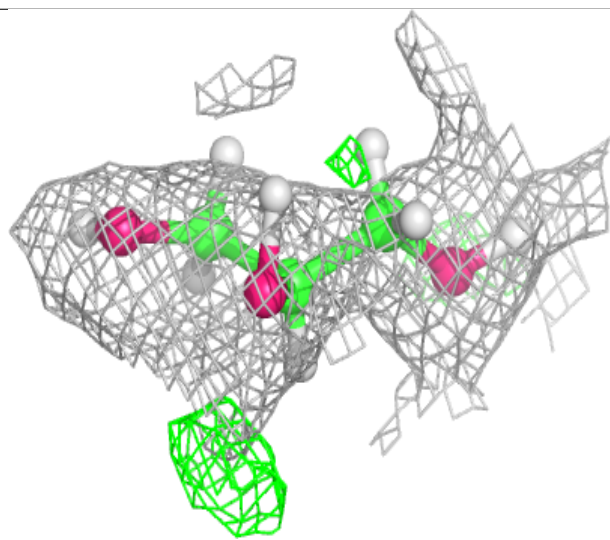
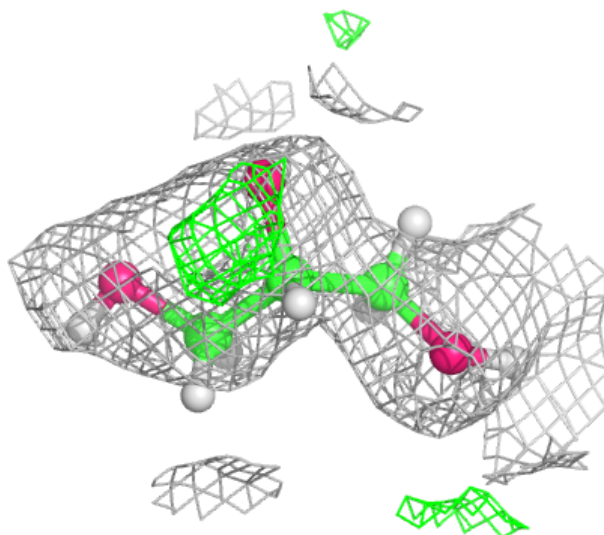
Electron density around GOL B 1302:

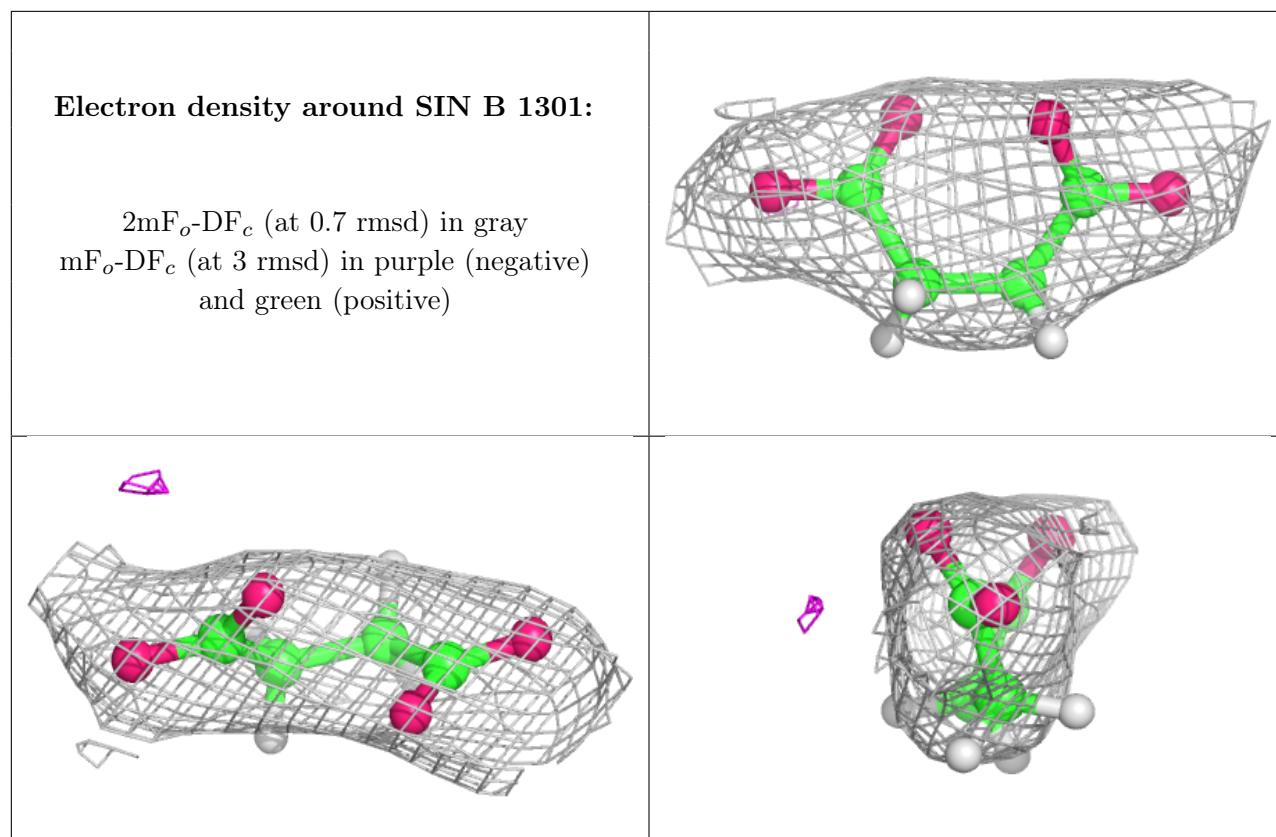
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL B 1305:

$2mF_o-DF_c$ (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.