



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:26 PM UTC

PDB ID : 7ZB2 / pdb_00007zb2
Title : apo macrocyclase OphP
Authors : Song, H.; Naismith, J.H.
Deposited on : 2022-03-23
Resolution : 1.94 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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

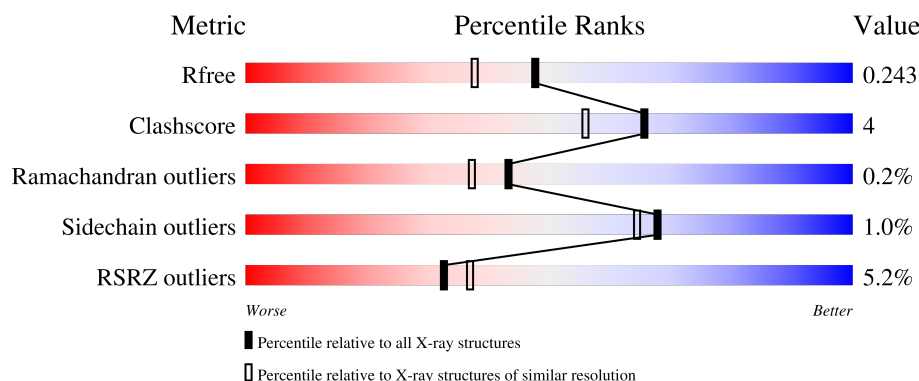
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	AAA	745	4% 88% 8% ..
1	BBB	745	4% 89% 7% .
1	CCC	745	4% 89% 8% .
1	DDD	745	5% 87% 9% .
1	EEE	745	6% 90% 7% .

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Mol	Chain	Length	Quality of chain
1	FFF	745	
1	GGG	745	
1	HHH	745	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 47221 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.

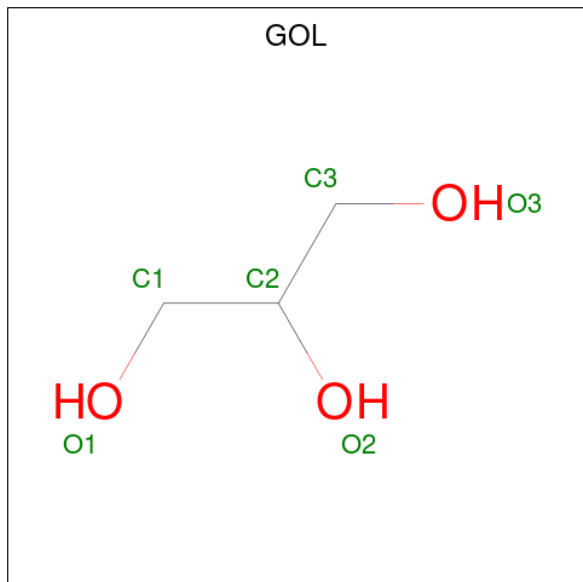
- Molecule 1 is a protein called OphP S580A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	724	Total	C	N	O	S	0	3	0
			5833	3726	983	1098	26			
1	BBB	718	Total	C	N	O	S	0	2	0
			5778	3693	971	1088	26			
1	CCC	720	Total	C	N	O	S	0	1	0
			5780	3696	971	1087	26			
1	DDD	717	Total	C	N	O	S	0	1	0
			5760	3678	971	1085	26			
1	EEE	721	Total	C	N	O	S	0	2	0
			5795	3700	976	1093	26			
1	FFF	718	Total	C	N	O	S	0	0	0
			5760	3681	968	1085	26			
1	GGG	714	Total	C	N	O	S	0	0	0
			5730	3661	961	1082	26			
1	HHH	723	Total	C	N	O	S	0	0	0
			5784	3694	971	1093	26			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Na	0	0
			1	1		
2	BBB	2	Total	Na	0	0
			2	2		
2	DDD	2	Total	Na	0	0
			2	2		
2	EEE	3	Total	Na	0	0
			3	3		
2	FFF	2	Total	Na	0	0
			2	2		
2	GGG	3	Total	Na	0	0
			3	3		

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

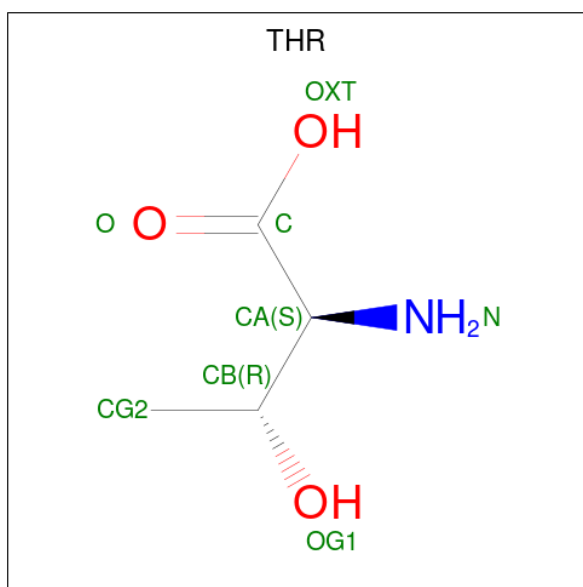


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	EEE	1	Total	C	O	0	0
			6	3	3		
3	HHH	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

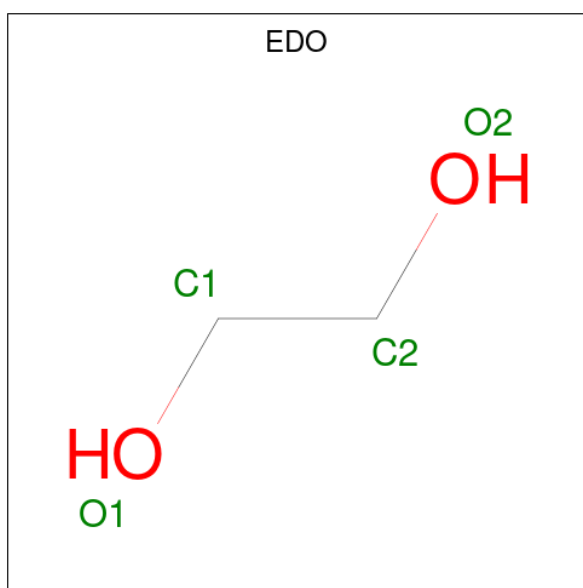
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	CCC	2	Total	Mg	0	0
			2	2		
4	FFF	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THREONINE (CCD ID: THR) (formula: $C_4H_9NO_3$).



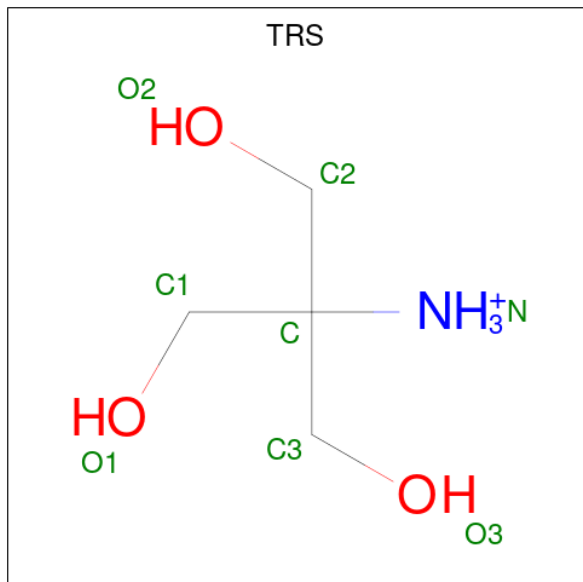
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	EEE	1	Total	C	N	O	0	0
			7	4	1	2		
5	FFF	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



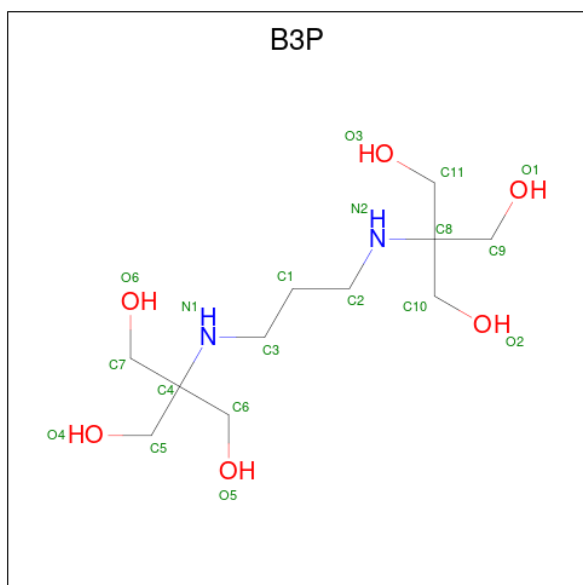
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	EEE	1	Total	C	O	0	0
			4	2	2		
6	GGG	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	FFF	1	Total	C	N	O	0	0
			8	4	1	3		
7	GGG	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	HHH	1	Total	C	N	O	0	0
			19	11	2	6		

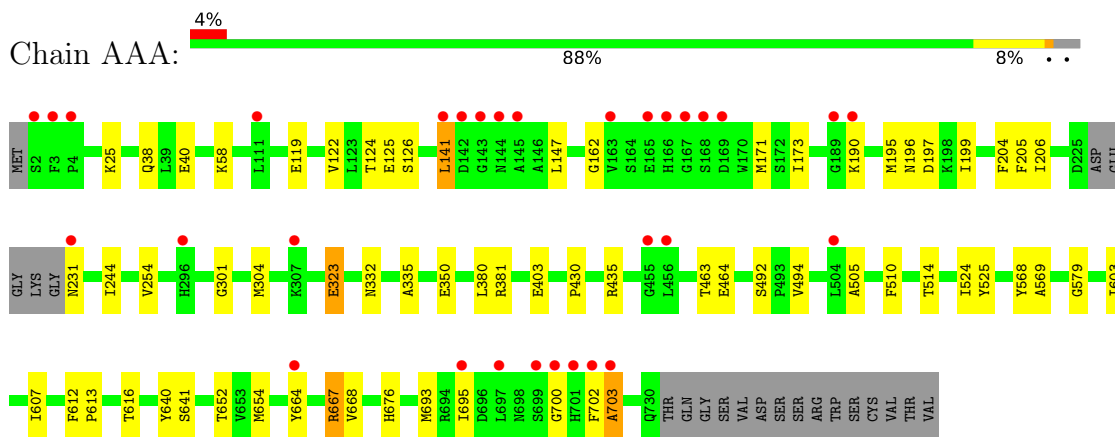
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	192	Total	O	0	0
			192	192		
9	BBB	110	Total	O	0	0
			110	110		
9	CCC	104	Total	O	0	0
			104	104		
9	DDD	141	Total	O	0	0
			141	141		
9	EEE	57	Total	O	0	0
			57	57		
9	FFF	80	Total	O	0	0
			80	80		
9	GGG	97	Total	O	0	0
			97	97		
9	HHH	117	Total	O	0	0
			117	117		

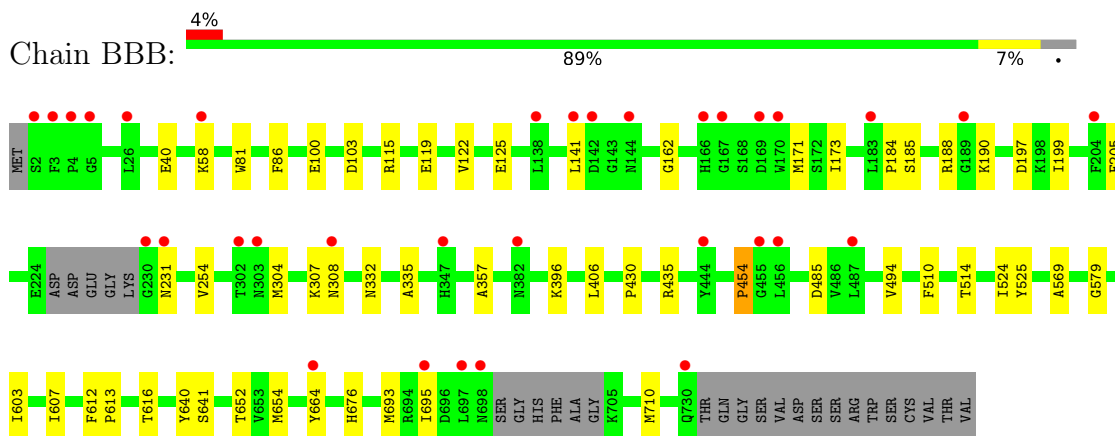
3 Residue-property plots [i](#)

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.

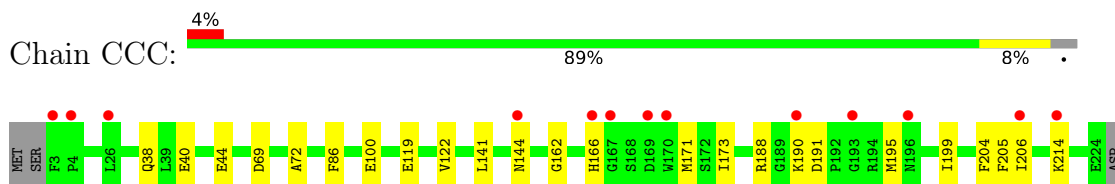
• Molecule 1: OphP S580A

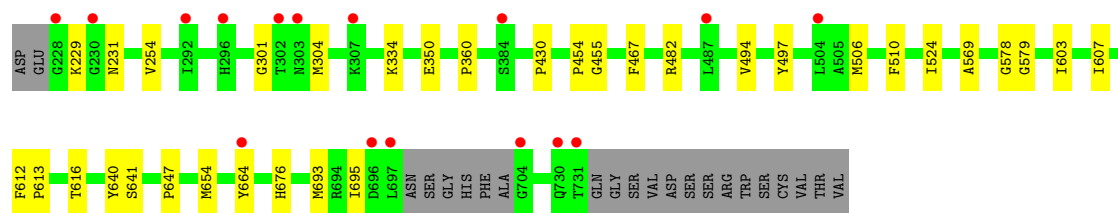


• Molecule 1: OphP S580A

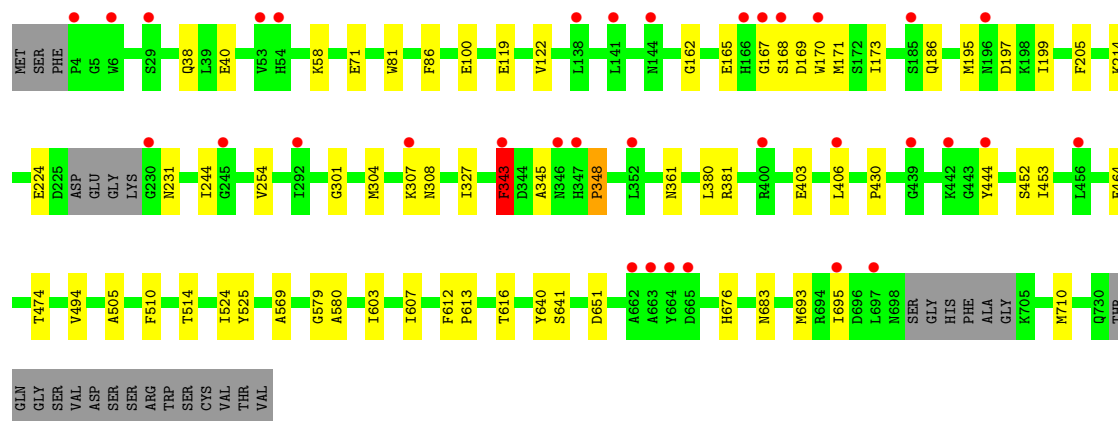
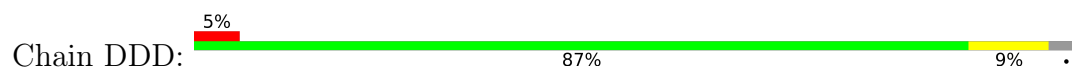


• Molecule 1: OphP S580A

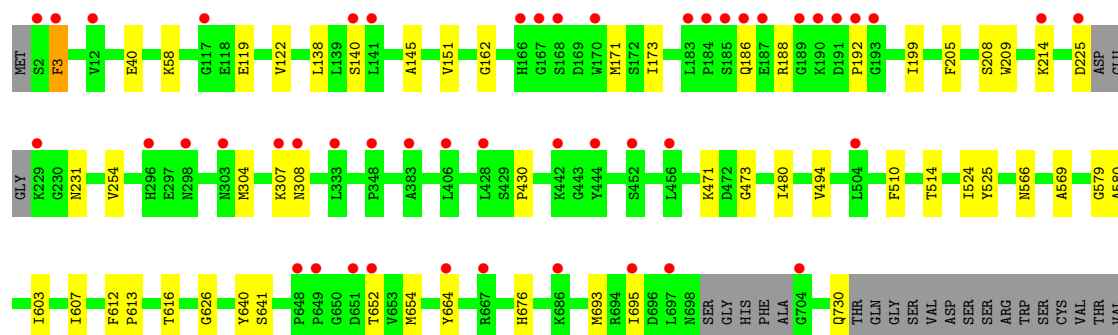




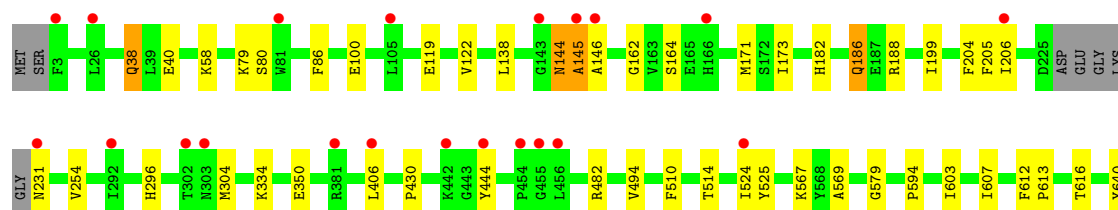
• Molecule 1: OphP S580A

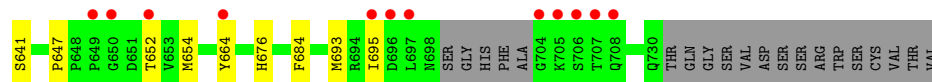


• Molecule 1: OphP S580A

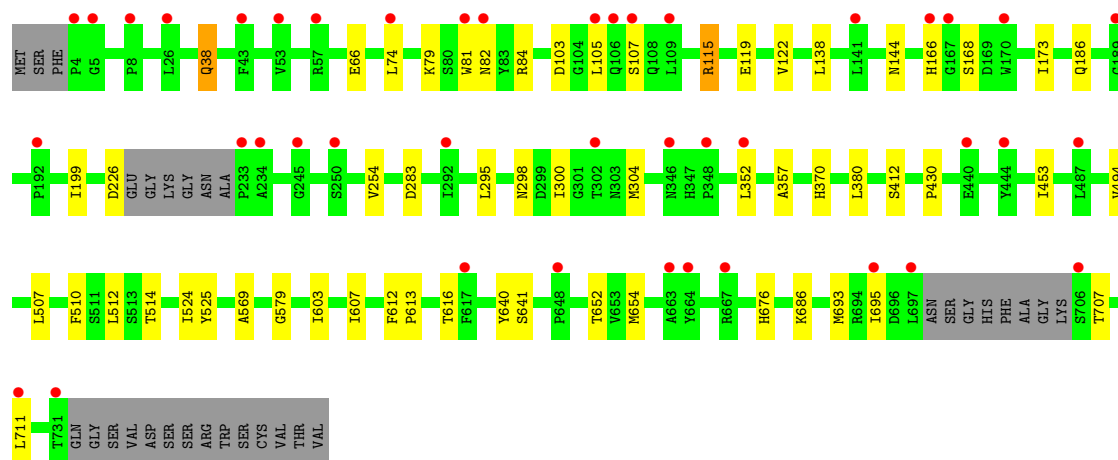
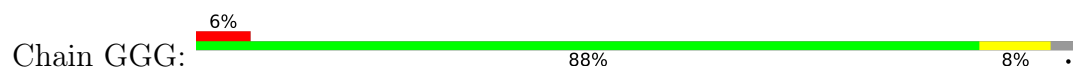


• Molecule 1: OphP S580A

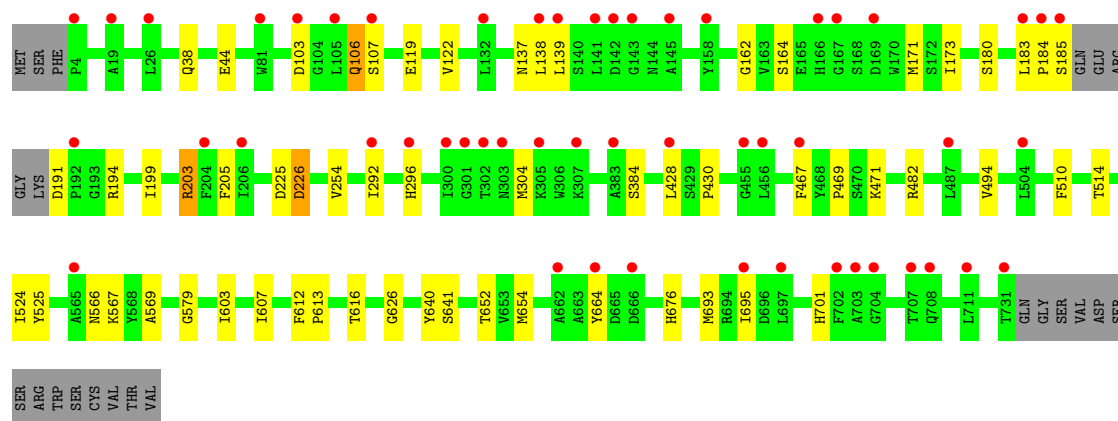




● Molecule 1: OphP S580A



● Molecule 1: OphP S580A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.86Å 113.43Å 186.32Å 83.97° 82.09° 76.93°	Depositor
Resolution (Å)	66.08 – 1.94 66.08 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.6 (66.08-1.94) 97.6 (66.08-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.241 0.212 , 0.243	Depositor DCC
R_{free} test set	19701 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	47221	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.78% 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: B3P, TRS, NA, MG, EDO, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AAA	0.99	0/6005	1.24	1/8146 (0.0%)
1	BBB	0.99	1/5947 (0.0%)	1.24	2/8067 (0.0%)
1	CCC	0.97	0/5949	1.23	3/8068 (0.0%)
1	DDD	1.00	0/5927	1.26	3/8038 (0.0%)
1	EEE	0.97	0/5963	1.24	1/8087 (0.0%)
1	FFF	1.00	1/5928 (0.0%)	1.24	0/8041
1	GGG	1.01	1/5897 (0.0%)	1.26	3/7999 (0.0%)
1	HHH	0.99	0/5954	1.26	3/8078 (0.0%)
All	All	0.99	3/47570 (0.0%)	1.24	16/64524 (0.0%)

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	FFF	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	182	HIS	CE1-NE2	7.26	1.39	1.32
1	BBB	454	PRO	C-O	-5.28	1.18	1.24
1	GGG	370	HIS	CE1-NE2	5.17	1.37	1.32

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	165	GLU	CA-C-O	-7.66	112.96	121.00
1	DDD	343	PHE	CA-CB-CG	7.51	121.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	115	ARG	CB-CG-CD	-7.48	94.10	111.30
1	DDD	651	ASP	CA-C-O	-5.97	112.06	119.28
1	BBB	103	ASP	CA-CB-CG	5.68	118.28	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	FFF	144	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	5833	0	5561	46	1
1	BBB	5778	0	5515	52	0
1	CCC	5780	0	5524	44	0
1	DDD	5760	0	5505	66	1
1	EEE	5795	0	5531	42	0
1	FFF	5760	0	5501	44	3
1	GGG	5730	0	5472	40	1
1	HHH	5784	0	5516	45	2
2	AAA	1	0	0	0	0
2	BBB	2	0	0	0	0
2	DDD	2	0	0	0	0
2	EEE	3	0	0	0	0
2	FFF	2	0	0	0	0
2	GGG	3	0	0	0	0
3	BBB	6	0	8	0	0
3	CCC	6	0	8	0	0
3	DDD	6	0	8	1	0
3	EEE	6	0	8	1	0
3	HHH	6	0	8	0	0
4	CCC	2	0	0	0	0
4	FFF	1	0	0	0	0
5	EEE	7	0	6	1	0
5	FFF	7	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	EEE	4	0	6	3	0
6	GGG	4	0	6	0	0
7	FFF	8	0	12	0	0
7	GGG	8	0	12	0	0
8	HHH	19	0	26	1	0
9	AAA	192	0	0	2	0
9	BBB	110	0	0	4	0
9	CCC	104	0	0	1	0
9	DDD	141	0	0	1	0
9	EEE	57	0	0	0	0
9	FFF	80	0	0	1	0
9	GGG	97	0	0	2	0
9	HHH	117	0	0	2	0
All	All	47221	0	44239	343	4

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.

The worst 5 of 343 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:HHH:103:ASP:HB3	1:HHH:106:GLN:HE22	1.13	1.09
1:EEE:140:SER:OG	1:EEE:145:ALA:HB2	1.61	1.00
1:HHH:103:ASP:CB	1:HHH:106:GLN:HE22	1.74	1.00
1:DDD:381:ARG:HG2	1:HHH:566:ASN:OD1	1.63	0.97
1:EEE:138:LEU:O	1:EEE:188:ARG:O	1.83	0.96

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:188:ARG:NH1	1:GGG:79:LYS:O[1_546]	2.07	0.13
1:AAA:196:ASN:OD1	1:HHH:44:GLU:OE1[1_554]	2.13	0.07
1:FFF:296:HIS:O	1:HHH:296:HIS:ND1[1_655]	2.16	0.04
1:DDD:474:THR:OG1	1:FFF:567:LYS:NZ[1_565]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	723/745 (97%)	702 (97%)	18 (2%)	3 (0%)	30	22
1	BBB	714/745 (96%)	695 (97%)	18 (2%)	1 (0%)	48	41
1	CCC	715/745 (96%)	695 (97%)	19 (3%)	1 (0%)	48	41
1	DDD	712/745 (96%)	691 (97%)	19 (3%)	2 (0%)	36	30
1	EEE	717/745 (96%)	696 (97%)	20 (3%)	1 (0%)	48	41
1	FFF	712/745 (96%)	692 (97%)	17 (2%)	3 (0%)	30	22
1	GGG	708/745 (95%)	691 (98%)	15 (2%)	2 (0%)	36	30
1	HHH	719/745 (96%)	701 (98%)	17 (2%)	1 (0%)	48	41
All	All	5720/5960 (96%)	5563 (97%)	143 (2%)	14 (0%)	43	37

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	168	SER
1	FFF	145	ALA
1	FFF	146	ALA
1	GGG	168	SER
1	AAA	700	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	AAA	629/644 (98%)	619 (98%)	10 (2%)	55	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BBB	624/644 (97%)	619 (99%)	5 (1%)	73	71
1	CCC	623/644 (97%)	619 (99%)	4 (1%)	78	78
1	DDD	622/644 (97%)	617 (99%)	5 (1%)	73	71
1	EEE	626/644 (97%)	618 (99%)	8 (1%)	61	54
1	FFF	622/644 (97%)	616 (99%)	6 (1%)	68	64
1	GGG	620/644 (96%)	612 (99%)	8 (1%)	61	54
1	HHH	624/644 (97%)	617 (99%)	7 (1%)	65	60
All	All	4990/5152 (97%)	4937 (99%)	53 (1%)	68	60

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	307	LYS
1	FFF	186	GLN
1	HHH	226	ASP
1	EEE	308[A]	ASN
1	FFF	38	GLN

Sometimes 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 ⓘ

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 ⓘ

Of 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 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	GOL	CCC	801	-	5,5,5	0.14	0	5,5,5	0.34	0
5	THR	EEE	801	-	5,6,7	0.53	0	5,7,9	1.01	0
5	THR	FFF	801	-	5,6,7	0.63	0	5,7,9	0.61	0
8	B3P	HHH	802	-	18,18,18	0.24	0	23,23,23	0.64	0
7	TRS	GGG	802	-	7,7,7	0.20	0	9,9,9	0.28	0
3	GOL	BBB	801	-	5,5,5	0.10	0	5,5,5	0.33	0
3	GOL	DDD	801	-	5,5,5	0.16	0	5,5,5	0.44	0
3	GOL	HHH	801	-	5,5,5	0.15	0	5,5,5	0.54	0
6	EDO	EEE	803	-	3,3,3	0.18	0	2,2,2	0.18	0
7	TRS	FFF	802	-	7,7,7	0.22	0	9,9,9	0.26	0
3	GOL	EEE	802	-	5,5,5	0.15	0	5,5,5	0.49	0
6	EDO	GGG	801	-	3,3,3	0.20	0	2,2,2	0.21	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	CCC	801	-	-	0/4/4/4	-
5	THR	EEE	801	-	-	0/5/6/8	-
5	THR	FFF	801	-	-	0/5/6/8	-
8	B3P	HHH	802	-	-	9/28/28/28	-
7	TRS	GGG	802	-	-	9/9/9/9	-
3	GOL	BBB	801	-	-	2/4/4/4	-
3	GOL	DDD	801	-	-	0/4/4/4	-
3	GOL	HHH	801	-	-	2/4/4/4	-
6	EDO	EEE	803	-	-	1/1/1/1	-
7	TRS	FFF	802	-	-	8/9/9/9	-
3	GOL	EEE	802	-	-	2/4/4/4	-
6	EDO	GGG	801	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

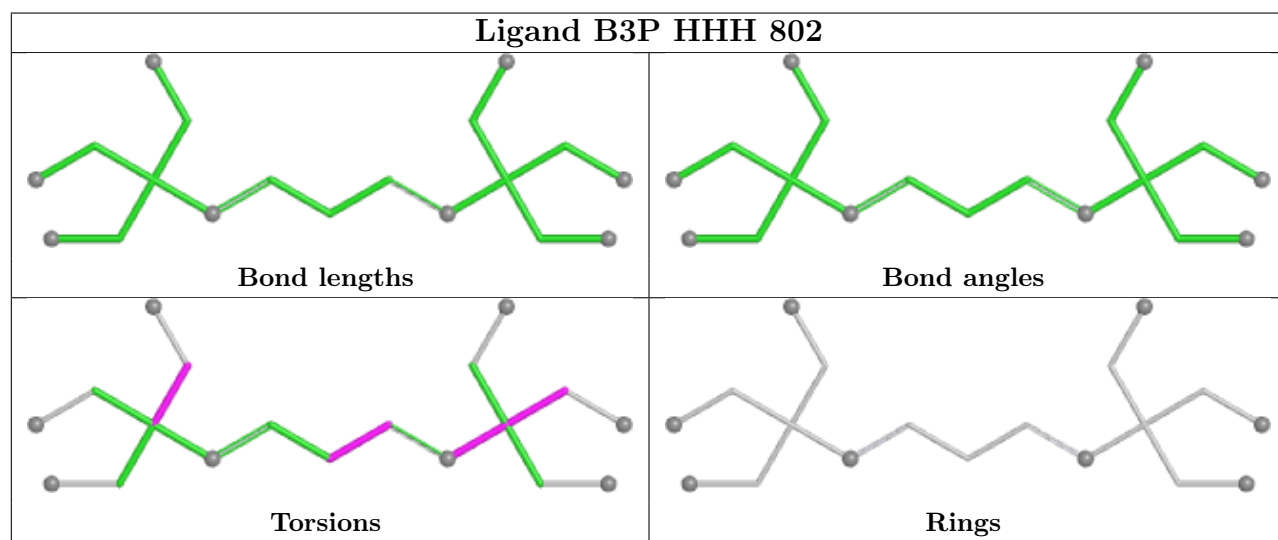
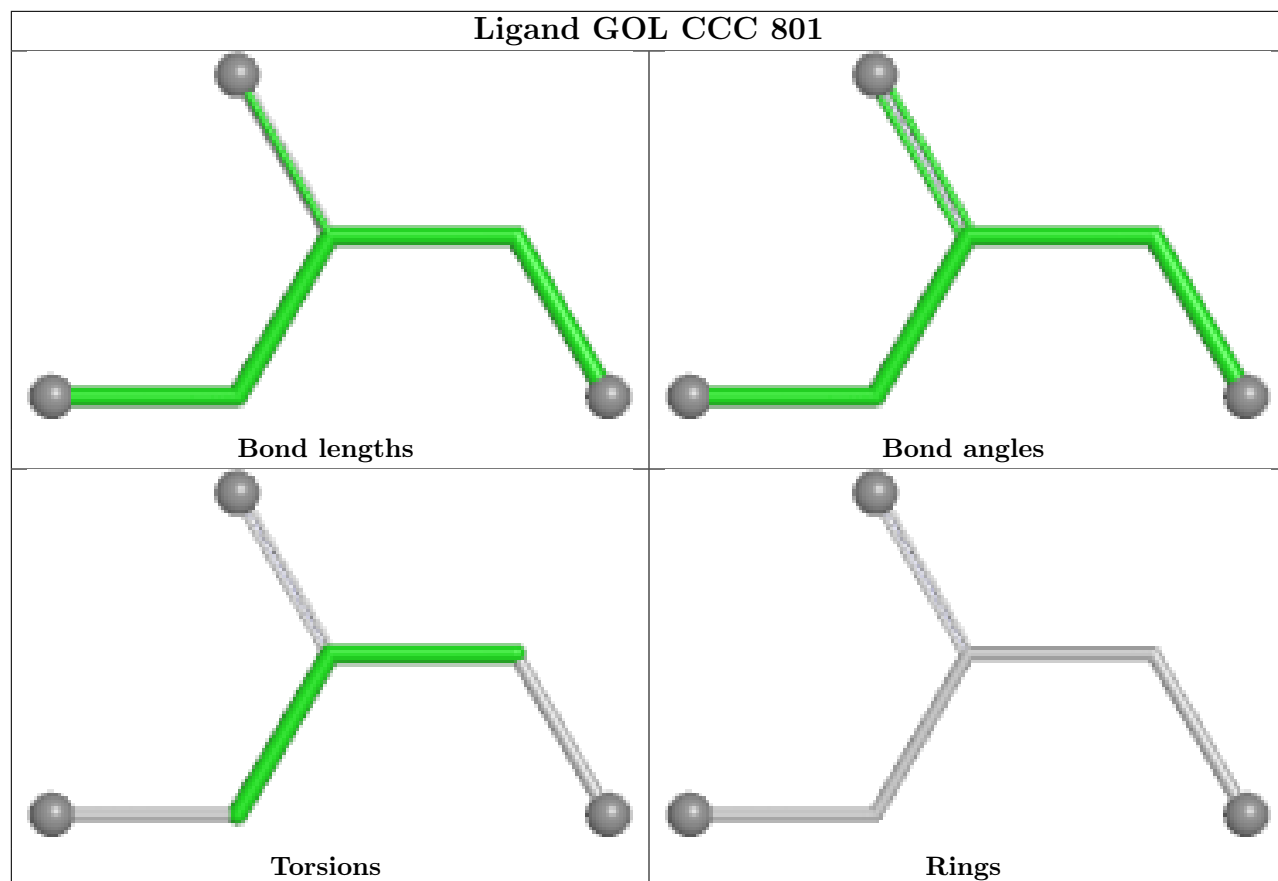
Mol	Chain	Res	Type	Atoms
3	BBB	801	GOL	C1-C2-C3-O3
3	BBB	801	GOL	O2-C2-C3-O3
3	EEE	802	GOL	C1-C2-C3-O3
3	HHH	801	GOL	O1-C1-C2-C3
7	FFF	802	TRS	C3-C-C1-O1

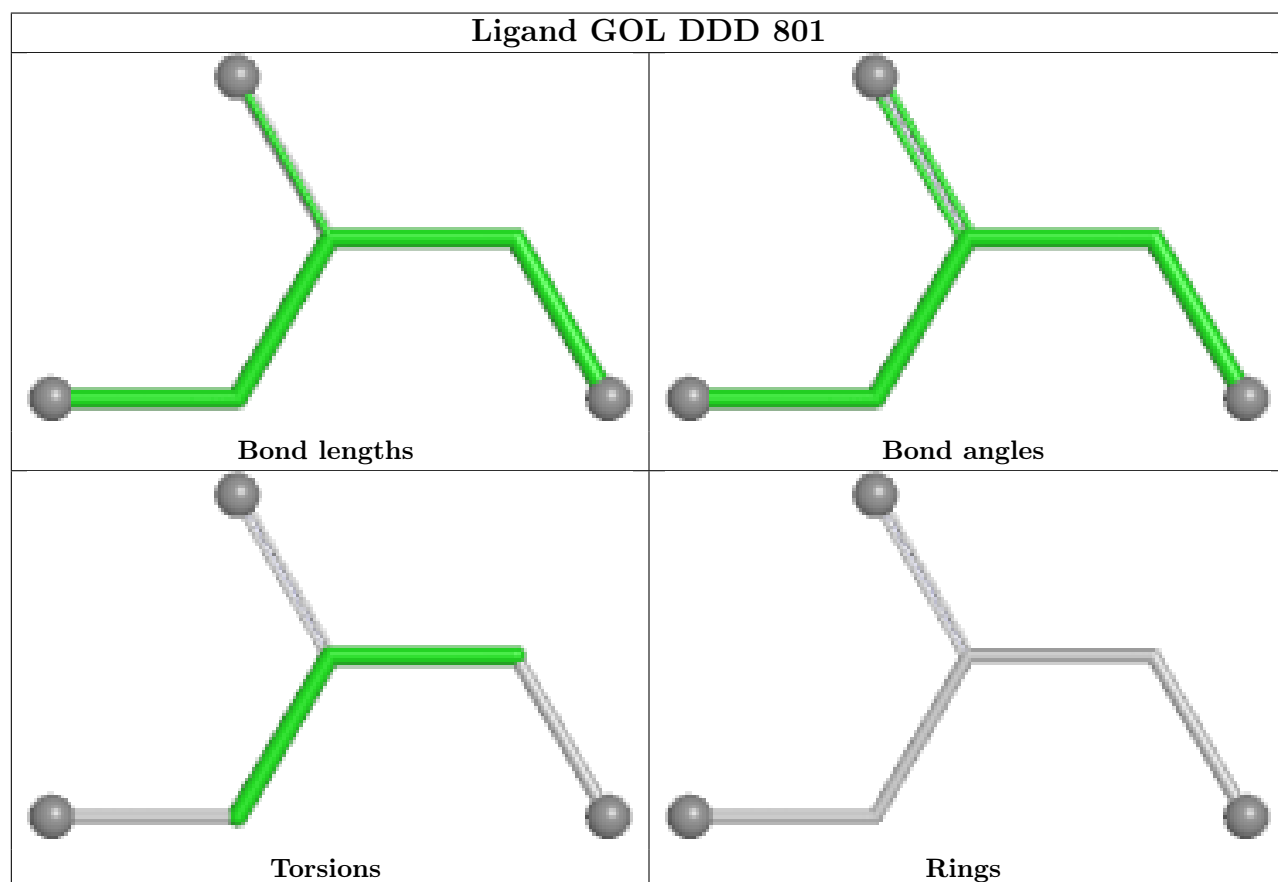
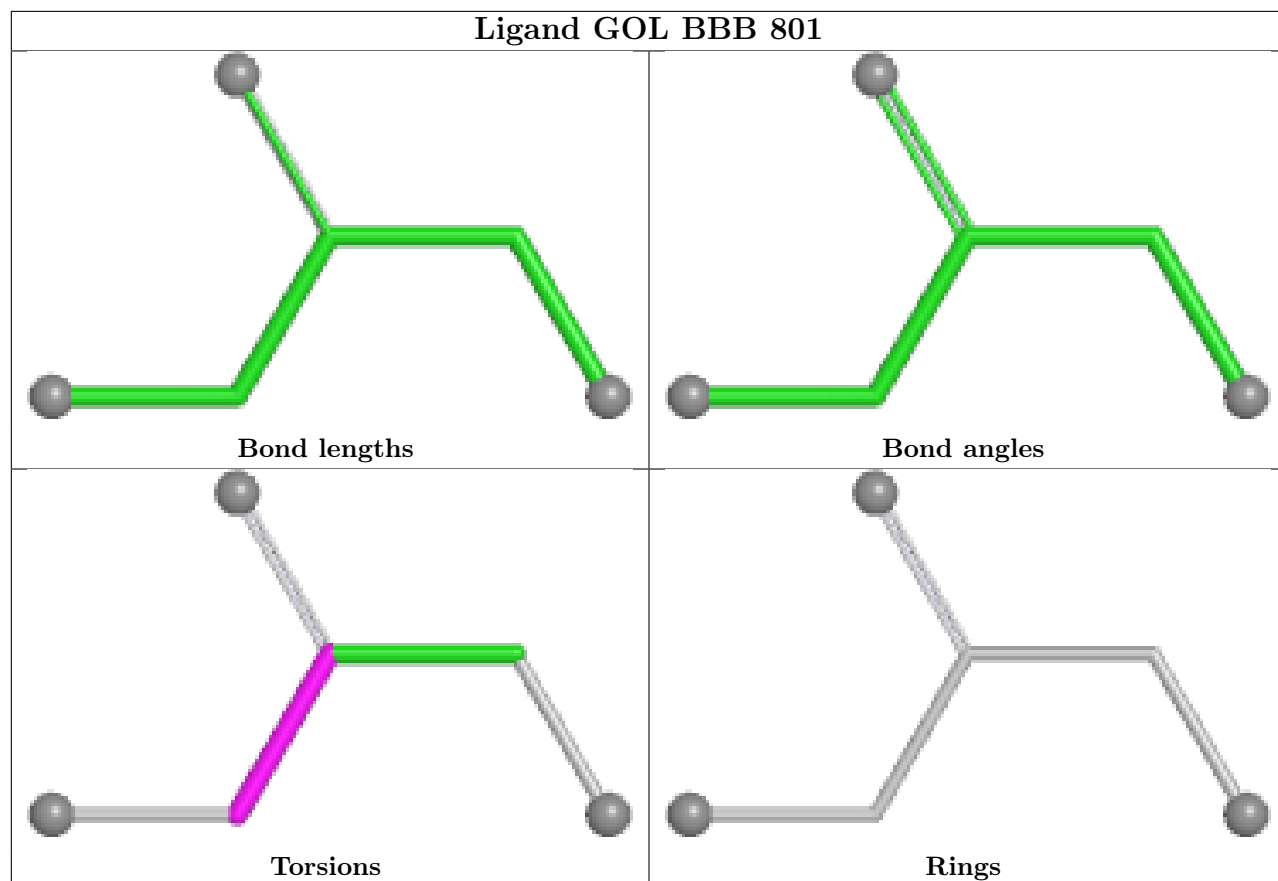
There are no ring outliers.

5 monomers are involved in 7 short contacts:

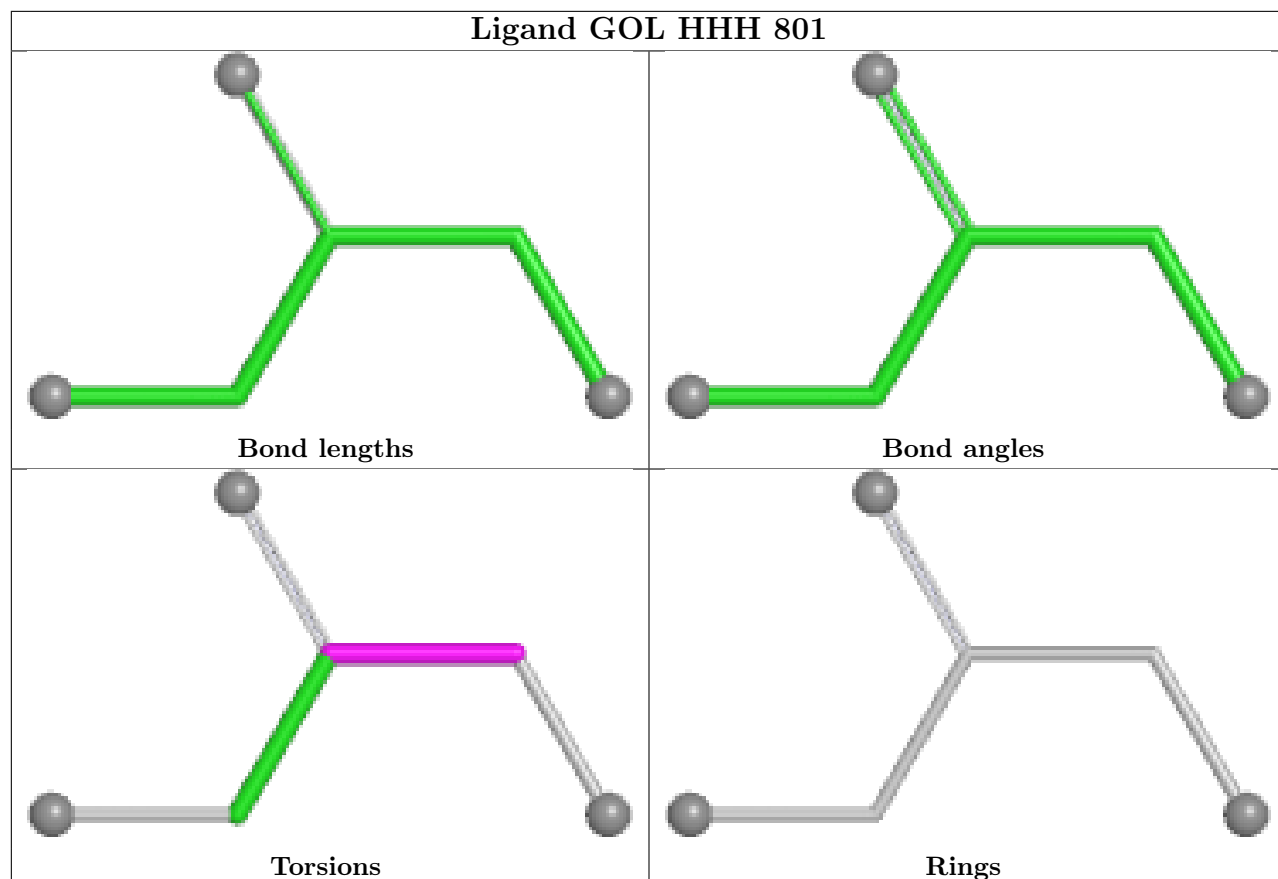
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EEE	801	THR	1	0
8	HHH	802	B3P	1	0
3	DDD	801	GOL	1	0
6	EEE	803	EDO	3	0
3	EEE	802	GOL	1	0

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

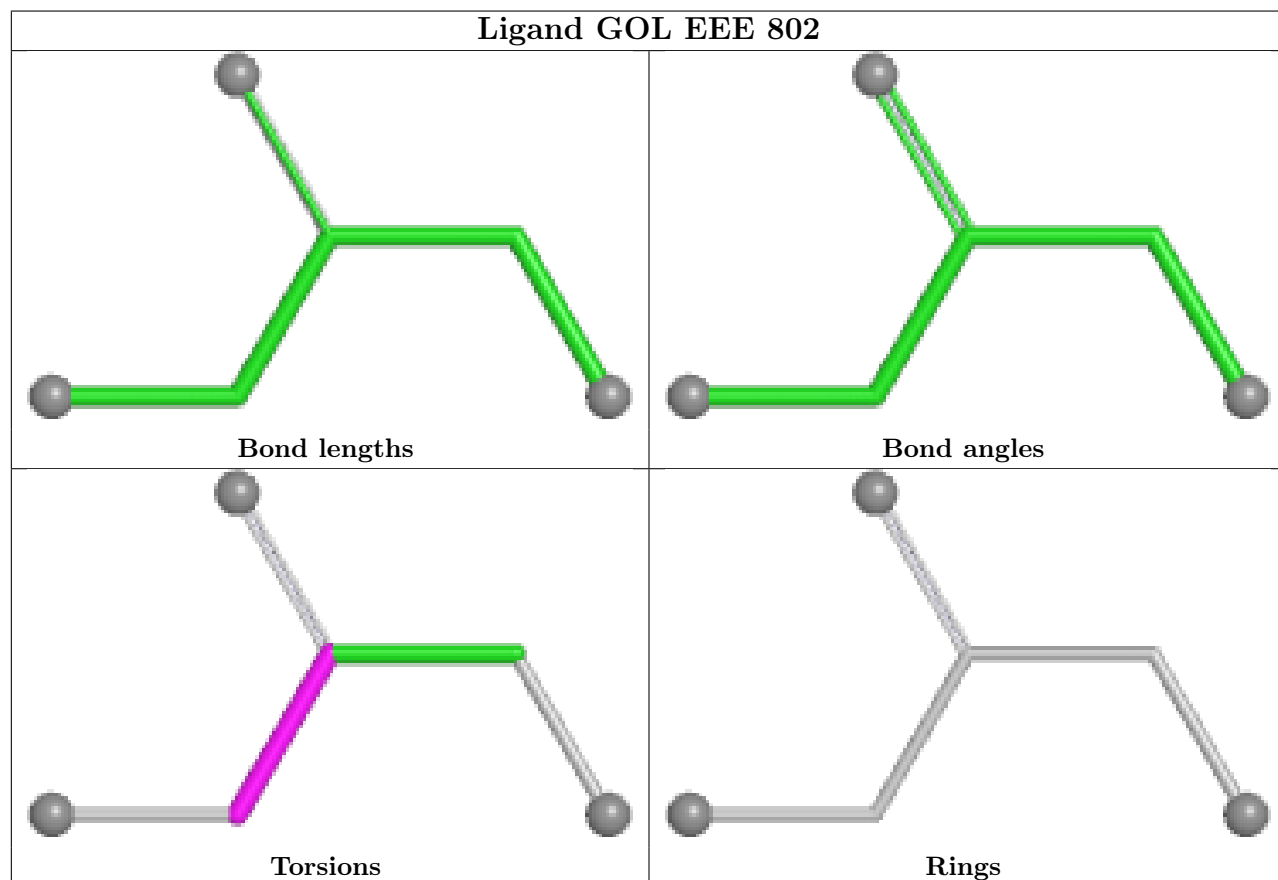




Ligand GOL HHH 801



Ligand GOL EEE 802



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AAA	724/745 (97%)	0.16	31 (4%)	40	44	15, 34, 66, 130	3 (0%)
1	BBB	718/745 (96%)	0.30	33 (4%)	37	42	20, 40, 69, 133	2 (0%)
1	CCC	720/745 (96%)	0.31	29 (4%)	42	47	20, 40, 75, 121	1 (0%)
1	DDD	717/745 (96%)	0.39	34 (4%)	36	41	17, 39, 74, 144	1 (0%)
1	EEE	721/745 (96%)	0.64	48 (6%)	24	27	18, 48, 83, 138	2 (0%)
1	FFF	718/745 (96%)	0.48	33 (4%)	37	42	29, 43, 74, 129	0
1	GGG	714/745 (95%)	0.48	42 (5%)	28	31	30, 42, 78, 123	0
1	HHH	723/745 (97%)	0.51	52 (7%)	21	24	27, 44, 76, 128	0
All	All	5755/5960 (96%)	0.41	302 (5%)	33	37	15, 41, 76, 144	9 (0%)

The worst 5 of 302 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GGG	487	LEU	6.6
1	HHH	383	ALA	6.6
1	AAA	3	PHE	6.2
1	CCC	3	PHE	5.9
1	HHH	166	HIS	5.7

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

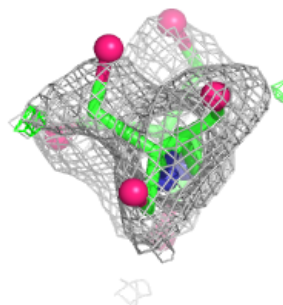
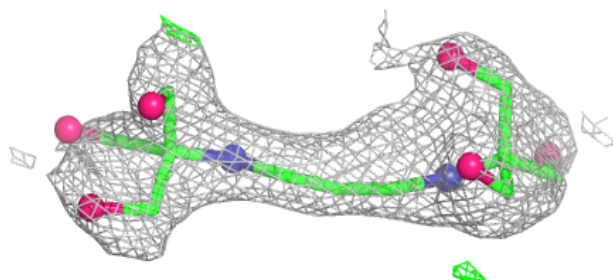
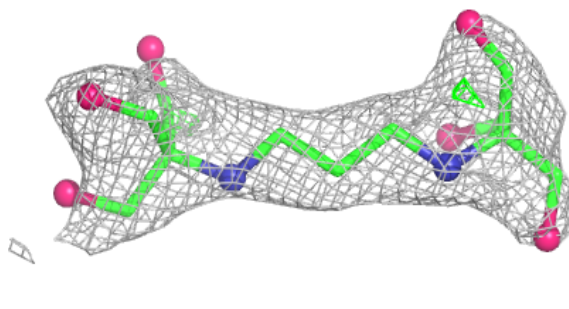
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	EEE	804	1/1	0.67	0.21	62,62,62,62	0
5	THR	EEE	801	7/8	0.67	0.15	83,108,120,125	0
5	THR	FFF	801	7/8	0.74	0.19	75,102,115,129	0
8	B3P	HHH	802	19/19	0.80	0.14	49,69,83,86	0
2	NA	DDD	803	1/1	0.81	0.14	64,64,64,64	0
7	TRS	GGG	802	8/8	0.83	0.16	45,63,74,80	0
7	TRS	FFF	802	8/8	0.83	0.15	50,65,72,75	0
3	GOL	HHH	801	6/6	0.84	0.15	41,61,72,79	0
3	GOL	CCC	801	6/6	0.84	0.14	40,58,64,70	0
3	GOL	EEE	802	6/6	0.86	0.13	41,61,73,77	0
3	GOL	BBB	801	6/6	0.86	0.14	46,57,66,71	0
6	EDO	EEE	803	4/4	0.86	0.15	42,50,52,64	0
3	GOL	DDD	801	6/6	0.87	0.13	36,49,56,64	0
2	NA	AAA	801	1/1	0.88	0.23	55,55,55,55	0
2	NA	BBB	803	1/1	0.89	0.20	46,46,46,46	0
2	NA	DDD	802	1/1	0.89	0.25	54,54,54,54	0
6	EDO	GGG	801	4/4	0.89	0.11	47,50,51,57	0
2	NA	EEE	805	1/1	0.90	0.10	61,61,61,61	0
2	NA	GGG	804	1/1	0.90	0.12	46,46,46,46	0
2	NA	GGG	805	1/1	0.91	0.19	46,46,46,46	0
2	NA	FFF	804	1/1	0.92	0.14	44,44,44,44	0
2	NA	BBB	802	1/1	0.92	0.21	47,47,47,47	0
2	NA	EEE	806	1/1	0.92	0.28	49,49,49,49	0
2	NA	GGG	803	1/1	0.93	0.11	48,48,48,48	0
4	MG	CCC	803	1/1	0.94	0.14	42,42,42,42	0
4	MG	CCC	802	1/1	0.94	0.11	43,43,43,43	0
2	NA	FFF	805	1/1	0.95	0.18	53,53,53,53	0
4	MG	FFF	803	1/1	0.98	0.25	43,43,43,43	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.

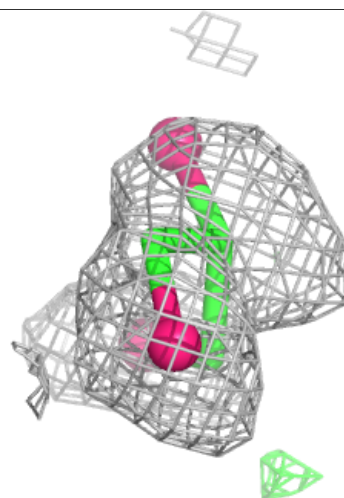
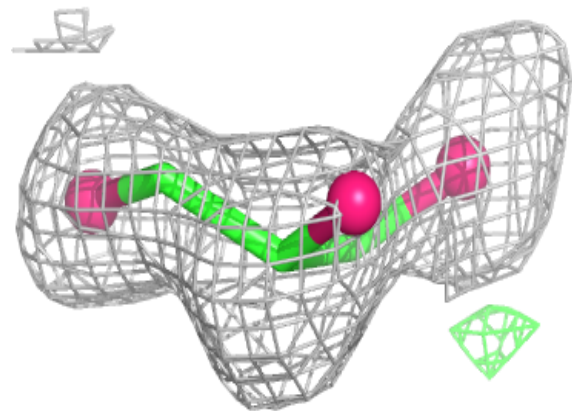
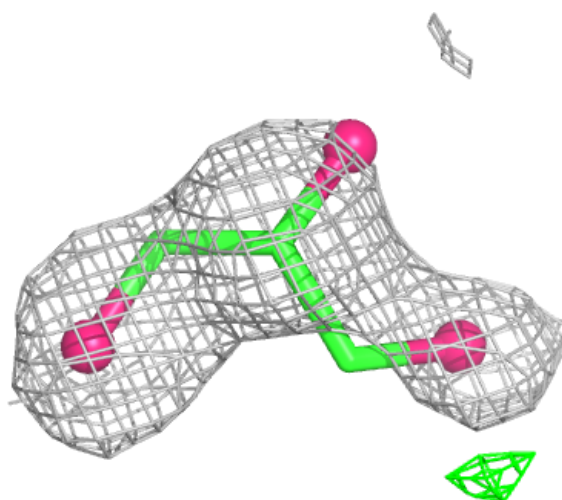
Electron density around B3P HHH 802:

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



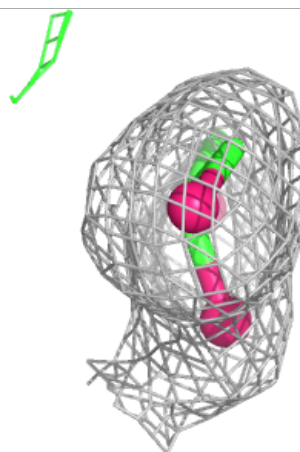
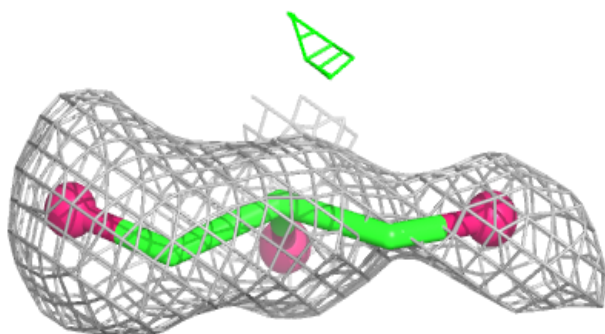
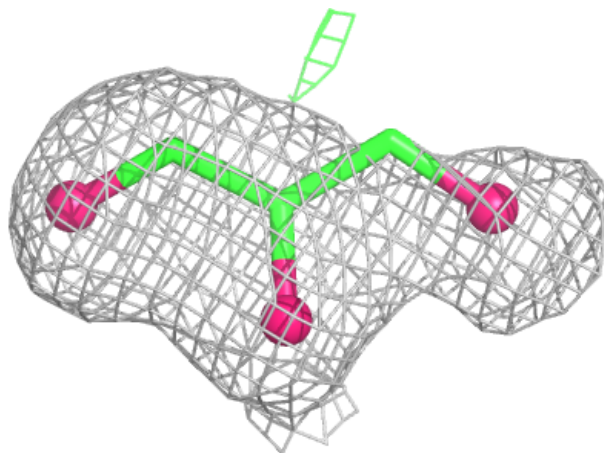
Electron density around GOL HHH 801:

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



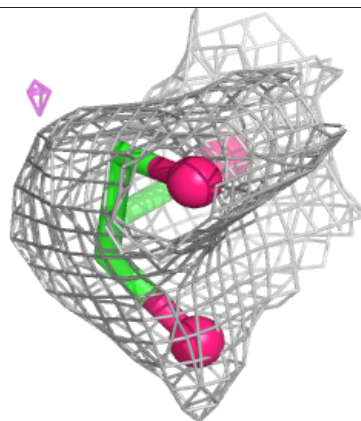
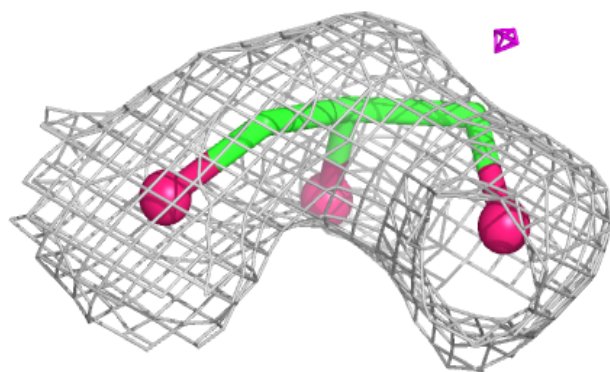
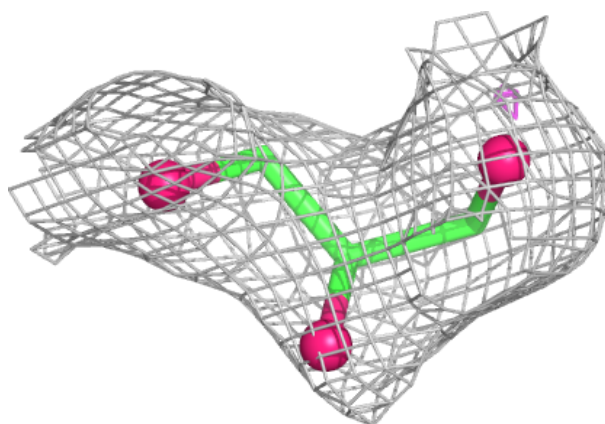
Electron density around GOL CCC 801:

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



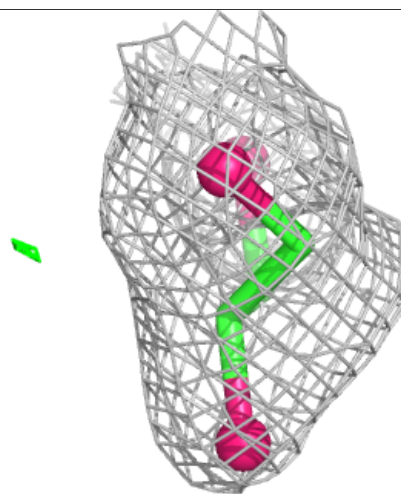
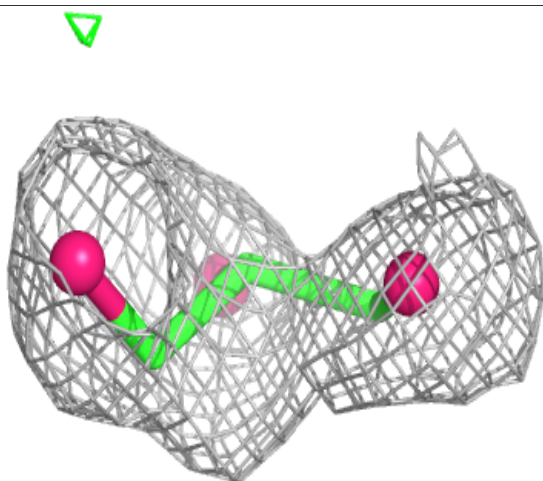
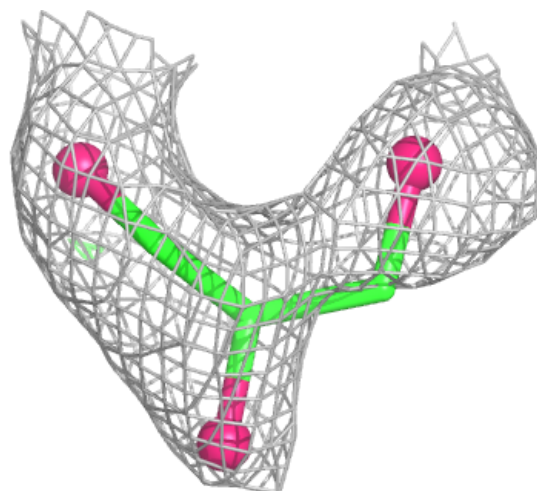
Electron density around GOL EEE 802:

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



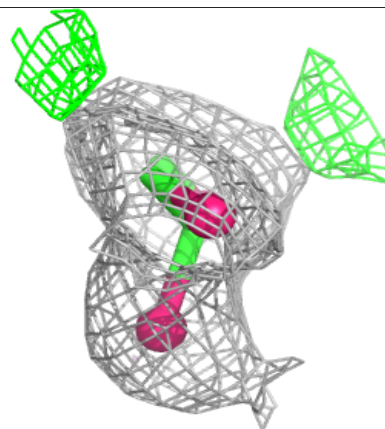
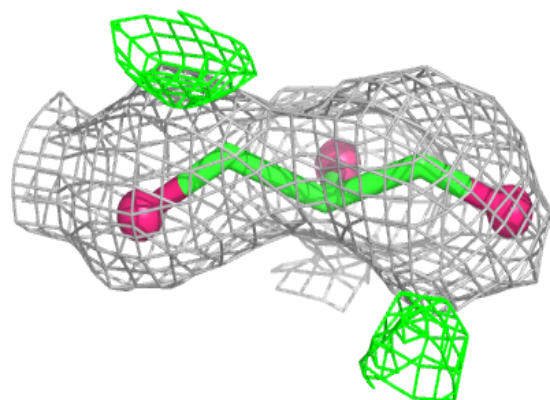
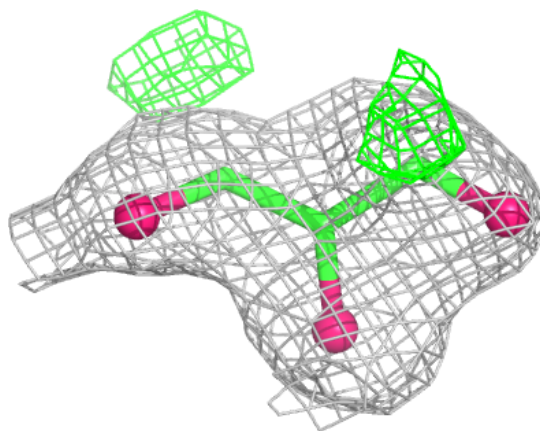
Electron density around GOL BBB 801:

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



Electron density around GOL DDD 801:

$2mF_o-DF_c$ (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.