



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:29 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 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 : 4-5-2 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

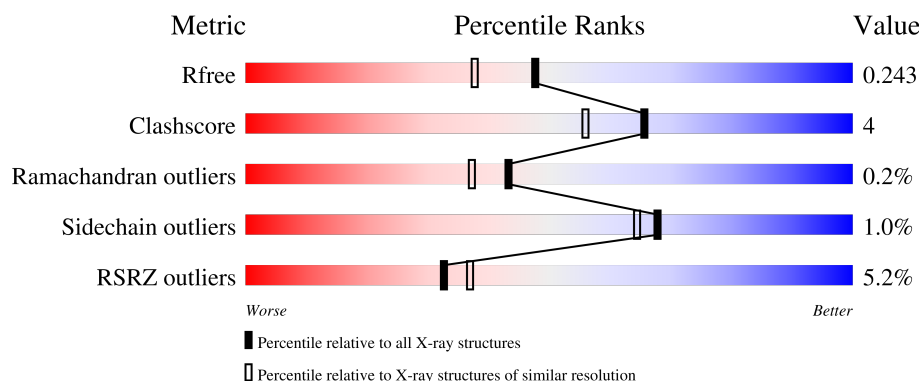
1 Overall quality at a glance

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	4% 89% 7%
1	GGG	745	6% 88% 8%
1	HHH	745	7% 89% 8%

2 Entry composition [i](#)

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.

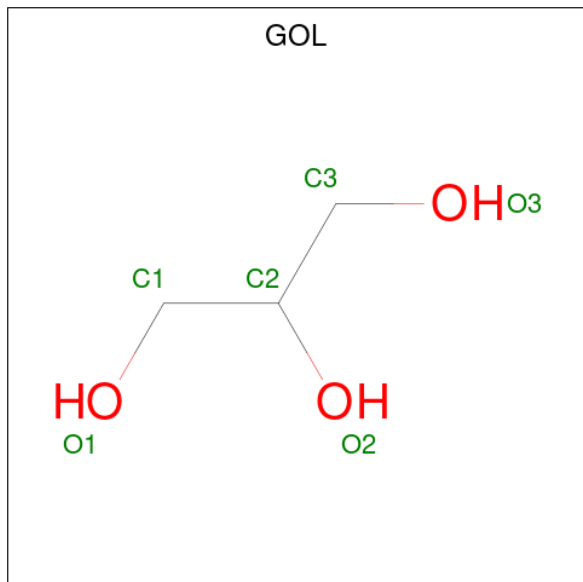
- Molecule 1 is a protein called OphP S580A.

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).

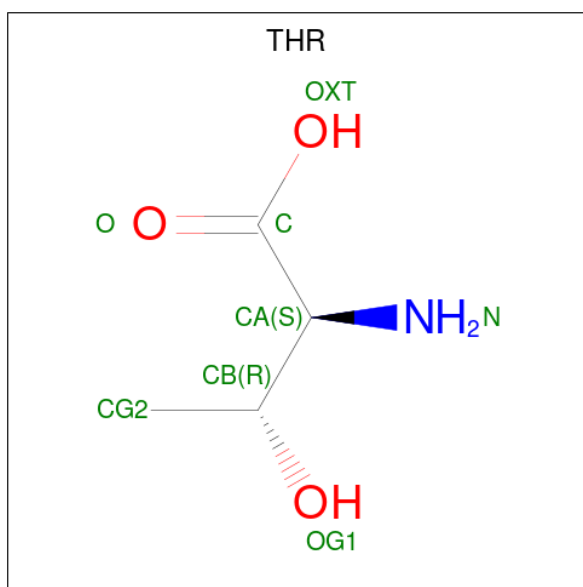


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	EEE	1	Total	C	O	0	0
			6	3	3		
3	HHH	1	Total	C	O	0	0
			6	3	3		

- 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: $C_4H_9NO_3$).



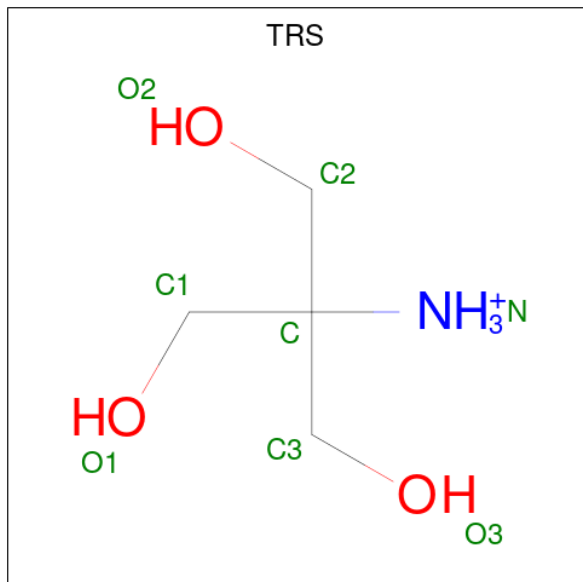
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	EEE	1	Total	C	N	O	0	0
			7	4	1	2		
5	FFF	1	Total	C	N	O	0	0
			7	4	1	2		

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



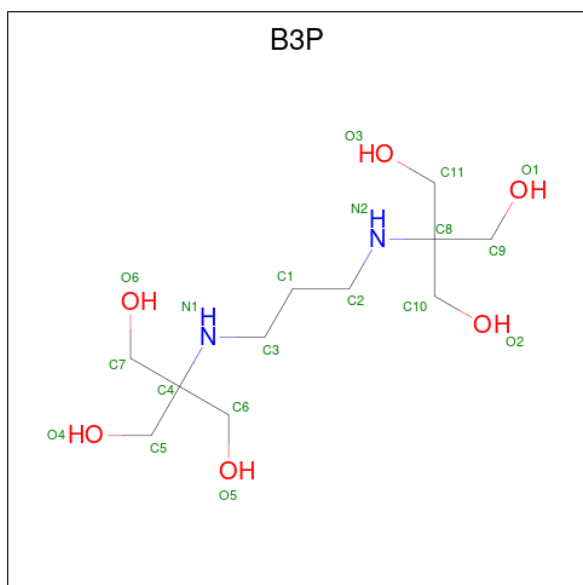
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	EEE	1	Total	C	O	0	0
			4	2	2		
6	GGG	1	Total	C	O	0	0
			4	2	2		

- 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		

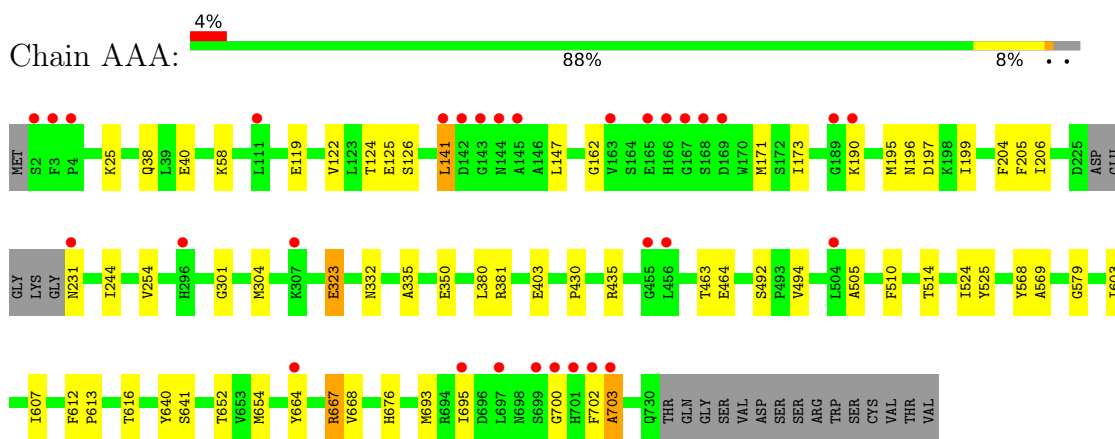
- Molecule 9 is water.

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		

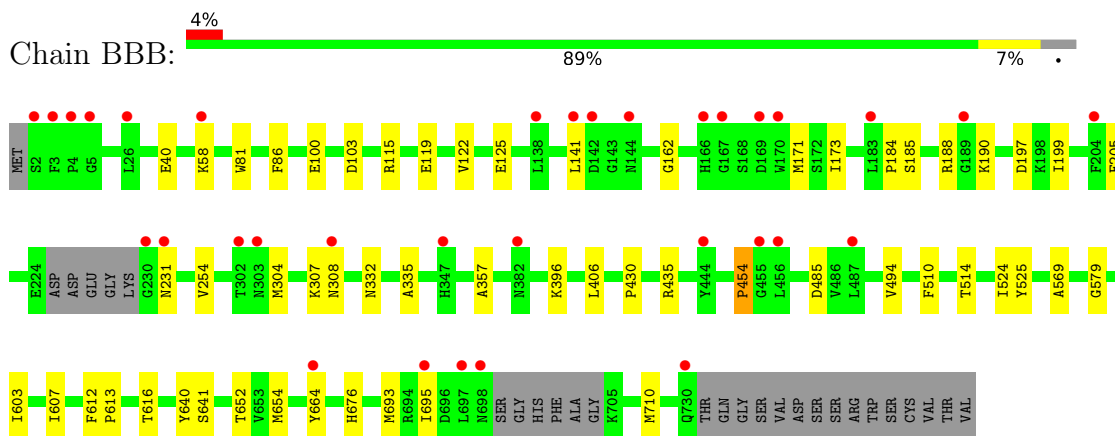
3 Residue-property plots [i](#)

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.

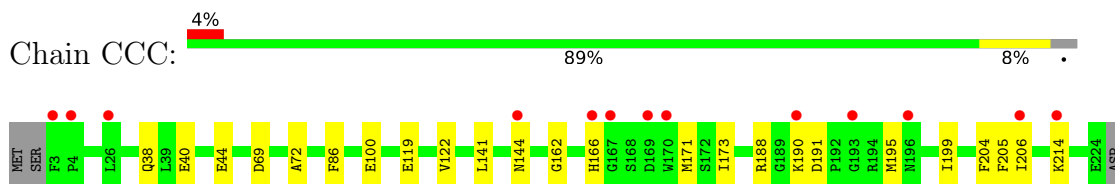
• Molecule 1: OphP S580A

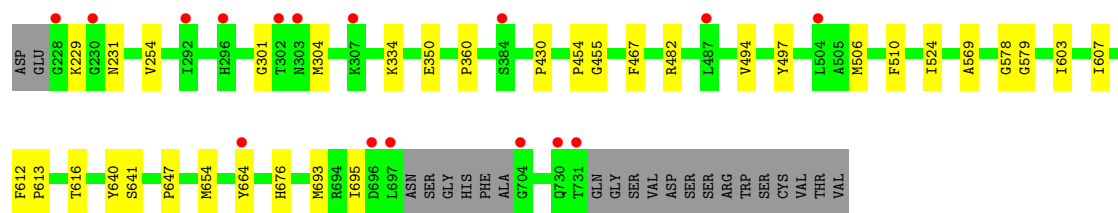


• Molecule 1: OphP S580A

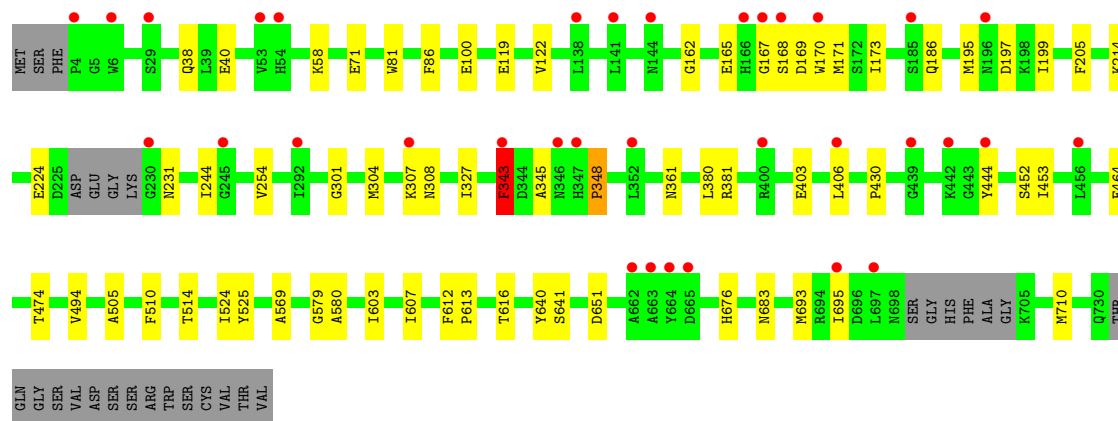
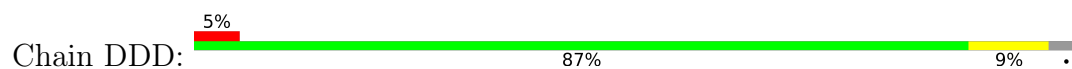


• Molecule 1: OphP S580A

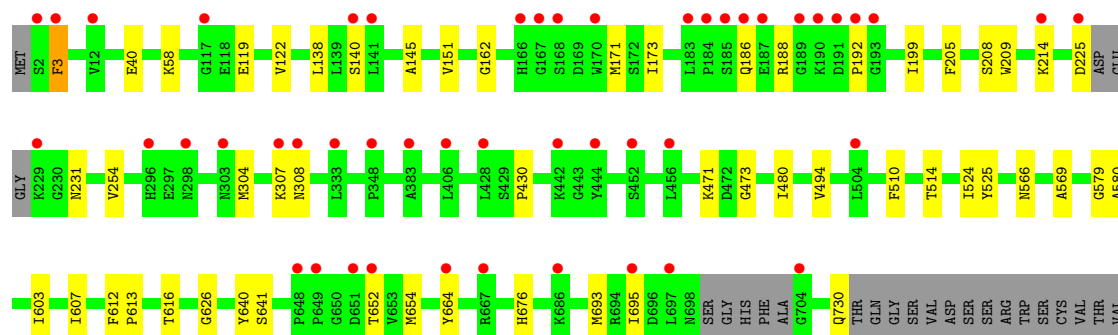




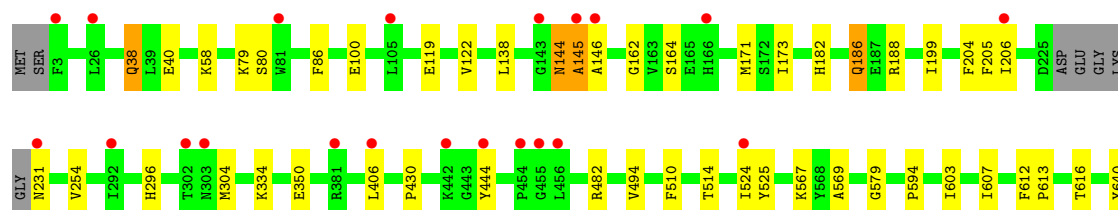
• Molecule 1: OphP S580A

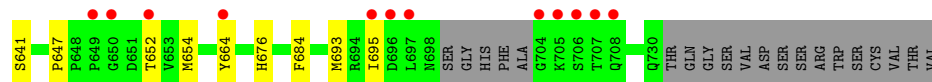


• Molecule 1: OphP S580A

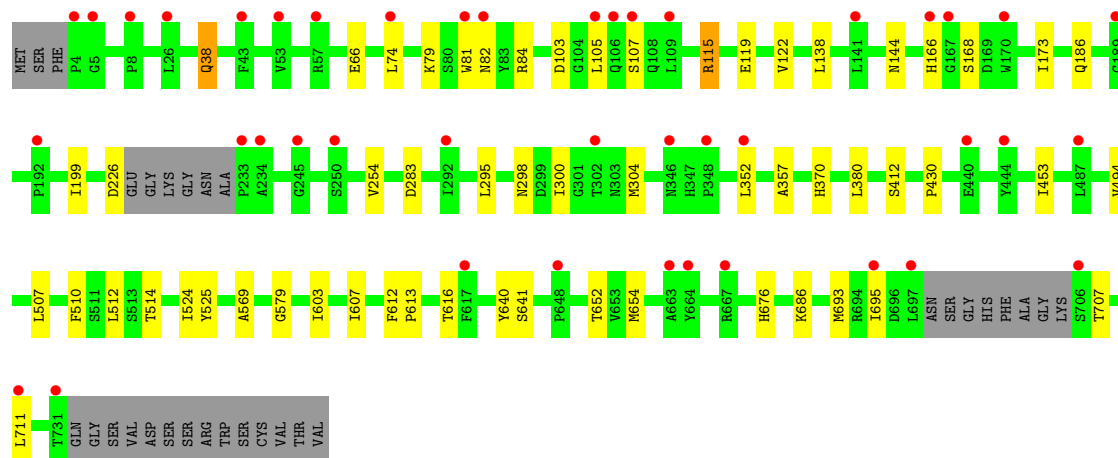
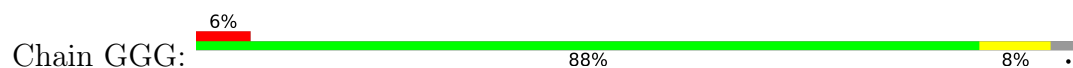


• Molecule 1: OphP S580A

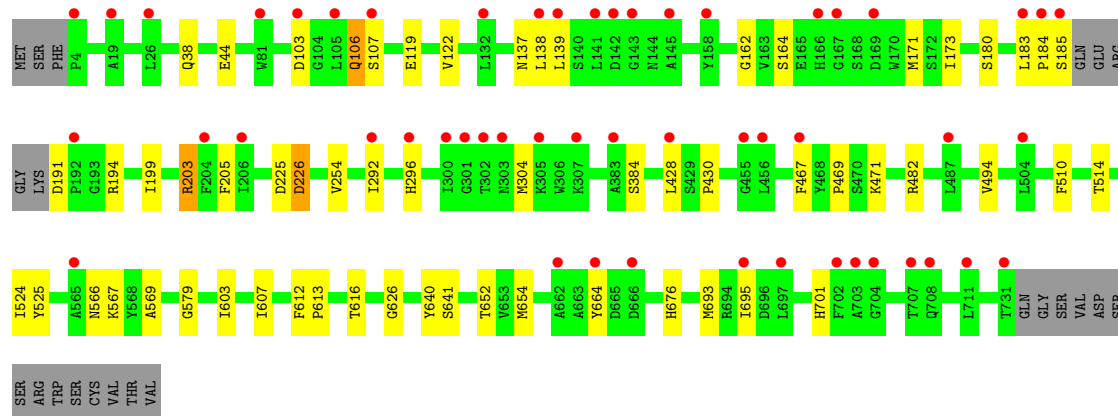




● Molecule 1: OphP S580A



● 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

All (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
1	AAA	435	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	EEE	626	GLY	CA-C-O	-5.56	118.45	122.45
1	HHH	203	ARG	CB-CG-CD	-5.45	98.76	111.30
1	GGG	82	ASN	CA-C-O	-5.32	115.77	122.63
1	CCC	578	GLY	CA-C-N	5.24	125.21	121.65
1	CCC	578	GLY	C-N-CA	5.24	125.21	121.65
1	HHH	626	GLY	CA-C-O	-5.23	118.69	122.45
1	BBB	435	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	HHH	225	ASP	CB-CA-C	5.20	120.14	111.83
1	GGG	283	ASP	CA-C-O	-5.15	115.64	121.05
1	CCC	647	PRO	N-CA-CB	5.07	105.85	103.22

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:BBB:710:MET:HE2	9:BBB:913:HOH:O	1.68	0.93
1:HHH:103:ASP:HB3	1:HHH:106:GLN:NE2	1.85	0.92
1:DDD:464:GLU:HA	1:HHH:471:LYS:O	1.70	0.91
1:DDD:167:GLY:O	1:DDD:169:ASP:N	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:307:LYS:HG2	1:DDD:348:PRO:HG2	1.62	0.82
1:CCC:334:LYS:HB3	1:GGG:357:ALA:HB1	1.62	0.82
1:EEE:140:SER:OG	1:EEE:145:ALA:CB	2.27	0.81
1:DDD:343:PHE:CE2	1:DDD:345:ALA:HA	2.18	0.79
1:DDD:343:PHE:HE1	1:DDD:348:PRO:HA	1.48	0.78
1:DDD:307:LYS:CG	1:DDD:348:PRO:HG2	2.15	0.77
1:FFF:171:MET:HE1	1:FFF:205:PHE:HB2	1.66	0.77
1:DDD:307:LYS:HG2	1:DDD:348:PRO:CG	2.15	0.76
1:AAA:171:MET:HE1	1:AAA:205:PHE:HB2	1.68	0.76
1:HHH:171:MET:HE1	1:HHH:205:PHE:HB2	1.68	0.76
1:HHH:138:LEU:HD13	1:HHH:184:PRO:HG3	1.67	0.76
1:EEE:171:MET:HE1	1:EEE:205:PHE:HB2	1.69	0.74
1:DDD:343:PHE:CE1	1:DDD:348:PRO:HA	2.21	0.74
1:FFF:145:ALA:O	1:FFF:164:SER:OG	2.06	0.73
1:AAA:323:GLU:HG3	9:AAA:967:HOH:O	1.86	0.73
1:DDD:406:LEU:HD13	1:HHH:469:PRO:HB3	1.71	0.73
1:BBB:357:ALA:CB	1:FFF:334:LYS:HG2	2.18	0.73
1:AAA:492:SER:OG	1:AAA:568:TYR:O	2.08	0.72
1:BBB:171:MET:HE1	1:BBB:205:PHE:HB2	1.72	0.72
1:CCC:171:MET:HE1	1:CCC:205:PHE:HB2	1.70	0.72
1:CCC:334:LYS:HB3	1:GGG:357:ALA:CB	2.19	0.72
1:DDD:171:MET:HE1	1:DDD:205:PHE:HB2	1.71	0.71
1:GGG:84:ARG:HG3	9:GGG:922:HOH:O	1.89	0.71
1:DDD:514:THR:HG21	1:DDD:525:TYR:CD2	2.26	0.71
1:DDD:307:LYS:HG2	1:DDD:348:PRO:CD	2.22	0.69
1:DDD:381:ARG:CG	1:HHH:566:ASN:OD1	2.37	0.69
1:AAA:514:THR:HG21	1:AAA:525:TYR:CD2	2.29	0.68
1:DDD:307:LYS:HG2	1:DDD:348:PRO:HD2	1.75	0.68
1:DDD:343:PHE:CZ	1:DDD:345:ALA:HA	2.29	0.68
1:CCC:144:ASN:CB	1:CCC:166:HIS:HB2	2.24	0.67
1:BBB:485:ASP:HB2	1:DDD:452:SER:HB2	1.77	0.66
1:CCC:144:ASN:HB3	1:CCC:166:HIS:HB2	1.76	0.66
1:CCC:360:PRO:HG3	1:GGG:352:LEU:O	1.96	0.66
1:DDD:343:PHE:HE1	1:DDD:348:PRO:CA	2.08	0.66
1:DDD:254:VAL:HG13	1:DDD:304:MET:CE	2.25	0.65
1:EEE:514:THR:HG21	1:EEE:525:TYR:CD2	2.32	0.64
1:GGG:514:THR:HG21	1:GGG:525:TYR:CD2	2.32	0.64
1:HHH:107:SER:OG	1:HHH:137:ASN:OD1	2.15	0.64
1:GGG:380:LEU:HD21	1:GGG:507:LEU:HD21	1.77	0.64
1:FFF:514:THR:HG21	1:FFF:525:TYR:CD2	2.33	0.64
1:BBB:357:ALA:HB2	1:FFF:334:LYS:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:514:THR:HG21	1:HHH:525:TYR:CD2	2.33	0.63
1:CCC:190:LYS:HB2	1:DDD:71:GLU:HG3	1.79	0.63
1:DDD:464:GLU:CA	1:HHH:471:LYS:O	2.47	0.62
1:AAA:254:VAL:HG13	1:AAA:304:MET:CE	2.30	0.61
1:AAA:125:GLU:H	1:AAA:125:GLU:CD	2.08	0.61
1:BBB:514:THR:HG21	1:BBB:525:TYR:CD2	2.36	0.60
1:AAA:381:ARG:HG2	1:EEE:566:ASN:OD1	2.01	0.60
1:AAA:204:PHE:HD1	1:AAA:206:ILE:HD13	1.67	0.60
1:DDD:343:PHE:CE1	1:DDD:348:PRO:HG3	2.37	0.60
1:GGG:380:LEU:HD21	1:GGG:507:LEU:CD2	2.32	0.59
1:HHH:254:VAL:HG13	1:HHH:304:MET:CE	2.33	0.59
1:FFF:254:VAL:HG13	1:FFF:304:MET:CE	2.32	0.59
1:CCC:204:PHE:HD1	1:CCC:206:ILE:HD13	1.68	0.59
1:GGG:254:VAL:HG13	1:GGG:304:MET:CE	2.32	0.59
1:AAA:464:GLU:HA	1:EEE:471:LYS:O	2.03	0.58
1:BBB:406:LEU:C	1:BBB:406:LEU:HD23	2.28	0.58
1:FFF:162:GLY:HA3	1:FFF:171:MET:HE3	1.85	0.58
1:EEE:494:VAL:CG2	1:EEE:569:ALA:HB2	2.34	0.58
1:EEE:254:VAL:HG13	1:EEE:304:MET:CE	2.33	0.58
1:GGG:494:VAL:CG2	1:GGG:569:ALA:HB2	2.33	0.58
1:DDD:343:PHE:CZ	1:DDD:348:PRO:HG3	2.39	0.58
1:CCC:494:VAL:CG2	1:CCC:569:ALA:HB2	2.34	0.57
1:DDD:170:TRP:CZ3	1:DDD:224:GLU:HG2	2.40	0.57
1:DDD:494:VAL:CG2	1:DDD:569:ALA:HB2	2.34	0.57
1:BBB:494:VAL:CG2	1:BBB:569:ALA:HB2	2.34	0.57
1:GGG:144:ASN:OD1	1:GGG:144:ASN:C	2.47	0.57
1:DDD:307:LYS:HE3	1:DDD:348:PRO:HB2	1.87	0.57
1:AAA:464:GLU:HB3	1:EEE:471:LYS:O	2.04	0.57
1:DDD:327:ILE:CD1	1:DDD:345:ALA:HB2	2.35	0.56
1:GGG:81:TRP:CE3	1:GGG:711:LEU:HD12	2.40	0.56
1:CCC:38:GLN:HG2	9:CCC:953:HOH:O	2.03	0.56
1:BBB:125:GLU:HG3	1:CCC:188:ARG:HG3	1.87	0.56
1:HHH:38:GLN:HG2	9:HHH:961:HOH:O	2.06	0.56
1:FFF:494:VAL:CG2	1:FFF:569:ALA:HB2	2.36	0.56
1:HHH:162:GLY:HA3	1:HHH:171:MET:HE3	1.88	0.55
1:DDD:254:VAL:HG13	1:DDD:304:MET:HE1	1.88	0.55
1:FFF:594:PRO:CG	1:FFF:652:THR:HG23	2.36	0.55
1:HHH:494:VAL:CG2	1:HHH:569:ALA:HB2	2.36	0.55
1:AAA:38:GLN:HG2	9:AAA:1058:HOH:O	2.06	0.55
1:AAA:494:VAL:HG22	1:AAA:524:ILE:HG12	1.87	0.55
1:EEE:208:SER:HA	6:EEE:803:EDO:H12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:480:ILE:HG23	1:EEE:524:ILE:CG2	2.36	0.55
1:BBB:710:MET:CE	9:BBB:913:HOH:O	2.40	0.55
1:AAA:380:LEU:HD21	1:AAA:505:ALA:HB2	1.88	0.54
1:DDD:162:GLY:HA3	1:DDD:171:MET:HE3	1.89	0.54
1:AAA:494:VAL:CG2	1:AAA:569:ALA:HB2	2.37	0.54
1:HHH:226:ASP:HB2	8:HHH:802:B3P:HN1	1.71	0.54
1:EEE:162:GLY:HA3	1:EEE:171:MET:HE3	1.88	0.54
1:CCC:204:PHE:CD1	1:CCC:206:ILE:HD13	2.42	0.54
1:HHH:164:SER:HB2	1:HHH:701:HIS:HB2	1.90	0.54
1:AAA:204:PHE:CD1	1:AAA:206:ILE:HD13	2.42	0.54
1:CCC:162:GLY:HA3	1:CCC:171:MET:HE3	1.89	0.53
1:DDD:494:VAL:HG22	1:DDD:524:ILE:HG12	1.91	0.53
1:BBB:162:GLY:HA3	1:BBB:171:MET:HE3	1.90	0.53
1:HHH:693:MET:HE3	1:HHH:695:ILE:HG13	1.91	0.53
1:AAA:162:GLY:HA3	1:AAA:171:MET:HE3	1.90	0.53
1:DDD:494:VAL:HG22	1:DDD:524:ILE:CG1	2.39	0.53
1:BBB:254:VAL:HG13	1:BBB:304:MET:CE	2.39	0.52
1:CCC:195:MET:HB3	1:DDD:58:LYS:HE3	1.91	0.52
1:DDD:38:GLN:HG2	9:DDD:996:HOH:O	2.10	0.52
1:GGG:494:VAL:HG22	1:GGG:524:ILE:CG1	2.40	0.52
1:DDD:307:LYS:CG	1:DDD:348:PRO:CG	2.84	0.52
1:EEE:730:GLN:C	5:EEE:801:THR:HA	2.35	0.51
1:AAA:173:ILE:HB	1:AAA:199:ILE:HB	1.92	0.51
1:BBB:173:ILE:HB	1:BBB:199:ILE:HB	1.91	0.51
1:DDD:380:LEU:HD21	1:DDD:505:ALA:HB2	1.93	0.51
1:FFF:204:PHE:HD1	1:FFF:206:ILE:HD13	1.75	0.51
1:DDD:173:ILE:HB	1:DDD:199:ILE:HB	1.93	0.51
1:EEE:173:ILE:HB	1:EEE:199:ILE:HB	1.92	0.51
1:HHH:482:ARG:HB3	1:HHH:524:ILE:HG13	1.92	0.51
1:DDD:514:THR:CG2	1:DDD:525:TYR:CG	2.94	0.51
1:FFF:204:PHE:CD1	1:FFF:206:ILE:HD13	2.46	0.51
1:DDD:170:TRP:CE3	1:DDD:224:GLU:HG2	2.46	0.51
1:CCC:254:VAL:HG13	1:CCC:304:MET:CE	2.41	0.51
1:CCC:482:ARG:HB3	1:CCC:524:ILE:HG13	1.91	0.51
1:GGG:652:THR:HG21	1:GGG:654:MET:HE3	1.92	0.51
1:BBB:494:VAL:HG22	1:BBB:524:ILE:HG12	1.91	0.50
1:EEE:119:GLU:O	1:EEE:122:VAL:HG22	2.11	0.50
1:FFF:173:ILE:HB	1:FFF:199:ILE:HB	1.93	0.50
1:AAA:464:GLU:CB	1:EEE:471:LYS:O	2.58	0.50
1:AAA:494:VAL:HG22	1:AAA:524:ILE:CG1	2.40	0.50
1:BBB:494:VAL:HG22	1:BBB:524:ILE:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:119:GLU:O	1:BBB:122:VAL:HG22	2.12	0.50
1:HHH:119:GLU:O	1:HHH:122:VAL:HG22	2.12	0.50
1:AAA:124:THR:OG1	1:AAA:126:SER:OG	2.30	0.50
1:CCC:44:GLU:HG3	1:DDD:186:GLN:HG3	1.93	0.50
1:BBB:115:ARG:HD2	9:BBB:987:HOH:O	2.11	0.50
1:CCC:119:GLU:O	1:CCC:122:VAL:HG22	2.12	0.50
1:HHH:164:SER:CB	1:HHH:701:HIS:HB2	2.42	0.50
1:BBB:185:SER:HB3	1:CCC:455:GLY:CA	2.40	0.50
1:DDD:119:GLU:O	1:DDD:122:VAL:HG22	2.11	0.50
1:GGG:74:LEU:CD1	1:GGG:711:LEU:HD23	2.42	0.50
1:AAA:119:GLU:O	1:AAA:122:VAL:HG22	2.11	0.50
1:GGG:173:ILE:HB	1:GGG:199:ILE:HB	1.93	0.50
1:EEE:140:SER:HG	1:EEE:145:ALA:HB2	1.70	0.49
1:GGG:81:TRP:CD1	1:GGG:707:THR:HG23	2.47	0.49
1:AAA:514:THR:CG2	1:AAA:525:TYR:CG	2.95	0.49
1:BBB:357:ALA:CB	1:FFF:334:LYS:CG	2.87	0.49
1:CCC:173:ILE:HB	1:CCC:199:ILE:HB	1.93	0.49
1:DDD:514:THR:HG21	1:DDD:525:TYR:CE2	2.48	0.49
1:GGG:138:LEU:HD13	1:GGG:186:GLN:HG2	1.94	0.49
1:GGG:579:GLY:HA2	1:GGG:603:ILE:O	2.13	0.49
1:FFF:119:GLU:O	1:FFF:122:VAL:HG22	2.13	0.49
1:AAA:693:MET:HE3	1:AAA:695:ILE:HG13	1.95	0.49
1:HHH:173:ILE:HB	1:HHH:199:ILE:HB	1.94	0.49
1:CCC:579:GLY:HA2	1:CCC:603:ILE:O	2.13	0.48
1:GGG:652:THR:HG21	1:GGG:654:MET:CE	2.44	0.48
1:AAA:430:PRO:HA	1:AAA:510:PHE:CG	2.49	0.48
1:BBB:579:GLY:HA2	1:BBB:603:ILE:O	2.13	0.48
1:GGG:494:VAL:HG22	1:GGG:524:ILE:HG12	1.94	0.48
1:AAA:254:VAL:HG13	1:AAA:304:MET:HE1	1.95	0.48
1:AAA:514:THR:HG21	1:AAA:525:TYR:CE2	2.48	0.48
1:AAA:667:ARG:HD3	1:AAA:668:VAL:HG23	1.96	0.48
1:BBB:485:ASP:HB3	1:DDD:453:ILE:C	2.38	0.48
1:FFF:594:PRO:HG3	1:FFF:652:THR:HG23	1.96	0.48
1:FFF:79:LYS:HG3	1:FFF:80:SER:N	2.28	0.48
1:GGG:119:GLU:O	1:GGG:122:VAL:HG22	2.13	0.48
1:DDD:514:THR:HG21	1:DDD:525:TYR:CG	2.49	0.48
1:EEE:430:PRO:HA	1:EEE:510:PHE:CG	2.49	0.48
1:FFF:138:LEU:HD13	1:FFF:186:GLN:HG2	1.94	0.48
1:FFF:579:GLY:HA2	1:FFF:603:ILE:O	2.14	0.48
1:GGG:514:THR:CG2	1:GGG:525:TYR:CG	2.97	0.48
1:GGG:693:MET:HE3	1:GGG:695:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:357:ALA:HB1	1:FFF:334:LYS:HG2	1.95	0.47
1:DDD:361:ASN:CG	1:HHH:567:LYS:HB2	2.39	0.47
1:FFF:652:THR:HG21	1:FFF:654:MET:CE	2.44	0.47
1:AAA:579:GLY:HA2	1:AAA:603:ILE:O	2.14	0.47
1:DDD:40:GLU:O	1:DDD:231:ASN:ND2	2.47	0.47
1:FFF:607:ILE:HG21	1:FFF:676:HIS:CG	2.49	0.47
1:HHH:514:THR:CG2	1:HHH:525:TYR:CG	2.97	0.47
1:FFF:254:VAL:HG13	1:FFF:304:MET:HE1	1.95	0.47
1:CCC:497:TYR:CE2	1:CCC:506:MET:HE1	2.50	0.47
1:EEE:652:THR:HG21	1:EEE:654:MET:HE3	1.97	0.47
1:EEE:693:MET:HE3	1:EEE:695:ILE:HG13	1.96	0.47
1:FFF:514:THR:CG2	1:FFF:525:TYR:CG	2.97	0.47
1:HHH:254:VAL:HG13	1:HHH:304:MET:HE1	1.97	0.47
1:BBB:693:MET:HE3	1:BBB:695:ILE:HG13	1.97	0.47
1:EEE:151:VAL:HG11	6:EEE:803:EDO:O1	2.14	0.47
1:HHH:579:GLY:HA2	1:HHH:603:ILE:O	2.15	0.47
1:EEE:579:GLY:HA2	1:EEE:603:ILE:O	2.15	0.47
1:HHH:183:LEU:HD12	1:HHH:191:ASP:HB2	1.96	0.47
1:EEE:209:TRP:H	6:EEE:803:EDO:H12	1.80	0.47
1:EEE:514:THR:CG2	1:EEE:525:TYR:CG	2.97	0.47
1:CCC:40:GLU:O	1:CCC:231:ASN:ND2	2.49	0.46
1:DDD:308:ASN:O	1:DDD:348:PRO:HB3	2.15	0.46
1:DDD:579:GLY:HA2	1:DDD:603:ILE:O	2.14	0.46
1:DDD:693:MET:HE3	1:DDD:695:ILE:HG13	1.96	0.46
1:GGG:453:ILE:HG21	1:GGG:512:LEU:HD13	1.96	0.46
1:BBB:40:GLU:O	1:BBB:231:ASN:ND2	2.49	0.46
1:GGG:693:MET:HE3	1:GGG:695:ILE:CG1	2.46	0.46
1:AAA:464:GLU:CA	1:EEE:471:LYS:O	2.63	0.46
1:GGG:514:THR:HG21	1:GGG:525:TYR:CE2	2.51	0.46
1:AAA:693:MET:HE3	1:AAA:695:ILE:CG1	2.46	0.46
1:FFF:693:MET:HE3	1:FFF:695:ILE:HG13	1.97	0.46
1:HHH:430:PRO:HA	1:HHH:510:PHE:CG	2.51	0.46
1:HHH:514:THR:HG21	1:HHH:525:TYR:CE2	2.51	0.46
1:CCC:693:MET:HE3	1:CCC:695:ILE:HG13	1.97	0.46
1:FFF:640:TYR:O	1:FFF:641:SER:C	2.59	0.46
1:BBB:693:MET:HE3	1:BBB:695:ILE:CG1	2.46	0.46
1:DDD:693:MET:HE3	1:DDD:695:ILE:CG1	2.46	0.46
1:AAA:40:GLU:O	1:AAA:231:ASN:ND2	2.49	0.46
1:HHH:640:TYR:O	1:HHH:641:SER:C	2.59	0.45
1:AAA:652:THR:HG21	1:AAA:654:MET:HE3	1.98	0.45
1:DDD:430:PRO:HA	1:DDD:510:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:652:THR:HG21	1:HHH:654:MET:CE	2.47	0.45
1:BBB:188:ARG:HD3	1:CCC:72:ALA:HB1	1.99	0.45
1:GGG:254:VAL:HG13	1:GGG:304:MET:HE1	1.98	0.45
1:FFF:40:GLU:O	1:FFF:231:ASN:ND2	2.49	0.45
1:BBB:406:LEU:C	1:BBB:406:LEU:CD2	2.89	0.45
1:BBB:607:ILE:HG21	1:BBB:676:HIS:CG	2.52	0.45
1:CCC:430:PRO:HA	1:CCC:510:PHE:CG	2.51	0.45
1:EEE:40:GLU:O	1:EEE:231:ASN:ND2	2.50	0.45
1:EEE:640:TYR:O	1:EEE:641:SER:C	2.60	0.45
1:FFF:430:PRO:HA	1:FFF:510:PHE:CG	2.52	0.45
1:GGG:607:ILE:HG21	1:GGG:676:HIS:CG	2.52	0.45
1:AAA:652:THR:HG21	1:AAA:654:MET:CE	2.47	0.45
1:CCC:607:ILE:HG21	1:CCC:676:HIS:CG	2.52	0.45
1:FFF:482:ARG:HB3	1:FFF:524:ILE:HG12	1.99	0.45
1:AAA:514:THR:HG21	1:AAA:525:TYR:CG	2.51	0.45
1:BBB:184:PRO:HG2	1:CCC:454:PRO:HB2	1.98	0.45
1:CCC:693:MET:HE3	1:CCC:695:ILE:CG1	2.47	0.45
1:DDD:640:TYR:O	1:DDD:641:SER:C	2.59	0.45
1:EEE:607:ILE:HG21	1:EEE:676:HIS:CG	2.52	0.45
1:EEE:693:MET:HE3	1:EEE:695:ILE:CG1	2.47	0.45
1:GGG:640:TYR:O	1:GGG:641:SER:C	2.59	0.45
1:BBB:81:TRP:CZ2	1:BBB:710:MET:HE1	2.52	0.44
1:BBB:430:PRO:HA	1:BBB:510:PHE:CG	2.52	0.44
1:BBB:652:THR:HG21	1:BBB:654:MET:HE3	1.99	0.44
1:DDD:607:ILE:HG21	1:DDD:676:HIS:CG	2.52	0.44
1:HHH:607:ILE:HG21	1:HHH:676:HIS:CG	2.52	0.44
1:CCC:640:TYR:O	1:CCC:641:SER:C	2.59	0.44
1:DDD:195:MET:HE1	1:DDD:244:ILE:CG2	2.47	0.44
1:EEE:514:THR:HG21	1:EEE:525:TYR:CE2	2.52	0.44
1:FFF:693:MET:HE3	1:FFF:695:ILE:CG1	2.47	0.44
1:GGG:298:ASN:HB2	9:GGG:968:HOH:O	2.17	0.44
1:AAA:607:ILE:HG21	1:AAA:676:HIS:CG	2.53	0.44
1:FFF:514:THR:HG21	1:FFF:525:TYR:CG	2.53	0.44
1:BBB:640:TYR:O	1:BBB:641:SER:C	2.60	0.44
1:HHH:652:THR:HG21	1:HHH:654:MET:HE3	1.99	0.44
1:EEE:186:GLN:HB3	1:EEE:192:PRO:HG3	2.00	0.44
1:HHH:428:LEU:HD12	9:HHH:1017:HOH:O	2.16	0.44
1:BBB:171:MET:HE1	1:BBB:205:PHE:CD1	2.52	0.44
1:BBB:396:LYS:HE2	1:FFF:350:GLU:HG3	1.99	0.44
1:EEE:514:THR:HG21	1:EEE:525:TYR:CG	2.53	0.44
1:AAA:640:TYR:O	1:AAA:641:SER:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:514:THR:CG2	1:BBB:525:TYR:CG	3.01	0.44
1:GGG:494:VAL:HG23	1:GGG:569:ALA:CB	2.48	0.44
1:BBB:171:MET:HE1	1:BBB:205:PHE:HD1	1.82	0.43
1:BBB:188:ARG:NH2	1:CCC:69:ASP:OD1	2.50	0.43
1:EEE:652:THR:HG21	1:EEE:654:MET:CE	2.48	0.43
1:HHH:693:MET:HE3	1:HHH:695:ILE:CG1	2.47	0.43
1:HHH:191:ASP:OD2	1:HHH:194:ARG:HG3	2.17	0.43
1:FFF:38:GLN:O	1:FFF:38:GLN:NE2	2.51	0.43
1:HHH:514:THR:HG21	1:HHH:525:TYR:CG	2.52	0.43
1:BBB:652:THR:HG21	1:BBB:654:MET:CE	2.49	0.43
1:FFF:514:THR:HG21	1:FFF:525:TYR:CE2	2.53	0.43
1:GGG:514:THR:HG21	1:GGG:525:TYR:CG	2.53	0.43
1:EEE:254:VAL:HG13	1:EEE:304:MET:HE1	1.99	0.43
1:HHH:612:PHE:CG	1:HHH:613:PRO:HD3	2.54	0.43
1:CCC:612:PHE:CG	1:CCC:613:PRO:HD3	2.54	0.43
1:GGG:105:LEU:N	1:GGG:105:LEU:HD22	2.34	0.43
1:HHH:103:ASP:CB	1:HHH:106:GLN:NE2	2.56	0.43
1:BBB:190:LYS:HD2	1:EEE:3:PHE:O	2.18	0.43
1:BBB:612:PHE:CG	1:BBB:613:PRO:HD3	2.54	0.43
1:CCC:494:VAL:HG23	1:CCC:569:ALA:CB	2.49	0.43
1:BBB:514:THR:HG21	1:BBB:525:TYR:CE2	2.54	0.42
1:AAA:301:GLY:O	1:AAA:304:MET:HE2	2.20	0.42
1:BBB:494:VAL:HG23	1:BBB:569:ALA:CB	2.50	0.42
1:DDD:580:ALA:CB	3:DDD:801:GOL:H12	2.49	0.42
1:AAA:612:PHE:CG	1:AAA:613:PRO:HD3	2.54	0.42
1:CCC:171:MET:HE1	1:CCC:205:PHE:CD1	2.54	0.42
1:FFF:652:THR:CG2	1:FFF:654:MET:HE2	2.48	0.42
1:EEE:494:VAL:HG23	1:EEE:569:ALA:CB	2.49	0.42
1:DDD:86:PHE:HA	1:DDD:100:GLU:O	2.19	0.42
1:DDD:494:VAL:CG2	1:DDD:569:ALA:CB	2.98	0.42
1:EEE:612:PHE:CG	1:EEE:613:PRO:HD3	2.54	0.42
1:AAA:25:LYS:HE2	1:CCC:467:PHE:CD2	2.55	0.42
1:DDD:81:TRP:CZ2	1:DDD:710:MET:HE1	2.54	0.42
1:EEE:188:ARG:HA	1:EEE:188:ARG:HD3	1.90	0.42
1:FFF:406:LEU:HA	9:FFF:955:HOH:O	2.18	0.42
1:BBB:141:LEU:HA	1:BBB:188:ARG:HD2	2.02	0.42
1:DDD:494:VAL:HG23	1:DDD:569:ALA:CB	2.50	0.42
1:AAA:702:PHE:O	1:AAA:703:ALA:HB3	2.19	0.42
1:GGG:430:PRO:HA	1:GGG:510:PHE:CG	2.55	0.42
1:CCC:190:LYS:HG2	1:CCC:191:ASP:N	2.35	0.42
1:GGG:38:GLN:O	1:GGG:38:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:494:VAL:HG23	1:GGG:569:ALA:HB2	2.02	0.42
1:CCC:44:GLU:OE1	1:CCC:229:LYS:HB2	2.20	0.41
1:GGG:295:LEU:HD22	1:GGG:300:ILE:CD1	2.49	0.41
1:FFF:654:MET:HG2	1:FFF:684:PHE:CE2	2.55	0.41
1:CCC:144:ASN:HB2	1:CCC:166:HIS:HB2	2.01	0.41
1:DDD:612:PHE:CG	1:DDD:613:PRO:HD3	2.54	0.41
1:HHH:185:SER:HB2	1:HHH:194:ARG:NH1	2.34	0.41
1:GGG:612:PHE:CG	1:GGG:613:PRO:HD3	2.54	0.41
1:FFF:594:PRO:HB3	1:FFF:654:MET:CE	2.51	0.41
1:FFF:647:PRO:HG2	1:FFF:654:MET:HE3	2.01	0.41
1:AAA:494:VAL:HG23	1:AAA:569:ALA:CB	2.51	0.41
1:BBB:357:ALA:HB2	1:FFF:334:LYS:CB	2.51	0.41
1:BBB:454:PRO:HD2	9:BBB:927:HOH:O	2.19	0.41
1:GGG:74:LEU:HD12	1:GGG:711:LEU:HD23	2.02	0.41
1:BBB:188:ARG:HD3	1:CCC:72:ALA:CB	2.51	0.41
1:BBB:332:ASN:HA	1:BBB:335:ALA:O	2.21	0.41
1:DDD:171:MET:HE1	1:DDD:205:PHE:CD1	2.55	0.41
1:GGG:686:LYS:O	1:GGG:686:LYS:HG2	2.20	0.41
1:HHH:138:LEU:HD13	1:HHH:184:PRO:CG	2.42	0.41
1:BBB:86:PHE:HA	1:BBB:100:GLU:O	2.21	0.41
1:BBB:357:ALA:HB3	1:FFF:334:LYS:HE3	2.03	0.41
1:CCC:86:PHE:HA	1:CCC:100:GLU:O	2.21	0.41
1:CCC:141:LEU:HD12	1:CCC:141:LEU:N	2.35	0.41
1:CCC:171:MET:HE1	1:CCC:205:PHE:HD1	1.86	0.41
1:CCC:494:VAL:HG23	1:CCC:569:ALA:HB2	2.03	0.41
1:DDD:403:GLU:HB3	1:HHH:467:PHE:CD1	2.56	0.41
1:FFF:612:PHE:N	1:FFF:613:PRO:CD	2.84	0.41
1:FFF:612:PHE:CG	1:FFF:613:PRO:HD3	2.55	0.41
1:HHH:494:VAL:HG23	1:HHH:569:ALA:CB	2.51	0.41
1:BBB:171:MET:CE	1:BBB:205:PHE:HD1	2.33	0.41
1:CCC:301:GLY:O	1:CCC:304:MET:HE2	2.21	0.41
1:EEE:138:LEU:C	1:EEE:188:ARG:O	2.60	0.41
1:AAA:141:LEU:N	1:AAA:141:LEU:HD13	2.36	0.40
1:AAA:332:ASN:HA	1:AAA:335:ALA:O	2.21	0.40
1:FFF:86:PHE:HA	1:FFF:100:GLU:O	2.21	0.40
1:DDD:171:MET:HE1	1:DDD:205:PHE:HD1	1.86	0.40
1:DDD:214:LYS:HD3	1:DDD:214:LYS:HA	1.87	0.40
1:FFF:494:VAL:HG23	1:FFF:569:ALA:CB	2.51	0.40
1:AAA:463:THR:O	1:EEE:473:GLY:HA3	2.21	0.40
1:DDD:167:GLY:C	1:DDD:169:ASP:H	2.28	0.40
1:HHH:139:LEU:HD23	1:HHH:139:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:195:MET:HE1	1:AAA:244:ILE:CG2	2.52	0.40
1:AAA:380:LEU:HD21	1:AAA:505:ALA:CB	2.51	0.40
1:BBB:612:PHE:N	1:BBB:613:PRO:CD	2.85	0.40
1:DDD:167:GLY:C	1:DDD:169:ASP:N	2.77	0.40
1:DDD:301:GLY:O	1:DDD:304:MET:HE2	2.21	0.40
1:EEE:580:ALA:HB1	3:EEE:802:GOL:H11	2.03	0.40

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

All (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
1	EEE	616	THR
1	GGG	616	THR
1	AAA	616	THR
1	AAA	703	ALA
1	BBB	616	THR
1	CCC	616	THR
1	DDD	616	THR
1	FFF	616	THR
1	HHH	616	THR

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	AAA	629/644 (98%)	619 (98%)	10 (2%)	55	46
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

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	58	LYS
1	AAA	141	LEU
1	AAA	147	LEU
1	AAA	190	LYS
1	AAA	197	ASP
1	AAA	323	GLU
1	AAA	350	GLU
1	AAA	403	GLU
1	AAA	664	TYR
1	AAA	667	ARG
1	BBB	58	LYS
1	BBB	197	ASP
1	BBB	307	LYS
1	BBB	308	ASN
1	BBB	664	TYR
1	CCC	214	LYS
1	CCC	350	GLU
1	CCC	654	MET
1	CCC	664	TYR
1	DDD	197	ASP
1	DDD	343	PHE
1	DDD	348	PRO
1	DDD	444	TYR
1	DDD	683	ASN
1	EEE	3	PHE
1	EEE	58	LYS
1	EEE	214	LYS
1	EEE	225	ASP
1	EEE	307	LYS
1	EEE	308[A]	ASN
1	EEE	308[B]	ASN
1	EEE	664	TYR
1	FFF	38	GLN
1	FFF	58	LYS
1	FFF	144	ASN
1	FFF	186	GLN
1	FFF	444	TYR
1	FFF	664	TYR
1	GGG	38	GLN
1	GGG	66	GLU
1	GGG	103	ASP
1	GGG	107	SER
1	GGG	115	ARG

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Mol	Chain	Res	Type
1	GGG	166	HIS
1	GGG	226	ASP
1	GGG	412	SER
1	HHH	106	GLN
1	HHH	180	SER
1	HHH	203	ARG
1	HHH	226	ASP
1	HHH	292	ILE
1	HHH	384	SER
1	HHH	664	TYR

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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.

All (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

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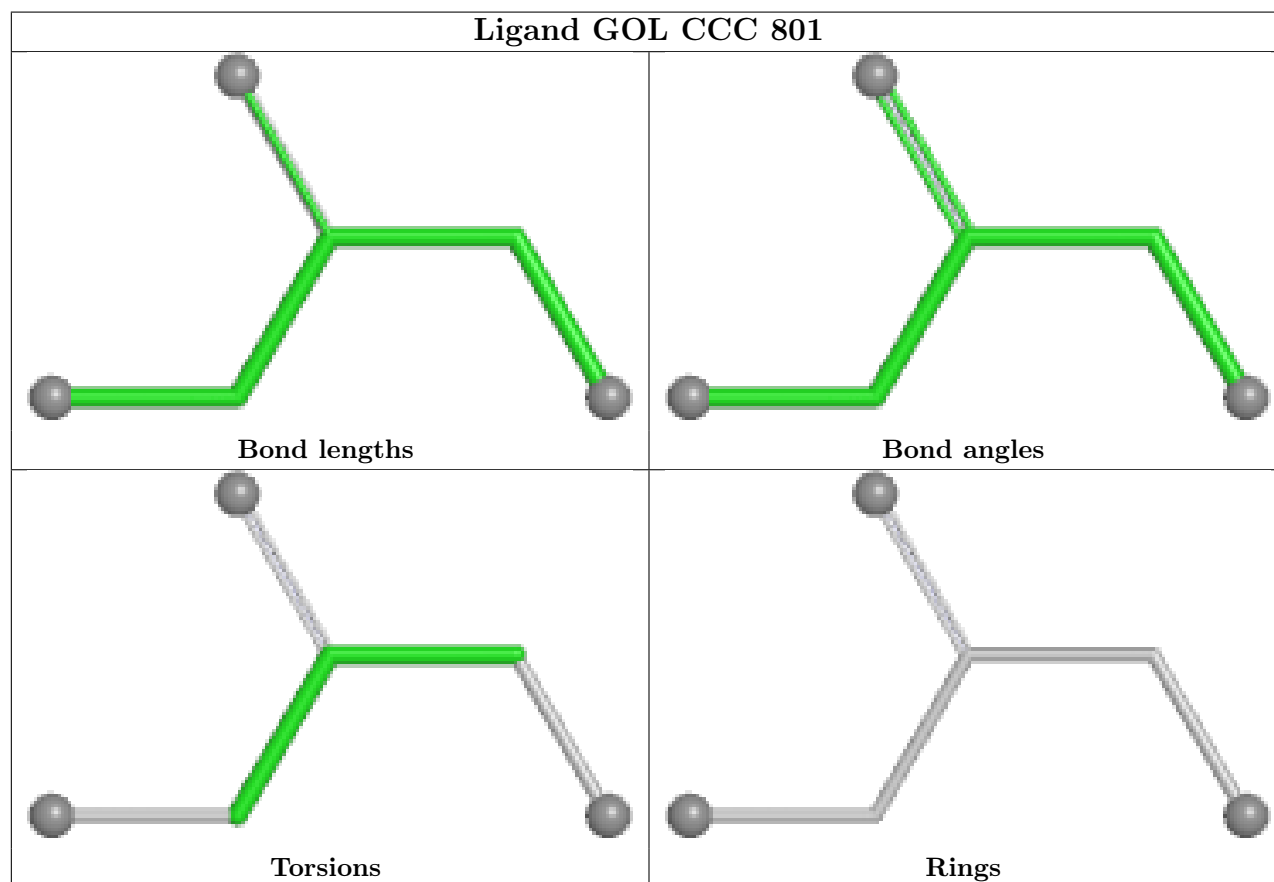
Mol	Chain	Res	Type	Atoms
3	EEE	802	GOL	C1-C2-C3-O3
3	HHH	801	GOL	O1-C1-C2-C3
7	FFF	802	TRS	C3-C-C1-O1
7	FFF	802	TRS	C1-C-C2-O2
7	FFF	802	TRS	N-C-C3-O3
7	GGG	802	TRS	C2-C-C1-O1
7	GGG	802	TRS	C1-C-C2-O2
7	GGG	802	TRS	C3-C-C2-O2
7	GGG	802	TRS	N-C-C2-O2
8	HHH	802	B3P	N1-C4-C5-O4
8	HHH	802	B3P	C6-C4-C5-O4
8	HHH	802	B3P	C7-C4-C5-O4
8	HHH	802	B3P	O2-C10-C8-N2
8	HHH	802	B3P	O2-C10-C8-C9
8	HHH	802	B3P	O2-C10-C8-C11
3	HHH	801	GOL	O1-C1-C2-O2
7	FFF	802	TRS	C2-C-C1-O1
7	FFF	802	TRS	C3-C-C2-O2
7	GGG	802	TRS	C3-C-C1-O1
3	EEE	802	GOL	O2-C2-C3-O3
8	HHH	802	B3P	C9-C8-N2-C2
8	HHH	802	B3P	C11-C8-N2-C2
6	EEE	803	EDO	O1-C1-C2-O2
6	GGG	801	EDO	O1-C1-C2-O2
7	GGG	802	TRS	N-C-C3-O3
7	GGG	802	TRS	C1-C-C3-O3
7	GGG	802	TRS	C2-C-C3-O3
8	HHH	802	B3P	C3-C1-C2-N2
7	FFF	802	TRS	N-C-C1-O1
7	FFF	802	TRS	N-C-C2-O2
7	GGG	802	TRS	N-C-C1-O1
7	FFF	802	TRS	C1-C-C3-O3

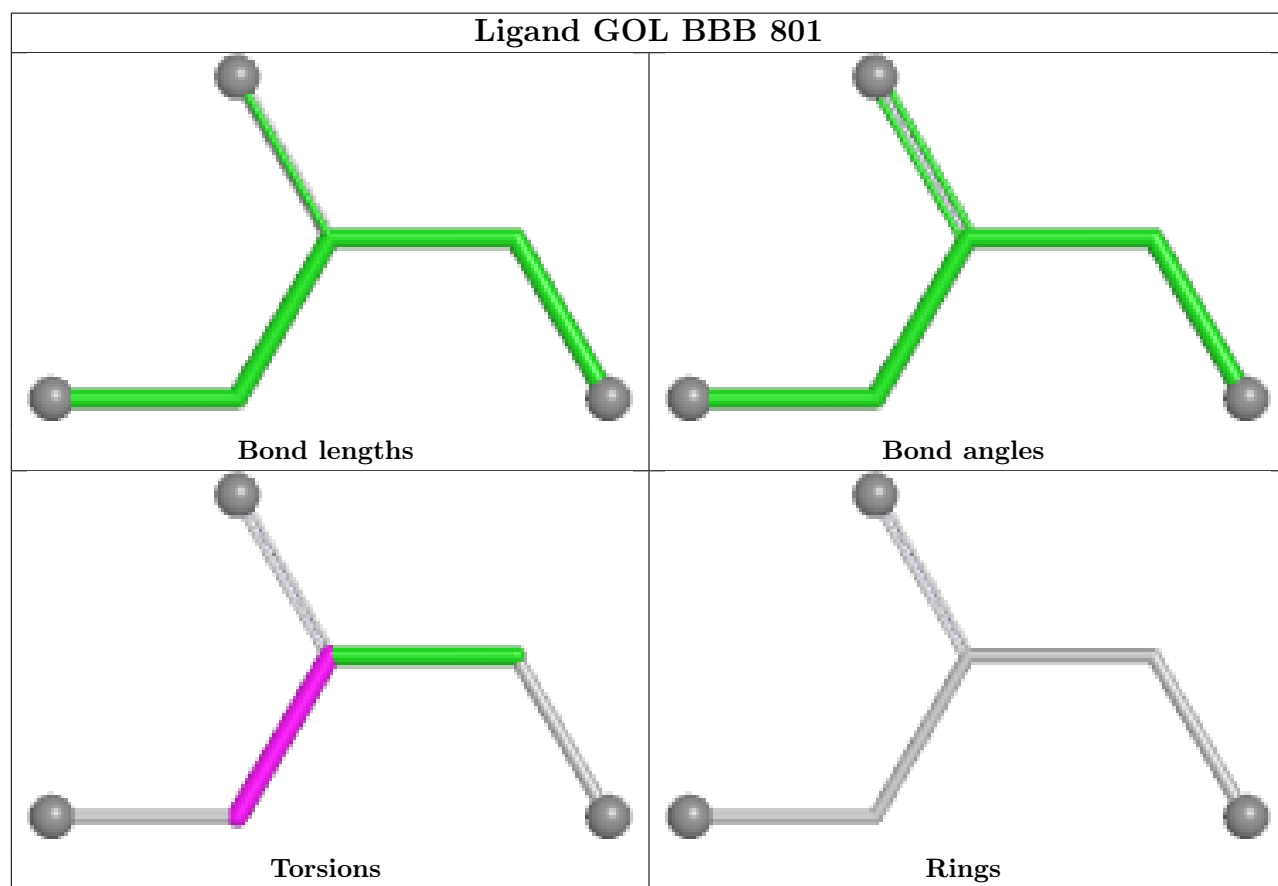
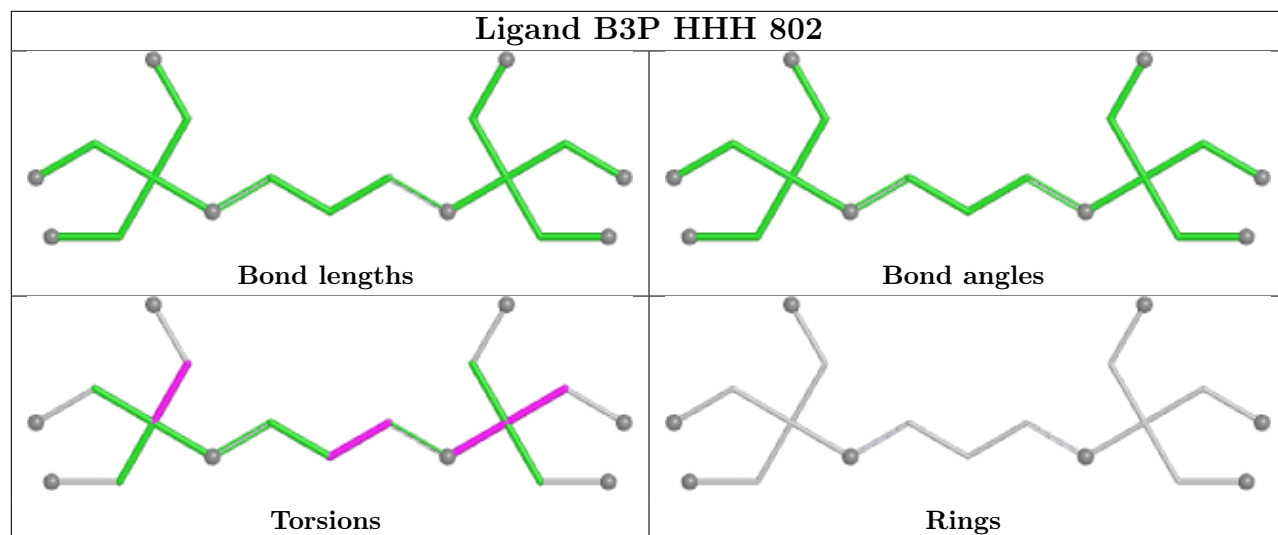
There are no ring outliers.

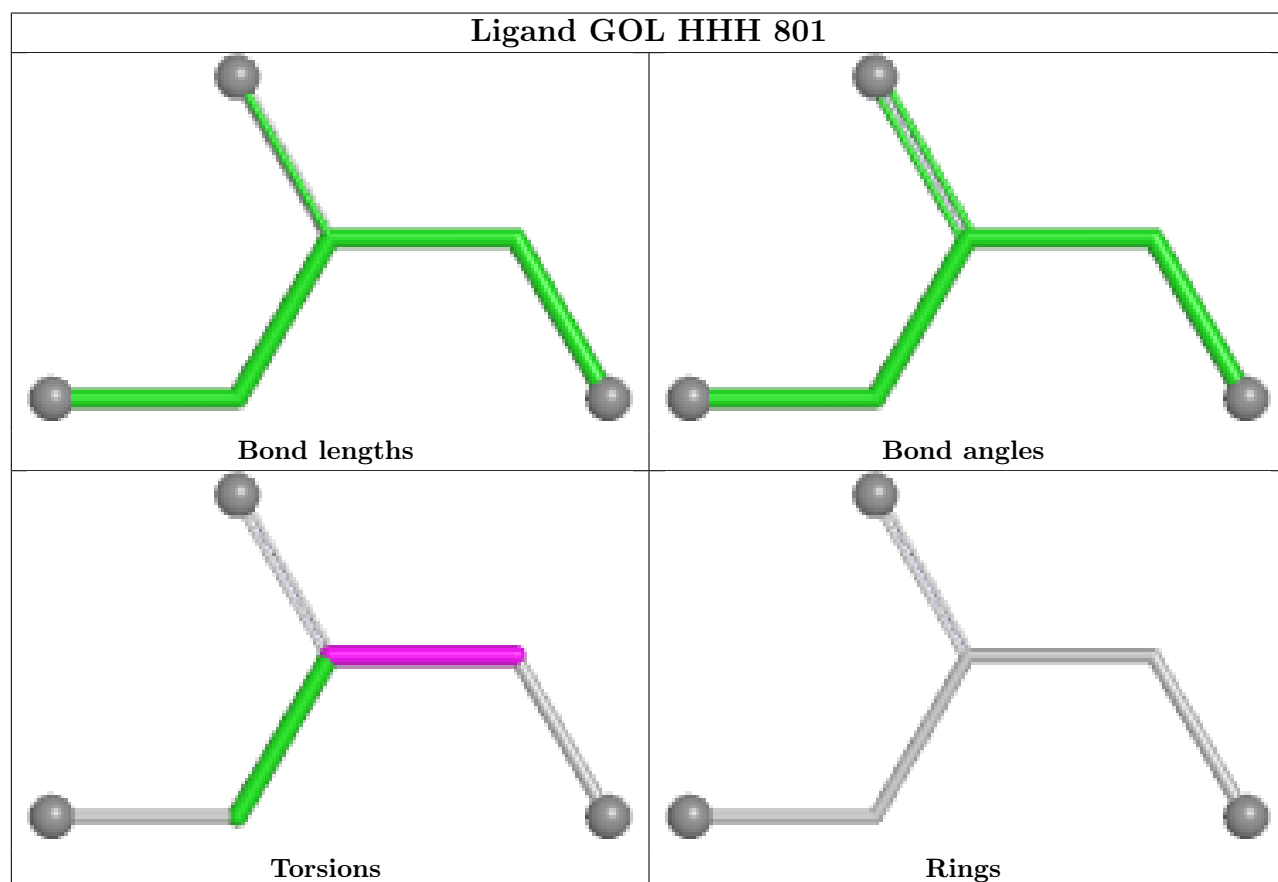
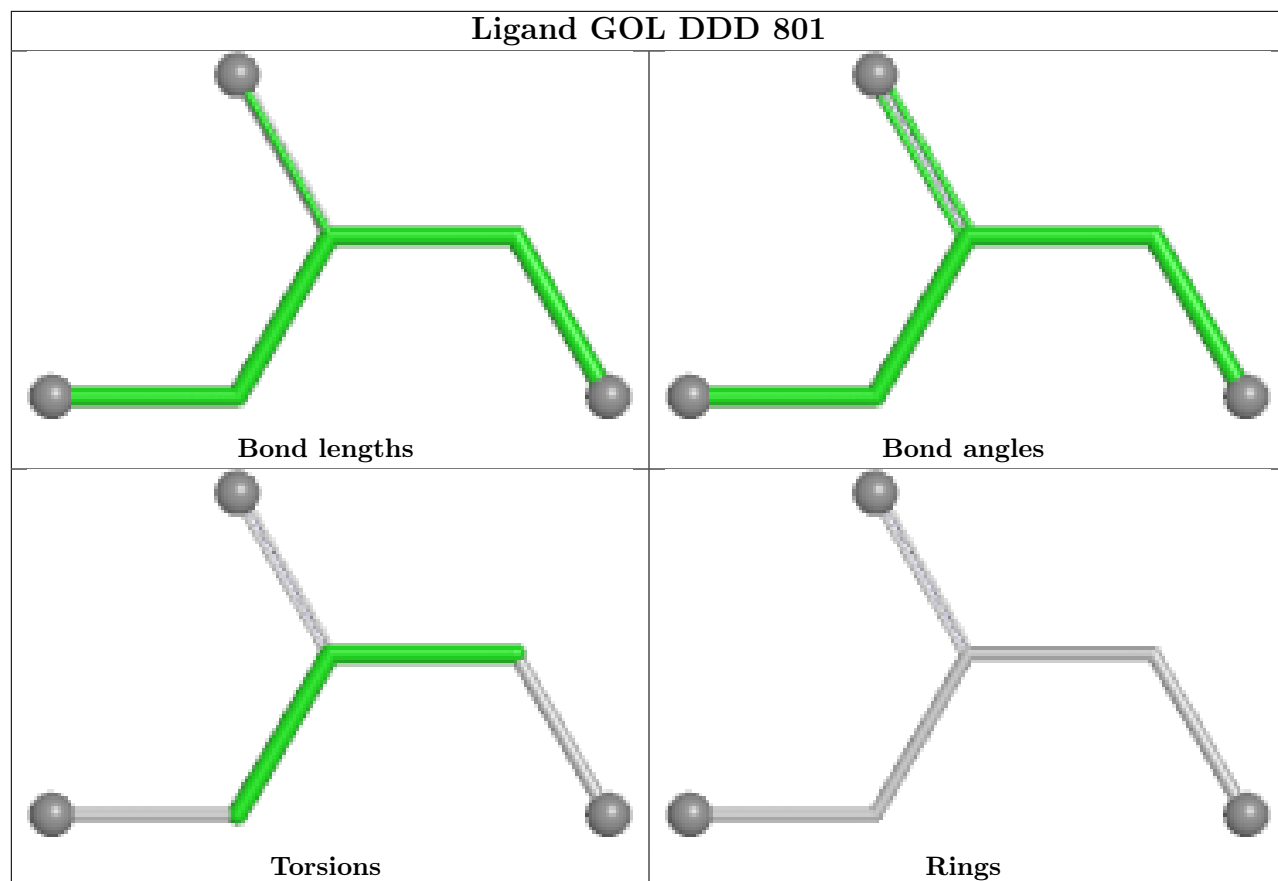
5 monomers are involved in 7 short contacts:

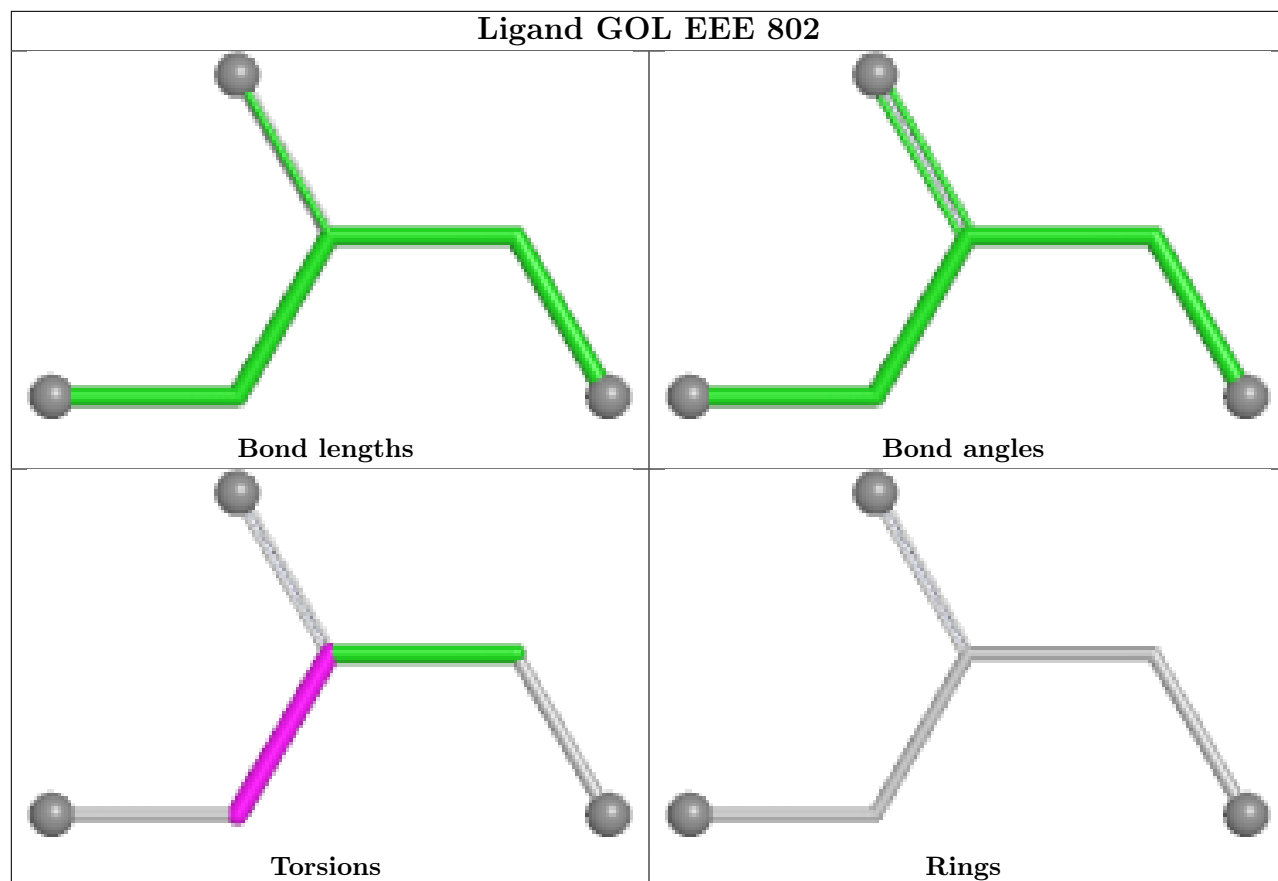
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EEE	801	THR	1	0
8	HHH	802	B3P	1	0
3	DDD	801	GOL	1	0
6	EEE	803	EDO	3	0
3	EEE	802	GOL	1	0

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.









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	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%)

All (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
1	AAA	702	PHE	5.6
1	BBB	3	PHE	5.5
1	DDD	343	PHE	5.4
1	DDD	168	SER	5.3
1	DDD	167	GLY	5.1
1	DDD	141	LEU	5.1
1	EEE	3	PHE	4.9
1	DDD	664	TYR	4.8
1	FFF	145	ALA	4.6
1	FFF	704	GLY	4.6
1	GGG	4	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	EEE	444	TYR	4.5
1	CCC	664	TYR	4.5
1	EEE	383	ALA	4.4
1	CCC	697	LEU	4.3
1	GGG	233	PRO	4.3
1	HHH	184	PRO	4.3
1	DDD	166	HIS	4.2
1	HHH	105	LEU	4.2
1	DDD	4	PRO	4.1
1	BBB	697	LEU	4.1
1	AAA	700	GLY	4.0
1	EEE	456	LEU	4.0
1	AAA	143	GLY	4.0
1	FFF	650	GLY	4.0
1	AAA	144	ASN	4.0
1	AAA	664	TYR	3.9
1	HHH	138	LEU	3.9
1	FFF	664	TYR	3.9
1	AAA	703	ALA	3.9
1	FFF	166	HIS	3.9
1	AAA	141	LEU	3.8
1	GGG	711	LEU	3.8
1	EEE	166	HIS	3.8
1	DDD	444	TYR	3.8
1	FFF	707	THR	3.7
1	EEE	664	TYR	3.7
1	BBB	302	THR	3.7
1	FFF	3	PHE	3.6
1	EEE	141	LEU	3.6
1	DDD	245	GLY	3.6
1	GGG	663	ALA	3.6
1	FFF	231	ASN	3.6
1	CCC	228	GLY	3.6
1	HHH	204	PHE	3.6
1	HHH	707	THR	3.5
1	GGG	302	THR	3.5
1	EEE	170	TRP	3.4
1	GGG	664	TYR	3.4
1	BBB	698	ASN	3.4
1	GGG	43	PHE	3.4
1	GGG	697	LEU	3.4
1	BBB	166	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	GGG	706	SER	3.3
1	HHH	731	THR	3.3
1	AAA	166	HIS	3.2
1	FFF	206	ILE	3.2
1	DDD	352	LEU	3.2
1	BBB	308	ASN	3.2
1	AAA	701	HIS	3.2
1	BBB	170	TRP	3.2
1	DDD	695	ILE	3.2
1	EEE	649	PRO	3.2
1	BBB	303	ASN	3.2
1	FFF	697	LEU	3.2
1	GGG	26	LEU	3.2
1	BBB	230	GLY	3.2
1	GGG	107	SER	3.2
1	GGG	167	GLY	3.2
1	GGG	617	PHE	3.2
1	CCC	166	HIS	3.2
1	HHH	703	ALA	3.1
1	HHH	107	SER	3.1
1	HHH	702	PHE	3.1
1	AAA	307	LYS	3.1
1	EEE	348	PRO	3.1
1	CCC	704	GLY	3.1
1	GGG	82	ASN	3.1
1	GGG	444	TYR	3.0
1	AAA	699	SER	3.0
1	BBB	487	LEU	3.0
1	GGG	170	TRP	3.0
1	HHH	142	ASP	3.0
1	BBB	231	ASN	3.0
1	FFF	406	LEU	2.9
1	HHH	697	LEU	2.9
1	FFF	143	GLY	2.9
1	CCC	303	ASN	2.9
1	GGG	234	ALA	2.9
1	HHH	292	ILE	2.9
1	GGG	141	LEU	2.9
1	DDD	230	GLY	2.9
1	FFF	146	ALA	2.9
1	AAA	456	LEU	2.9
1	BBB	167	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	FFF	649	PRO	2.8
1	DDD	662	ALA	2.8
1	EEE	308[A]	ASN	2.8
1	CCC	302	THR	2.8
1	EEE	186	GLN	2.8
1	GGG	53	VAL	2.8
1	HHH	103	ASP	2.8
1	EEE	189	GLY	2.8
1	HHH	455	GLY	2.8
1	BBB	141	LEU	2.8
1	EEE	190	LYS	2.8
1	CCC	169	ASP	2.8
1	CCC	384	SER	2.8
1	CCC	26	LEU	2.8
1	AAA	168	SER	2.7
1	EEE	229	LYS	2.7
1	EEE	704	GLY	2.7
1	HHH	302	THR	2.7
1	FFF	706	SER	2.7
1	HHH	664	TYR	2.7
1	CCC	731	THR	2.7
1	FFF	26	LEU	2.7
1	EEE	193	GLY	2.7
1	BBB	2	SER	2.7
1	HHH	26	LEU	2.7
1	HHH	301	GLY	2.6
1	CCC	214	LYS	2.6
1	AAA	695	ILE	2.6
1	AAA	167	GLY	2.6
1	AAA	145	ALA	2.6
1	BBB	444[A]	TYR	2.6
1	EEE	214	LYS	2.6
1	AAA	296	HIS	2.6
1	DDD	347	HIS	2.6
1	FFF	456	LEU	2.6
1	GGG	105	LEU	2.6
1	HHH	711	LEU	2.6
1	CCC	170	TRP	2.6
1	HHH	81	TRP	2.6
1	EEE	504	LEU	2.6
1	AAA	165	GLU	2.6
1	DDD	292	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	CCC	167	GLY	2.5
1	EEE	298	ASN	2.5
1	EEE	2	SER	2.5
1	HHH	185	SER	2.5
1	FFF	705	LYS	2.5
1	HHH	456	LEU	2.5
1	GGG	346	ASN	2.5
1	HHH	145	ALA	2.5
1	BBB	169	ASP	2.5
1	CCC	504	LEU	2.5
1	DDD	346	ASN	2.5
1	HHH	169	ASP	2.5
1	AAA	231	ASN	2.4
1	BBB	664	TYR	2.4
1	GGG	106	GLN	2.4
1	HHH	206	ILE	2.4
1	CCC	307	LYS	2.4
1	AAA	142	ASP	2.4
1	GGG	8	PRO	2.4
1	EEE	167	GLY	2.4
1	FFF	455	GLY	2.4
1	DDD	406	LEU	2.4
1	HHH	183	LEU	2.4
1	EEE	651	ASP	2.4
1	FFF	696	ASP	2.4
1	HHH	695	ILE	2.4
1	HHH	143	GLY	2.4
1	HHH	167	GLY	2.4
1	AAA	697	LEU	2.4
1	DDD	307	LYS	2.4
1	EEE	307	LYS	2.4
1	EEE	406	LEU	2.4
1	BBB	142	ASP	2.4
1	DDD	663	ALA	2.4
1	DDD	144	ASN	2.4
1	EEE	303	ASN	2.4
1	FFF	303	ASN	2.4
1	HHH	704	GLY	2.4
1	GGG	81	TRP	2.4
1	GGG	352	LEU	2.3
1	HHH	487	LEU	2.3
1	EEE	652	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	730	GLN	2.3
1	CCC	730	GLN	2.3
1	EEE	184	PRO	2.3
1	GGG	166	HIS	2.3
1	AAA	169	ASP	2.3
1	EEE	225	ASP	2.3
1	DDD	697	LEU	2.3
1	FFF	708	GLN	2.3
1	HHH	708	GLN	2.3
1	BBB	204	PHE	2.3
1	CCC	196	ASN	2.3
1	BBB	455	GLY	2.3
1	EEE	117	GLY	2.3
1	FFF	442	LYS	2.3
1	EEE	667	ARG	2.3
1	GGG	667	ARG	2.3
1	DDD	665	ASP	2.3
1	EEE	428	LEU	2.3
1	HHH	132	LEU	2.3
1	BBB	382	ASN	2.3
1	CCC	190	LYS	2.3
1	HHH	192	PRO	2.3
1	CCC	193	GLY	2.3
1	GGG	245	GLY	2.3
1	EEE	168	SER	2.3
1	EEE	296	HIS	2.3
1	BBB	138	LEU	2.3
1	BBB	183	LEU	2.3
1	BBB	456	LEU	2.3
1	DDD	442	LYS	2.3
1	HHH	141	LEU	2.3
1	GGG	57	ARG	2.2
1	BBB	5	GLY	2.2
1	EEE	648	PRO	2.2
1	GGG	192	PRO	2.2
1	GGG	648	PRO	2.2
1	HHH	662	ALA	2.2
1	CCC	292	ILE	2.2
1	FFF	292	ILE	2.2
1	CCC	296	HIS	2.2
1	FFF	652	THR	2.2
1	AAA	504	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	2	SER	2.2
1	AAA	4	PRO	2.2
1	BBB	189	GLY	2.2
1	EEE	185	SER	2.2
1	HHH	4	PRO	2.2
1	BBB	347	HIS	2.2
1	HHH	303	ASN	2.2
1	DDD	53	VAL	2.2
1	GGG	731	THR	2.2
1	EEE	183	LEU	2.2
1	CCC	4	PRO	2.2
1	GGG	348	PRO	2.2
1	BBB	695	ILE	2.2
1	FFF	695	ILE	2.2
1	BBB	58	LYS	2.2
1	EEE	686	LYS	2.2
1	FFF	381	ARG	2.2
1	CCC	696	ASP	2.2
1	GGG	189	GLY	2.2
1	DDD	170	TRP	2.1
1	FFF	81	TRP	2.1
1	FFF	302	THR	2.1
1	EEE	452	SER	2.1
1	CCC	230	GLY	2.1
1	GGG	5	GLY	2.1
1	CCC	487	LEU	2.1
1	DDD	138	LEU	2.1
1	EEE	442	LYS	2.1
1	HHH	307	LYS	2.1
1	EEE	187	GLU	2.1
1	CCC	144	ASN	2.1
1	HHH	565	ALA	2.1
1	CCC	206	ILE	2.1
1	HHH	300	ILE	2.1
1	DDD	6	TRP	2.1
1	DDD	185	SER	2.1
1	EEE	140	SER	2.1
1	AAA	111	LEU	2.1
1	BBB	26	LEU	2.1
1	BBB	144	ASN	2.1
1	DDD	456	LEU	2.1
1	GGG	74	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	GGG	109	LEU	2.1
1	HHH	428	LEU	2.1
1	EEE	191	ASP	2.1
1	FFF	444	TYR	2.1
1	AAA	190	LYS	2.1
1	AAA	189	GLY	2.1
1	AAA	455	GLY	2.1
1	DDD	439	GLY	2.1
1	DDD	196	ASN	2.1
1	BBB	4	PRO	2.1
1	EEE	333	LEU	2.1
1	FFF	105	LEU	2.1
1	HHH	139	LEU	2.1
1	HHH	666	ASP	2.1
1	GGG	292	ILE	2.0
1	GGG	440	GLU	2.0
1	HHH	467	PHE	2.0
1	AAA	163	VAL	2.0
1	EEE	192	PRO	2.0
1	FFF	454	PRO	2.0
1	EEE	697	LEU	2.0
1	HHH	504	LEU	2.0
1	DDD	400	ARG	2.0
1	HHH	19	ALA	2.0
1	HHH	305	LYS	2.0
1	DDD	29	SER	2.0
1	GGG	250	SER	2.0
1	DDD	54	HIS	2.0
1	EEE	695	ILE	2.0
1	FFF	524	ILE	2.0
1	GGG	695	ILE	2.0
1	HHH	296	HIS	2.0
1	HHH	158	TYR	2.0
1	EEE	12	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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.

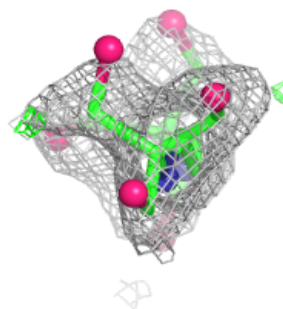
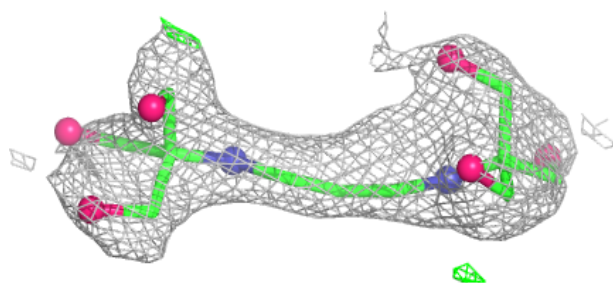
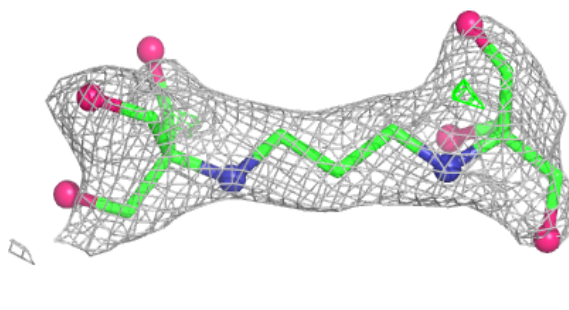
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	EEE	804	1/1	0.67	0.21	62,62,62,62	0
5	THR	EEE	801	7/8	0.67	0.15	83,108,120,125	0
5	THR	FFF	801	7/8	0.74	0.19	75,102,115,129	0
8	B3P	HHH	802	19/19	0.80	0.14	49,69,83,86	0
2	NA	DDD	803	1/1	0.81	0.14	64,64,64,64	0
7	TRS	GGG	802	8/8	0.83	0.16	45,63,74,80	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.

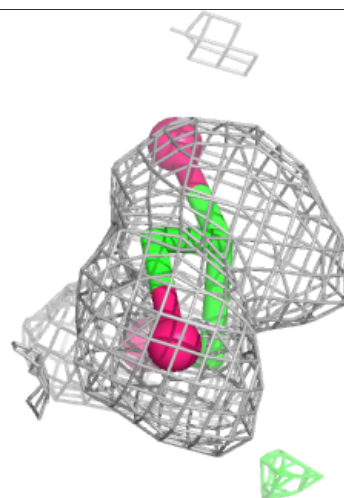
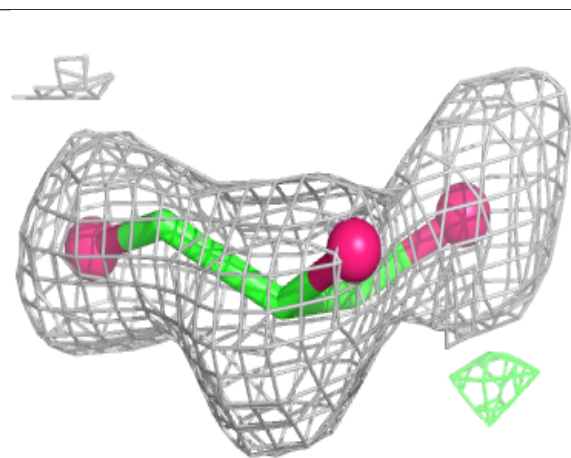
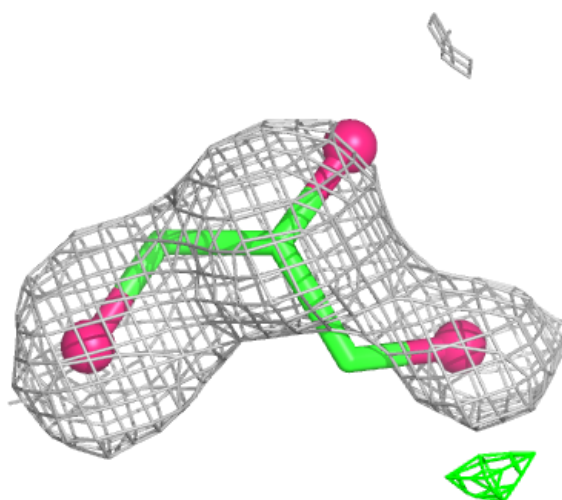
Electron density around B3P HHH 802:

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



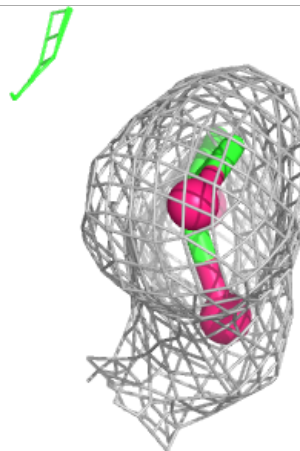
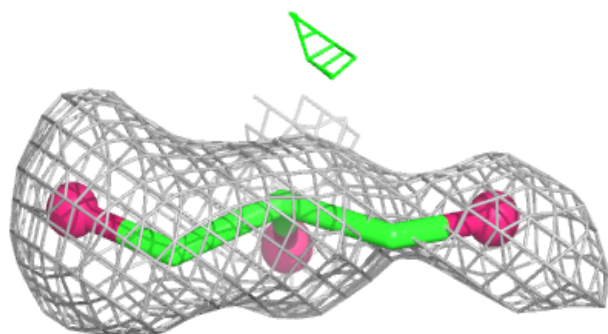
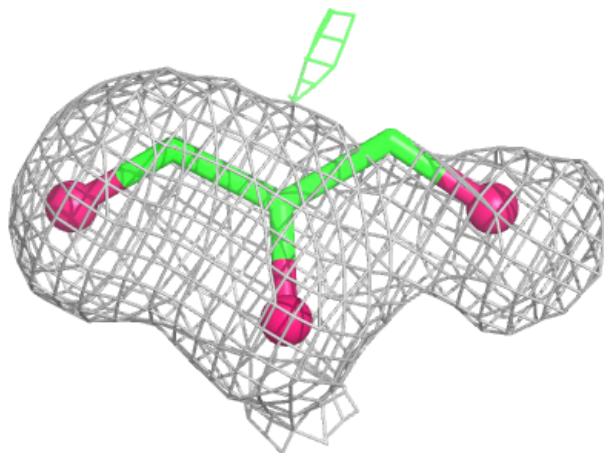
Electron density around GOL HHH 801:

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



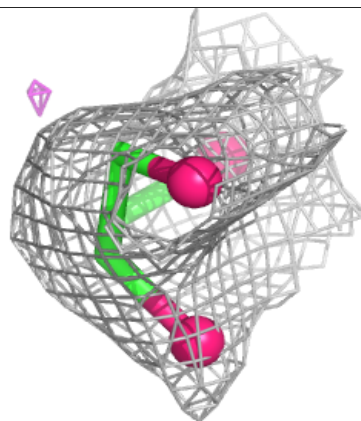
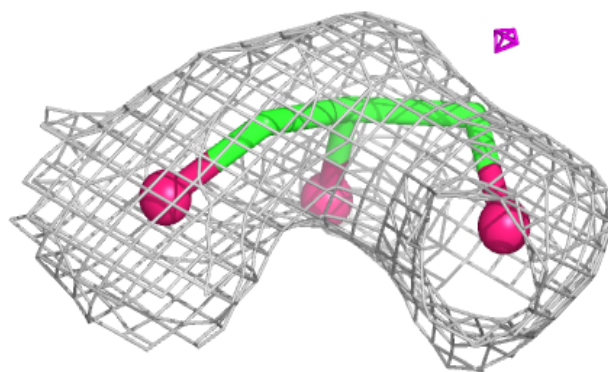
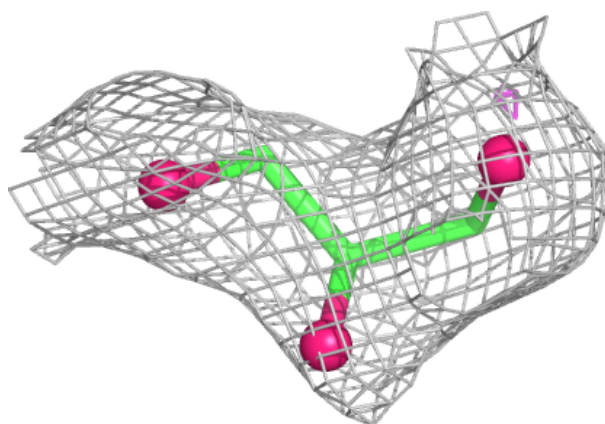
Electron density around GOL CCC 801:

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



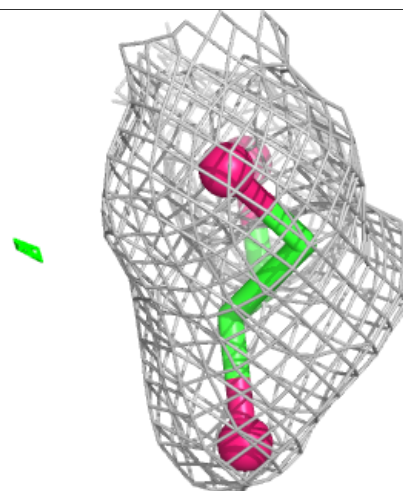
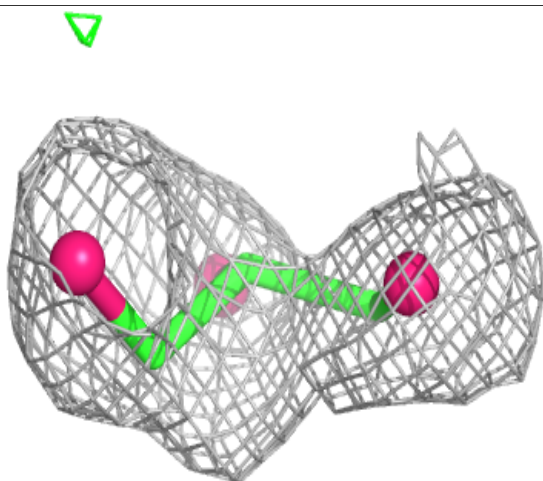
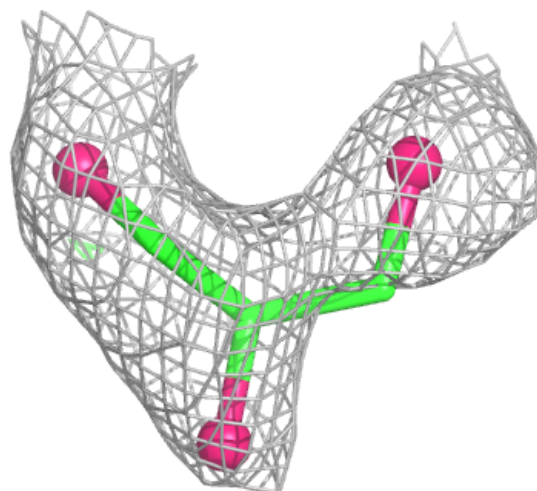
Electron density around GOL EEE 802:

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



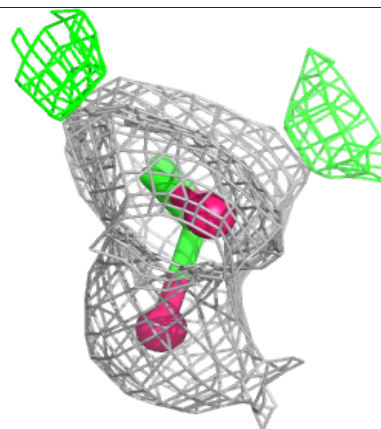
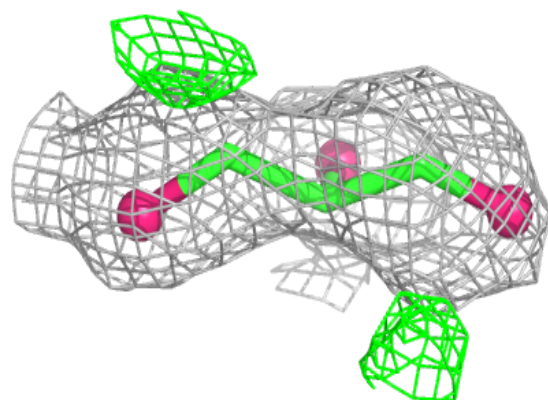
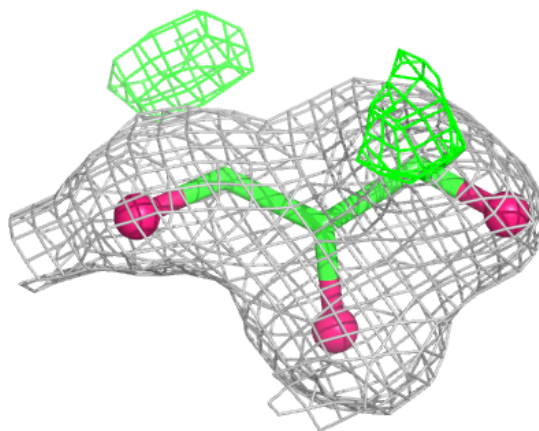
Electron density around GOL BBB 801:

$2mF_o-DF_c$ (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.