Full wwPDB X-ray Structure Validation Report (i)

Jun 30, 2022 – 01:36 am BST

PDB ID	:	7ZB2
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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

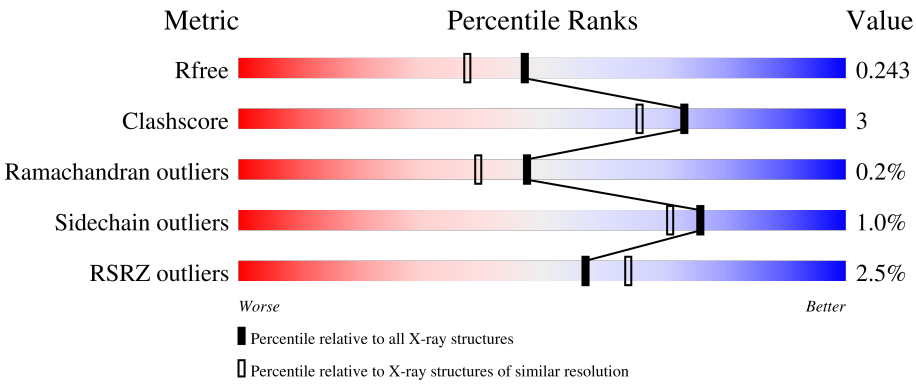
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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

Mol	Chain	Length	Quality of chain
1	AAA	745	2% 89% 7%
1	BBB	745	% 90% 7%
1	CCC	745	2% 90% 7%
1	DDD	745	3% 89% 7%
1	EEE	745	3% 90% 7%

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Mol	Chain	Length	Quality of chain
1	FFF	745	2% 89% 7%
1	GGG	745	3% 89% 7%
1	HHH	745	3% 90% 7%

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.

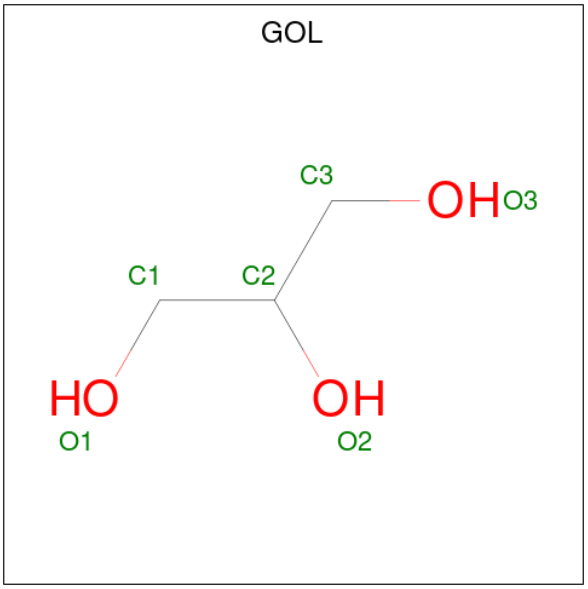
- Molecule 1 is a protein called OphP S580A.

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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

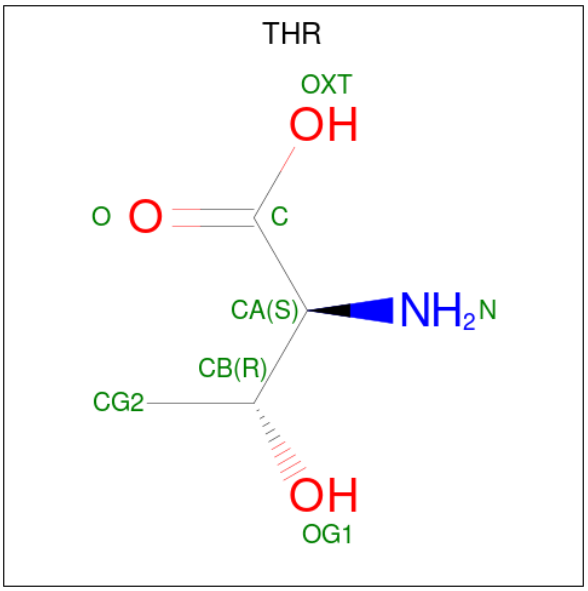


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	BBB	1	6	3	3	0	0
			Total	C	O		
3	CCC	1	6	3	3	0	0
			Total	C	O		
3	DDD	1	6	3	3	0	0
			Total	C	O		
3	EEE	1	6	3	3	0	0
			Total	C	O		
3	HHH	1	6	3	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

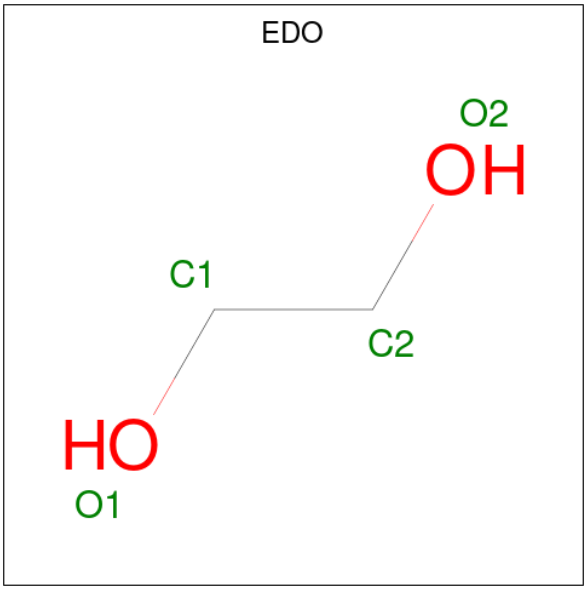
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	CCC	2	2	2	0	0
			Total	Mg		
4	FFF	1	1	1	0	0

- Molecule 5 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$).



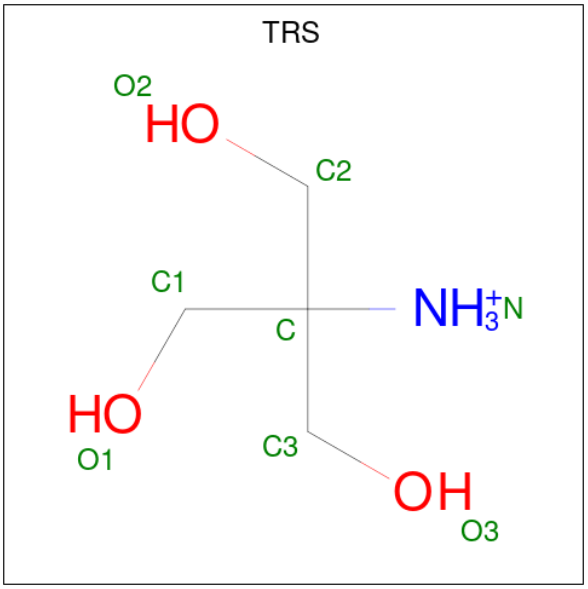
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	EEE	1	7	4	1	2	0	0
5	FFF	1	7	4	1	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



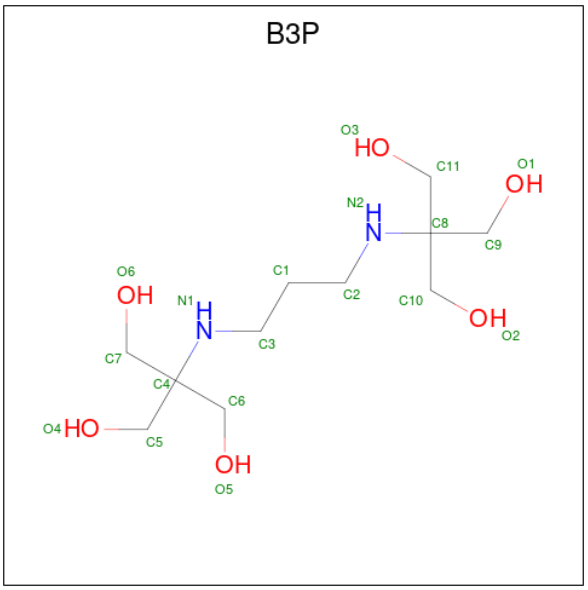
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	EEE	1	4	2	2		0	0
6	GGG	1	4	2	2		0	0

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



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

- Molecule 8 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



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

- Molecule 9 is water.

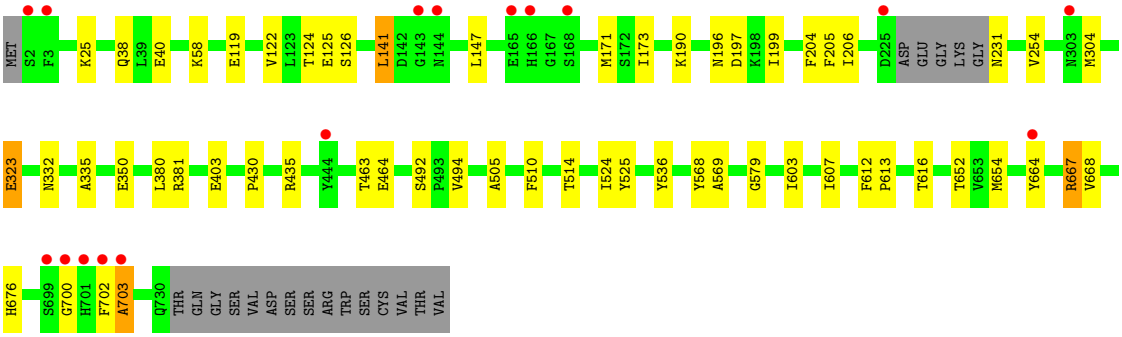
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	AAA	192	192	192	0	0
9	BBB	110	110	110	0	0
9	CCC	104	104	104	0	0
9	DDD	141	141	141	0	0
9	EEE	57	57	57	0	0
9	FFF	80	80	80	0	0
9	GGG	97	97	97	0	0
9	HHH	117	117	117	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

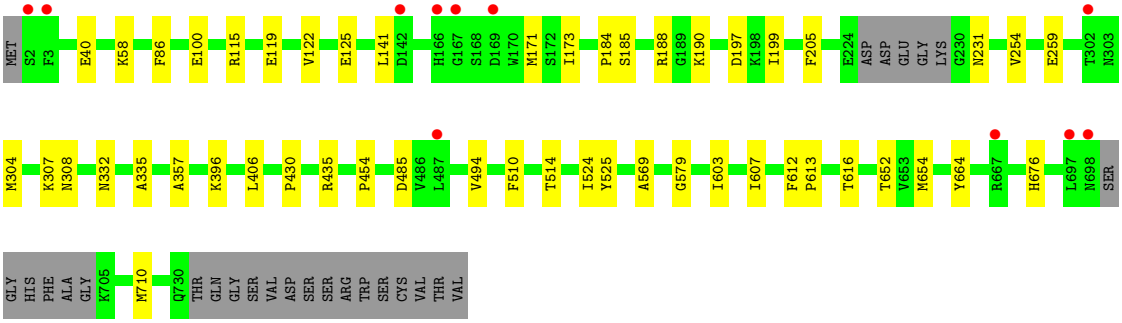
• Molecule 1: OphP S580A

Chain AAA:



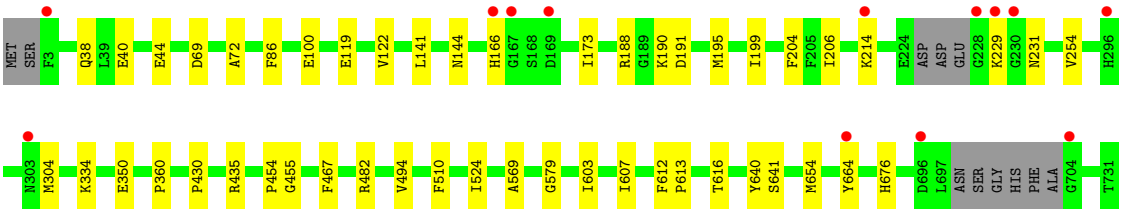
• Molecule 1: OphP S580A

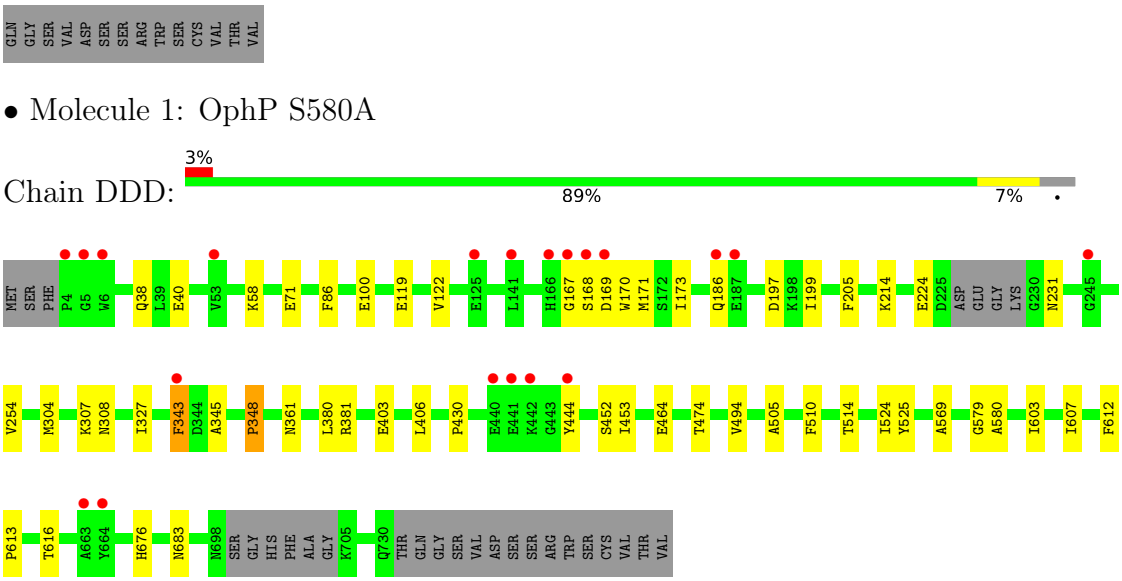
Chain BBB:

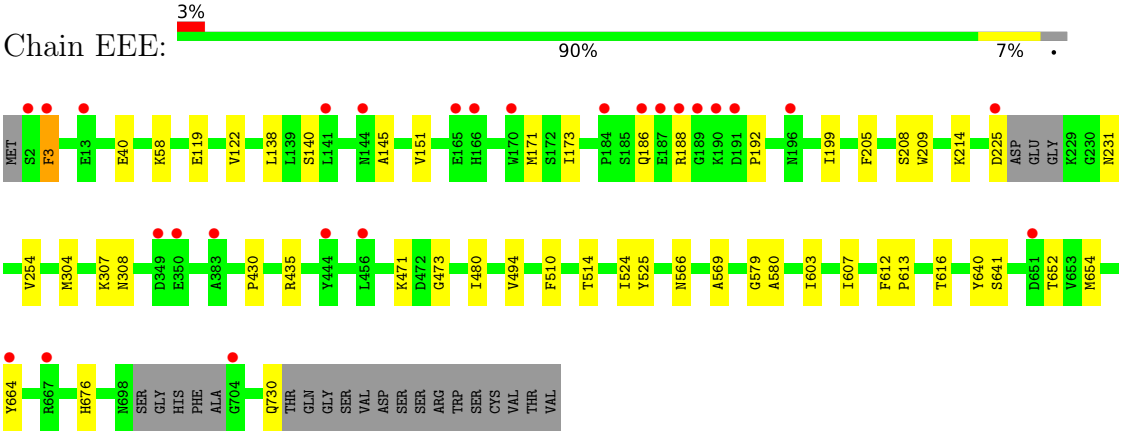


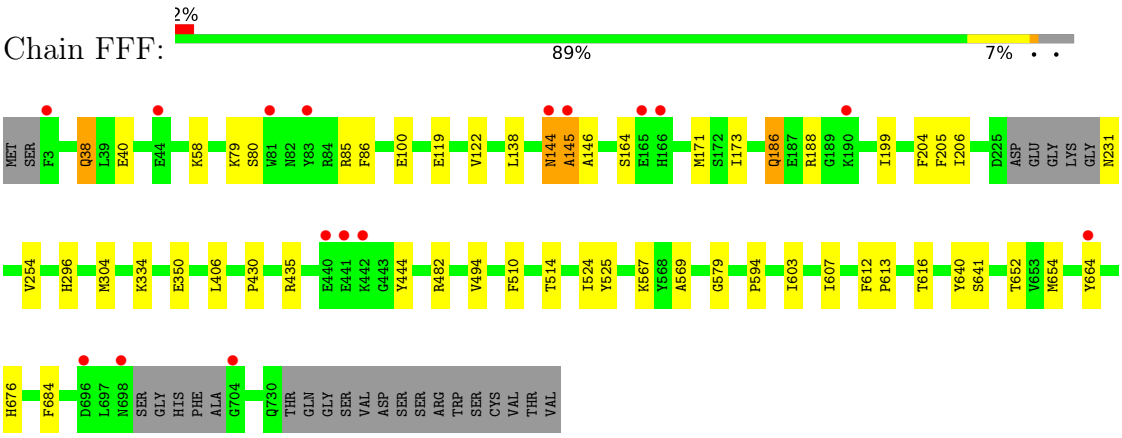
• Molecule 1: OphP S580A

Chain CCC:

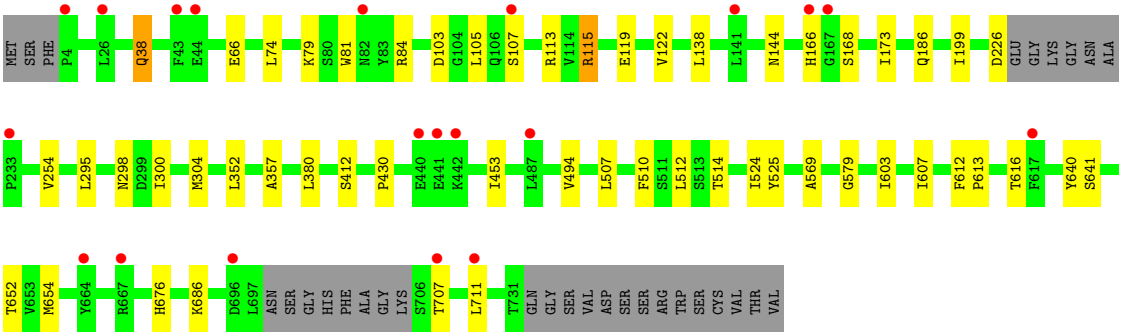



GLN GLY SER VAL ASP SER SER ARG TRP SER CYS VAL THR VAL
• Molecule 1: OphP S580A
Chain DDD:
3%
89%
7%
MET SER PHE P4 G5 W6 Q38 L39 E40 V53 K58 E71 F86 E100 E119 V122 E125 L141 H166 G167 S168 D169 W170 M171 S172 I173 Q186 E187 D197 K198 I199 F205 K214 E224 D225 ASP GLU GLY LYS G230 N231 G245
V254 M304 K307 N308 I327 F343 D344 A345 P348 N361 L380 R381 E403 L406 P430 E440 E441 K442 G443 Y444 S452 I453 E464 T474 V494 A505 F510 T514 I524 Y525 A569 G579 A580 I603 I607 F612
P613 T616 A663 Y664 H676 N683 N698 SER GLY HIS PHE ALA GLY K705 Q730 THR GLN GLY SER VAL ASP SER SER ARG TRP SER CYS VAL THR VAL


• Molecule 1: OphP S580A
Chain EEE:
3%
90%
7%
MET S2 F3 E13 E40 K58 E119 V122 L138 L139 S140 L141 N144 A145 V151 E165 H166 W170 M171 S172 I173 P184 S185 Q186 E187 R188 G189 K190 D191 P192 N196 I199 F205 S208 W209 K214 D225 ASP GLU GLY K229 G230 N231
V254 M304 K307 N308 D349 E350 A383 P430 R435 Y444 L456 K471 D472 G473 I480 V494 F510 T514 I524 Y525 N566 A569 G579 A580 I603 I607 F612 P613 T616 Y640 S641 D651 T652 V653 M654
Y664 R667 H676 N698 SER GLY HIS PHE ALA G704 Q730 THR GLN GLY SER VAL ASP SER SER ARG TRP SER CYS VAL THR VAL

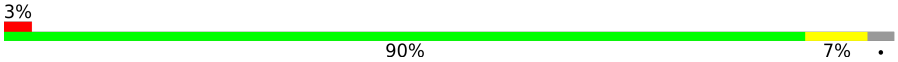

• Molecule 1: OphP S580A
Chain FFF:
2%
89%
7%
MET SER F3 Q38 L39 E40 E44 K58 K79 S80 W81 N82 Y83 R84 R85 F86 E100 E119 V122 L138 N144 A145 A146 S164 E165 H166 M171 S172 I173 Q186 E187 R188 G189 K190 I199 F204 F205 I206 D225 ASP GLU GLY LYS GLY N231
V254 H296 M304 K334 E350 L406 P430 R435 E440 E441 K442 G443 Y444 R482 V494 F510 T514 I524 Y525 K567 Y568 A569 G579 P594 I603 I607 F612 P613 T616 Y640 S641 T652 V653 M654 Y664
H676 F684 D696 L697 N698 SER GLY HIS PHE ALA G704 Q730 THR GLN GLY SER VAL ASP SER SER ARG TRP SER CYS VAL THR VAL

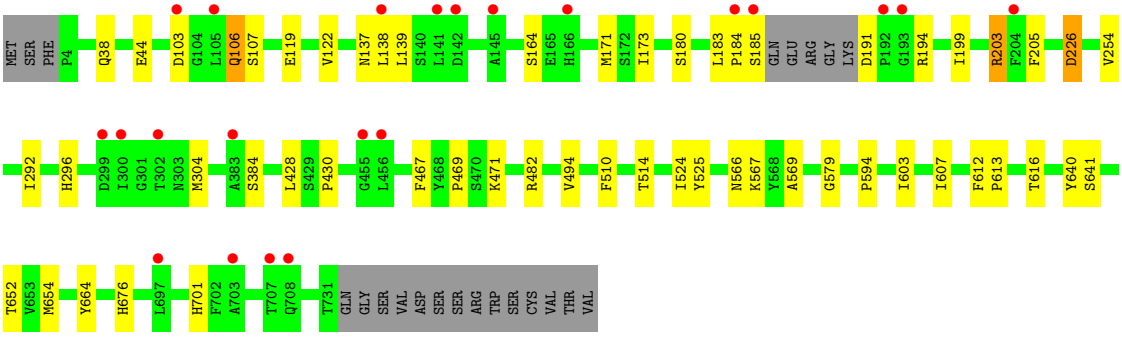
• Molecule 1: OphP S580A
Chain GGG:
3%
89%
7%



- Molecule 1: OphP S580A

Chain HHH:





4 Data and refinement statistics (i)

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 66.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.6 (66.08-1.94) 97.6 (66.00-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.96%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, B3P, TRS, GOL, EDO, NA

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	0.66	0/6005	0.78	3/8146 (0.0%)
1	BBB	0.66	1/5947 (0.0%)	0.77	1/8067 (0.0%)
1	CCC	0.64	0/5949	0.75	1/8068 (0.0%)
1	DDD	0.66	0/5927	0.78	0/8038
1	EEE	0.65	0/5963	0.76	1/8087 (0.0%)
1	FFF	0.66	0/5928	0.77	2/8041 (0.0%)
1	GGG	0.67	0/5897	0.79	3/7999 (0.0%)
1	HHH	0.66	0/5954	0.78	2/8078 (0.0%)
All	All	0.66	1/47570 (0.0%)	0.77	13/64524 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	259	GLU	CD-OE1	-5.44	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	435	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	BBB	435	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	HHH	203	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	FFF	435	ARG	NE-CZ-NH1	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	GGG	115	ARG	CB-CG-CD	-6.73	94.10	111.60
1	HHH	203	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	GGG	113	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	AAA	435	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	GGG	113	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	AAA	536	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	FFF	85	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	EEE	435	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	CCC	435	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	40	1
1	BBB	5778	0	5515	44	0
1	CCC	5780	0	5524	36	0
1	DDD	5760	0	5505	56	1
1	EEE	5795	0	5531	37	0
1	FFF	5760	0	5501	39	3
1	GGG	5730	0	5472	37	1
1	HHH	5784	0	5516	42	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	295	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 3.

All (295) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:307:LYS:HG2	1:DDD:348:PRO:CG	2.15	0.76
1:HHH:138:LEU:HD13	1:HHH:184:PRO:HG3	1.67	0.76
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:CCC:334:LYS:HB3	1:GGG:357:ALA:CB	2.19	0.72
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:BBB:710:MET:CE	9:BBB:913:HOH:O	2.40	0.68
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
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:BBB:710:MET:HE2	9:BBB:913:HOH:O	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:AAA:125:GLU:H	1:AAA:125:GLU:CD	2.08	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: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
1:EEE:480:ILE:HG23	1:EEE:524:ILE:CG2	2.36	0.55
1:AAA:380:LEU:HD21	1:AAA:505:ALA:HB2	1.88	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:BBB:710:MET:HE1	9:BBB:913:HOH:O	2.04	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:BBB:406:LEU:C	1:BBB:406:LEU:HD23	2.28	0.54
1:DDD:494:VAL:HG22	1:DDD:524:ILE:HG12	1.91	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:GGG:144:ASN:OD1	1:GGG:144:ASN:C	2.47	0.52
1:AAA:652:THR:HG21	1:AAA:654:MET:HE3	1.91	0.52
1:DDD:38:GLN:HG2	9:DDD:996:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:652:THR:HG21	1:HHH:654:MET:HE3	1.92	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:EEE:652:THR:HG21	1:EEE:654:MET:HE3	1.95	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: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: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:BBB:357:ALA:HB1	1:FFF:334:LYS:HG2	1.95	0.47
1:HHH:171:MET:HE1	1:HHH:205:PHE:HB2	1.96	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:171:MET:HE1	1:FFF:205:PHE:HB2	1.95	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:AAA:171:MET:HE1	1:AAA:205:PHE:HB2	1.96	0.47
1:FFF:514:THR:CG2	1:FFF:525:TYR:CG	2.97	0.47
1:EEE:151:VAL:HG11	6:EEE:803:EDO:O1	2.14	0.47
1:EEE:730:GLN:C	5:EEE:801:THR:HA	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:EEE:171:MET:HE1	1:EEE:205:PHE:HB2	1.98	0.46
1:AAA:40:GLU:O	1:AAA:231:ASN:ND2	2.49	0.46
1:BBB:652:THR:HG21	1:BBB:654:MET:HE3	1.97	0.46
1:DDD:430:PRO:HA	1:DDD:510:PHE:CG	2.51	0.45
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:FFF:40:GLU:O	1:FFF:231:ASN:ND2	2.49	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: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: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:EEE:607:ILE:HG21	1:EEE:676:HIS:CG	2.52	0.45
1:BBB:430:PRO:HA	1:BBB:510:PHE:CG	2.52	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:EEE:514:THR:HG21	1:EEE:525:TYR:CE2	2.52	0.44
1:FFF:594:PRO:HB3	1:FFF:654:MET:HE2	1.99	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: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: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: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:AAA:652:THR:HG21	1:AAA:654:MET:CE	2.47	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:DDD:254:VAL:HG13	1:DDD:304:MET:HE1	2.00	0.43
1:DDD:254:VAL:HG13	1:DDD:304:MET:HE2	2.00	0.43
1:HHH:191:ASP:OD2	1:HHH:194:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:485:ASP:HB3	1:DDD:453:ILE:C	2.38	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: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:DDD:361:ASN:CG	1:HHH:567:LYS:HB2	2.39	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:BBB:494:VAL:HG23	1:BBB:569:ALA:CB	2.50	0.42
1:DDD:171:MET:HE1	1:DDD:205:PHE:HB2	2.02	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: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: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
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:AAA:254:VAL:HG13	1:AAA:304:MET:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:594:PRO:HB3	1:FFF:654:MET:CE	2.51	0.41
1:FFF:640:TYR:O	1:FFF:641:SER:C	2.59	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:GGG:640:TYR:O	1:GGG:641:SER:C	2.59	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: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:HHH:640:TYR:O	1:HHH:641:SER:C	2.59	0.41
1:BBB:171:MET:CE	1:BBB:205:PHE:HD1	2.33	0.41
1:HHH:594:PRO:HB3	1:HHH:654:MET:HE2	2.03	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: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:HHH:139:LEU:HD23	1:HHH:139:LEU:HA	1.97	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:CCC:640:TYR:O	1:CCC:641:SER:C	2.59	0.40
1:EEE:640:TYR:O	1:EEE:641:SER:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	24
1	BBB	714/745 (96%)	695 (97%)	18 (2%)	1 (0%)	51	43
1	CCC	715/745 (96%)	695 (97%)	19 (3%)	1 (0%)	51	43
1	DDD	712/745 (96%)	691 (97%)	19 (3%)	2 (0%)	41	32
1	EEE	717/745 (96%)	696 (97%)	20 (3%)	1 (0%)	51	43
1	FFF	712/745 (96%)	692 (97%)	17 (2%)	3 (0%)	34	24
1	GGG	708/745 (95%)	691 (98%)	15 (2%)	2 (0%)	41	32
1	HHH	719/745 (96%)	701 (98%)	17 (2%)	1 (0%)	51	43
All	All	5720/5960 (96%)	5563 (97%)	143 (2%)	14 (0%)	47	39

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

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Mol	Chain	Res	Type
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 (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%)	62	52
1	BBB	624/644 (97%)	619 (99%)	5 (1%)	81	78
1	CCC	623/644 (97%)	619 (99%)	4 (1%)	86	85
1	DDD	622/644 (97%)	617 (99%)	5 (1%)	81	78
1	EEE	626/644 (97%)	618 (99%)	8 (1%)	69	62
1	FFF	622/644 (97%)	616 (99%)	6 (1%)	76	71
1	GGG	620/644 (96%)	612 (99%)	8 (1%)	69	62
1	HHH	624/644 (97%)	617 (99%)	7 (1%)	73	67
All	All	4990/5152 (97%)	4937 (99%)	53 (1%)	76	67

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 monosaccharides 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	DDD	801	-	5,5,5	0.16	0	5,5,5	0.43	0
3	GOL	HHH	801	-	5,5,5	0.16	0	5,5,5	0.53	0
3	GOL	CCC	801	-	5,5,5	0.15	0	5,5,5	0.34	0
3	GOL	EEE	802	-	5,5,5	0.16	0	5,5,5	0.49	0
5	THR	EEE	801	-	5,6,7	0.50	0	6,7,9	1.07	0
7	TRS	FFF	802	-	7,7,7	0.19	0	9,9,9	0.22	0
7	TRS	GGG	802	-	7,7,7	0.18	0	9,9,9	0.22	0
6	EDO	GGG	801	-	3,3,3	0.20	0	2,2,2	0.16	0
5	THR	FFF	801	-	5,6,7	0.59	0	6,7,9	0.57	0
3	GOL	BBB	801	-	5,5,5	0.10	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	B3P	HHH	802	-	18,18,18	0.24	0	21,23,23	0.68	0
6	EDO	EEE	803	-	3,3,3	0.18	0	2,2,2	0.24	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	DDD	801	-	-	0/4/4/4	-
3	GOL	HHH	801	-	-	2/4/4/4	-
3	GOL	CCC	801	-	-	0/4/4/4	-
3	GOL	EEE	802	-	-	2/4/4/4	-
5	THR	EEE	801	-	-	0/5/6/8	-
7	TRS	FFF	802	-	-	7/9/9/9	-
7	TRS	GGG	802	-	-	9/9/9/9	-
6	EDO	GGG	801	-	-	1/1/1/1	-
5	THR	FFF	801	-	-	0/5/6/8	-
3	GOL	BBB	801	-	-	2/4/4/4	-
8	B3P	HHH	802	-	-	9/28/28/28	-
6	EDO	EEE	803	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) 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
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

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

There are no ring outliers.

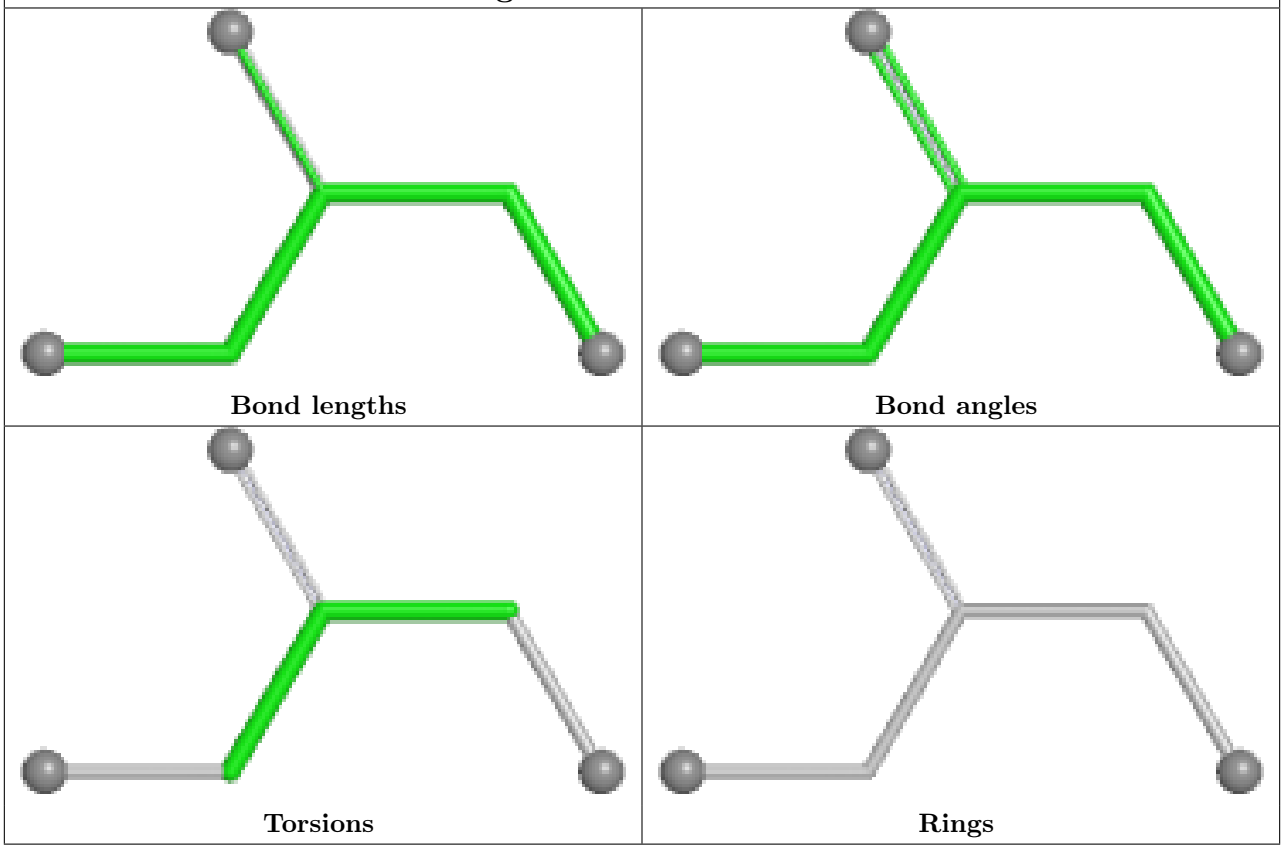
5 monomers are involved in 7 short contacts:

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

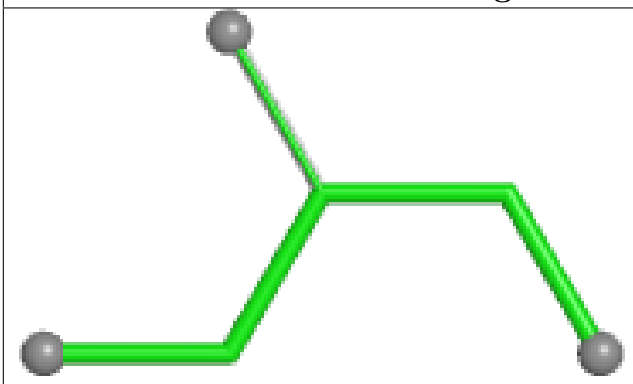
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

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.

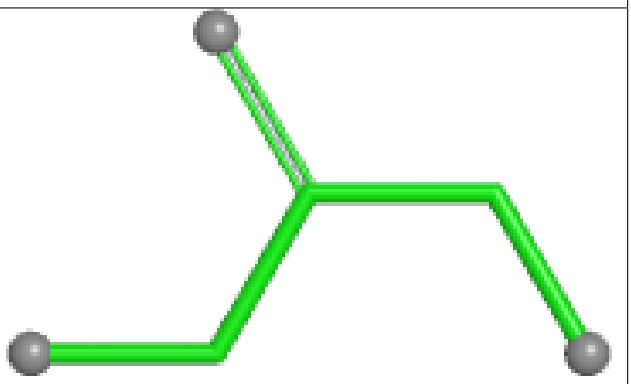
Ligand GOL DDD 801



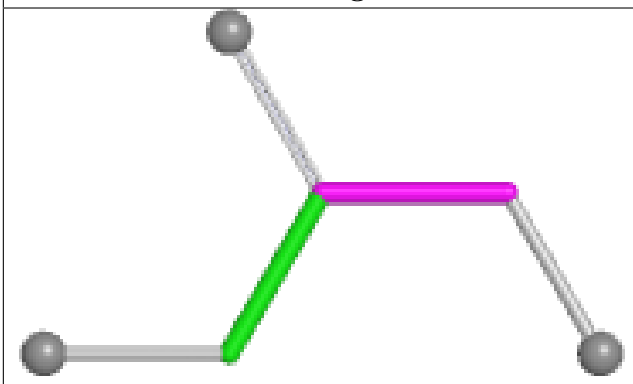
Ligand GOL HHH 801



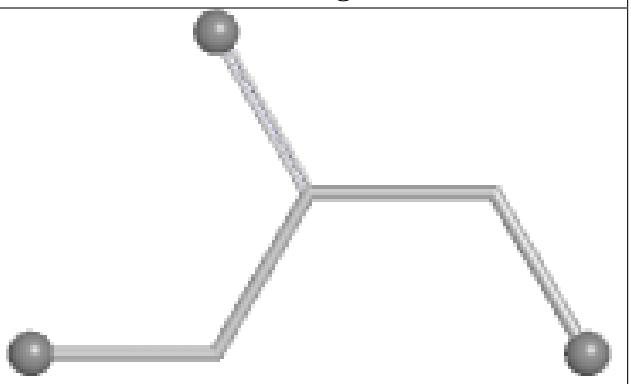
Bond lengths



Bond angles

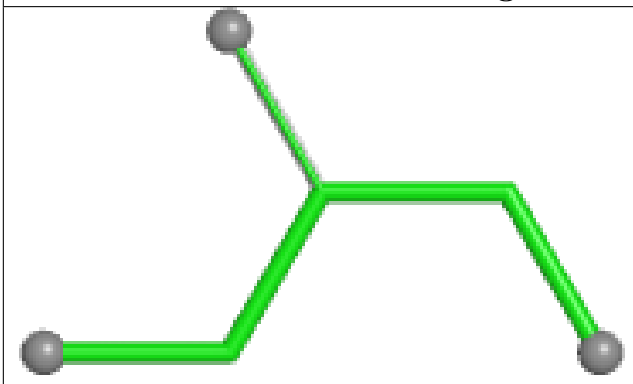


Torsions



Rings

Ligand GOL CCC 801



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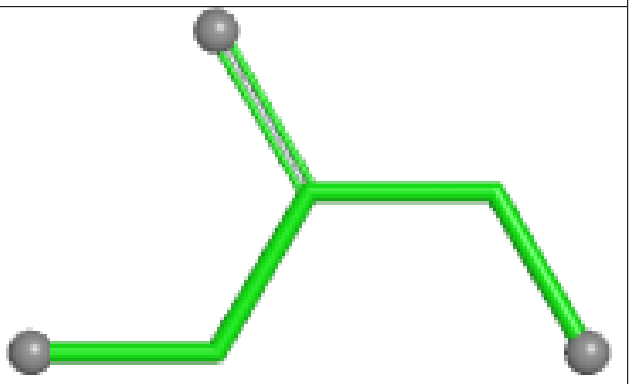
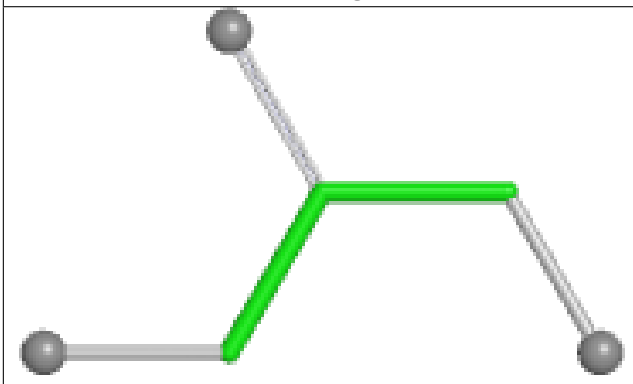


Bond angles



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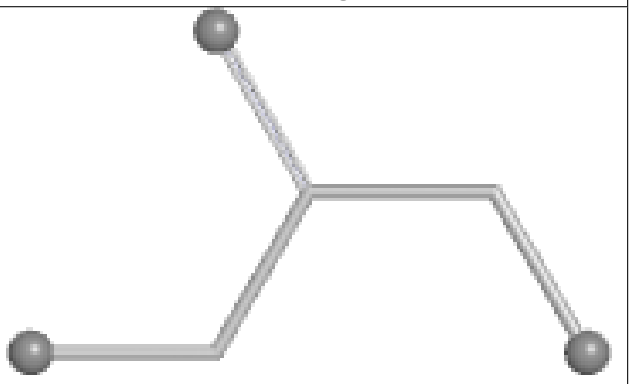
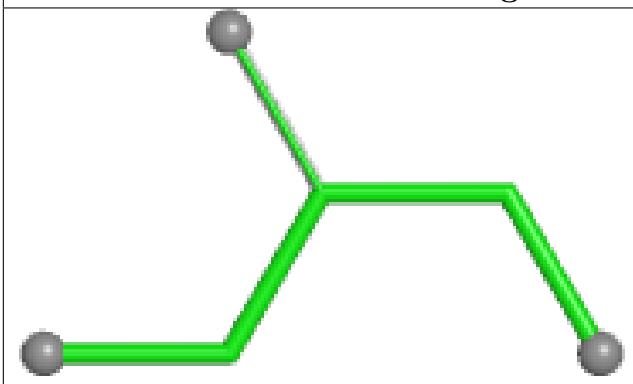
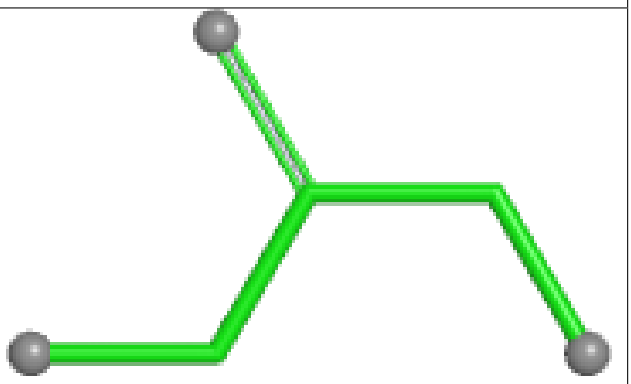


Rings

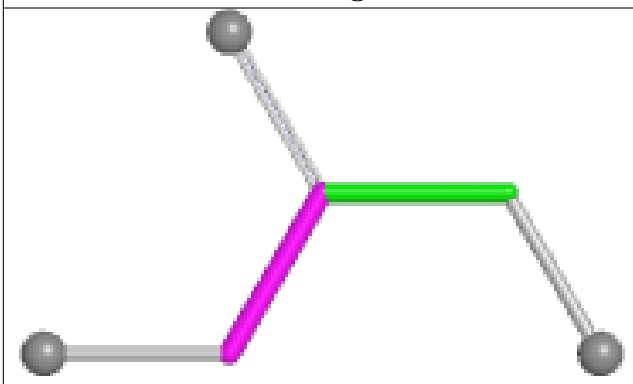
Ligand GOL EEE 802



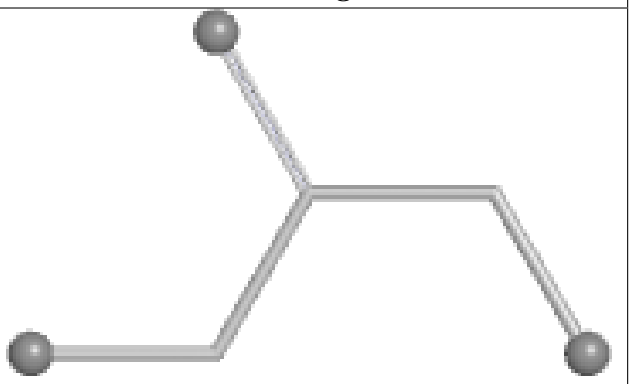
Bond lengths



Bond angles

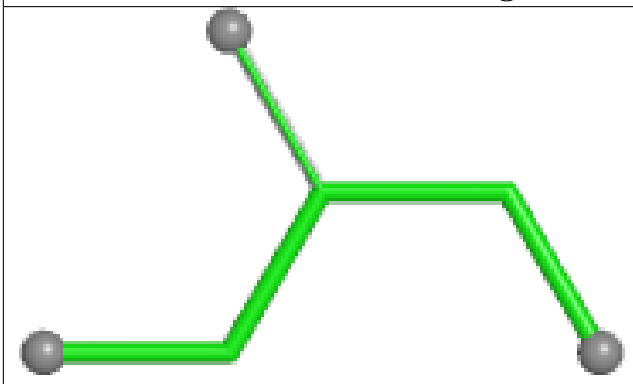


Torsions

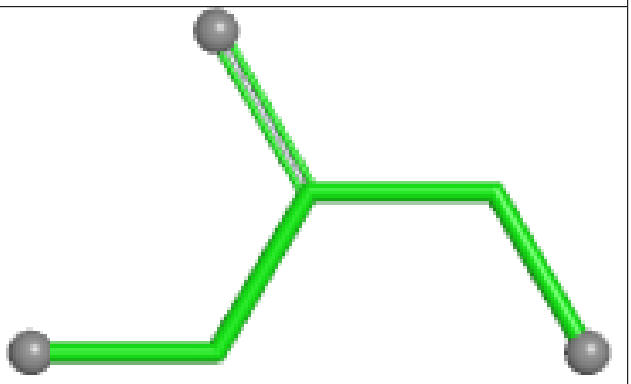


Rings

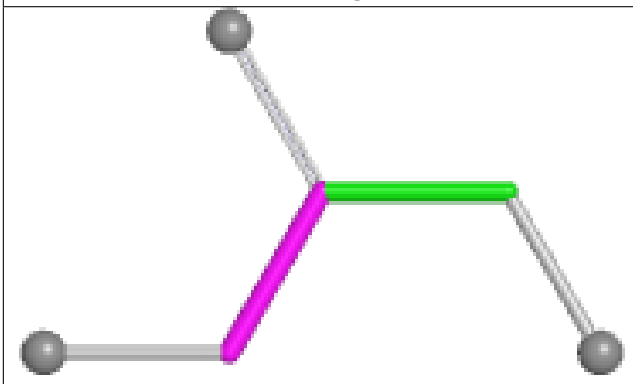
Ligand GOL BBB 801



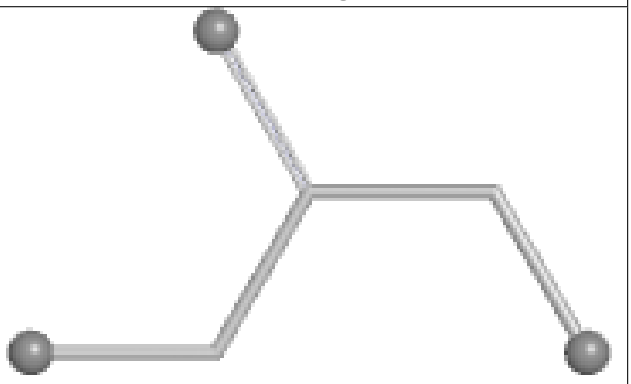
Bond lengths



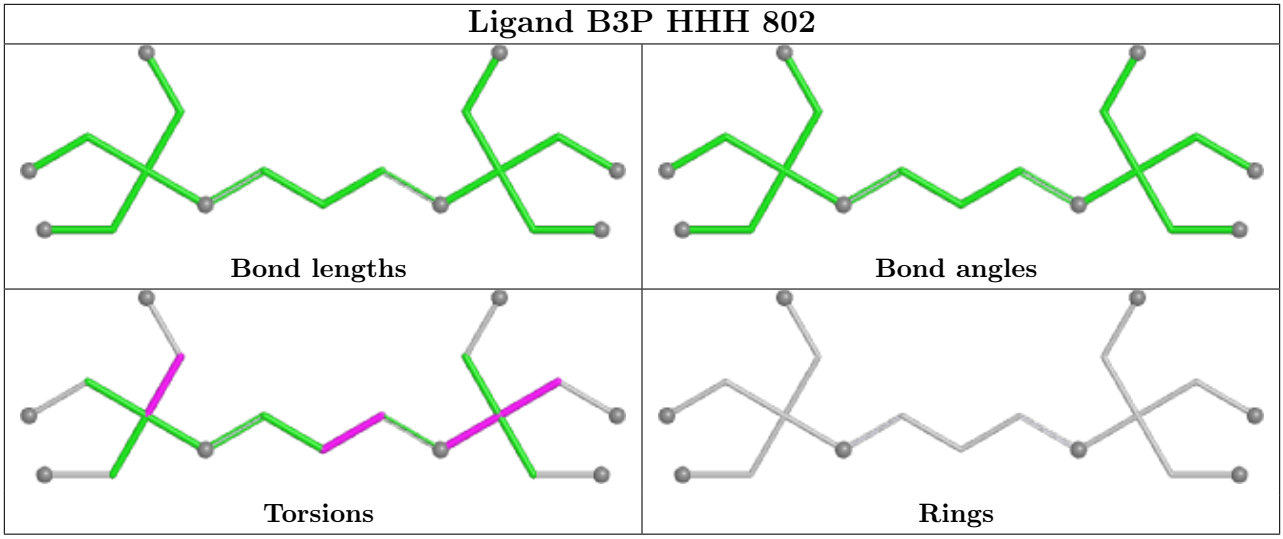
Bond angles



Torsions



Rings



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%)	-0.03	16 (2%)	62	69	24, 35, 66, 130	0
1	BBB	718/745 (96%)	-0.02	11 (1%)	73	79	29, 40, 69, 133	0
1	CCC	720/745 (96%)	0.01	13 (1%)	68	74	25, 40, 75, 121	0
1	DDD	717/745 (96%)	0.07	20 (2%)	53	60	24, 39, 74, 144	0
1	EEE	721/745 (96%)	0.22	26 (3%)	42	50	30, 49, 83, 138	0
1	FFF	718/745 (96%)	0.05	16 (2%)	62	69	29, 43, 74, 129	0
1	GGG	714/745 (95%)	0.09	20 (2%)	53	60	30, 42, 78, 123	0
1	HHH	723/745 (97%)	0.08	22 (3%)	50	57	27, 44, 76, 128	0
All	All	5755/5960 (96%)	0.06	144 (2%)	57	64	24, 41, 76, 144	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	3	PHE	10.5
1	AAA	3	PHE	9.3
1	AAA	702	PHE	9.2
1	FFF	166	HIS	8.5
1	BBB	2	SER	7.9
1	BBB	166	HIS	7.8
1	CCC	3	PHE	7.1
1	DDD	441	GLU	6.5
1	EEE	187	GLU	6.5
1	CCC	664	TYR	6.1
1	EEE	3	PHE	5.9
1	CCC	166	HIS	5.8
1	HHH	166	HIS	5.7
1	GGG	664	TYR	5.6
1	DDD	664	TYR	5.5
1	HHH	184	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	FFF	664	TYR	5.2
1	AAA	166	HIS	5.2
1	EEE	444	TYR	5.0
1	FFF	440	GLU	5.0
1	DDD	440	GLU	4.9
1	EEE	186	GLN	4.7
1	AAA	144	ASN	4.6
1	AAA	700	GLY	4.6
1	DDD	343	PHE	4.6
1	GGG	166	HIS	4.4
1	EEE	651	ASP	4.4
1	DDD	187	GLU	4.3
1	GGG	487	LEU	4.2
1	HHH	142	ASP	4.2
1	FFF	442	LYS	4.2
1	EEE	383	ALA	4.1
1	HHH	302	THR	4.0
1	DDD	168	SER	4.0
1	DDD	444	TYR	3.9
1	GGG	82	ASN	3.9
1	DDD	186	GLN	3.9
1	FFF	704	GLY	3.9
1	GGG	141	LEU	3.8
1	EEE	166	HIS	3.8
1	HHH	383	ALA	3.7
1	GGG	43	PHE	3.7
1	GGG	711	LEU	3.7
1	HHH	192	PRO	3.6
1	FFF	165	GLU	3.6
1	DDD	663	ALA	3.4
1	EEE	188	ARG	3.4
1	EEE	456	LEU	3.4
1	EEE	704	GLY	3.3
1	CCC	169	ASP	3.3
1	HHH	703	ALA	3.3
1	BBB	167	GLY	3.3
1	HHH	185	SER	3.3
1	EEE	141	LEU	3.2
1	HHH	105	LEU	3.2
1	GGG	617	PHE	3.2
1	AAA	143	GLY	3.2
1	DDD	5	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	HHH	193	GLY	3.2
1	AAA	664	TYR	3.2
1	GGG	4	PRO	3.2
1	GGG	667	ARG	3.2
1	EEE	196	ASN	3.2
1	GGG	440	GLU	3.1
1	BBB	169	ASP	3.1
1	GGG	167	GLY	3.1
1	EEE	184	PRO	3.1
1	GGG	107	SER	3.1
1	HHH	707	THR	3.0
1	AAA	699	SER	3.0
1	FFF	441	GLU	3.0
1	EEE	225	ASP	3.0
1	FFF	145	ALA	3.0
1	DDD	166	HIS	3.0
1	BBB	142	ASP	3.0
1	AAA	2	SER	3.0
1	GGG	44	GLU	2.9
1	EEE	190	LYS	2.9
1	GGG	707	THR	2.9
1	EEE	350	GLU	2.9
1	AAA	165	GLU	2.8
1	CCC	230	GLY	2.8
1	AAA	225	ASP	2.8
1	GGG	442	LYS	2.8
1	AAA	703	ALA	2.7
1	HHH	455	GLY	2.7
1	GGG	441	GLU	2.7
1	EEE	189	GLY	2.7
1	DDD	169	ASP	2.6
1	GGG	696	ASP	2.6
1	EEE	170	TRP	2.6
1	DDD	245	GLY	2.5
1	BBB	487	LEU	2.5
1	AAA	701	HIS	2.5
1	GGG	233	PRO	2.5
1	EEE	349	ASP	2.5
1	FFF	3	PHE	2.5
1	EEE	2	SER	2.5
1	DDD	53	VAL	2.4
1	EEE	165	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	697	LEU	2.4
1	BBB	698	ASN	2.4
1	FFF	698	ASN	2.4
1	BBB	302	THR	2.4
1	EEE	191	ASP	2.4
1	DDD	167	GLY	2.4
1	FFF	696	ASP	2.3
1	AAA	303	ASN	2.3
1	CCC	704	GLY	2.3
1	FFF	190	LYS	2.3
1	CCC	228	GLY	2.3
1	DDD	442	LYS	2.3
1	DDD	141	LEU	2.3
1	CCC	303	ASN	2.3
1	FFF	81	TRP	2.3
1	HHH	300	ILE	2.3
1	EEE	144	ASN	2.3
1	HHH	456	LEU	2.3
1	AAA	444[A]	TYR	2.2
1	HHH	103	ASP	2.3
1	HHH	299	ASP	2.3
1	CCC	229	LYS	2.2
1	EEE	667	ARG	2.2
1	GGG	26	LEU	2.2
1	DDD	6	TRP	2.2
1	BBB	667	ARG	2.2
1	CCC	296	HIS	2.2
1	CCC	167	GLY	2.2
1	EEE	664	TYR	2.1
1	HHH	141	LEU	2.1
1	HHH	697	LEU	2.1
1	EEE	13	GLU	2.1
1	FFF	83	TYR	2.1
1	DDD	4	PRO	2.1
1	DDD	125	GLU	2.1
1	CCC	214	LYS	2.1
1	CCC	696	ASP	2.1
1	HHH	708	GLN	2.1
1	FFF	44	GLU	2.1
1	AAA	168	SER	2.1
1	HHH	138	LEU	2.1
1	HHH	204	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	HHH	145	ALA	2.0
1	FFF	144	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	THR	FFF	801	7/8	0.59	0.28	75,102,115,129	0
2	NA	DDD	803	1/1	0.64	0.18	64,64,64,64	0
2	NA	EEE	804	1/1	0.67	0.35	62,62,62,62	0
5	THR	EEE	801	7/8	0.68	0.23	83,108,120,125	0
3	GOL	EEE	802	6/6	0.76	0.16	41,61,73,77	0
3	GOL	CCC	801	6/6	0.82	0.18	40,58,64,70	0
8	B3P	HHH	802	19/19	0.83	0.20	49,69,83,86	0
7	TRS	GGG	802	8/8	0.84	0.17	45,63,74,80	0
3	GOL	HHH	801	6/6	0.84	0.26	41,61,72,79	0
2	NA	AAA	801	1/1	0.85	0.28	55,55,55,55	0
3	GOL	DDD	801	6/6	0.85	0.15	36,49,56,64	0
2	NA	GGG	805	1/1	0.87	0.19	46,46,46,46	0
7	TRS	FFF	802	8/8	0.89	0.14	50,65,72,75	0
3	GOL	BBB	801	6/6	0.89	0.16	46,57,66,71	0
6	EDO	EEE	803	4/4	0.89	0.30	42,50,52,64	0
2	NA	BBB	803	1/1	0.90	0.26	46,46,46,46	0
2	NA	GGG	804	1/1	0.90	0.13	46,46,46,46	0
2	NA	EEE	806	1/1	0.91	0.26	49,49,49,49	0
2	NA	GGG	803	1/1	0.91	0.12	48,48,48,48	0
2	NA	DDD	802	1/1	0.91	0.42	54,54,54,54	0
6	EDO	GGG	801	4/4	0.92	0.10	47,50,51,57	0

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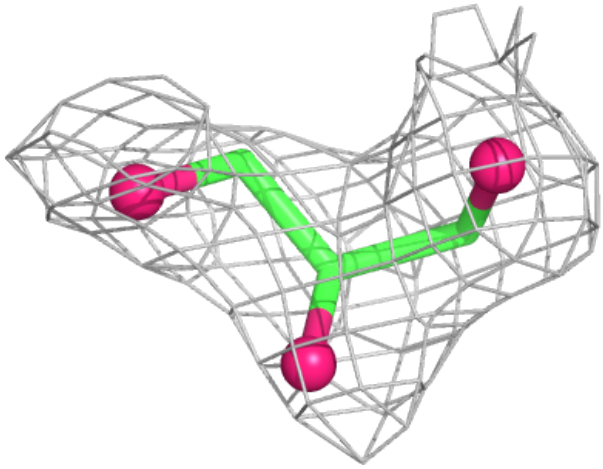
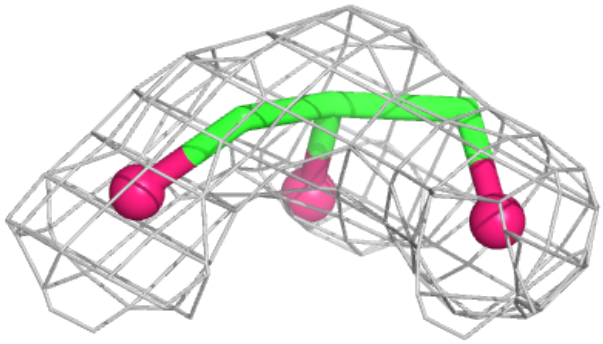
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	CCC	803	1/1	0.93	0.11	42,42,42,42	0
2	NA	BBB	802	1/1	0.94	0.26	47,47,47,47	0
4	MG	CCC	802	1/1	0.94	0.08	43,43,43,43	0
2	NA	FFF	804	1/1	0.95	0.16	44,44,44,44	0
2	NA	EEE	805	1/1	0.95	0.13	61,61,61,61	0
4	MG	FFF	803	1/1	0.97	0.17	43,43,43,43	0
2	NA	FFF	805	1/1	0.98	0.24	53,53,53,53	0

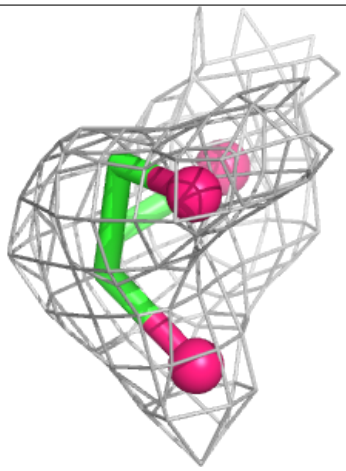
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOL 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)

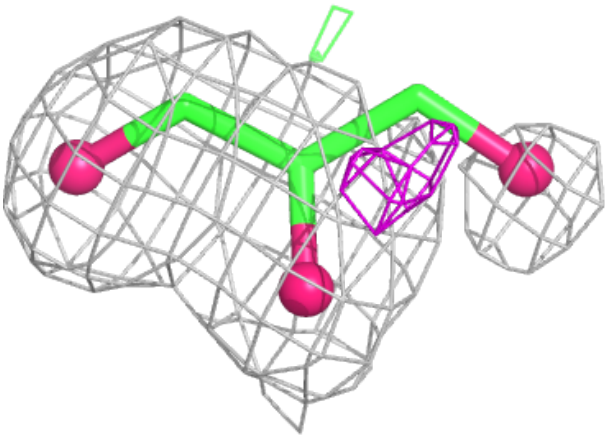


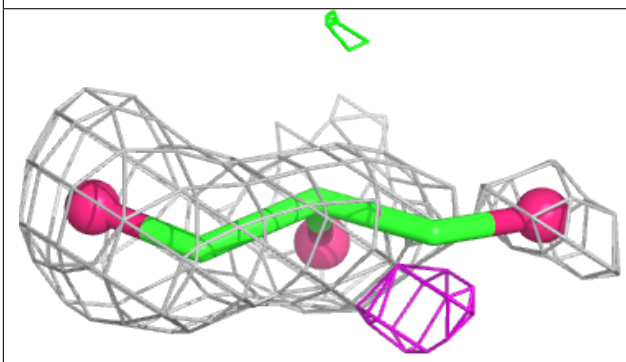


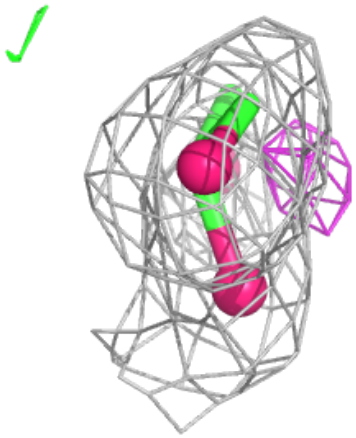


Electron density around GOL CCC 801:

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

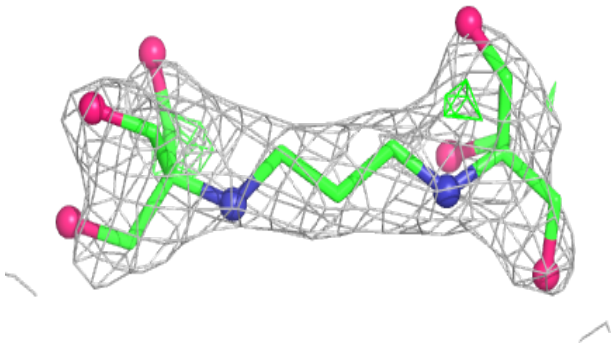


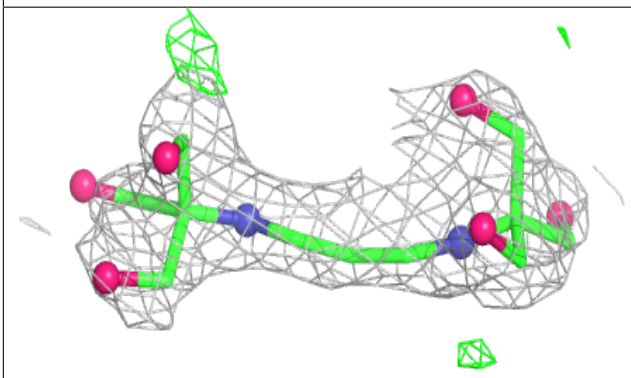


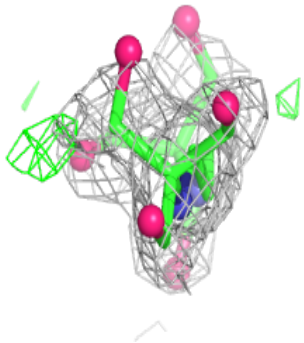


Electron density around B3P HHH 802:

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

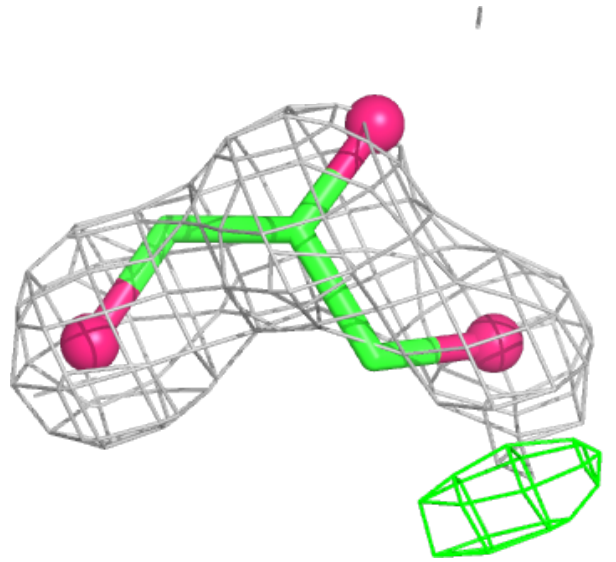


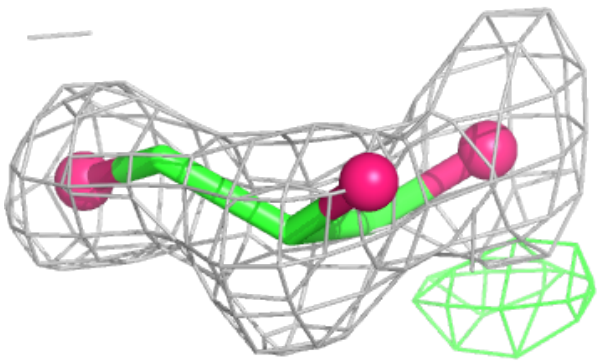


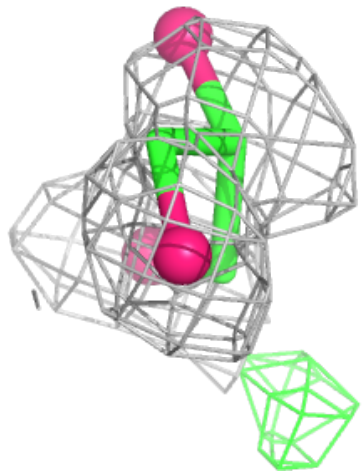


Electron density around GOL HHH 801:

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

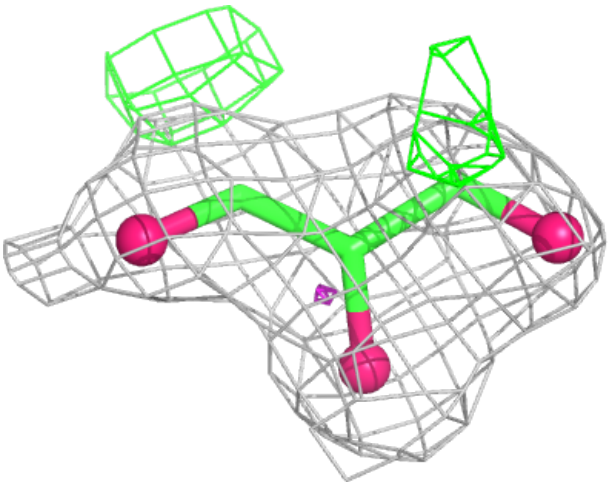


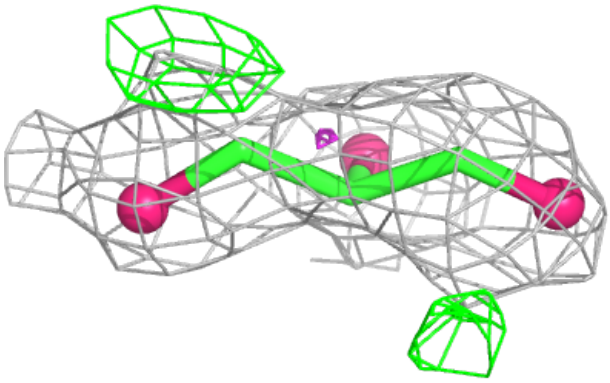


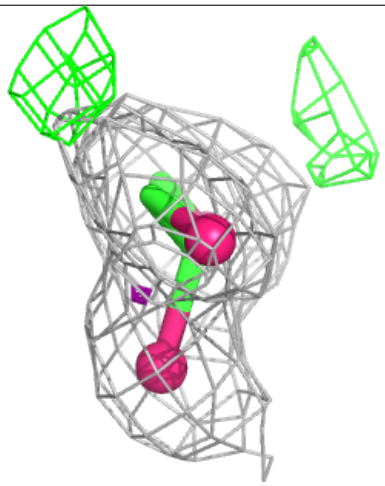


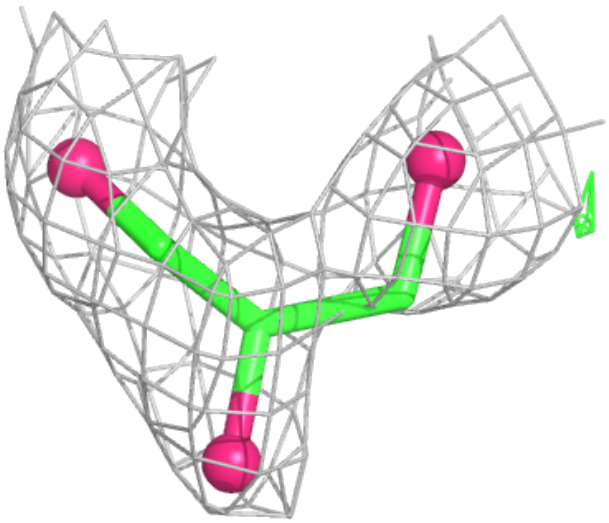
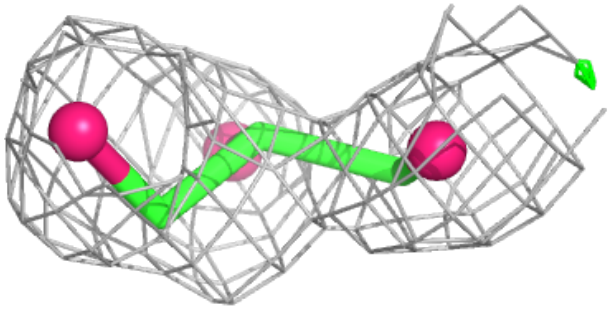
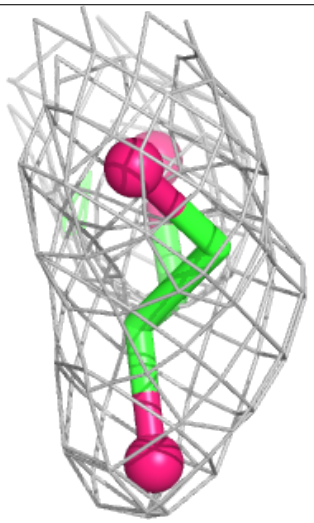
Electron density around GOL DDD 801:

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







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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.