



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 4BWI / pdb_00004bwi
Title : Structure of the phytochrome Cph2 from Synechocystis sp. PCC6803
Authors : Anders, K.; Angerer, V.; Widany, G.D.; Mroginiski, M.A.; von Stetten, D.;
Essen, L.-O.
Deposited on : 2013-07-03
Resolution : 2.60 Å(reported)

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

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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

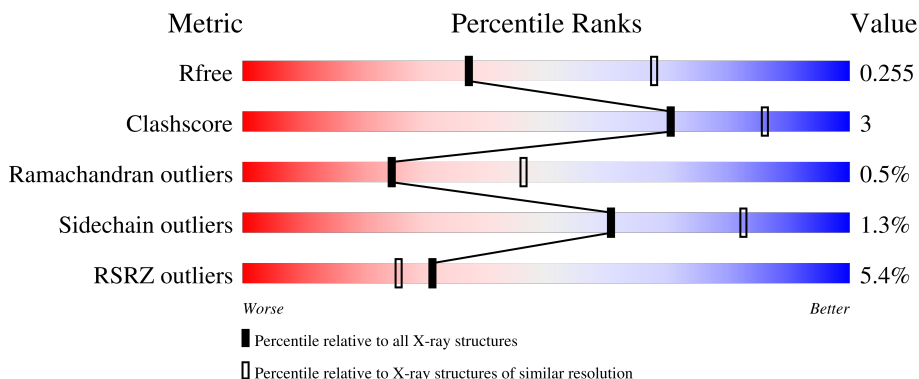
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6311 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.

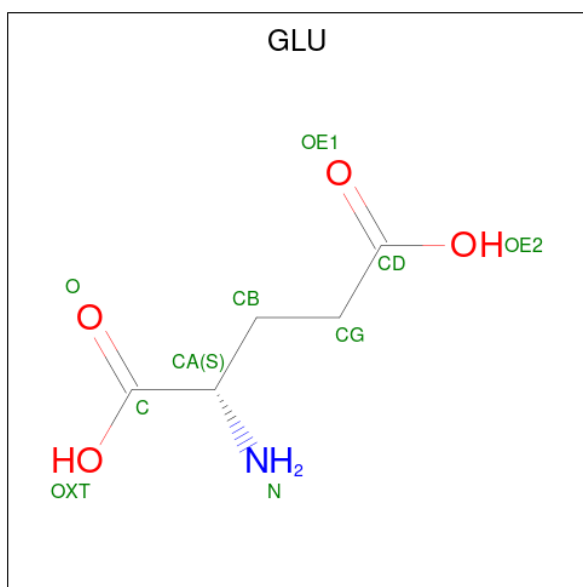
- Molecule 1 is a protein called PHYTOCHROME-LIKE PROTEIN CPH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	1	0
			3009	1910	540	550	9			
1	B	377	Total	C	N	O	S	0	0	0
			2992	1898	542	544	8			

There are 18 discrepancies between the modelled and reference sequences:

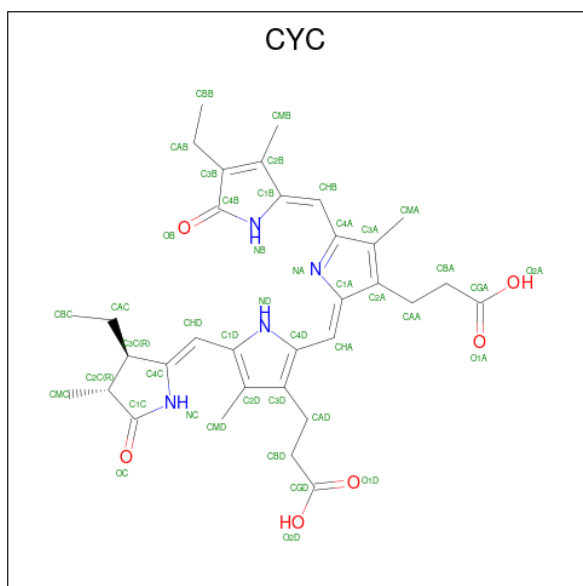
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q55434
A	425	ALA	-	expression tag	UNP Q55434
A	426	SER	-	expression tag	UNP Q55434
A	427	HIS	-	expression tag	UNP Q55434
A	428	HIS	-	expression tag	UNP Q55434
A	429	HIS	-	expression tag	UNP Q55434
A	430	HIS	-	expression tag	UNP Q55434
A	431	HIS	-	expression tag	UNP Q55434
A	432	HIS	-	expression tag	UNP Q55434
B	1	SER	-	expression tag	UNP Q55434
B	425	ALA	-	expression tag	UNP Q55434
B	426	SER	-	expression tag	UNP Q55434
B	427	HIS	-	expression tag	UNP Q55434
B	428	HIS	-	expression tag	UNP Q55434
B	429	HIS	-	expression tag	UNP Q55434
B	430	HIS	-	expression tag	UNP Q55434
B	431	HIS	-	expression tag	UNP Q55434
B	432	HIS	-	expression tag	UNP Q55434

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



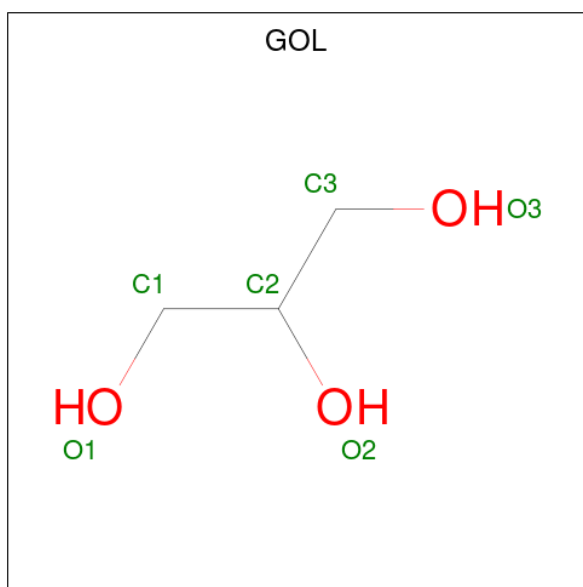
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



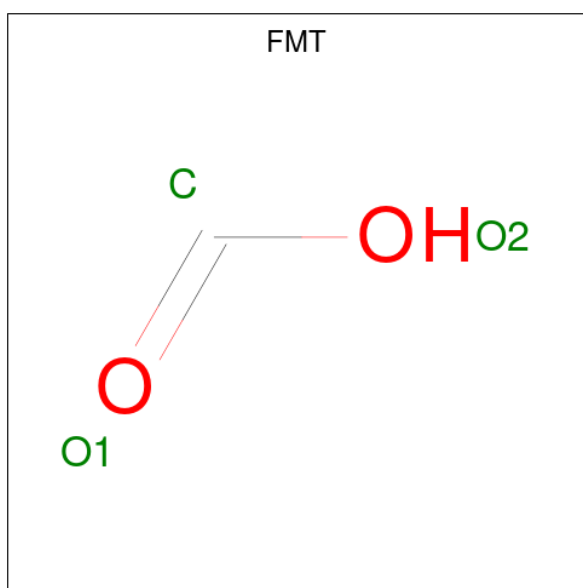
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0

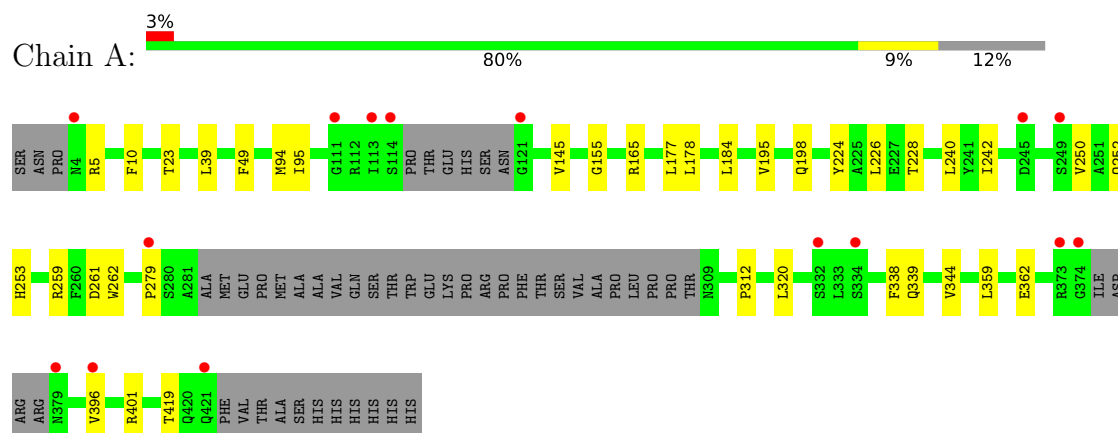
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	89	Total O 89 89	0	0
6	B	92	Total O 92 92	0	0

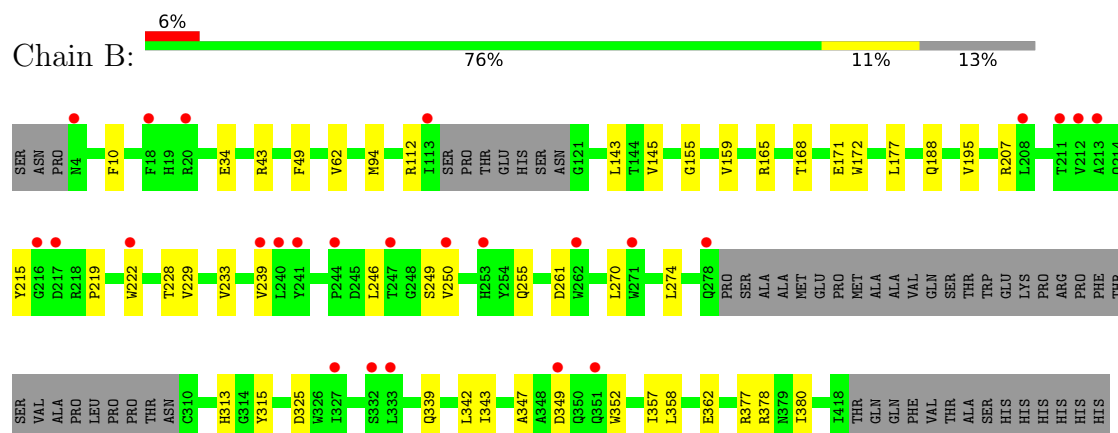
3 Residue-property plots

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

• Molecule 1: PHYTOCHROME-LIKE PROTEIN CPH2



• Molecule 1: PHYTOCHROME-LIKE PROTEIN CPH2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.43Å 88.46Å 84.87Å 90.00° 109.85° 90.00°	Depositor
Resolution (Å)	29.63 – 2.60 29.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.63-2.60) 98.4 (29.63-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.200 , 0.253 0.205 , 0.255	Depositor DCC
R_{free} test set	1624 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/3078	0.69	0/4181
1	B	0.27	0/3057	0.70	1/4151 (0.0%)
All	All	0.28	0/6135	0.69	1/8332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	LEU	CB-CA-C	-5.36	110.41	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3009	0	2929	21	0
1	B	2992	0	2941	27	0
2	A	10	0	5	0	0
3	A	43	0	37	1	0
3	B	43	0	37	0	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
5	A	9	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	12	0	4	0	0
6	A	89	0	0	1	0
6	B	92	0	0	1	0
All	All	6311	0	5972	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ARG:NH1	1:B:34:GLU:OE1	2.34	0.60
1:B:219:PRO:HA	1:B:222:TRP:HD1	1.67	0.60
1:A:259:ARG:HH22	1:A:338:PHE:HE2	1.50	0.59
1:A:177:LEU:HD11	1:B:195:VAL:HG22	1.86	0.57
1:A:94:MET:HE3	1:A:145:VAL:HG22	1.86	0.57
1:B:339:GLN:HG3	1:B:362:GLU:HB2	1.87	0.56
1:B:347:ALA:HB2	1:B:352:TRP:HD1	1.74	0.52
1:B:94:MET:HE3	1:B:145:VAL:HG22	1.92	0.52
1:B:255:GLN:HE22	1:B:261:ASP:HA	1.75	0.51
1:A:401:ARG:NH1	6:A:2086:HOH:O	2.43	0.51
1:B:239:VAL:HB	1:B:357:ILE:HB	1.93	0.50
1:A:253:HIS:NE2	1:A:261:ASP:OD1	2.45	0.50
1:A:95:ILE:HD12	3:A:1422:CYC:HBA1	1.92	0.50
1:B:49:PHE:CD2	1:B:155:GLY:HA2	2.47	0.49
1:A:339:GLN:HG3	1:A:362:GLU:HB2	1.93	0.49
1:A:39:LEU:O	1:A:165:ARG:NH2	2.47	0.48
1:A:224:TYR:O	1:A:228:THR:OG1	2.28	0.47
1:B:219:PRO:HA	1:B:222:TRP:CD1	2.48	0.46
1:B:377:ARG:HH21	1:B:380:ILE:HG21	1.80	0.46
1:A:312:PRO:HB3	1:A:344:VAL:HG22	1.97	0.46
1:A:178:LEU:HD11	1:B:10:PHE:HZ	1.82	0.44
1:A:10:PHE:HE1	1:B:34:GLU:HB3	1.82	0.44
1:A:242:ILE:HB	1:A:252:GLN:HB2	1.99	0.44
1:B:168:THR:O	1:B:172:TRP:HD1	2.00	0.44
1:B:274:LEU:HB3	1:B:343:ILE:HD13	2.00	0.44
1:A:195:VAL:HG22	1:B:177:LEU:HD11	2.00	0.43
1:B:43:ARG:HG3	1:B:62:VAL:HB	2.00	0.43
1:A:184:LEU:HD11	1:B:188:GLN:HG3	2.01	0.42
1:A:49:PHE:CD2	1:A:155:GLY:HA2	2.55	0.42
1:B:342:LEU:HB3	1:B:358:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HD21	1:B:188:GLN:HG2	2.02	0.42
1:B:313:HIS:HD2	1:B:315:TYR:CZ	2.37	0.42
1:B:229:VAL:O	1:B:233:VAL:HG23	2.20	0.42
1:B:143:LEU:HB3	1:B:159:VAL:HB	2.01	0.42
1:A:224:TYR:CE2	4:A:1423:GOL:H11	2.54	0.41
1:A:262:TRP:CH2	1:A:359:LEU:HD21	2.55	0.41
1:B:165:ARG:NH1	1:B:171:GLU:OE1	2.51	0.41
1:B:270:LEU:HA	1:B:325:ASP:OD2	2.21	0.41
1:B:207:ARG:HG2	1:B:228:THR:HG21	2.03	0.41
1:A:226:LEU:HD13	1:A:240:LEU:HB2	2.03	0.40
1:B:378:ARG:NH2	6:B:2084:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/432 (87%)	353 (94%)	19 (5%)	2 (0%)	24	46
1	B	371/432 (86%)	357 (96%)	12 (3%)	2 (0%)	24	46
All	All	745/864 (86%)	710 (95%)	31 (4%)	4 (0%)	24	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	PRO
1	B	349	ASP
1	A	250	VAL
1	B	249	SER

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	A	310/375 (83%)	305 (98%)	5 (2%)	55	79
1	B	311/375 (83%)	308 (99%)	3 (1%)	68	86
All	All	621/750 (83%)	613 (99%)	8 (1%)	61	82

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	198	GLN
1	A	320	LEU
1	A	396	VAL
1	A	419	THR
1	B	112	ARG
1	B	215	TYR
1	B	250	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	313	HIS
1	B	74	HIS
1	B	132	GLN
1	B	190	GLN
1	B	255	GLN
1	B	313	HIS
1	B	337	ASN

5.3.3 RNA ⓘ

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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	1420	-	5,5,5	0.37	0	5,5,5	0.28	0
5	FMT	B	1421	-	2,2,2	0.74	0	1,1,1	0.23	0
2	GLU	A	1427	-	8,9,9	1.10	1 (12%)	8,11,11	1.21	1 (12%)
5	FMT	A	1426	-	2,2,2	0.75	0	1,1,1	0.24	0
3	CYC	B	1419	1	46,46,46	3.15	21 (45%)	63,67,67	3.20	18 (28%)
5	FMT	B	1424	-	2,2,2	0.75	0	1,1,1	0.24	0
5	FMT	B	1422	-	2,2,2	0.74	0	1,1,1	0.23	0
4	GOL	A	1423	-	5,5,5	0.36	0	5,5,5	0.29	0
5	FMT	A	1425	-	2,2,2	0.74	0	1,1,1	0.22	0
5	FMT	A	1424	-	2,2,2	0.74	0	1,1,1	0.22	0
5	FMT	B	1423	-	2,2,2	0.72	0	1,1,1	0.23	0
3	CYC	A	1422	1	46,46,46	3.14	21 (45%)	63,67,67	3.18	20 (31%)

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
4	GOL	B	1420	-	-	2/4/4/4	-
2	GLU	A	1427	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	B	1419	1	-	14/26/74/74	0/4/4/4
4	GOL	A	1423	-	-	2/4/4/4	-
3	CYC	A	1422	1	-	12/26/74/74	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1419	CYC	C3B-C2B	9.73	1.57	1.36
3	A	1422	CYC	C3B-C2B	9.60	1.57	1.36
3	A	1422	CYC	CHD-C1D	7.37	1.57	1.40
3	B	1419	CYC	CHD-C1D	7.33	1.57	1.40
3	A	1422	CYC	CHA-C4D	6.93	1.56	1.40
3	B	1419	CYC	CHA-C4D	6.91	1.56	1.40
3	A	1422	CYC	C4A-NA	5.25	1.48	1.36
3	B	1419	CYC	C4A-NA	5.16	1.48	1.36
3	B	1419	CYC	C4A-C3A	5.15	1.56	1.45
3	A	1422	CYC	C2A-C3A	5.12	1.47	1.36
3	A	1422	CYC	C4A-C3A	5.08	1.56	1.45
3	B	1419	CYC	C2A-C3A	4.95	1.47	1.36
3	B	1419	CYC	CHB-C4A	4.78	1.51	1.40
3	A	1422	CYC	CHB-C4A	4.75	1.51	1.40
3	B	1419	CYC	CAC-C3C	-4.34	1.45	1.54
3	A	1422	CYC	CAC-C3C	-4.28	1.45	1.54
3	B	1419	CYC	CHA-C1A	3.95	1.46	1.38
3	A	1422	CYC	C1C-NC	3.83	1.42	1.37
3	A	1422	CYC	CHA-C1A	3.81	1.45	1.38
3	B	1419	CYC	C1C-NC	3.59	1.42	1.37
3	A	1422	CYC	O1A-CGA	3.38	1.33	1.22
3	B	1419	CYC	C1B-C2B	3.36	1.51	1.45
3	A	1422	CYC	C1B-C2B	3.35	1.51	1.45
3	A	1422	CYC	CMB-C2B	3.23	1.57	1.50
3	B	1419	CYC	CMB-C2B	3.18	1.57	1.50
3	B	1419	CYC	O1A-CGA	2.99	1.31	1.22
3	B	1419	CYC	C2C-C3C	2.86	1.62	1.54
3	A	1422	CYC	C2C-C3C	2.69	1.61	1.54
3	B	1419	CYC	O2D-CGD	-2.67	1.22	1.30
3	B	1419	CYC	O1D-CGD	2.64	1.30	1.22
3	A	1422	CYC	O2D-CGD	-2.63	1.22	1.30
3	B	1419	CYC	C1A-C2A	-2.62	1.41	1.45
3	A	1422	CYC	O1D-CGD	2.60	1.30	1.22
3	A	1422	CYC	C1A-C2A	-2.56	1.41	1.45
3	B	1419	CYC	OB-C4B	-2.52	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1422	CYC	CHD-C4C	2.52	1.40	1.36
3	A	1422	CYC	OB-C4B	-2.48	1.18	1.23
3	B	1419	CYC	C4C-NC	2.45	1.42	1.37
3	A	1422	CYC	C4C-NC	2.44	1.42	1.37
3	B	1419	CYC	CHD-C4C	2.32	1.40	1.36
2	A	1427	GLU	OXT-C	-2.25	1.23	1.30
3	A	1422	CYC	CAD-C3D	2.19	1.57	1.51
3	B	1419	CYC	CAD-C3D	2.04	1.56	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1422	CYC	C3B-C4B-NB	10.82	115.39	106.77
3	B	1419	CYC	C3B-C4B-NB	10.61	115.23	106.77
3	B	1419	CYC	C2C-C1C-NC	9.77	116.42	108.29
3	A	1422	CYC	C2C-C1C-NC	9.67	116.33	108.29
3	B	1419	CYC	C1C-NC-C4C	-8.59	102.64	113.41
3	A	1422	CYC	C1C-NC-C4C	-8.53	102.70	113.41
3	B	1419	CYC	C3C-C4C-NC	7.00	116.95	107.94
3	A	1422	CYC	C3C-C4C-NC	6.37	116.15	107.94
3	B	1419	CYC	C1B-C2B-C3B	-6.27	101.42	107.86
3	A	1422	CYC	C1B-C2B-C3B	-5.99	101.71	107.86
3	B	1419	CYC	OC-C1C-C2C	-5.85	121.52	126.17
3	A	1422	CYC	OC-C1C-C2C	-5.80	121.56	126.17
3	A	1422	CYC	C2B-C1B-NB	5.70	115.28	106.97
3	B	1419	CYC	C2B-C1B-NB	5.68	115.25	106.97
3	A	1422	CYC	CAB-C3B-C4B	5.51	129.88	121.37
3	A	1422	CYC	OB-C4B-C3B	-5.48	122.28	128.03
3	B	1419	CYC	OB-C4B-C3B	-5.25	122.52	128.03
3	B	1419	CYC	CAB-C3B-C4B	5.00	129.10	121.37
3	A	1422	CYC	C2A-C1A-NA	4.73	116.74	110.04
3	B	1419	CYC	C2A-C1A-NA	4.63	116.59	110.04
3	B	1419	CYC	CMB-C2B-C1B	4.45	129.57	124.16
3	A	1422	CYC	CMB-C2B-C1B	4.16	129.22	124.16
3	A	1422	CYC	C1B-NB-C4B	-3.69	106.13	110.66
3	B	1419	CYC	C1B-NB-C4B	-3.44	106.44	110.66
3	B	1419	CYC	C1B-CHB-C4A	-3.32	119.89	128.06
3	A	1422	CYC	CHB-C1B-C2B	-2.94	121.11	126.97
2	A	1427	GLU	OXT-C-O	-2.77	117.80	124.08
3	A	1422	CYC	CHD-C1D-C2D	-2.64	121.06	127.53
3	A	1422	CYC	CHA-C4D-C3D	-2.46	121.93	127.22
3	B	1419	CYC	OC-C1C-NC	-2.43	122.06	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1419	CYC	CMA-C3A-C4A	2.43	128.88	125.10
3	A	1422	CYC	OC-C1C-NC	-2.40	122.10	124.93
3	A	1422	CYC	CHD-C1D-ND	2.34	130.59	125.29
3	B	1419	CYC	CHD-C1D-C2D	-2.32	121.84	127.53
3	B	1419	CYC	CHB-C1B-C2B	-2.16	122.67	126.97
3	B	1419	CYC	CHA-C4D-C3D	-2.15	122.60	127.22
3	A	1422	CYC	CHA-C4D-ND	2.10	130.03	125.29
3	A	1422	CYC	C1B-CHB-C4A	-2.10	122.91	128.06
3	A	1422	CYC	CMA-C3A-C4A	2.09	128.35	125.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1422	CYC	NA-C4A-CHB-C1B
3	A	1422	CYC	C3A-C4A-CHB-C1B
3	B	1419	CYC	NA-C4A-CHB-C1B
3	B	1419	CYC	C3A-C4A-CHB-C1B
4	B	1420	GOL	C1-C2-C3-O3
4	B	1420	GOL	O2-C2-C3-O3
4	A	1423	GOL	C1-C2-C3-O3
3	B	1419	CYC	NA-C1A-CHA-C4D
3	A	1422	CYC	C2B-C3B-CAB-CBB
4	A	1423	GOL	O2-C2-C3-O3
3	B	1419	CYC	NB-C1B-CHB-C4A
3	A	1422	CYC	NA-C1A-CHA-C4D
3	B	1419	CYC	C2A-C1A-CHA-C4D
3	B	1419	CYC	C2B-C1B-CHB-C4A
3	A	1422	CYC	ND-C1D-CHD-C4C
3	B	1419	CYC	ND-C1D-CHD-C4C
3	A	1422	CYC	NB-C1B-CHB-C4A
3	A	1422	CYC	C2A-C1A-CHA-C4D
3	A	1422	CYC	C3D-CAD-CBD-CGD
3	B	1419	CYC	CAA-CBA-CGA-O1A
3	A	1422	CYC	C2B-C1B-CHB-C4A
3	B	1419	CYC	C2B-C3B-CAB-CBB
3	B	1419	CYC	CAA-CBA-CGA-O2A
3	B	1419	CYC	C4B-C3B-CAB-CBB
3	B	1419	CYC	C2D-C1D-CHD-C4C
3	A	1422	CYC	CAA-CBA-CGA-O2A
3	A	1422	CYC	C2D-C1D-CHD-C4C
3	B	1419	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	B	1419	CYC	CAD-CBD-CGD-O1D
3	A	1422	CYC	CAA-CBA-CGA-O1A

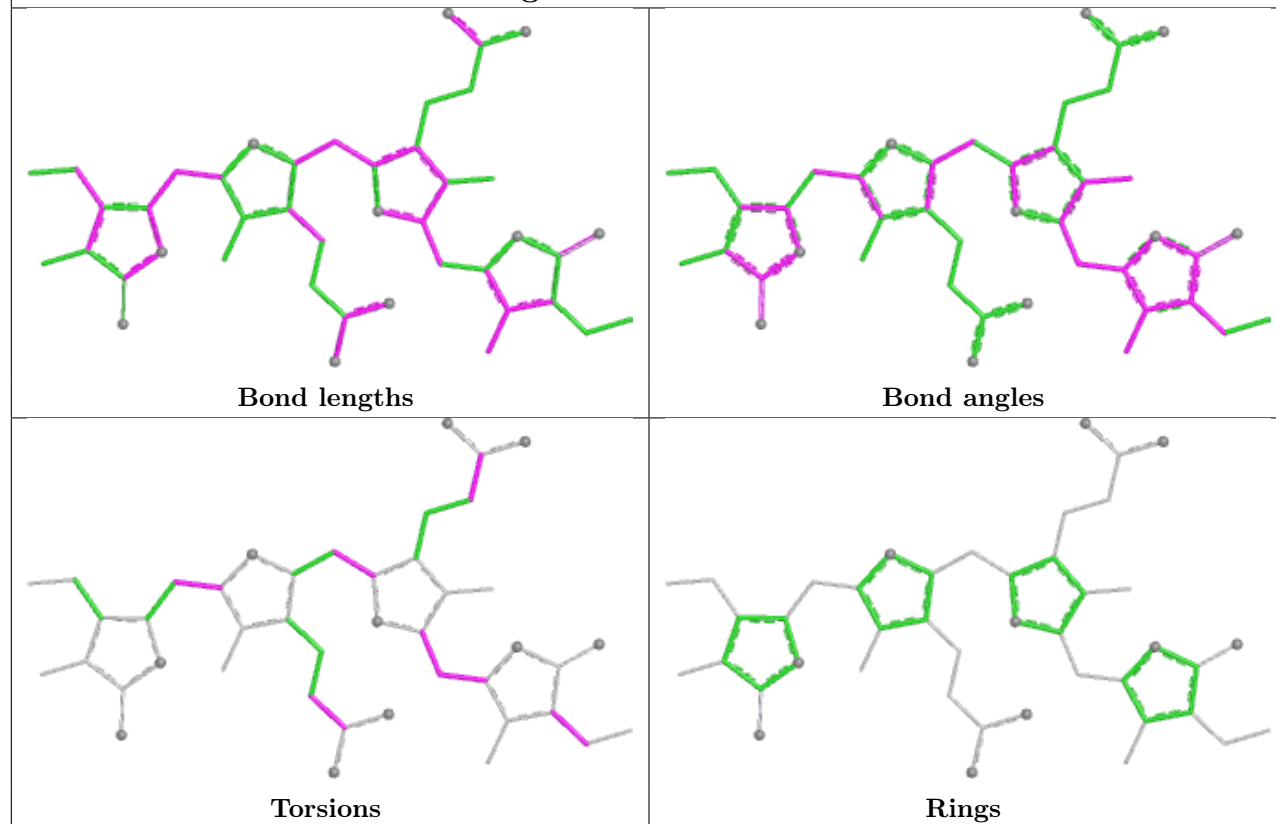
There are no ring outliers.

2 monomers are involved in 2 short contacts:

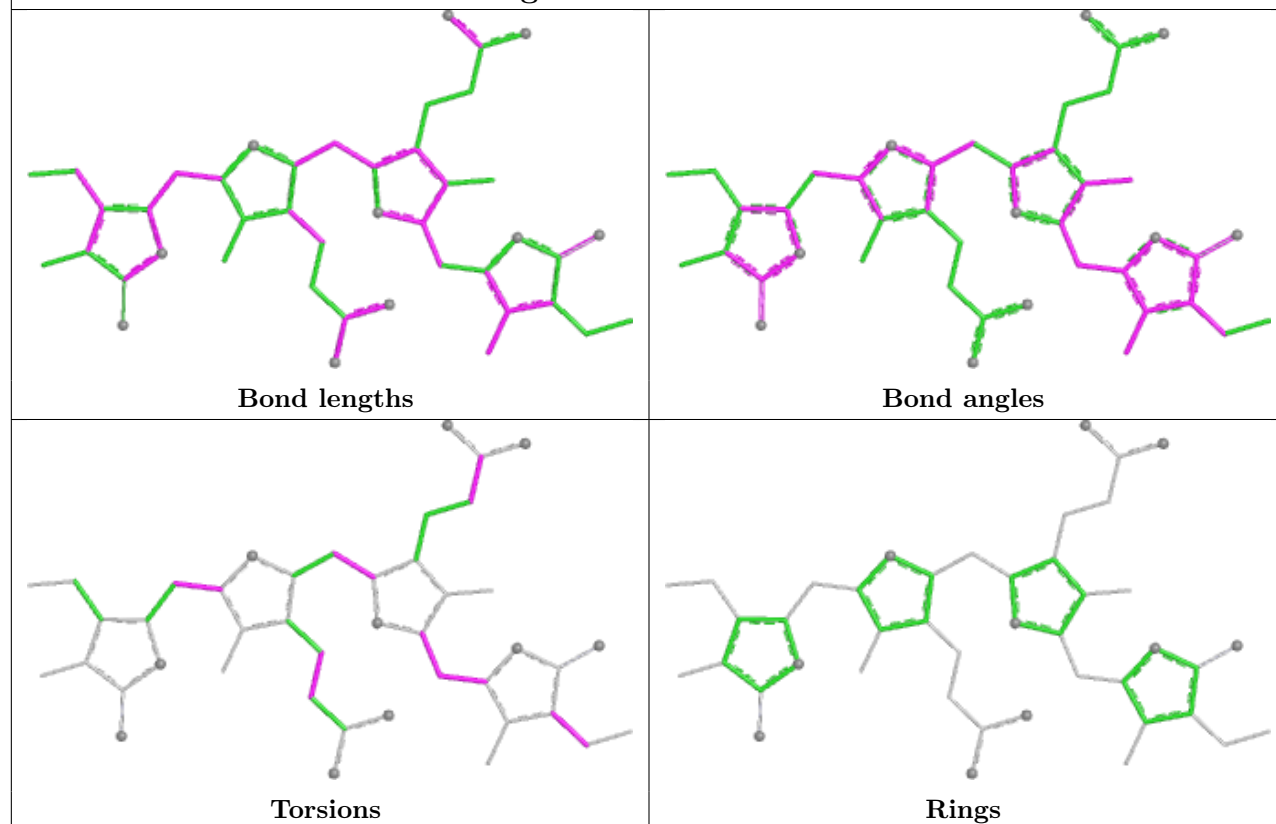
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1423	GOL	1	0
3	A	1422	CYC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CYC B 1419



Ligand CYC A 1422



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/432 (88%)	0.05	15 (3%) 43 38	22, 53, 113, 153	1 (0%)
1	B	377/432 (87%)	0.32	26 (6%) 23 18	22, 70, 143, 196	0
All	All	758/864 (87%)	0.19	41 (5%) 31 26	22, 59, 130, 196	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	THR	4.3
1	A	421	GLN	3.6
1	B	4	ASN	3.5
1	A	113	ILE	3.1
1	A	114	SER	3.0
1	B	212	VAL	3.0
1	B	222	TRP	2.9
1	A	332	SER	2.9
1	B	113	ILE	2.9
1	A	334	SER	2.8
1	A	121	GLY	2.8
1	A	374	GLY	2.8
1	B	240	LEU	2.8
1	A	396	VAL	2.8
1	B	327	ILE	2.8
1	A	249	SER	2.7
1	B	332	SER	2.7
1	A	111	GLY	2.7
1	A	379	ASN	2.7
1	A	373	ARG	2.7
1	B	333	LEU	2.6
1	B	216	GLY	2.6
1	B	244	PRO	2.6
1	B	253	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	250	VAL	2.5
1	B	213	ALA	2.5
1	B	241	TYR	2.4
1	B	208	LEU	2.3
1	B	20	ARG	2.3
1	B	351	GLN	2.3
1	B	239	VAL	2.3
1	A	245	ASP	2.3
1	B	271	TRP	2.2
1	A	4	ASN	2.1
1	B	217	ASP	2.1
1	B	349	ASP	2.1
1	B	278	GLN	2.1
1	B	18	PHE	2.0
1	B	262	TRP	2.0
1	A	279	PRO	2.0
1	B	211	THR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	FMT	B	1424	3/3	0.44	0.21	103,103,105,106	0
5	FMT	B	1421	3/3	0.62	0.14	75,75,80,83	0
2	GLU	A	1427	10/10	0.67	0.16	79,87,90,91	0
5	FMT	A	1424	3/3	0.77	0.18	83,83,87,88	0
5	FMT	A	1426	3/3	0.80	0.11	86,86,88,88	0
5	FMT	B	1422	3/3	0.82	0.11	81,81,85,85	0

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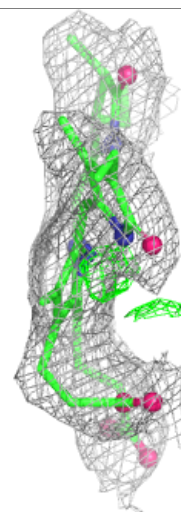
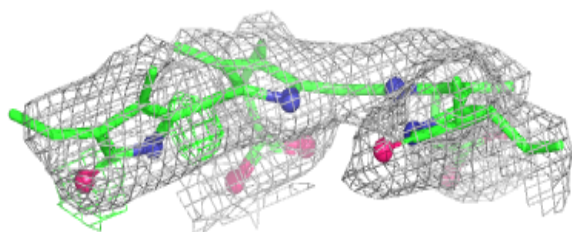
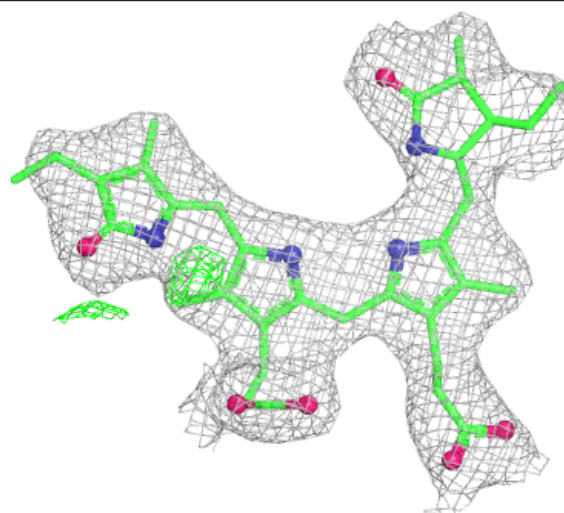
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	B	1423	3/3	0.84	0.12	52,52,62,67	0
5	FMT	A	1425	3/3	0.84	0.24	70,70,71,72	0
4	GOL	B	1420	6/6	0.91	0.12	44,50,61,61	0
4	GOL	A	1423	6/6	0.91	0.13	58,63,78,82	0
3	CYC	A	1422	43/43	0.94	0.09	26,40,54,66	0
3	CYC	B	1419	43/43	0.96	0.08	18,31,53,60	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.

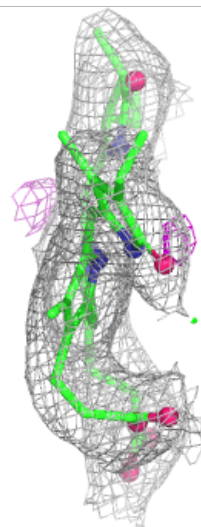
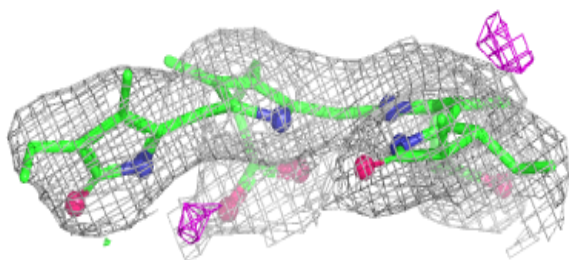
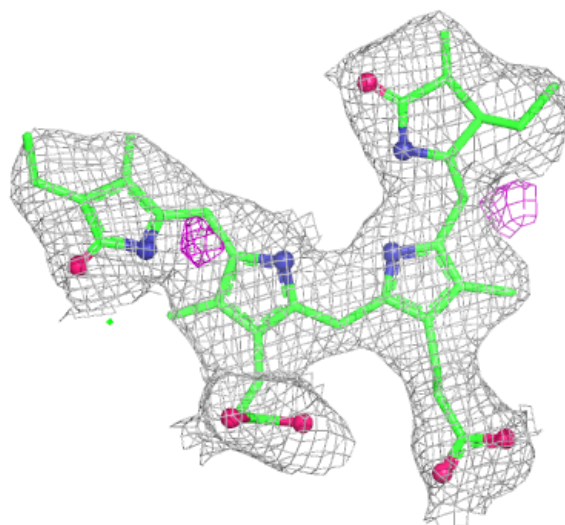
Electron density around CYC A 1422:

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 CYC B 1419:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.