



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:58 am BST

PDB ID : 6HRN
Title : C-Phycocyanin from heterocyst forming filamentous cyanobacterium Nostoc sp. WR13
Authors : Patel, H.M.; Roszak, A.W.; Madamwar, D.; Cogdell, R.J.
Deposited on : 2018-09-27
Resolution : 1.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

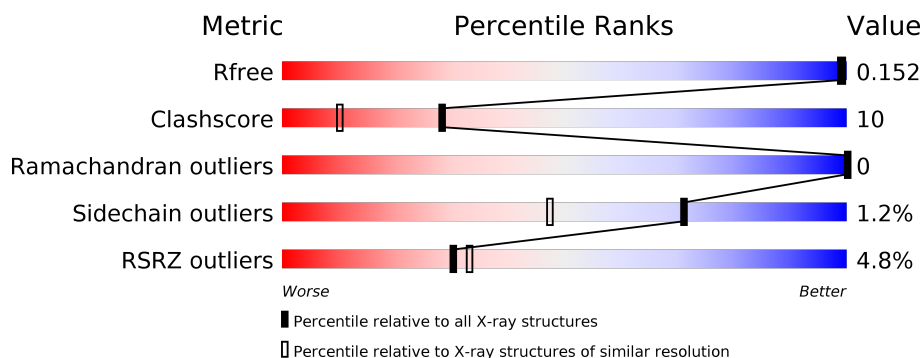
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 on 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	162	<div> <div>10%</div> <div> <div></div> <div>94%</div> <div>6% •</div> </div> </div>
2	B	172	<div> <div>95%</div> <div>5%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PG4	B	206	-	-	X	-
4	PG4	B	207	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3170 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.

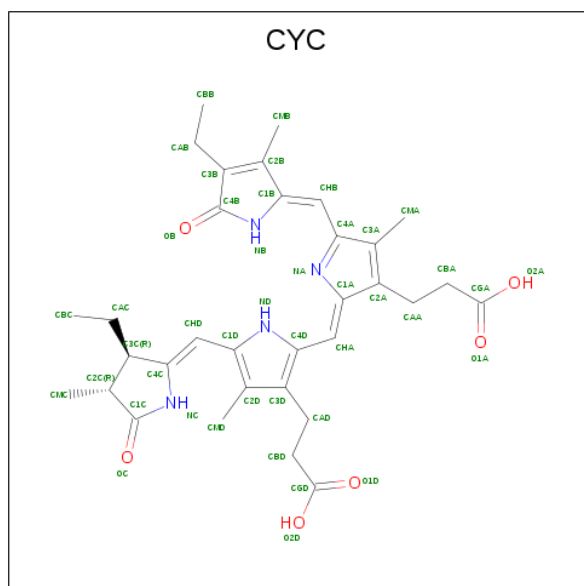
- Molecule 1 is a protein called Alpha Subunit of Cyanobacterial Phycocyanin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	5	0
			1243	786	206	247	4			

- Molecule 2 is a protein called Beta Subunit of Cyanobacterial Phycocyanin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	7	0
			1305	806	233	255	11			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: 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		

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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



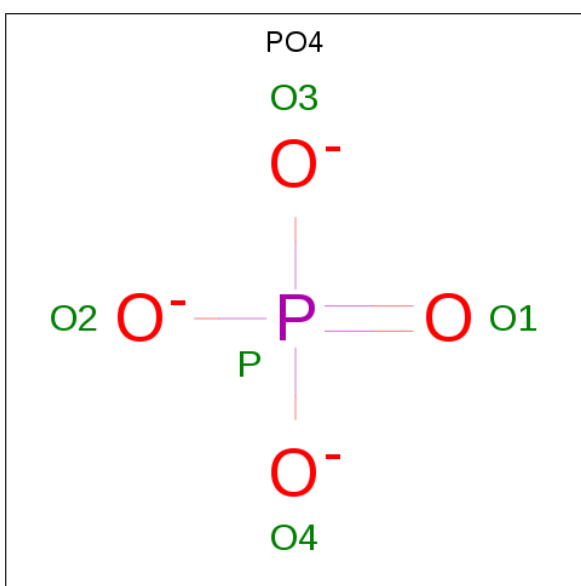
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



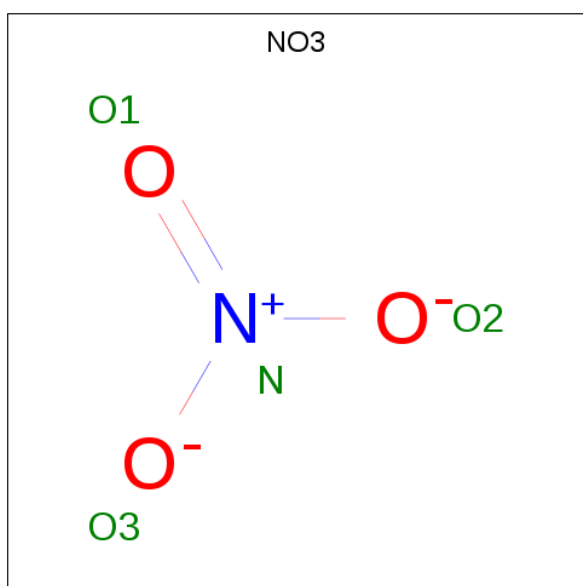
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

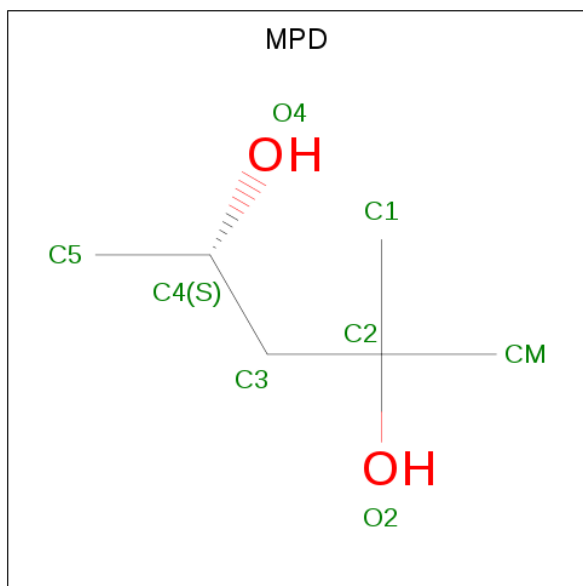
- Molecule 8 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	1
			16	12	4		

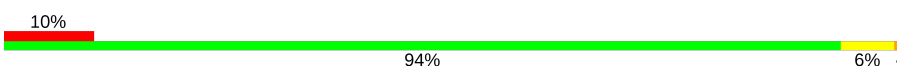
- Molecule 10 is water.

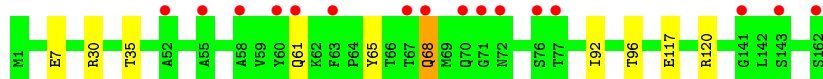
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	134	Total	O	0	0
			134	134		
10	B	235	Total	O	0	0
			235	235		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

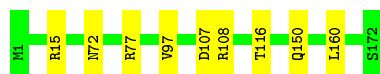
- Molecule 1: Alpha Subunit of Cyanobacterial Phycocyanin protein

Chain A: 



- Molecule 2: Beta Subunit of Cyanobacterial Phycocyanin protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	151.47Å 151.47Å 39.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.75 – 1.51 75.74 – 1.51	Depositor EDS
% Data completeness (in resolution range)	89.6 (75.75-1.51) 89.6 (75.74-1.51)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.115 , 0.154 0.125 , 0.152	Depositor DCC
R_{free} test set	2535 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3170	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MPD, PGE, PO4, MEN, CYC, PG4, PEG, NO3

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	0.72	0/1282	0.84	0/1739
2	B	0.78	0/1329	0.88	0/1793
All	All	0.75	0/2611	0.86	0/3532

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1243	0	1226	8	0
2	B	1305	0	1319	15	0
3	A	43	0	37	1	0
3	B	86	0	74	7	0
4	A	13	0	18	5	0
4	B	52	0	72	22	0
5	A	7	0	10	2	0
5	B	7	0	10	1	0
6	B	5	0	0	0	0
7	B	20	0	28	2	0
8	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	16	0	28	3	0
10	A	134	0	0	5	0
10	B	235	0	0	18	0
All	All	3170	0	2822	55	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 10.

All (55) 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)
4:B:204:PG4:H72	10:B:303:HOH:O	1.37	1.20
4:B:204:PG4:C7	10:B:303:HOH:O	1.93	1.06
4:A:202:PG4:H82	4:A:202:PG4:H52	1.46	0.96
4:B:204:PG4:H12	10:B:397:HOH:O	1.70	0.89
4:B:207:PG4:H21	10:B:353:HOH:O	1.73	0.87
4:A:202:PG4:C5	4:A:202:PG4:H82	2.05	0.86
2:B:116:THR:HA	4:B:207:PG4:C4	2.06	0.86
2:B:116:THR:HA	4:B:207:PG4:H41	1.60	0.82
9:B:212[A]:MPD:O2	9:B:212[A]:MPD:H52	1.84	0.78
10:A:323:HOH:O	4:B:206:PG4:H41	1.83	0.77
10:A:312:HOH:O	4:B:204:PG4:H62	1.84	0.76
4:B:204:PG4:C1	10:B:397:HOH:O	2.34	0.69
1:A:7[A]:GLU:OE2	10:A:301:HOH:O	2.10	0.68
2:B:116:THR:HA	4:B:207:PG4:H42	1.75	0.67
4:B:205:PG4:H22	4:B:207:PG4:H81	1.76	0.67
2:B:77[A]:ARG:NH2	10:B:301:HOH:O	1.96	0.67
4:A:202:PG4:C5	4:A:202:PG4:C8	2.72	0.65
2:B:77[A]:ARG:NH2	3:B:201:CYC:O2D	2.29	0.64
1:A:117:GLU:HG3	5:A:203:PEG:H41	1.80	0.63
10:A:323:HOH:O	4:B:206:PG4:C4	2.45	0.63
4:B:206:PG4:H82	10:B:465:HOH:O	1.99	0.62
2:B:116:THR:HG23	4:B:207:PG4:H62	1.81	0.61
4:B:205:PG4:H81	10:B:462:HOH:O	2.00	0.61
3:B:201:CYC:HMD2	3:B:201:CYC:HC	1.66	0.60
4:B:206:PG4:H32	10:B:331:HOH:O	2.04	0.57
2:B:77[C]:ARG:NE	10:B:308:HOH:O	2.37	0.56
7:B:209:PGE:H4	10:B:433:HOH:O	2.07	0.53
4:B:206:PG4:H41	10:B:331:HOH:O	2.08	0.53
2:B:15:ARG:NH2	10:B:307:HOH:O	2.35	0.53
2:B:150[A]:GLN:NE2	10:B:310:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:HG3	5:A:203:PEG:C4	2.39	0.52
3:B:202:CYC:HMA1	3:B:202:CYC:NB	2.24	0.52
3:A:201:CYC:HC	3:A:201:CYC:HMD2	1.75	0.52
2:B:108:ARG:O	3:B:201:CYC:HBB1	2.09	0.52
4:B:205:PG4:C2	4:B:207:PG4:H81	2.40	0.50
4:B:206:PG4:H52	4:B:206:PG4:H21	1.93	0.49
1:A:92:ILE:O	1:A:96:THR:HG23	2.12	0.49
2:B:72:MEN:HE21	5:B:208:PEG:H12	1.96	0.47
9:B:212[A]:MPD:H12	10:B:318:HOH:O	2.13	0.47
3:B:202:CYC:HMD2	3:B:202:CYC:NC	2.30	0.47
4:A:202:PG4:H51	4:A:202:PG4:C8	2.47	0.44
7:B:209:PGE:H1	10:B:313:HOH:O	2.16	0.44
1:A:65:TYR:HA	1:A:68:GLN:HG2	2.00	0.44
9:B:212[A]:MPD:H13	9:B:212[A]:MPD:H4	1.83	0.43
3:B:202:CYC:HMD2	3:B:202:CYC:HC	1.83	0.43
2:B:116:THR:HG23	4:B:207:PG4:H42	2.00	0.43
3:B:201:CYC:HMA1	3:B:201:CYC:NB	2.34	0.42
1:A:68:GLN:HB3	1:A:68:GLN:HE21	1.68	0.42
2:B:107:ASP:O	4:B:206:PG4:H12	2.20	0.42
4:B:206:PG4:C4	10:B:331:HOH:O	2.66	0.41
2:B:77[B]:ARG:HG2	10:B:302:HOH:O	2.20	0.41
1:A:35[B]:THR:HG23	10:A:313:HOH:O	2.21	0.41
2:B:97:VAL:HG21	2:B:160:LEU:HD13	2.03	0.40
4:A:202:PG4:H51	4:A:202:PG4:H82	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	165/162 (102%)	161 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	177/172 (103%)	174 (98%)	3 (2%)	0	100	100
All	All	342/334 (102%)	335 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	129/124 (104%)	126 (98%)	3 (2%)	50	20
2	B	133/125 (106%)	133 (100%)	0	100	100
All	All	262/249 (105%)	259 (99%)	3 (1%)	71	52

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	68	GLN
1	A	120	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	68	GLN
2	B	11	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	MEN	B	72	2	7,8,9	0.72	0	6,9,11	1.07	1 (16%)

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
2	MEN	B	72	2	-	2/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	MEN	OD1-CG-CB	2.29	124.85	121.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
9	MPD	B	212[A]	-	7,7,7	0.18	0	9,10,10	0.51	0
6	PO4	B	203	-	4,4,4	1.14	1 (25%)	6,6,6	0.54	0
4	PG4	B	206	-	12,12,12	0.22	0	11,11,11	0.15	0
4	PG4	A	202	-	12,12,12	0.19	0	11,11,11	0.16	0
4	PG4	B	207	-	12,12,12	0.49	0	11,11,11	0.35	0
3	CYC	B	201	2	36,46,46	1.26	1 (2%)	44,67,67	1.12	5 (11%)
7	PGE	B	209	-	9,9,9	0.19	0	8,8,8	0.12	0
4	PG4	B	204	-	12,12,12	0.43	0	11,11,11	0.45	0
8	NO3	B	211	-	1,3,3	0.83	0	0,3,3	0.00	-
5	PEG	B	208	-	6,6,6	0.21	0	5,5,5	0.10	0
7	PGE	B	210	-	9,9,9	0.29	0	8,8,8	0.18	0
3	CYC	B	202	2	36,46,46	1.55	3 (8%)	44,67,67	0.99	2 (4%)
4	PG4	B	205	-	12,12,12	0.15	0	11,11,11	0.25	0
5	PEG	A	203	-	6,6,6	0.13	0	5,5,5	0.16	0
9	MPD	B	212[B]	-	7,7,7	0.23	0	9,10,10	0.38	0
3	CYC	A	201	1	36,46,46	1.45	2 (5%)	44,67,67	1.05	3 (6%)

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
9	MPD	B	212[A]	-	-	1/5/5/5	-
5	PEG	B	208	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	B	206	-	-	8/10/10/10	-
4	PG4	A	202	-	-	6/10/10/10	-
4	PG4	B	207	-	-	6/10/10/10	-
3	CYC	B	201	2	-	4/21/74/74	0/4/4/4
7	PGE	B	209	-	-	5/7/7/7	-
4	PG4	B	204	-	-	7/10/10/10	-
7	PGE	B	210	-	-	4/7/7/7	-
3	CYC	B	202	2	-	3/21/74/74	0/4/4/4
4	PG4	B	205	-	-	10/10/10/10	-
5	PEG	A	203	-	-	1/4/4/4	-
9	MPD	B	212[B]	-	-	0/5/5/5	-
3	CYC	A	201	1	-	7/21/74/74	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	CYC	CHA-C1A	7.49	1.41	1.35
3	A	201	CYC	CHA-C1A	7.37	1.41	1.35
3	B	201	CYC	CHA-C1A	6.43	1.40	1.35
3	A	201	CYC	C1B-C2B	-3.00	1.39	1.45
3	B	202	CYC	C4C-NC	2.46	1.42	1.37
3	B	202	CYC	C1B-NB	-2.26	1.34	1.37
6	B	203	PO4	P-O1	2.05	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	CYC	CAA-CBA-CGA	2.63	117.08	112.67
3	A	201	CYC	C3B-C4B-NB	-2.62	104.66	106.78
3	B	201	CYC	C2C-C3C-C4C	2.46	105.02	101.34
3	B	202	CYC	CHD-C4C-NC	-2.43	122.31	125.20
3	A	201	CYC	CHA-C1A-NA	-2.39	125.52	128.83
3	B	201	CYC	C4D-CHA-C1A	2.26	131.51	128.81
3	B	201	CYC	CHD-C4C-NC	2.11	127.72	125.20
3	B	201	CYC	CHA-C1A-NA	-2.10	125.92	128.83
3	B	202	CYC	CHA-C1A-NA	-2.09	125.93	128.83
3	A	201	CYC	C4D-CHA-C1A	2.06	131.27	128.81

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	212[A]	MPD	C2-C3-C4-O4
3	B	201	CYC	NA-C4A-CHB-C1B
3	B	201	CYC	C3A-C4A-CHB-C1B
3	B	201	CYC	ND-C1D-CHD-C4C
3	B	201	CYC	C2D-C1D-CHD-C4C
3	B	202	CYC	NA-C4A-CHB-C1B
3	B	202	CYC	C3A-C4A-CHB-C1B
3	A	201	CYC	NA-C4A-CHB-C1B
3	A	201	CYC	C3A-C4A-CHB-C1B
3	A	201	CYC	C2C-C3C-CAC-CBC
3	A	201	CYC	C4C-C3C-CAC-CBC
3	A	201	CYC	ND-C1D-CHD-C4C
4	B	205	PG4	C6-C5-O3-C4
4	B	206	PG4	C8-C7-O4-C6
4	B	207	PG4	O3-C5-C6-O4
4	B	205	PG4	O2-C3-C4-O3
4	B	206	PG4	O3-C5-C6-O4
4	A	202	PG4	C5-C6-O4-C7
4	B	204	PG4	C5-C6-O4-C7
4	B	206	PG4	C4-C3-O2-C2
3	A	201	CYC	C2B-C3B-CAB-CBB
7	B	210	PGE	O2-C3-C4-O3
7	B	209	PGE	O3-C5-C6-O4
4	B	204	PG4	O4-C7-C8-O5
7	B	209	PGE	O2-C3-C4-O3
7	B	210	PGE	O1-C1-C2-O2
5	A	203	PEG	O2-C3-C4-O4
4	B	205	PG4	O3-C5-C6-O4
4	B	207	PG4	C3-C4-O3-C5
4	B	207	PG4	O1-C1-C2-O2
4	B	204	PG4	O1-C1-C2-O2
5	B	208	PEG	O1-C1-C2-O2
4	B	206	PG4	O1-C1-C2-O2
4	B	206	PG4	O4-C7-C8-O5
4	B	207	PG4	O4-C7-C8-O5
7	B	209	PGE	O1-C1-C2-O2
4	B	205	PG4	O1-C1-C2-O2
4	B	205	PG4	O4-C7-C8-O5
4	B	206	PG4	O2-C3-C4-O3
4	B	207	PG4	O2-C3-C4-O3
7	B	210	PGE	C3-C4-O3-C5
4	B	207	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
4	B	204	PG4	C6-C5-O3-C4
4	B	205	PG4	C5-C6-O4-C7
4	B	205	PG4	C1-C2-O2-C3
4	B	205	PG4	C8-C7-O4-C6
7	B	209	PGE	C1-C2-O2-C3
7	B	210	PGE	C6-C5-O3-C4
4	A	202	PG4	C6-C5-O3-C4
4	B	204	PG4	C8-C7-O4-C6
4	B	206	PG4	C3-C4-O3-C5
4	B	204	PG4	O2-C3-C4-O3
4	B	205	PG4	C4-C3-O2-C2
4	A	202	PG4	C1-C2-O2-C3
4	A	202	PG4	C4-C3-O2-C2
4	B	206	PG4	C5-C6-O4-C7
5	B	208	PEG	C4-C3-O2-C2
4	B	204	PG4	C3-C4-O3-C5
7	B	209	PGE	C6-C5-O3-C4
4	A	202	PG4	O2-C3-C4-O3
3	A	201	CYC	C4B-C3B-CAB-CBB
3	B	202	CYC	C4C-C3C-CAC-CBC
4	B	205	PG4	C3-C4-O3-C5
4	A	202	PG4	O3-C5-C6-O4

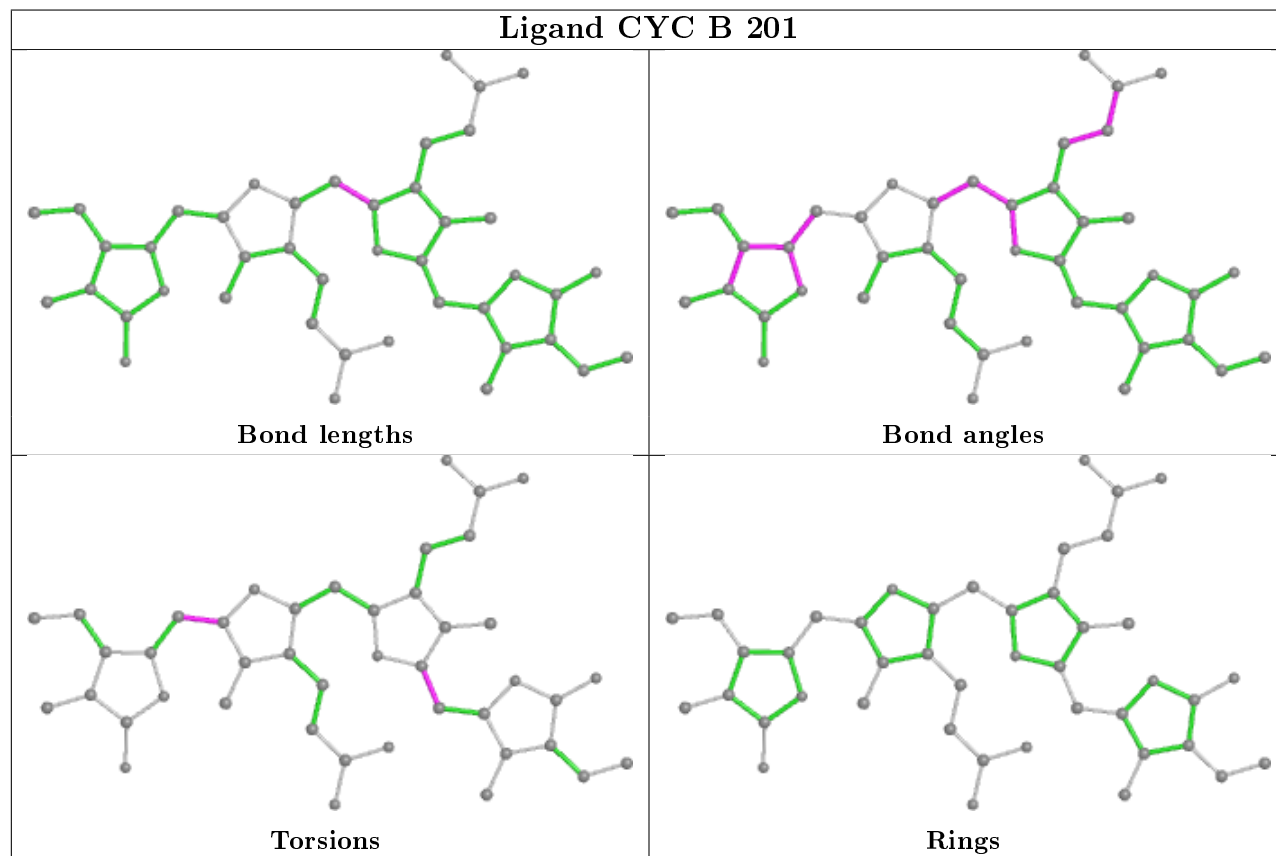
There are no ring outliers.

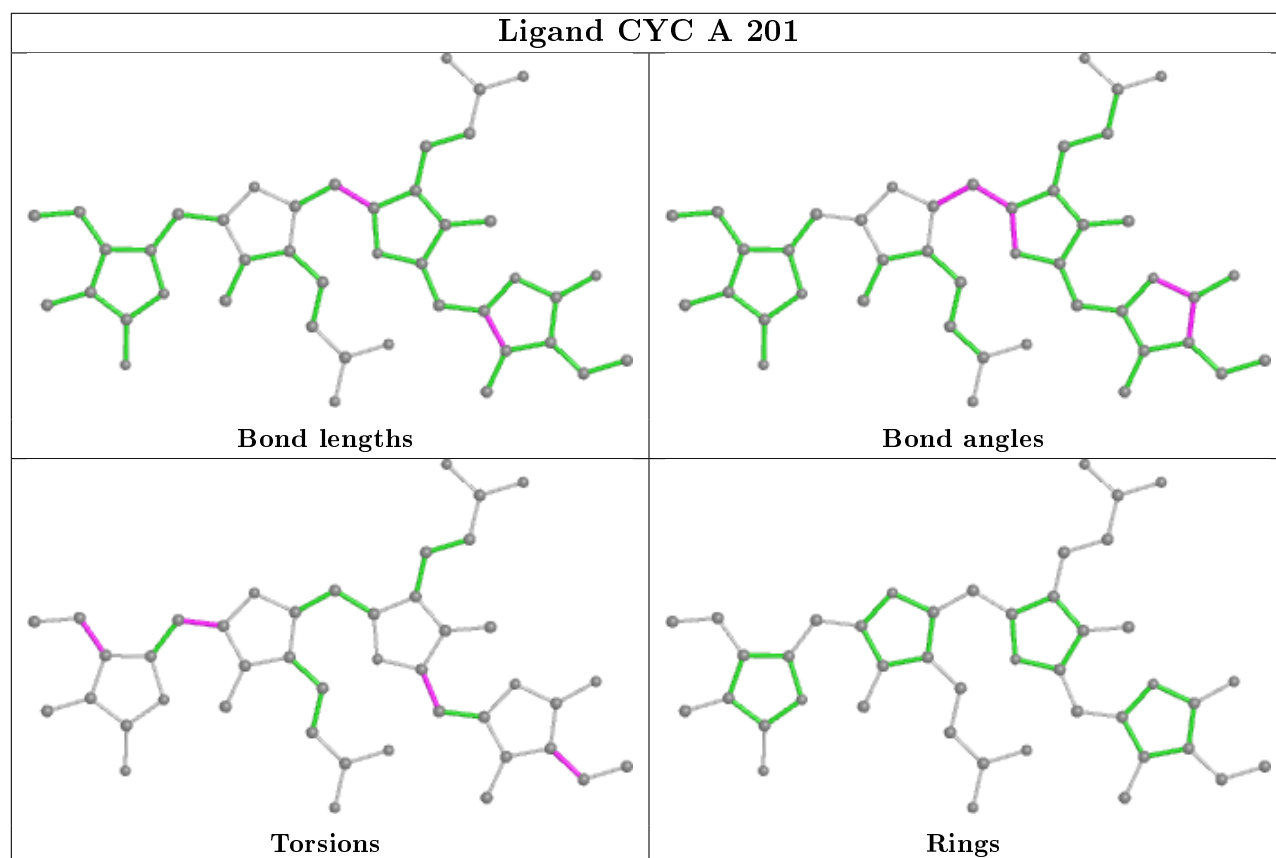
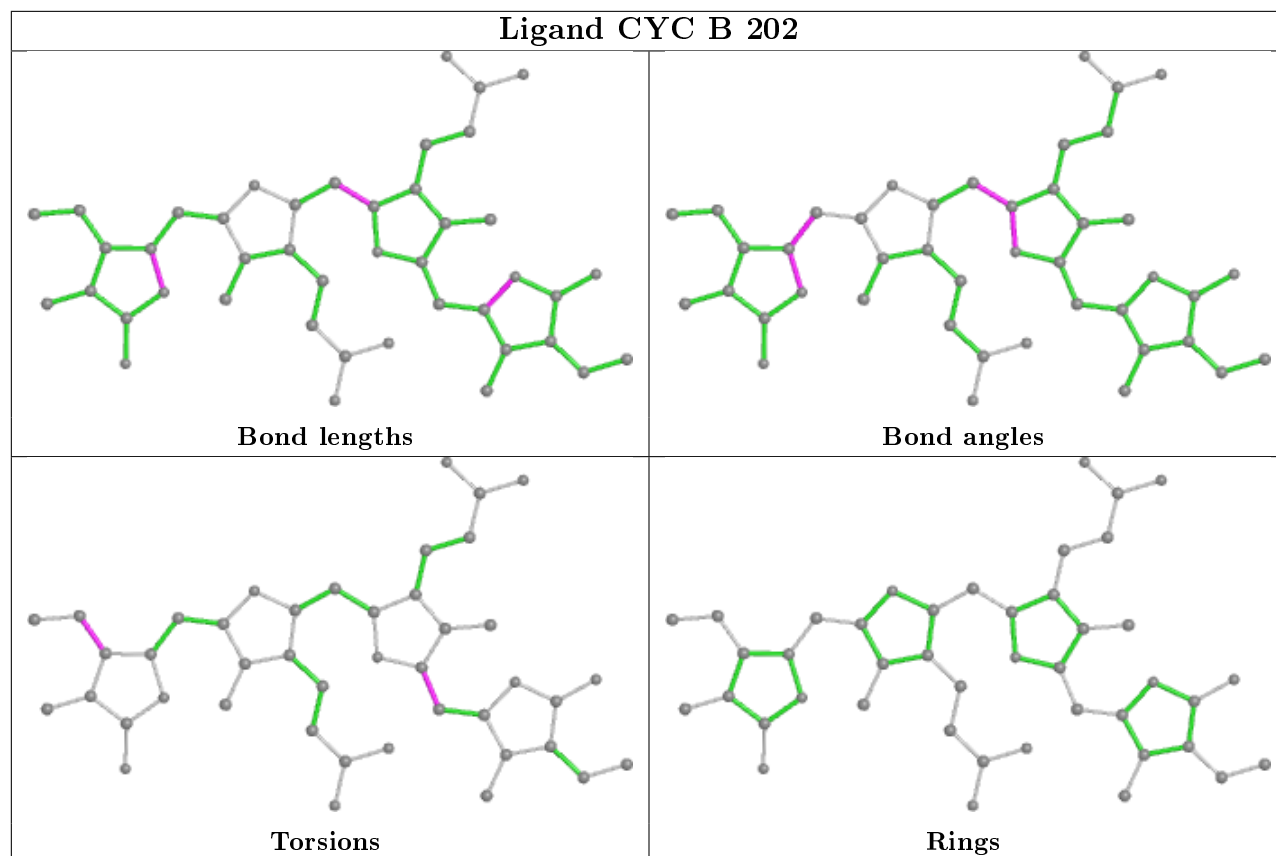
12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	212[A]	MPD	3	0
4	B	206	PG4	8	0
4	A	202	PG4	5	0
4	B	207	PG4	8	0
3	B	201	CYC	4	0
7	B	209	PGE	2	0
4	B	204	PG4	5	0
5	B	208	PEG	1	0
3	B	202	CYC	3	0
4	B	205	PG4	3	0
5	A	203	PEG	2	0
3	A	201	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.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	162/162 (100%)	0.43	16 (9%) 7 7	29, 54, 82, 106	0
2	B	171/172 (99%)	-0.07	0 100 100	26, 34, 49, 67	0
All	All	333/334 (99%)	0.17	16 (4%) 30 33	26, 39, 78, 106	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	SER	4.5
1	A	68	GLN	3.5
1	A	60	TYR	3.4
1	A	76	SER	3.2
1	A	70	GLN	3.2
1	A	55	ALA	3.1
1	A	63	PHE	2.9
1	A	143	SER	2.7
1	A	141	GLY	2.6
1	A	61	GLN	2.4
1	A	77	THR	2.2
1	A	58	ALA	2.2
1	A	52	ALA	2.1
1	A	72	ASN	2.1
1	A	67	THR	2.1
1	A	71	GLY	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MEN	B	72	9/10	0.95	0.09	33,36,43,46	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

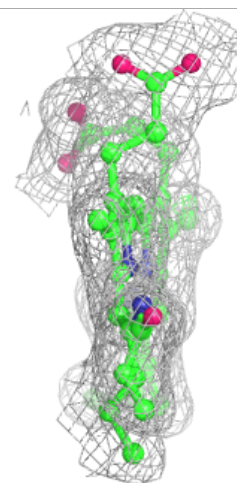
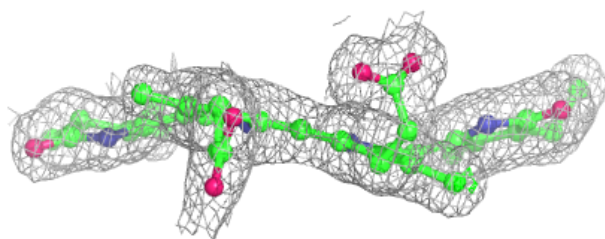
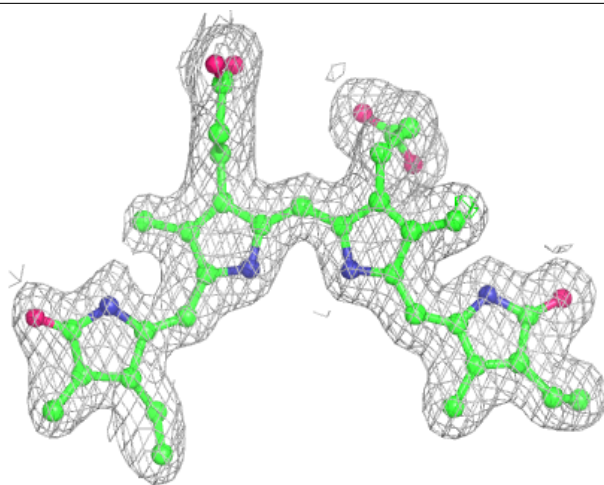
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PGE	B	209	10/10	0.65	0.26	47,60,68,71	10
4	PG4	B	207	13/13	0.75	0.38	44,54,64,68	13
5	PEG	B	208	7/7	0.78	0.28	51,59,64,72	7
4	PG4	A	202	13/13	0.78	0.19	58,61,70,73	13
5	PEG	A	203	7/7	0.81	0.30	60,61,69,71	7
4	PG4	B	205	13/13	0.85	0.51	46,51,61,65	13
4	PG4	B	204	13/13	0.85	0.26	31,48,58,62	13
7	PGE	B	210	10/10	0.87	0.29	69,80,102,104	0
9	MPD	B	212[A]	8/8	0.88	0.25	35,51,59,65	8
9	MPD	B	212[B]	8/8	0.88	0.25	33,46,53,57	8
4	PG4	B	206	13/13	0.90	0.40	37,57,70,72	13
3	CYC	A	201	43/43	0.93	0.08	37,46,57,64	0
3	CYC	B	201	43/43	0.95	0.08	30,36,62,72	0
8	NO3	B	211	4/4	0.96	0.23	49,56,58,62	4
3	CYC	B	202	43/43	0.96	0.08	24,27,34,41	0
6	PO4	B	203	5/5	0.99	0.12	35,36,38,44	5

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.

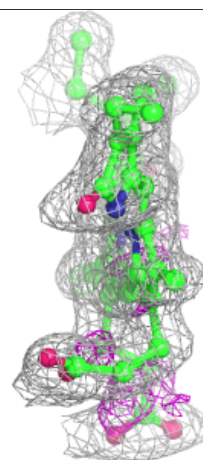
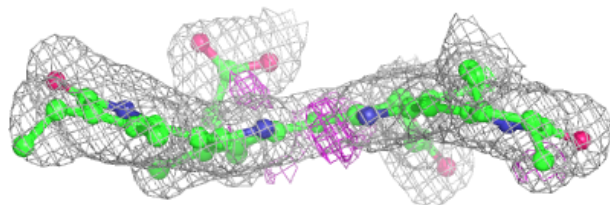
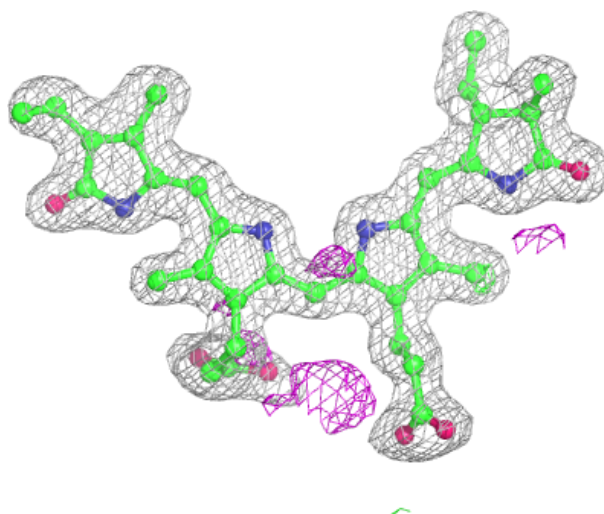
Electron density around CYC A 201:

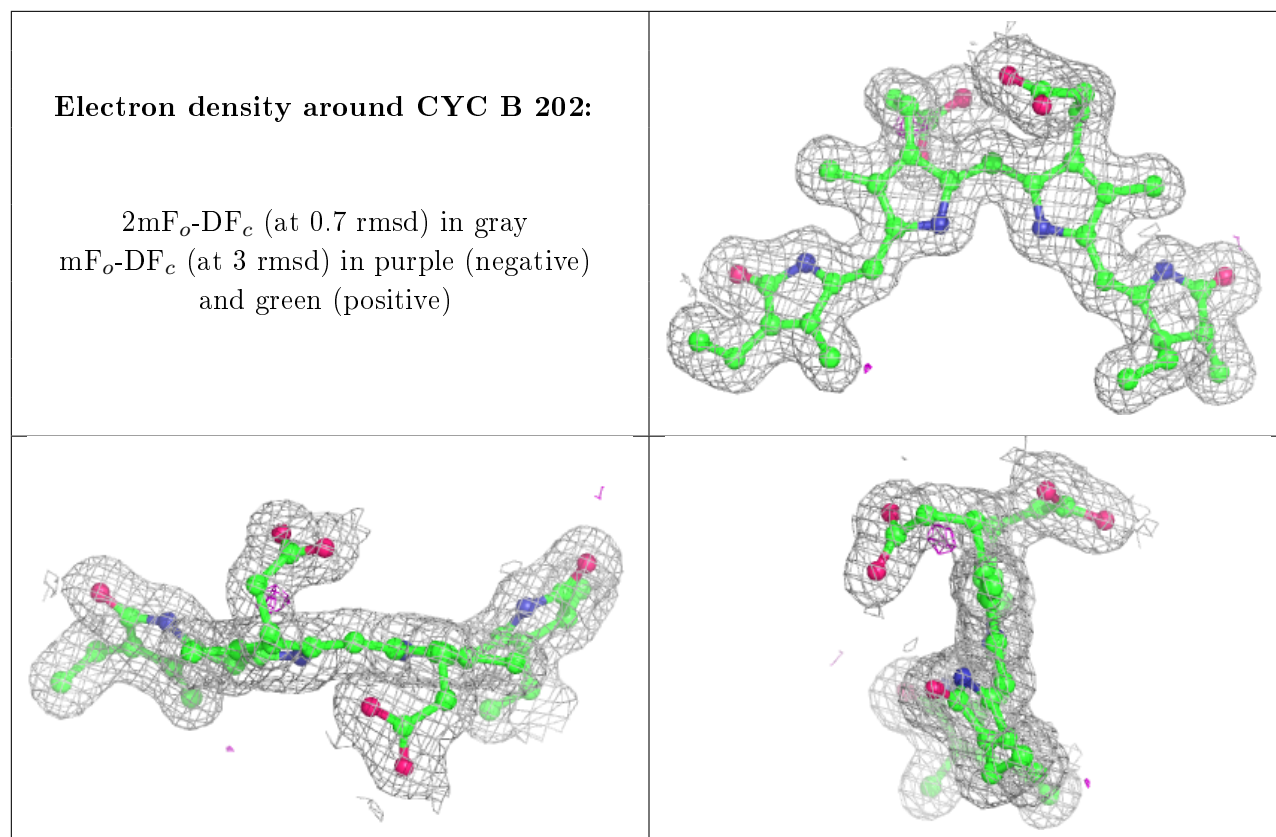
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CYC B 201:

$2mF_o-DF_c$ (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.