Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2024 – 11:09 am BST

PDB ID	:	8R44
Title	:	PAS-GAF bidomain of Glycine max phytochrome A
Deposited on	:	2023-11-13
Resolution	:	1.58 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

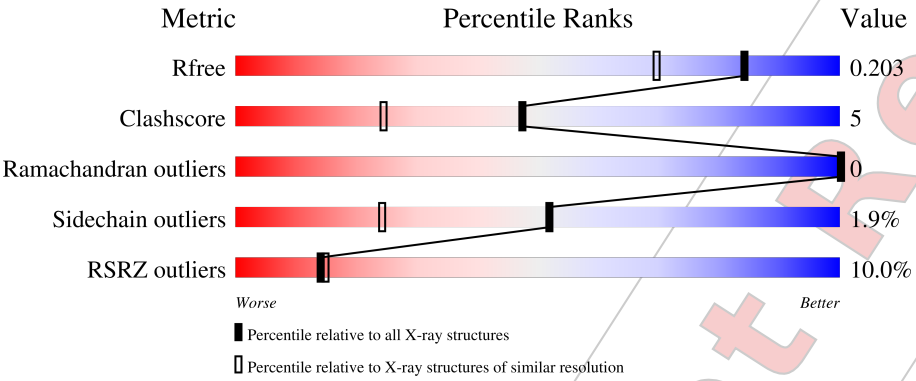
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.58 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}	164625	7165 (1.60-1.56)
Clashscore	180529	1026 (1.58-1.58)
Ramachandran outliers	177936	1005 (1.58-1.58)
Sidechain outliers	177891	1004 (1.58-1.58)
RSRZ outliers	164620	7163 (1.60-1.56)

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	A	359	10% 76% 11% • 13%
1	B	359	8% 83% 5% 13%

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:

Validation Pipeline (wwPDB-VP) : 2.38.2

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	501	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5669 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.

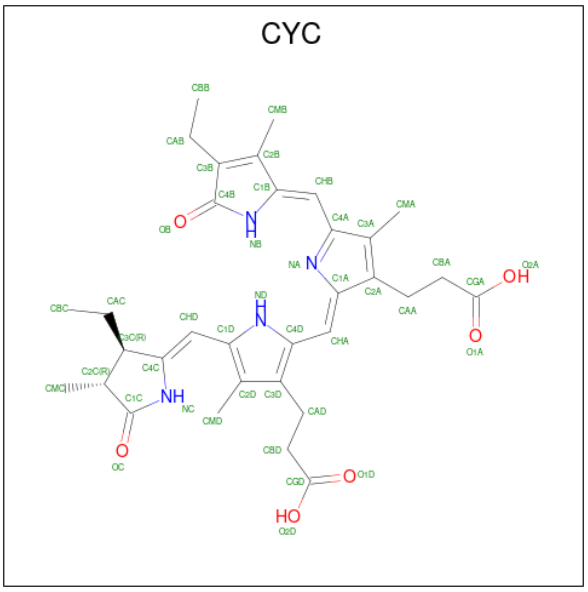
- Molecule 1 is a protein called Phytochrome A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2462	1585	420	434	23			
1	B	314	Total	C	N	O	S	0	0	0
			2462	1585	420	434	23			

There are 14 discrepancies between the modelled and reference sequences:

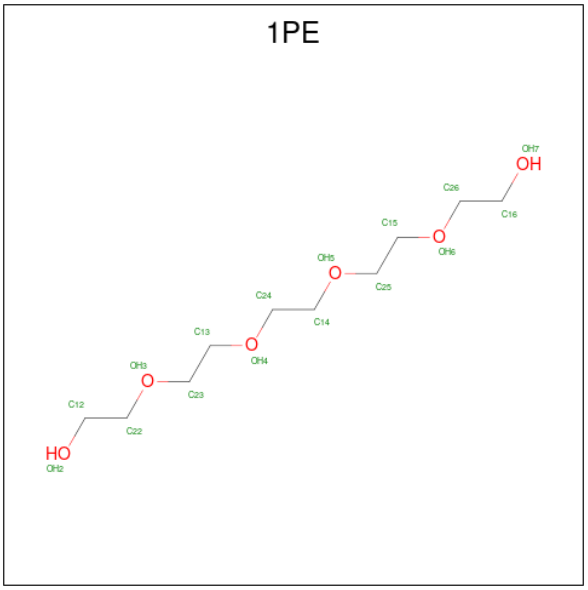
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	initiating methionine	UNP B4YB07
A	403	HIS	-	expression tag	UNP B4YB07
A	404	HIS	-	expression tag	UNP B4YB07
A	405	HIS	-	expression tag	UNP B4YB07
A	406	HIS	-	expression tag	UNP B4YB07
A	407	HIS	-	expression tag	UNP B4YB07
A	408	HIS	-	expression tag	UNP B4YB07
B	50	MET	-	initiating methionine	UNP B4YB07
B	403	HIS	-	expression tag	UNP B4YB07
B	404	HIS	-	expression tag	UNP B4YB07
B	405	HIS	-	expression tag	UNP B4YB07
B	406	HIS	-	expression tag	UNP B4YB07
B	407	HIS	-	expression tag	UNP B4YB07
B	408	HIS	-	expression tag	UNP B4YB07

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0

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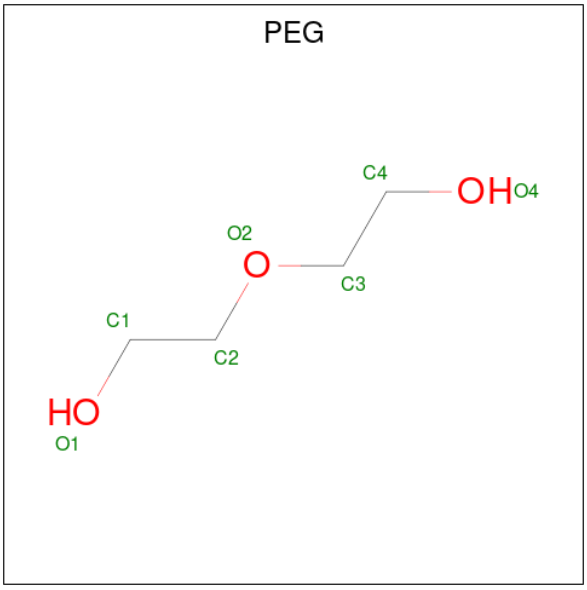
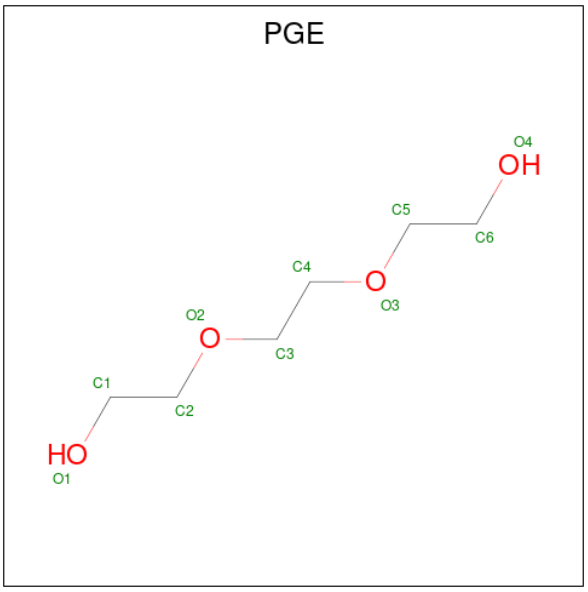
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 16 10 6	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0

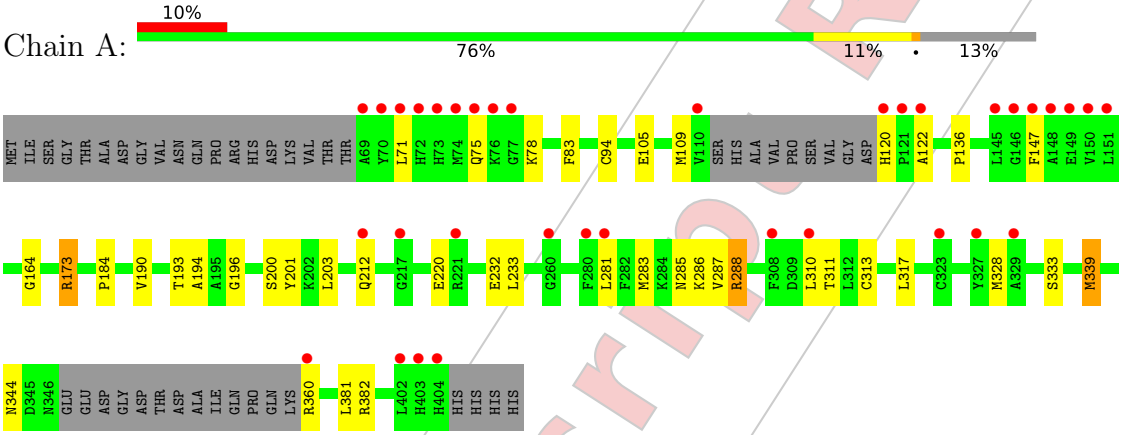
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	283	Total O 283 283	0	0
6	B	304	Total O 304 304	0	0

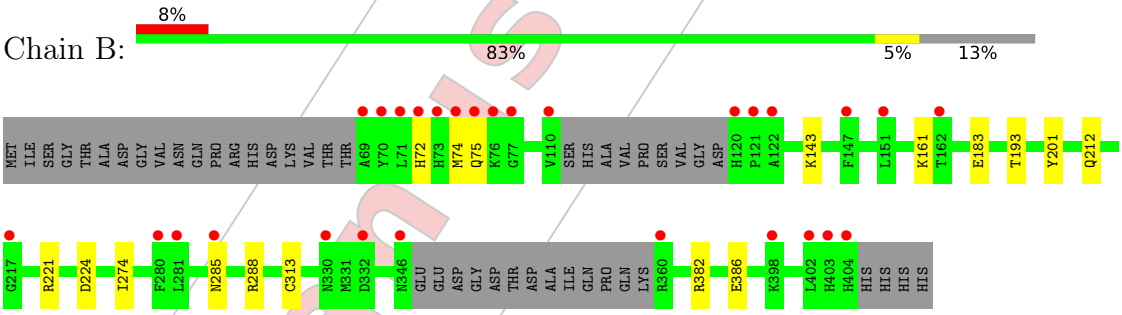
3 Residue-property plots (i)

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: Phytochrome A-2



• Molecule 1: Phytochrome A-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.29Å 111.81Å 68.27Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	43.84 – 1.58 43.84 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.84-1.58) 99.6 (43.84-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.175 , 0.195 0.186 , 0.203	Depositor DCC
R_{free} test set	5391 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: CYC, 1PE, PEG, PGE

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	0.52	1/2521 (0.0%)	0.82	3/3416 (0.1%)
1	B	0.52	1/2521 (0.0%)	0.78	1/3416 (0.0%)
All	All	0.52	2/5042 (0.0%)	0.80	4/6832 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	GLU	CD-OE2	7.35	1.33	1.25
1	A	220	GLU	CD-OE1	-5.27	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	382	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	339	MET	CG-SD-CE	-7.35	88.44	100.20
1	B	382	ARG	NE-CZ-NH2	-5.85	117.37	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain

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	2462	0	2493	31	0
1	B	2462	0	2493	12	0
2	A	43	0	37	4	0
2	B	43	0	37	2	0
3	A	32	0	44	9	0
3	B	16	0	22	2	0
4	A	14	0	20	1	0
5	A	10	0	14	5	0
6	A	283	0	0	17	0
6	B	304	0	0	9	0
All	All	5669	0	5160	56	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 5.

All (56) 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:288:ARG:NH1	6:A:601:HOH:O	1.76	1.13
6:A:688:HOH:O	1:B:193:THR:CG2	1.98	1.10
6:A:688:HOH:O	1:B:193:THR:HG22	1.66	0.83
1:A:147:PHE:O	1:A:173:ARG:NH2	2.11	0.82
1:B:221:ARG:NH2	1:B:224:ASP:OD2	2.12	0.81
2:A:500:CYC:CGD	6:A:601:HOH:O	2.29	0.81
1:B:386:GLU:OE1	6:B:601:HOH:O	2.00	0.79
1:A:184:PRO:HB2	3:A:501:1PE:H222	1.70	0.73
1:B:161:LYS:HE2	6:B:826:HOH:O	1.91	0.71
3:A:501:1PE:H142	6:A:816:HOH:O	1.92	0.69
6:A:688:HOH:O	1:B:193:THR:HG23	1.71	0.69
3:B:501:1PE:H132	6:B:646:HOH:O	1.91	0.68
3:B:501:1PE:H221	6:B:833:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:NH1	6:A:602:HOH:O	2.25	0.67
1:A:164:GLY:HA3	3:A:502:1PE:H222	1.76	0.66
1:A:184:PRO:HB2	3:A:501:1PE:C22	2.27	0.65
1:A:200:SER:OG	5:A:505:PGE:H5	1.97	0.64
1:A:232:GLU:O	5:A:505:PGE:H1	1.98	0.64
2:A:500:CYC:NB	2:A:500:CYC:HMA1	2.14	0.63
1:A:147:PHE:O	1:A:173:ARG:CZ	2.46	0.63
1:A:287:VAL:HG22	1:A:339:MET:HG3	1.83	0.59
3:A:501:1PE:H151	6:A:816:HOH:O	2.04	0.56
1:B:212:GLN:NE2	6:B:606:HOH:O	2.37	0.56
1:A:196:GLY:HA3	4:A:503:PEG:H11	1.89	0.54
1:A:311:THR:HG22	6:A:644:HOH:O	2.07	0.54
1:A:203:LEU:HD13	5:A:505:PGE:H12	1.90	0.53
3:A:501:1PE:H162	6:A:816:HOH:O	2.08	0.53
1:A:283:MET:O	1:A:286:LYS:HE3	2.09	0.53
1:A:75:GLN:HA	1:A:313:CYS:SG	2.49	0.52
1:A:83:PHE:CZ	1:A:317:LEU:HD23	2.45	0.52
1:B:143:LYS:HE3	6:B:699:HOH:O	2.09	0.52
1:A:281:LEU:HD22	6:A:763:HOH:O	2.09	0.52
1:A:105:GLU:HG3	6:A:801:HOH:O	2.08	0.51
1:B:285:ASN:ND2	6:B:603:HOH:O	2.32	0.51
1:A:344:ASN:ND2	1:A:360:ARG:HG3	2.27	0.49
1:A:194:ALA:HB2	1:B:193:THR:OG1	2.12	0.49
2:A:500:CYC:O1D	6:A:601:HOH:O	2.20	0.49
3:A:502:1PE:H221	6:A:749:HOH:O	2.13	0.48
1:B:74:MET:O	1:B:313:CYS:HB3	2.15	0.47
1:A:190:VAL:O	1:A:193:THR:HG23	2.14	0.47
1:A:212:GLN:HA	6:B:606:HOH:O	2.14	0.47
1:A:78:LYS:HE2	1:A:310:LEU:O	2.15	0.46
1:A:233:LEU:HG	1:A:381:LEU:HD11	1.98	0.46
2:A:500:CYC:HHA	2:A:500:CYC:HBA2	1.97	0.46
1:A:233:LEU:HA	5:A:505:PGE:H1	1.98	0.45
1:A:122:ALA:HB3	6:A:738:HOH:O	2.17	0.44
1:B:274:ILE:HG12	2:B:500:CYC:C4A	2.47	0.44
3:A:501:1PE:H222	3:A:501:1PE:H131	1.79	0.44
2:B:500:CYC:NB	2:B:500:CYC:HMA1	2.32	0.44
3:A:501:1PE:H131	6:A:808:HOH:O	2.17	0.43
5:A:505:PGE:H12	5:A:505:PGE:H32	1.73	0.43
1:A:281:LEU:CD2	1:A:285:ASN:HB2	2.49	0.43
1:A:212:GLN:CA	6:B:606:HOH:O	2.67	0.42
1:A:136:PRO:HA	6:A:620:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:HB3	1:A:333:SER:O	2.20	0.41
1:A:147:PHE:O	1:A:173:ARG:NE	2.54	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	308/359 (86%)	303 (98%)	5 (2%)	0	100	100
1	B	308/359 (86%)	306 (99%)	2 (1%)	0	100	100
All	All	616/718 (86%)	609 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	269/307 (88%)	263 (98%)	6 (2%)	47	19
1	B	269/307 (88%)	265 (98%)	4 (2%)	60	36
All	All	538/614 (88%)	528 (98%)	10 (2%)	52	24

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	94	CYS
1	A	109	MET
1	A	120	HIS
1	A	201	TYR
1	A	288	ARG
1	B	72	HIS
1	B	75	GLN
1	B	201	TYR
1	B	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	1PE	A	502	-	15,15,15	0.35	0	14,14,14	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	1PE	A	501	-	15,15,15	1.26	1 (6%)	14,14,14	0.91	0
4	PEG	A	504	-	6,6,6	0.33	0	5,5,5	0.23	0
2	CYC	B	500	1	42,46,46	1.47	5 (11%)	50,67,67	1.66	10 (20%)
3	1PE	B	501	-	15,15,15	0.26	0	14,14,14	0.28	0
5	PGE	A	505	-	9,9,9	0.33	0	8,8,8	0.27	0
4	PEG	A	503	-	6,6,6	0.52	0	5,5,5	0.31	0
2	CYC	A	500	1	42,46,46	1.59	7 (16%)	50,67,67	1.69	11 (22%)

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	1PE	A	502	-	-	3/13/13/13	-
3	1PE	A	501	-	-	7/13/13/13	-
4	PEG	A	504	-	-	3/4/4/4	-
2	CYC	B	500	1	-	8/25/74/74	0/4/4/4
3	1PE	B	501	-	-	8/13/13/13	-
5	PGE	A	505	-	-	4/7/7/7	-
4	PEG	A	503	-	-	4/4/4/4	-
2	CYC	A	500	1	-	9/25/74/74	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CYC	CHA-C1A	5.54	1.39	1.35
2	A	500	CYC	CHA-C1A	5.22	1.39	1.35
3	A	501	1PE	OH7-C16	3.90	1.62	1.42
2	A	500	CYC	O2A-CGA	-3.56	1.18	1.30
2	B	500	CYC	C2C-C1C	3.27	1.55	1.52
2	A	500	CYC	C3C-C4C	2.94	1.55	1.50
2	B	500	CYC	CHD-C4C	-2.64	1.31	1.38
2	B	500	CYC	C3C-C4C	2.43	1.54	1.50
2	A	500	CYC	C4B-C3B	2.38	1.52	1.48
2	A	500	CYC	C1C-NC	2.25	1.40	1.37
2	B	500	CYC	O2A-CGA	-2.20	1.23	1.30
2	A	500	CYC	O2D-CGD	-2.09	1.23	1.30
2	A	500	CYC	C3B-C2B	2.05	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	CYC	CAB-C3B-C2B	4.36	134.98	127.53
2	B	500	CYC	CBD-CAD-C3D	-4.19	105.47	112.62
2	A	500	CYC	CHA-C1A-NA	-4.13	123.09	128.83
2	B	500	CYC	OC-C1C-C2C	3.62	129.05	126.17
2	B	500	CYC	C4D-CHA-C1A	3.53	133.02	128.81
2	B	500	CYC	CAB-C3B-C2B	3.53	133.56	127.53
2	A	500	CYC	C4D-CHA-C1A	3.50	132.99	128.81
2	A	500	CYC	C1B-NB-C4B	-3.10	106.72	110.67
2	A	500	CYC	C3B-C4B-NB	3.10	109.28	106.78
2	A	500	CYC	C2B-C1B-NB	3.05	111.46	106.99
2	B	500	CYC	CHA-C1A-NA	-3.01	124.65	128.83
2	A	500	CYC	CBA-CAA-C2A	-2.98	104.34	112.63
2	B	500	CYC	O1A-CGA-CBA	-2.76	114.23	123.08
2	B	500	CYC	CBA-CAA-C2A	-2.75	104.99	112.63
2	A	500	CYC	CBD-CAD-C3D	-2.65	108.10	112.62
2	A	500	CYC	CHB-C1B-NB	-2.46	120.78	126.06
2	B	500	CYC	CHB-C4A-NA	-2.35	120.02	124.93
2	A	500	CYC	O1A-CGA-CBA	-2.25	115.86	123.08
2	B	500	CYC	O2D-CGD-O1D	2.21	128.81	123.30
2	B	500	CYC	OC-C1C-NC	-2.12	122.37	124.94
2	A	500	CYC	C2C-C3C-C4C	2.11	104.50	101.34

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	PGE	C1-C2-O2-C3
3	B	501	1PE	OH7-C16-C26-OH6
2	B	500	CYC	NB-C1B-CHB-C4A
3	B	501	1PE	OH5-C14-C24-OH4
4	A	503	PEG	O2-C3-C4-O4
2	A	500	CYC	NA-C4A-CHB-C1B
2	B	500	CYC	NA-C4A-CHB-C1B
2	A	500	CYC	C3A-C4A-CHB-C1B
2	B	500	CYC	C3A-C4A-CHB-C1B
2	A	500	CYC	C2B-C3B-CAB-CBB
4	A	504	PEG	C4-C3-O2-C2
2	A	500	CYC	NB-C1B-CHB-C4A
3	A	502	1PE	OH4-C13-C23-OH3
3	B	501	1PE	OH6-C15-C25-OH5
3	A	502	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
2	B	500	CYC	C2B-C3B-CAB-CBB
3	A	501	1PE	OH2-C12-C22-OH3
3	A	501	1PE	OH7-C16-C26-OH6
4	A	504	PEG	O1-C1-C2-O2
5	A	505	PGE	O1-C1-C2-O2
5	A	505	PGE	O3-C5-C6-O4
4	A	504	PEG	O2-C3-C4-O4
3	B	501	1PE	C14-C24-OH4-C13
4	A	503	PEG	O1-C1-C2-O2
5	A	505	PGE	O2-C3-C4-O3
2	A	500	CYC	C2B-C1B-CHB-C4A
3	B	501	1PE	C25-C15-OH6-C26
2	B	500	CYC	C2B-C1B-CHB-C4A
3	A	502	1PE	OH6-C15-C25-OH5
3	B	501	1PE	C13-C23-OH3-C22
4	A	503	PEG	C4-C3-O2-C2
3	B	501	1PE	C15-C25-OH5-C14
4	A	503	PEG	C1-C2-O2-C3
3	A	501	1PE	C16-C26-OH6-C15
2	B	500	CYC	CAA-CBA-CGA-O1A
3	A	501	1PE	C13-C23-OH3-C22
2	A	500	CYC	CAA-CBA-CGA-O2A
2	B	500	CYC	CAA-CBA-CGA-O2A
2	A	500	CYC	CAA-CBA-CGA-O1A
3	A	501	1PE	OH4-C13-C23-OH3
3	A	501	1PE	OH6-C15-C25-OH5
3	A	501	1PE	OH5-C14-C24-OH4
2	A	500	CYC	CAD-CBD-CGD-O2D
3	B	501	1PE	OH4-C13-C23-OH3
2	A	500	CYC	CAD-CBD-CGD-O1D
2	B	500	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	1PE	2	0
3	A	501	1PE	7	0
2	B	500	CYC	2	0
3	B	501	1PE	2	0
5	A	505	PGE	5	0
4	A	503	PEG	1	0

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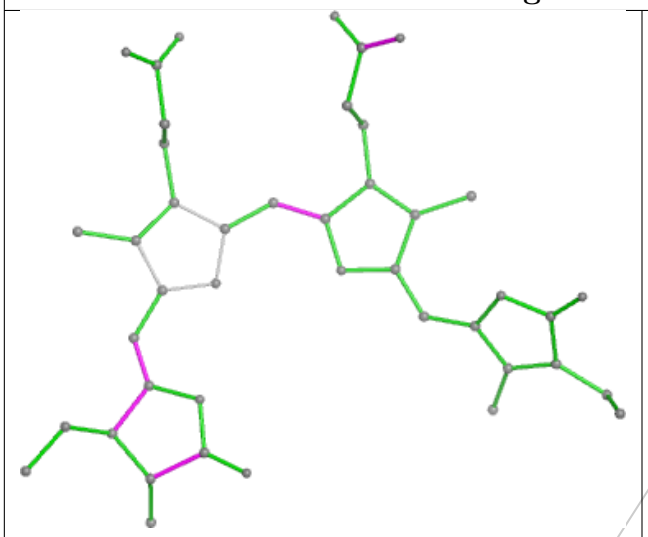
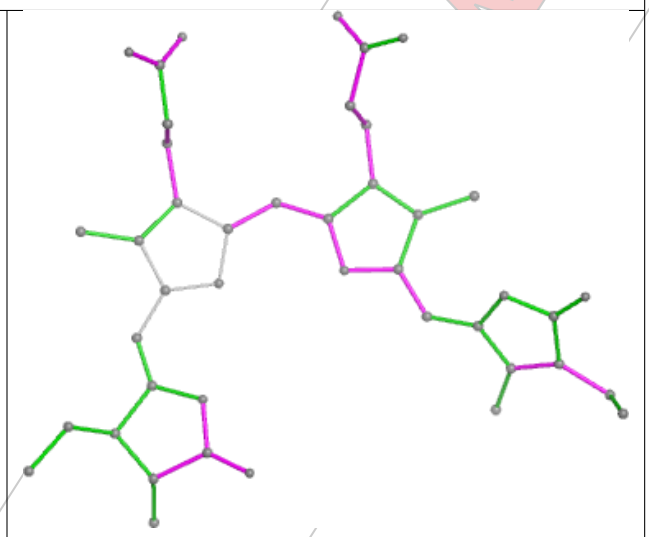
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	CYC	4	0

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.

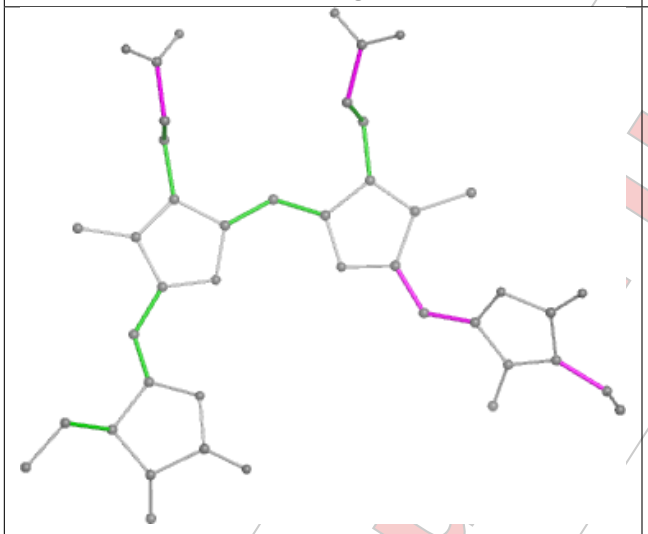
Ligand CYC B 500



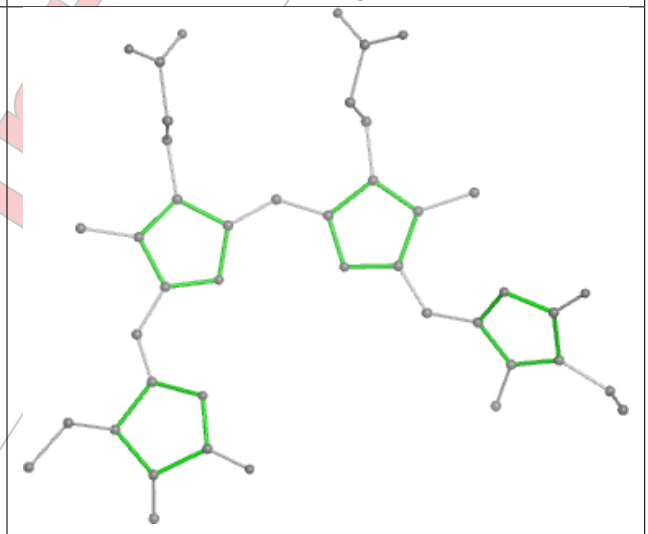
Bond lengths



Bond angles

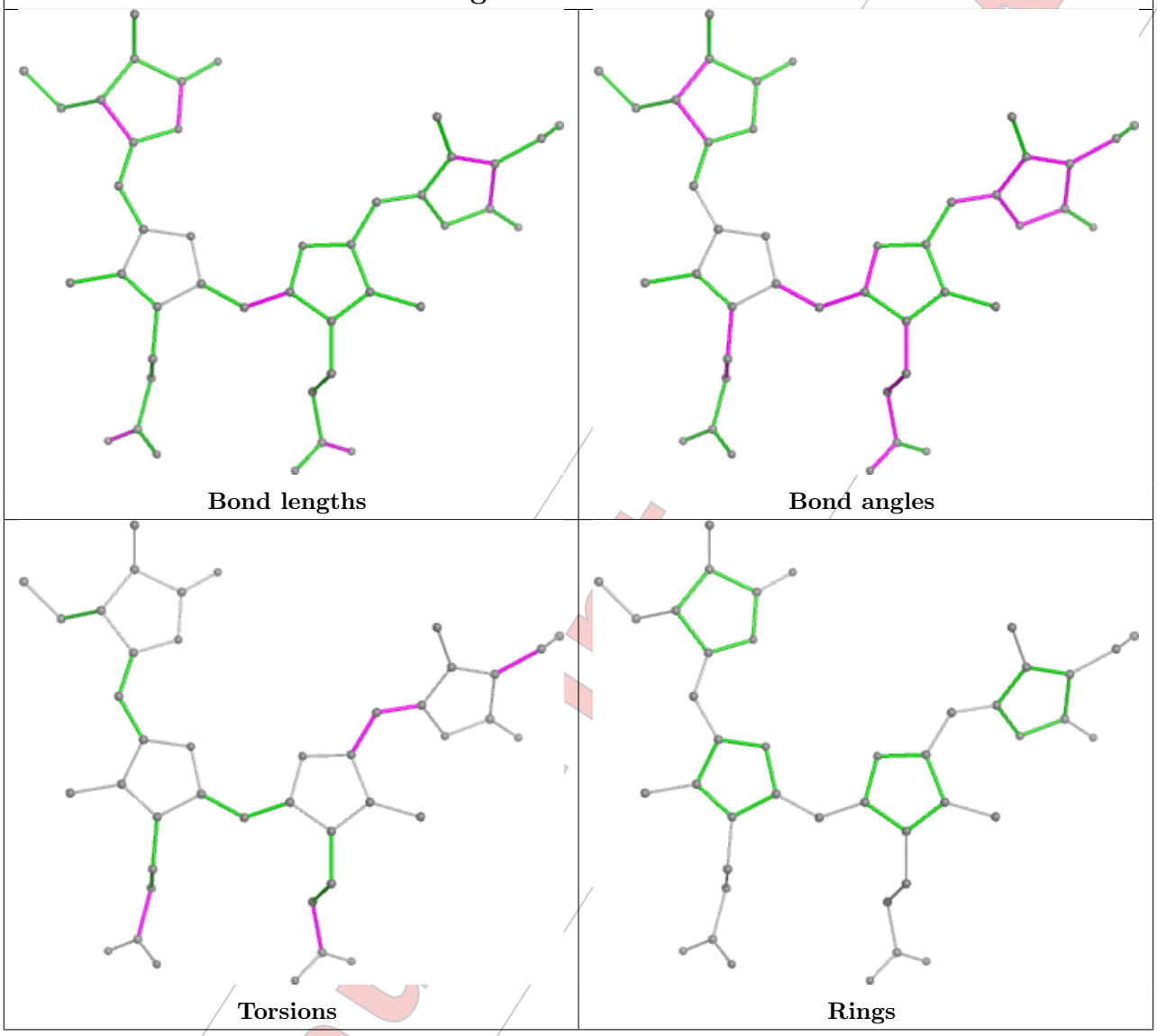


Torsions



Rings

Ligand CYC A 500



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, 95^{th} 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	314/359 (87%)	0.58	35 (11%) 12 12	14, 25, 70, 158	0
1	B	314/359 (87%)	0.41	28 (8%) 17 18	15, 24, 56, 120	0
All	All	628/718 (87%)	0.49	63 (10%) 14 15	14, 24, 65, 158	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	8.4
1	A	110	VAL	8.4
1	A	70	TYR	8.2
1	B	110	VAL	7.3
1	A	150	VAL	7.0
1	A	147	PHE	6.7
1	A	69	ALA	6.2
1	B	71	LEU	6.2
1	B	69	ALA	5.4
1	B	121	PRO	5.2
1	A	73	HIS	5.1
1	A	121	PRO	4.9
1	A	122	ALA	4.8
1	A	403	HIS	4.8
1	B	72	HIS	4.8
1	A	148	ALA	4.5
1	B	120	HIS	4.4
1	B	404	HIS	4.4
1	B	70	TYR	4.2
1	B	122	ALA	4.1
1	A	280	PHE	4.1
1	A	74	MET	3.7
1	B	75	GLN	3.6
1	A	77	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	281	LEU	3.6
1	A	120	HIS	3.5
1	A	72	HIS	3.5
1	A	151	LEU	3.4
1	B	402	LEU	3.4
1	A	402	LEU	3.3
1	A	75	GLN	3.2
1	B	73	HIS	3.0
1	A	146	GLY	3.0
1	A	76	LYS	2.9
1	A	323	CYS	2.9
1	A	149	GLU	2.9
1	A	260	GLY	2.8
1	B	346	ASN	2.7
1	A	404	HIS	2.7
1	A	310	LEU	2.7
1	B	217	GLY	2.6
1	B	403	HIS	2.6
1	B	147	PHE	2.6
1	A	308	PHE	2.5
1	B	280	PHE	2.5
1	A	212	GLN	2.5
1	B	332	ASP	2.5
1	A	221	ARG	2.4
1	B	285	ASN	2.4
1	B	330	ASN	2.4
1	B	281	LEU	2.3
1	A	217	GLY	2.3
1	B	162	THR	2.3
1	B	77	GLY	2.3
1	A	145	LEU	2.2
1	B	398	LYS	2.2
1	A	360	ARG	2.1
1	B	151	LEU	2.1
1	A	327	TYR	2.1
1	B	74	MET	2.1
1	A	329	ALA	2.1
1	B	76	LYS	2.1
1	B	360	ARG	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)

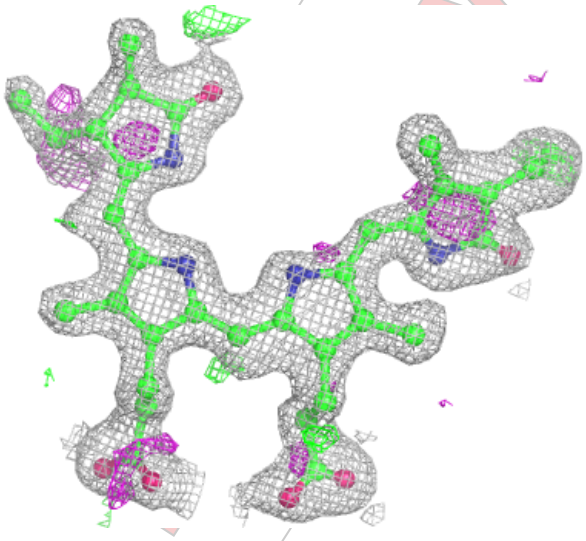
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

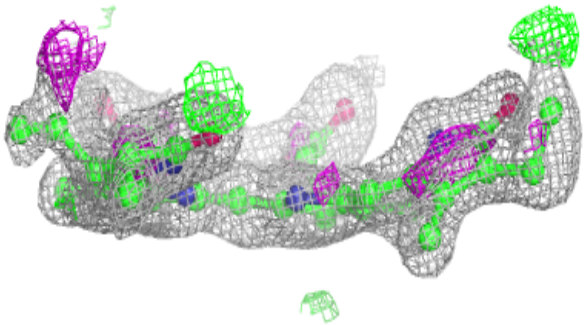
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CYC	A	500	43/43	0.82	0.14	27,43,49,52	0
4	PEG	A	504	7/7	0.83	0.20	62,65,69,71	0
5	PGE	A	505	10/10	0.83	0.15	37,47,59,59	0
3	1PE	B	501	16/16	0.84	0.16	33,45,57,61	0
4	PEG	A	503	7/7	0.88	0.13	29,39,47,48	0
2	CYC	B	500	43/43	0.89	0.11	27,38,45,47	0
3	1PE	A	501	16/16	0.91	0.10	18,27,32,35	0
3	1PE	A	502	16/16	0.91	0.12	26,36,50,53	0

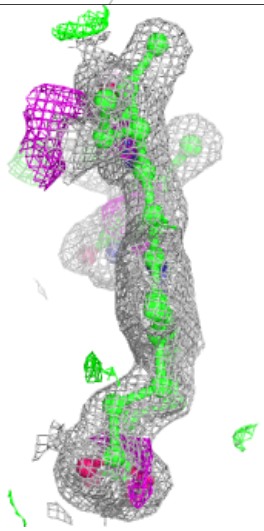
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC A 500:

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

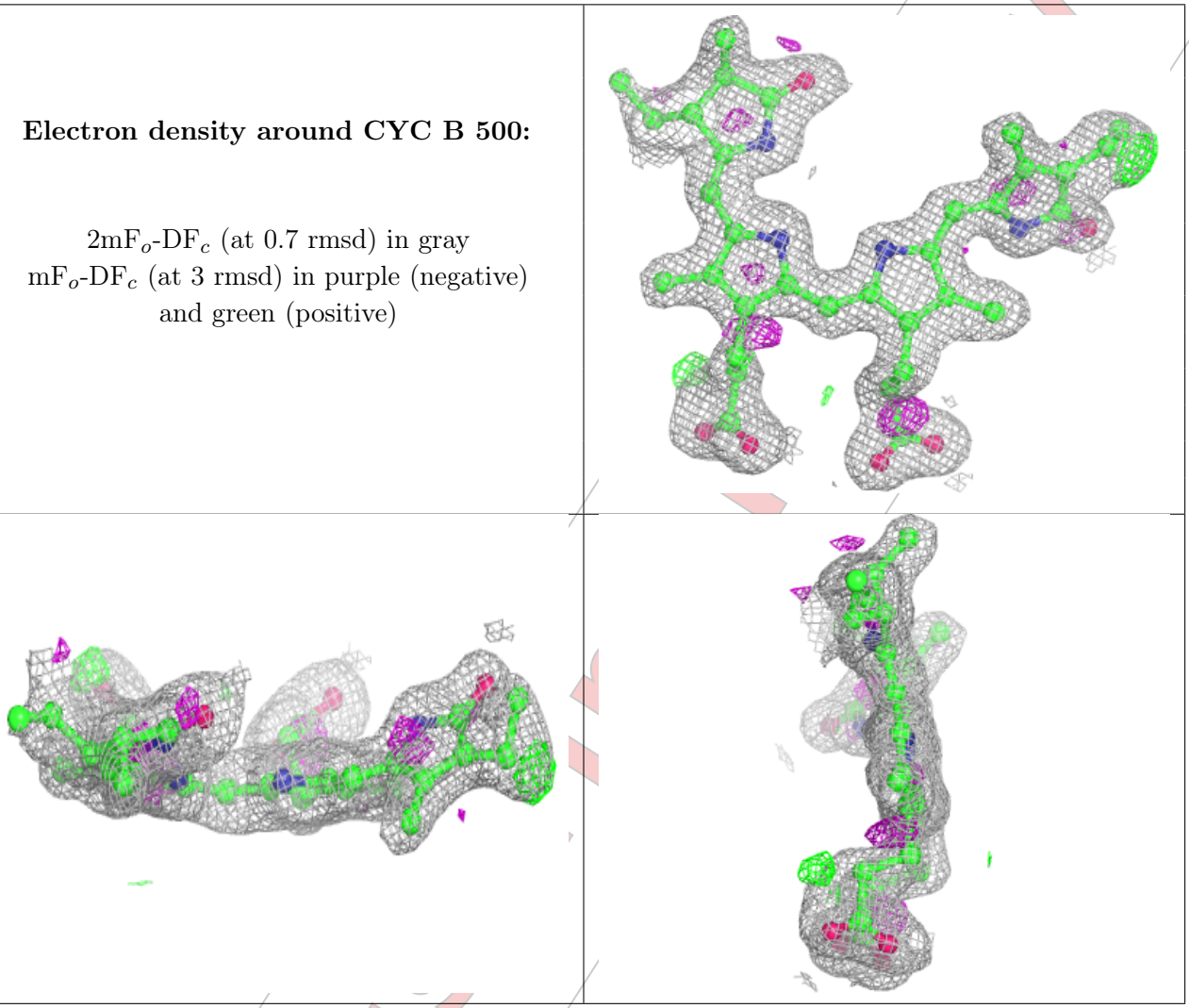






Electron density around CYC B 500:

$2mF_o$-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.