Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:58 am BST

PDB ID	:	2VEA
Title	:	The complete sensory module of the cyanobacterial phytochrome Cph1 in the Pr-state.
Authors	:	Essen, L.-O.; Mailliet, J.; Hughes, J.
Deposited on	:	2007-10-18
Resolution	:	2.21 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:

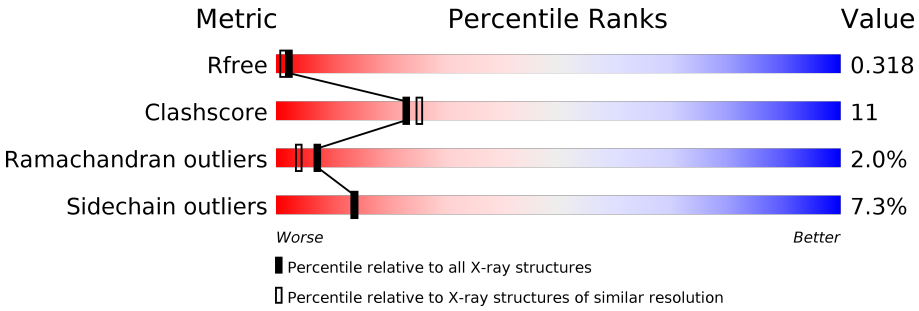
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	520	70% 24%

2 Entry composition

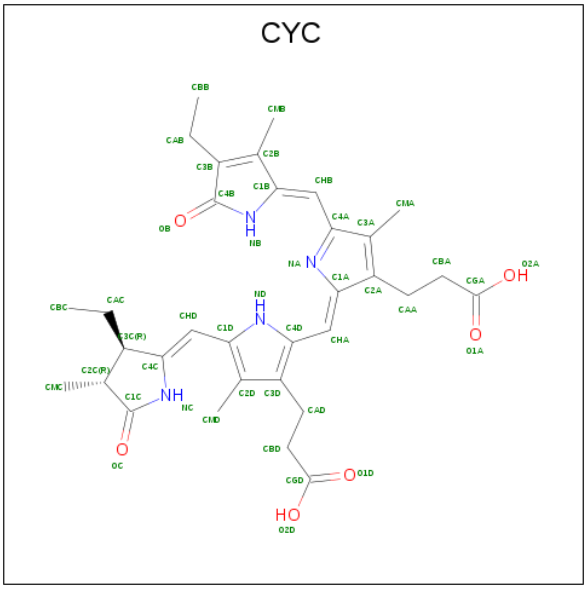
There are 3 unique types of molecules in this entry. The entry contains 4022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CPH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	2	0
			3950	2527	690	720	13			

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 3 is water.

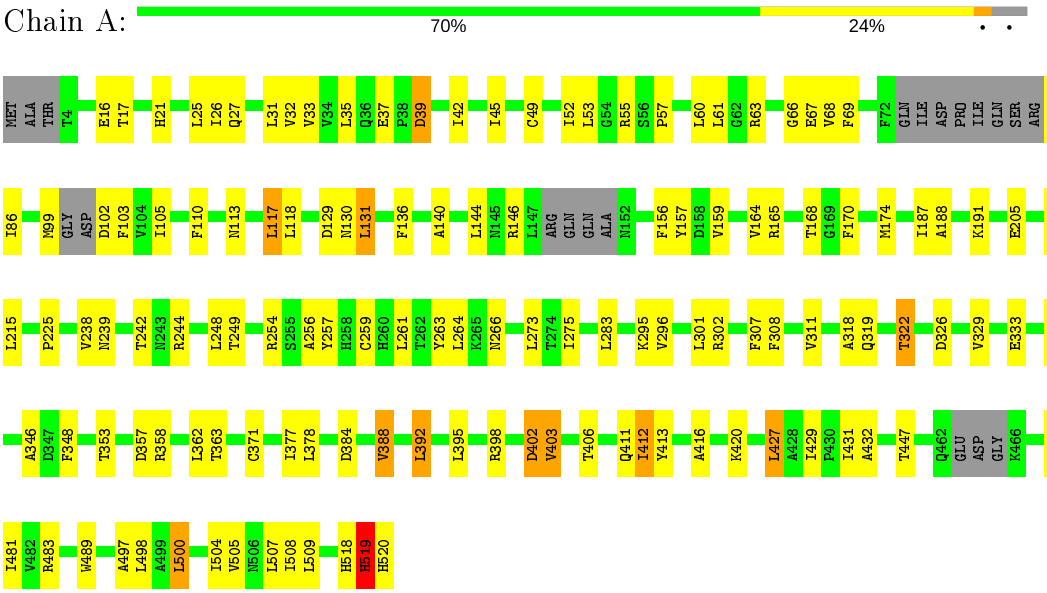
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		

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. 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. 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 CPH1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.18Å 77.18Å 249.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.68 – 2.21 24.68 – 2.21	Depositor EDS
% Data completeness (in resolution range)	68.1 (24.68-2.21) 68.1 (24.68-2.21)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.271 0.326 , 0.318	Depositor DCC
R_{free} test set	1097 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4022	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/4049	0.54	0/5510

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	518	HIS	Peptide
1	A	67	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3950	0	3873	85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	36	11	0
3	A	29	0	0	1	0
All	All	4022	0	3909	90	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 11.

All (90) 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:343:THR:HG22	1:A:507:LEU:HD21	1.42	0.98
1:A:215:LEU:HD12	1:A:249:THR:HG23	1.46	0.96
1:A:239:ASN:HB3	1:A:242:THR:HG22	1.62	0.82
1:A:318:ALA:O	1:A:322:THR:HG22	1.82	0.78
1:A:307:PHE:O	1:A:311:VAL:HG23	1.84	0.77
1:A:447:THR:HG22	1:A:481:ILE:HD12	1.69	0.75
1:A:263:TYR:OH	2:A:1521:CYC:HMB3	1.87	0.74
1:A:174:MET:CE	2:A:1521:CYC:HBB3	2.18	0.74
1:A:174:MET:HE3	2:A:1521:CYC:HBB3	1.69	0.74
1:A:403:VAL:HG21	1:A:498:LEU:HD11	1.74	0.69
2:A:1521:CYC:HMA1	2:A:1521:CYC:NB	2.09	0.68
1:A:378:LEU:HD11	1:A:388:VAL:HG11	1.77	0.67
1:A:37:GLU:CB	1:A:81:LEU:HD13	2.24	0.67
1:A:68:VAL:HG13	1:A:69:PHE:CD2	2.28	0.67
1:A:326:ASP:O	1:A:329:VAL:HG22	1.95	0.66
1:A:429:ILE:HD13	1:A:498:LEU:HD12	1.76	0.66
2:A:1521:CYC:HB	2:A:1521:CYC:HMA1	1.61	0.65
1:A:429:ILE:CD1	1:A:497:ALA:HB1	2.27	0.64
1:A:402:ASP:O	1:A:403:VAL:HG23	1.99	0.63
1:A:31:LEU:HD21	1:A:52:ILE:HD11	1.80	0.63
1:A:168:THR:HG23	1:A:170:PHE:H	1.64	0.62
1:A:31:LEU:CD2	1:A:52:ILE:HD11	2.33	0.59
1:A:371:CYS:HB2	1:A:392:LEU:HD21	1.84	0.58
1:A:81:LEU:HD11	1:A:118:LEU:HD22	1.84	0.58
1:A:429:ILE:HD12	1:A:497:ALA:HB1	1.86	0.58
1:A:16:GLU:HG3	1:A:17:THR:HG23	1.88	0.56
1:A:429:ILE:CD1	1:A:498:LEU:HD12	2.37	0.55
2:A:1521:CYC:HB	2:A:1521:CYC:CMA	2.19	0.55
1:A:49:CYS:HB2	1:A:53:LEU:HD12	1.87	0.55
1:A:86:ILE:HG23	1:A:110:PHE:HB2	1.91	0.53
1:A:256:ALA:HB3	1:A:261:LEU:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:THR:CG2	1:A:377:ILE:HG21	2.39	0.53
1:A:342:MET:CG	1:A:348:PHE:HB2	2.39	0.52
1:A:505:VAL:O	1:A:509:LEU:HD23	2.10	0.52
1:A:431:ILE:O	1:A:432:ALA:HB3	2.10	0.52
1:A:131:LEU:HD22	1:A:136:PHE:CZ	2.46	0.51
1:A:257:TYR:HD2	2:A:1521:CYC:HMD2	1.76	0.51
1:A:519:HIS:CG	1:A:520:HIS:N	2.79	0.51
1:A:429:ILE:HD11	1:A:497:ALA:CB	2.41	0.51
1:A:168:THR:O	1:A:295:LYS:NZ	2.43	0.51
1:A:337:VAL:HG21	1:A:358:ARG:CZ	2.42	0.50
1:A:504:ILE:O	1:A:508:ILE:HD12	2.11	0.50
1:A:429:ILE:HD11	1:A:497:ALA:HB1	1.93	0.50
1:A:413:TYR:HD1	1:A:416:ALA:HB2	1.77	0.49
1:A:481:ILE:O	1:A:481:ILE:HG23	2.12	0.49
1:A:42:ILE:HB	1:A:61:LEU:O	2.13	0.49
1:A:156:PHE:O	1:A:159:VAL:HG12	2.12	0.48
1:A:33:VAL:HG23	1:A:35:LEU:HD21	1.94	0.48
1:A:447:THR:HG22	1:A:481:ILE:CD1	2.40	0.48
1:A:481:ILE:HG21	1:A:483:ARG:HH21	1.78	0.48
1:A:174:MET:HE3	2:A:1521:CYC:OB	2.14	0.48
1:A:144:LEU:O	1:A:144:LEU:HD23	2.14	0.48
1:A:248:LEU:HB2	1:A:254:ARG:HD3	1.96	0.48
1:A:164:VAL:O	1:A:168:THR:HG22	2.14	0.47
1:A:296:VAL:O	1:A:296:VAL:HG23	2.13	0.47
1:A:33:VAL:HG12	1:A:45:ILE:HG13	1.96	0.47
1:A:157:TYR:CE1	1:A:187:ILE:HD12	2.50	0.47
1:A:26:ILE:HG21	1:A:32:VAL:HG23	1.96	0.46
1:A:406:THR:HG21	1:A:412:ILE:HD11	1.96	0.46
1:A:257:TYR:CD2	2:A:1521:CYC:HMD2	2.50	0.46
1:A:353:THR:HG21	1:A:377:ILE:HG21	1.98	0.46
1:A:384:ASP:O	1:A:388:VAL:HG12	2.16	0.45
1:A:238:VAL:HG23	1:A:244:ARG:C	2.37	0.45
1:A:33:VAL:HG23	1:A:35:LEU:CD2	2.47	0.45
1:A:105:ILE:HD12	1:A:105:ILE:N	2.31	0.45
2:A:1521:CYC:HBD2	2:A:1521:CYC:HMD1	1.97	0.45
2:A:1521:CYC:HBA2	2:A:1521:CYC:CMA	2.47	0.45
1:A:140:ALA:HB1	1:A:308:PHE:CE1	2.52	0.45
1:A:165:ARG:NE	1:A:170:PHE:O	2.50	0.44
1:A:165:ARG:HA	1:A:168:THR:HG22	2.00	0.44
1:A:55:ARG:HD2	1:A:68:VAL:HG23	2.00	0.44
1:A:256:ALA:HB3	1:A:261:LEU:CD1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HG2	1:A:283:LEU:HD23	1.99	0.44
1:A:319:GLN:HA	1:A:322:THR:HG23	2.00	0.43
1:A:403:VAL:CG2	1:A:498:LEU:HD11	2.46	0.43
1:A:130:ASN:HB3	1:A:131:LEU:HD23	2.01	0.43
1:A:157:TYR:HB3	1:A:188:ALA:HB2	2.01	0.42
1:A:371:CYS:CB	1:A:392:LEU:HD21	2.49	0.42
1:A:26:ILE:N	1:A:26:ILE:HD12	2.35	0.42
1:A:113:ASN:HB2	1:A:117:LEU:HD22	2.01	0.42
1:A:333:GLU:O	1:A:337:VAL:HG23	2.19	0.42
1:A:273:LEU:HD11	1:A:302:ARG:HG2	2.02	0.41
1:A:264:LEU:HD11	3:A:2029:HOH:O	2.19	0.41
1:A:130:ASN:CB	1:A:131:LEU:HD23	2.51	0.41
1:A:481:ILE:HG21	1:A:483:ARG:NH2	2.36	0.41
1:A:427:LEU:HB2	1:A:489:TRP:CH2	2.55	0.41
1:A:103:PHE:CD2	1:A:105:ILE:HD11	2.56	0.41
1:A:27:GLN:OE1	1:A:225:PRO:HD2	2.20	0.41
1:A:362:LEU:HD21	1:A:500:LEU:HB2	2.03	0.41
1:A:363:THR:HG21	1:A:497:ALA:HB2	2.04	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	492/520 (95%)	457 (93%)	25 (5%)	10 (2%)	7 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	346	ALA
1	A	83	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	519	HIS
1	A	60	LEU
1	A	146	ARG
1	A	402	ASP
1	A	66	GLY
1	A	403	VAL
1	A	57	PRO

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	425/453 (94%)	394 (93%)	31 (7%)	14 14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	25	LEU
1	A	39	ASP
1	A	63	ARG
1	A	99	MET
1	A	102	ASP
1	A	117	LEU
1	A	129	ASP
1	A	131	LEU
1	A	191	LYS
1	A	205	GLU
1	A	210	GLN
1	A	214	ARG
1	A	259	CYS
1	A	266	ASN
1	A	275	ILE
1	A	301	LEU
1	A	322	THR
1	A	357	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	388	VAL
1	A	392	LEU
1	A	395	LEU
1	A	398	ARG
1	A	411	GLN
1	A	412	ILE
1	A	420	LYS
1	A	427	LEU
1	A	469	LEU
1	A	473	GLN
1	A	500	LEU
1	A	519	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	85	GLN
1	A	138	HIS
1	A	266	ASN
1	A	290	HIS
1	A	319	GLN
1	A	330	GLN
1	A	397	ASN
1	A	411	GLN
1	A	435	ASN
1	A	449	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand 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	CYC	A	1521	1	36,46,46	4.21	16 (44%)	44,67,67	3.42	21 (47%)

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	CYC	A	1521	1	-	9/21/74/74	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1521	CYC	CHA-C1A	14.74	1.47	1.35
2	A	1521	CYC	OB-C4B	13.05	1.48	1.23
2	A	1521	CYC	C1C-NC	-8.03	1.27	1.37
2	A	1521	CYC	C2A-C3A	5.54	1.48	1.36
2	A	1521	CYC	OC-C1C	5.04	1.33	1.23
2	A	1521	CYC	C4B-C3B	-4.59	1.39	1.48
2	A	1521	CYC	CHB-C1B	4.37	1.48	1.38
2	A	1521	CYC	C1B-C2B	-3.70	1.38	1.45
2	A	1521	CYC	CHB-C4A	3.61	1.48	1.40
2	A	1521	CYC	C3D-C2D	3.33	1.47	1.37
2	A	1521	CYC	CBD-CAD	-3.00	1.32	1.53
2	A	1521	CYC	C4A-C3A	-2.53	1.40	1.45
2	A	1521	CYC	CAD-C3D	-2.43	1.48	1.52
2	A	1521	CYC	C1D-CHD	2.25	1.49	1.41
2	A	1521	CYC	C2C-C1C	-2.20	1.50	1.52
2	A	1521	CYC	C1A-NA	-2.08	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1521	CYC	C3B-C4B-NB	11.38	115.97	106.78
2	A	1521	CYC	C1B-NB-C4B	-7.02	101.73	110.67
2	A	1521	CYC	CAB-C3B-C4B	6.52	131.67	121.38
2	A	1521	CYC	C4D-CHA-C1A	6.06	136.04	128.81
2	A	1521	CYC	OB-C4B-C3B	-5.65	121.91	128.04
2	A	1521	CYC	C2C-C1C-NC	5.51	113.02	108.27
2	A	1521	CYC	CHB-C4A-NA	-4.92	114.63	124.93
2	A	1521	CYC	CAD-CBD-CGD	4.86	120.83	112.67
2	A	1521	CYC	OC-C1C-C2C	-4.31	122.75	126.17
2	A	1521	CYC	CBD-CAD-C3D	4.24	120.30	112.49
2	A	1521	CYC	C1A-C2A-C3A	-3.77	102.61	106.78
2	A	1521	CYC	C2B-C1B-NB	3.44	112.02	106.99
2	A	1521	CYC	CAA-CBA-CGA	-3.06	107.55	112.67
2	A	1521	CYC	CAA-C2A-C3A	2.95	133.37	127.88
2	A	1521	CYC	C4A-C3A-C2A	-2.87	103.22	106.51
2	A	1521	CYC	CMD-C2D-C3D	2.81	130.24	124.94
2	A	1521	CYC	C3A-C4A-NA	2.77	116.45	110.53
2	A	1521	CYC	C2A-C1A-NA	2.56	113.77	110.05
2	A	1521	CYC	CHA-C1A-C2A	-2.48	119.59	125.32
2	A	1521	CYC	CMA-C3A-C4A	2.43	128.81	125.06
2	A	1521	CYC	CHB-C1B-C2B	-2.16	122.67	126.95

There are no chirality outliers.

All (9) torsion outliers are listed below:

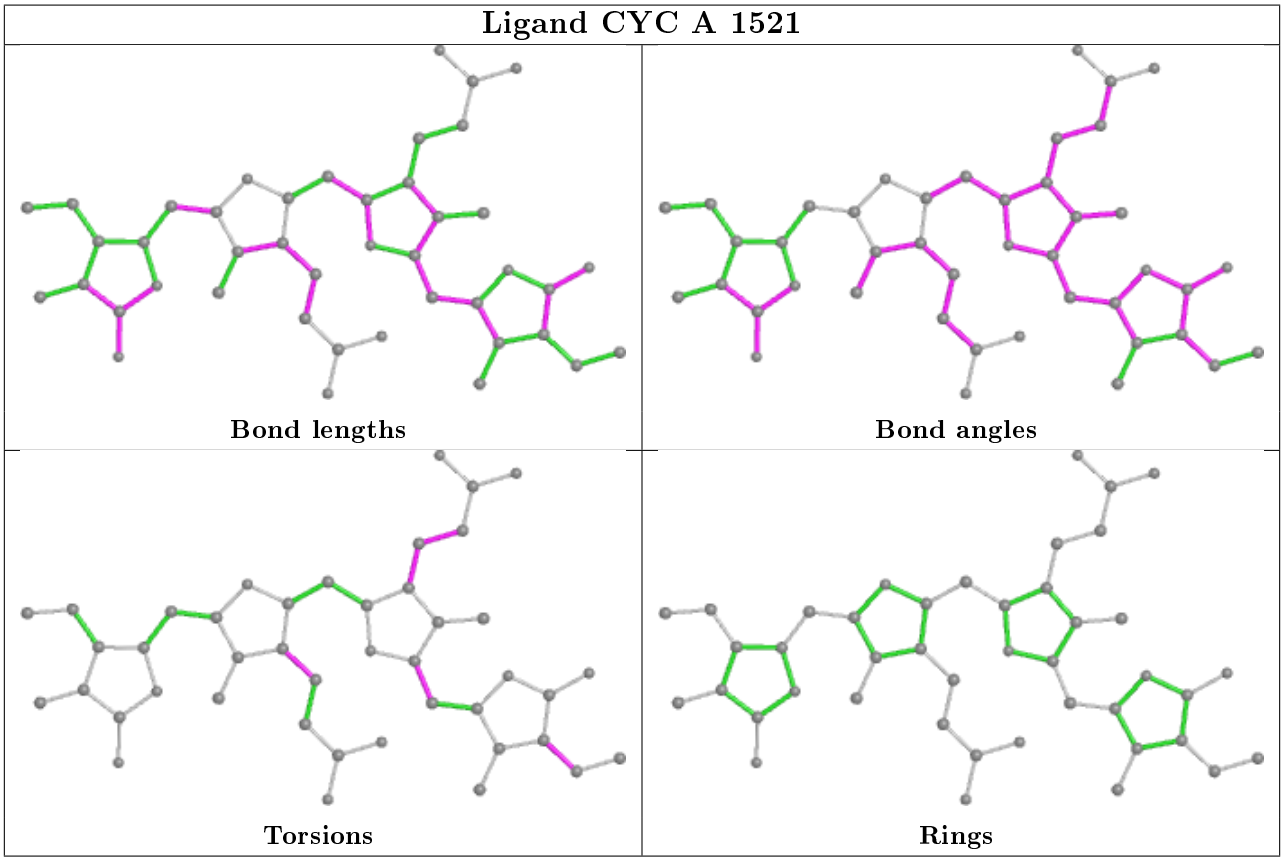
Mol	Chain	Res	Type	Atoms
2	A	1521	CYC	C3A-C2A-CAA-CBA
2	A	1521	CYC	NA-C4A-CHB-C1B
2	A	1521	CYC	C2D-C3D-CAD-CBD
2	A	1521	CYC	C4D-C3D-CAD-CBD
2	A	1521	CYC	C2B-C3B-CAB-CBB
2	A	1521	CYC	C1A-C2A-CAA-CBA
2	A	1521	CYC	C4B-C3B-CAB-CBB
2	A	1521	CYC	C3A-C4A-CHB-C1B
2	A	1521	CYC	C2A-CAA-CBA-CGA

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1521	CYC	11	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.



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

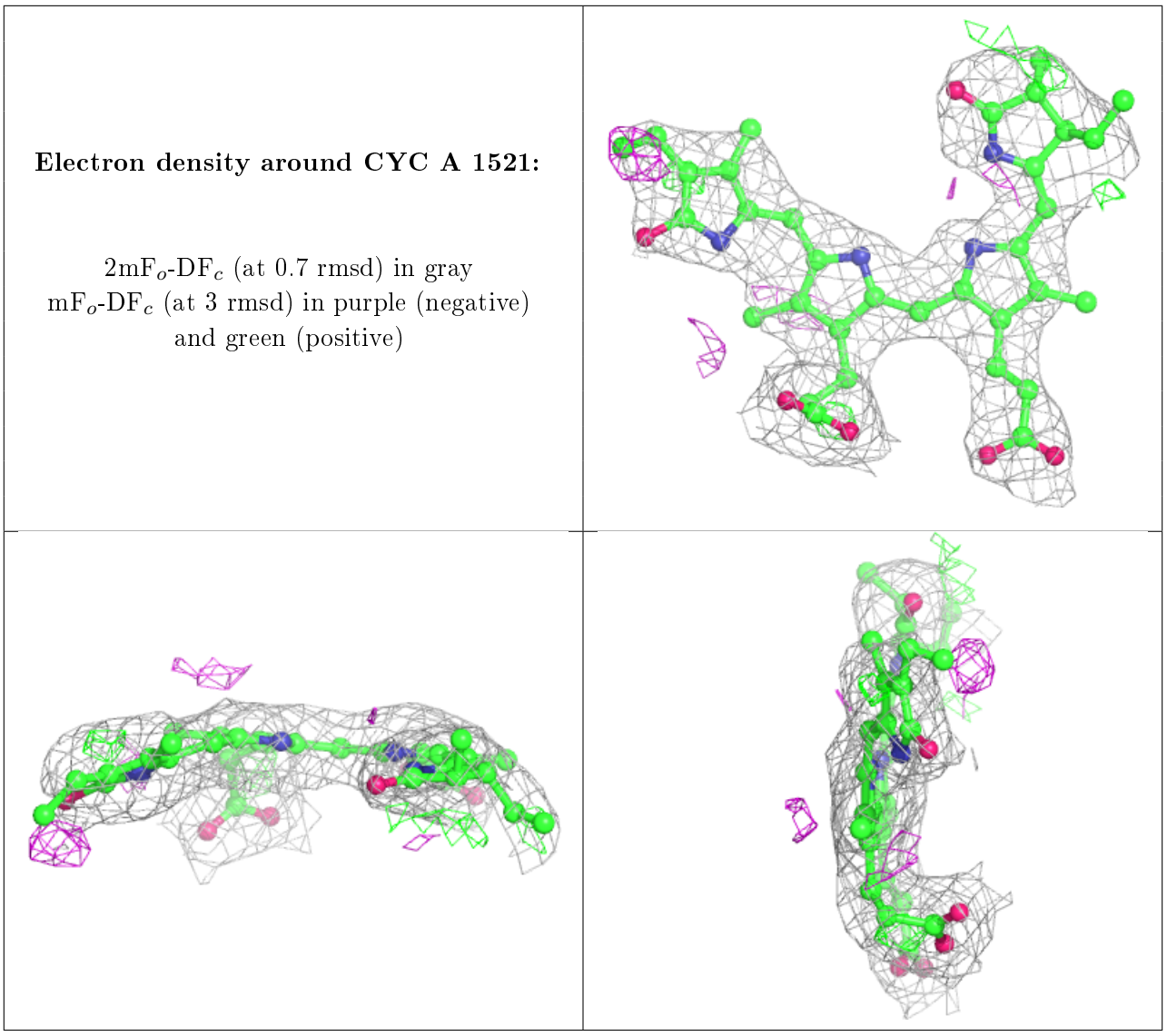
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 1521:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.