Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 05:17 PM EST

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 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:

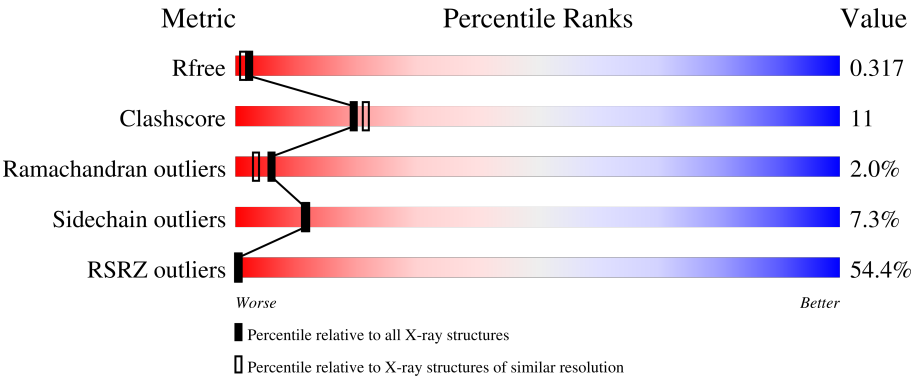
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (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 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%

Mol	Chain	Length	Quality of chain
1	A	520	52% 70% 24%

2 Entry composition

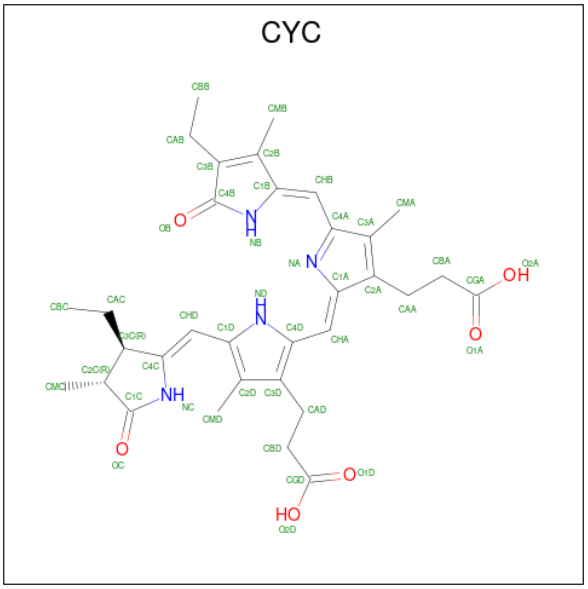
There are 3 unique types of molecules in this entry. The entry contains 4022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, 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. 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) 68.0 (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 , 0.317	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)	0.35 , 52.0	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

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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:NB	2:A:1521:CYC:HMA1	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:HMA1	2:A:1521:CYC:HB	1.61	0.65
1:A:429:ILE:CD1	1:A:497:ALA:HB1	2.27	0.64
1:A:31:LEU:HD21	1:A:52:ILE:HD11	1.80	0.63
1:A:402:ASP:O	1:A:403:VAL:HG23	1.99	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:81:LEU:HD11	1:A:118:LEU:HD22	1.84	0.58
1:A:371:CYS:HB2	1:A:392:LEU:HD21	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

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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:HD23	1:A:144:LEU:O	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:HMD1	2:A:1521:CYC:HBD2	1.97	0.45
1:A:140:ALA:HB1	1:A:308:PHE:CE1	2.52	0.45
2:A:1521:CYC:CMA	2:A:1521:CYC:HBA2	2.47	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:213:ARG:HG2	1:A:283:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:HB3	1:A:261:LEU:CD1	2.48	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:HD12	1:A:26:ILE:N	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%)	6 3

All (10) Ramachandran outliers are listed below:

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

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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%)	11 12

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

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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

Sometimes 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 oligosaccharides 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	42,46,46	3.78	16 (38%)	52,67,67	3.18	24 (46%)

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	-	13/25/74/74	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	OB-C4B	13.09	1.48	1.23
2	A	1521	CYC	CHA-C1A	12.76	1.47	1.35
2	A	1521	CYC	C1C-NC	-8.01	1.27	1.37
2	A	1521	CYC	C2A-C3A	5.44	1.48	1.36
2	A	1521	CYC	OC-C1C	5.21	1.33	1.23
2	A	1521	CYC	C4B-C3B	-4.75	1.39	1.48
2	A	1521	CYC	CHB-C1B	4.40	1.48	1.37
2	A	1521	CYC	CAD-CBD	-4.23	1.32	1.52
2	A	1521	CYC	C1B-C2B	-3.72	1.38	1.45
2	A	1521	CYC	CHB-C4A	3.58	1.48	1.40
2	A	1521	CYC	C3D-C2D	3.33	1.47	1.37
2	A	1521	CYC	C4A-C3A	-2.51	1.40	1.45
2	A	1521	CYC	C2C-C1C	-2.20	1.50	1.52
2	A	1521	CYC	C1A-NA	-2.11	1.34	1.38
2	A	1521	CYC	C4C-NC	-2.10	1.33	1.37
2	A	1521	CYC	C1D-CHD	2.06	1.49	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1521	CYC	C3B-C4B-NB	11.54	115.97	106.77
2	A	1521	CYC	C1B-NB-C4B	-7.28	101.73	110.66
2	A	1521	CYC	CAB-C3B-C4B	6.66	131.67	121.37
2	A	1521	CYC	OB-C4B-C3B	-5.83	121.91	128.03
2	A	1521	CYC	C2C-C1C-NC	5.69	113.02	108.29
2	A	1521	CYC	C4D-CHA-C1A	5.46	136.04	128.73
2	A	1521	CYC	CHB-C4A-NA	-4.78	114.63	124.95
2	A	1521	CYC	CBD-CAD-C3D	4.62	120.30	112.54
2	A	1521	CYC	OC-C1C-C2C	-4.31	122.75	126.17
2	A	1521	CYC	C1A-C2A-C3A	-3.80	102.61	106.73
2	A	1521	CYC	C2B-C1B-NB	3.47	112.02	106.97
2	A	1521	CYC	CAA-C2A-C3A	2.94	133.37	127.87
2	A	1521	CYC	C4A-C3A-C2A	-2.87	103.22	106.48
2	A	1521	CYC	CMD-C2D-C3D	2.81	130.24	124.94
2	A	1521	CYC	C3A-C4A-NA	2.68	116.45	110.58
2	A	1521	CYC	C2A-C1A-NA	2.63	113.77	110.04
2	A	1521	CYC	C3C-C4C-NC	2.61	111.31	107.94
2	A	1521	CYC	CAD-CBD-CGD	2.60	120.83	113.83
2	A	1521	CYC	CHA-C1A-C2A	-2.52	119.59	125.40
2	A	1521	CYC	CMA-C3A-C4A	2.39	128.81	125.10
2	A	1521	CYC	O1D-CGD-CBD	-2.34	115.66	123.09
2	A	1521	CYC	CAA-CBA-CGA	-2.31	107.55	113.67
2	A	1521	CYC	CHB-C1B-C2B	-2.16	122.67	126.97
2	A	1521	CYC	O2D-CGD-CBD	2.10	120.63	114.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

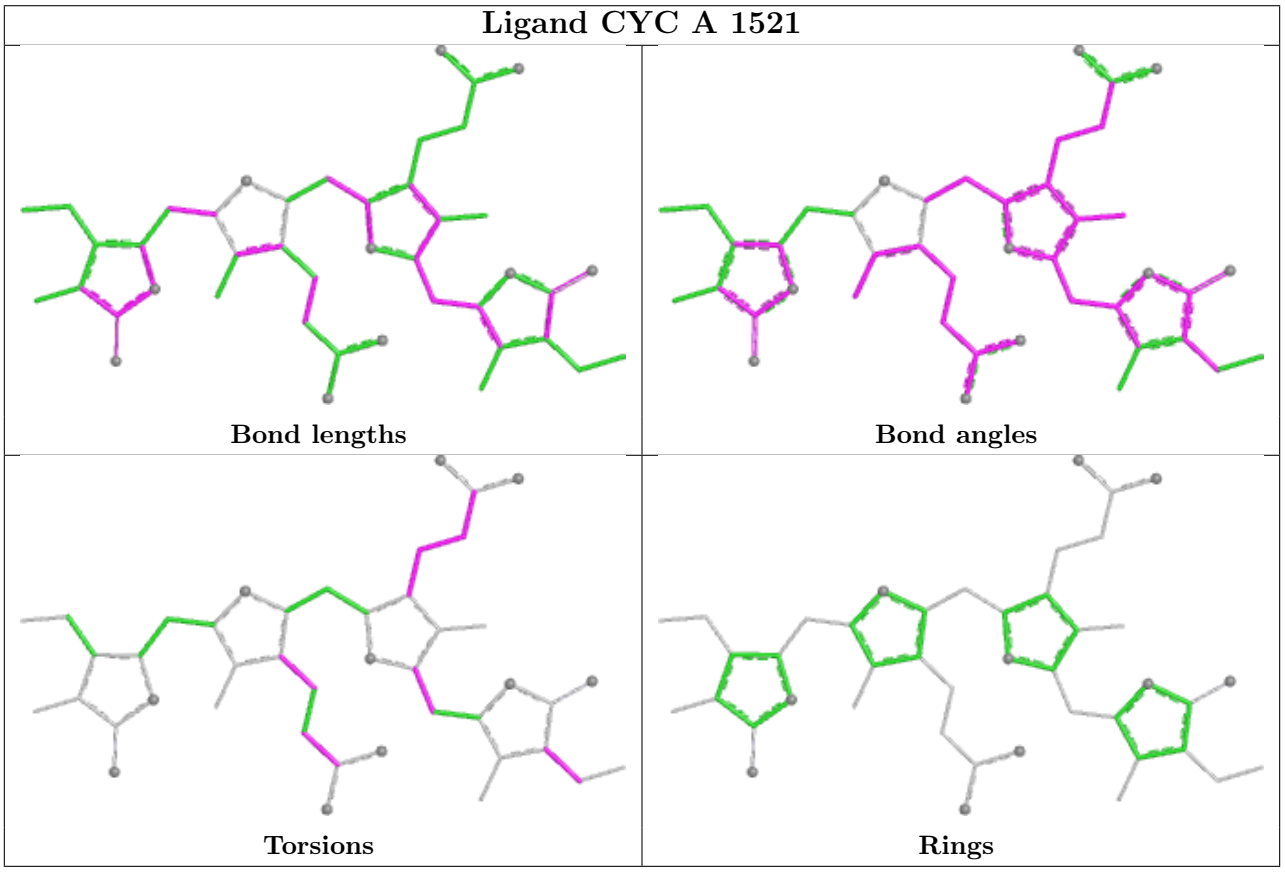
Mol	Chain	Res	Type	Atoms
2	A	1521	CYC	C3A-C2A-CAA-CBA
2	A	1521	CYC	NA-C4A-CHB-C1B
2	A	1521	CYC	C2D-C3D-CAD-CBD
2	A	1521	CYC	C4D-C3D-CAD-CBD
2	A	1521	CYC	C2B-C3B-CAB-CBB
2	A	1521	CYC	C1A-C2A-CAA-CBA
2	A	1521	CYC	C4B-C3B-CAB-CBB
2	A	1521	CYC	C3A-C4A-CHB-C1B
2	A	1521	CYC	C2A-CAA-CBA-CGA
2	A	1521	CYC	CAA-CBA-CGA-O2A
2	A	1521	CYC	CAA-CBA-CGA-O1A
2	A	1521	CYC	CAD-CBD-CGD-O2D
2	A	1521	CYC	CAD-CBD-CGD-O1D

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

Warning: The R factor obtained from EDS is 0.3318, which does not match the depositor's R factor of 0.244. Please interpret the results in this section carefully.

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	500/520 (96%)	2.25	272 (54%) 0 0	44, 79, 84, 90	2 (0%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	6.8
1	A	237	ALA	6.4
1	A	54	GLY	6.4
1	A	195	MET	6.3
1	A	238	VAL	6.1
1	A	351	GLY	5.9
1	A	142	ALA	5.6
1	A	393	GLN	5.5
1	A	245	ALA	5.1
1	A	82	THR	5.0
1	A	242	THR	4.8
1	A	61	LEU	4.7
1	A	353	THR	4.7
1	A	194	ASP	4.7
1	A	81	LEU	4.6
1	A	461	THR	4.6
1	A	239	ASN	4.6
1	A	186	VAL	4.5
1	A	329	VAL	4.5
1	A	98	VAL	4.4
1	A	175	LEU	4.4
1	A	36	GLN	4.4
1	A	283	LEU	4.4
1	A	453	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	144	LEU	4.4
1	A	132	PRO	4.3
1	A	37	GLU	4.3
1	A	232	VAL	4.3
1	A	38	PRO	4.2
1	A	21	HIS	4.2
1	A	50	THR	4.1
1	A	520	HIS	4.1
1	A	424	SER	4.1
1	A	298	PRO	4.0
1	A	41	THR	4.0
1	A	143	ALA	4.0
1	A	161	VAL	3.8
1	A	346	ALA	3.8
1	A	64	THR	3.8
1	A	304	ALA	3.7
1	A	113	ASN	3.7
1	A	214	ARG	3.7
1	A	285	GLY	3.7
1	A	395	LEU	3.7
1	A	199	LEU	3.7
1	A	240	PRO	3.7
1	A	129	ASP	3.7
1	A	135	GLY	3.7
1	A	7	LEU	3.6
1	A	12	LEU	3.6
1	A	56	SER	3.6
1	A	131	LEU	3.6
1	A	310[A]	ARG	3.6
1	A	475	PHE	3.6
1	A	49	CYS	3.5
1	A	411	GLN	3.5
1	A	145	ASN	3.5
1	A	418	ASN	3.5
1	A	86	ILE	3.5
1	A	307	PHE	3.5
1	A	34	VAL	3.5
1	A	116	GLY	3.5
1	A	402	ASP	3.5
1	A	200	GLY	3.4
1	A	513	GLU	3.4
1	A	360	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	130	ASN	3.4
1	A	396	GLU	3.4
1	A	170	PHE	3.4
1	A	422	VAL	3.4
1	A	426	LEU	3.4
1	A	84	GLY	3.4
1	A	196	GLU	3.4
1	A	188	ALA	3.4
1	A	85	GLN	3.3
1	A	137	TYR	3.3
1	A	273	LEU	3.3
1	A	96	ALA	3.3
1	A	217	ILE	3.2
1	A	352	LEU	3.2
1	A	427	LEU	3.2
1	A	316	ILE	3.2
1	A	246	VAL	3.2
1	A	284	TRP	3.2
1	A	439	TRP	3.2
1	A	146	ARG	3.2
1	A	257	TYR	3.2
1	A	350	GLU	3.2
1	A	282	HIS	3.1
1	A	22	THR	3.1
1	A	369	ALA	3.1
1	A	505	VAL	3.1
1	A	349	VAL	3.1
1	A	58	GLU	3.1
1	A	288	ALA	3.1
1	A	431	ILE	3.0
1	A	309	GLY	3.0
1	A	11	SER	3.0
1	A	178	PHE	3.0
1	A	367	GLY	3.0
1	A	180	GLU	3.0
1	A	136	PHE	3.0
1	A	348	PHE	3.0
1	A	274	THR	3.0
1	A	277	LEU	3.0
1	A	339	LEU	3.0
1	A	299	PHE	3.0
1	A	160	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	173	VAL	3.0
1	A	362	LEU	2.9
1	A	400	VAL	2.9
1	A	516	HIS	2.9
1	A	235	THR	2.9
1	A	139	MET	2.9
1	A	502	LYS	2.9
1	A	158	ASP	2.9
1	A	147	LEU	2.9
1	A	455	ASN	2.9
1	A	509	LEU	2.9
1	A	33	VAL	2.8
1	A	337	VAL	2.8
1	A	191	LYS	2.8
1	A	4	THR	2.8
1	A	25	LEU	2.8
1	A	354	ASN	2.8
1	A	10	GLN	2.8
1	A	71	SER	2.8
1	A	519	HIS	2.8
1	A	340	ASP	2.8
1	A	301	LEU	2.8
1	A	468	GLU	2.8
1	A	368	ALA	2.8
1	A	438	LEU	2.8
1	A	243	ASN	2.8
1	A	412	ILE	2.8
1	A	39	ASP	2.8
1	A	169	GLY	2.8
1	A	153	LEU	2.8
1	A	432	ALA	2.7
1	A	322	THR	2.7
1	A	390	TYR	2.7
1	A	440	PHE	2.7
1	A	112	ARG	2.7
1	A	510	ARG	2.7
1	A	407	SER	2.7
1	A	59	ASP	2.7
1	A	296	VAL	2.7
1	A	490	GLN	2.7
1	A	219	ASN	2.7
1	A	208	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	308	PHE	2.7
1	A	398	ARG	2.6
1	A	365	SER	2.6
1	A	57	PRO	2.6
1	A	247	ASP	2.6
1	A	295	LYS	2.6
1	A	379	VAL	2.6
1	A	287	ILE	2.6
1	A	377	ILE	2.6
1	A	488	PRO	2.6
1	A	363	THR	2.6
1	A	507	LEU	2.6
1	A	291	HIS	2.6
1	A	318	ALA	2.6
1	A	102	ASP	2.6
1	A	311	VAL	2.5
1	A	336	ALA	2.5
1	A	457	ALA	2.5
1	A	35	LEU	2.5
1	A	90	ASN	2.5
1	A	47	ALA	2.5
1	A	117	LEU	2.5
1	A	391	LEU	2.5
1	A	168	THR	2.5
1	A	138	HIS	2.5
1	A	126	TYR	2.5
1	A	220	PRO	2.5
1	A	460	ALA	2.5
1	A	491	SER	2.4
1	A	280	ASP	2.4
1	A	68	VAL	2.4
1	A	376	LEU	2.4
1	A	403	VAL	2.4
1	A	32	VAL	2.4
1	A	223	VAL	2.4
1	A	157	TYR	2.4
1	A	97	ARG	2.4
1	A	302	ARG	2.4
1	A	125	ALA	2.4
1	A	392	LEU	2.4
1	A	275	ILE	2.4
1	A	190	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	60	LEU	2.4
1	A	261	LEU	2.4
1	A	133	PHE	2.3
1	A	294	PRO	2.3
1	A	134	LEU	2.3
1	A	397	ASN	2.3
1	A	269	VAL	2.3
1	A	233	PRO	2.3
1	A	55	ARG	2.3
1	A	241	SER	2.3
1	A	518	HIS	2.3
1	A	292	GLN	2.3
1	A	359	LEU	2.3
1	A	423	ALA	2.3
1	A	297	ILE	2.3
1	A	511	GLN	2.3
1	A	16	GLU	2.3
1	A	388	VAL	2.3
1	A	216	PHE	2.3
1	A	258	HIS	2.3
1	A	394	TRP	2.3
1	A	127	THR	2.2
1	A	201	LEU	2.2
1	A	477	LEU	2.2
1	A	345	ALA	2.2
1	A	106	PHE	2.2
1	A	120	CYS	2.2
1	A	338	LEU	2.2
1	A	445	LEU	2.2
1	A	436	PHE	2.2
1	A	278	ILE	2.2
1	A	95	TRP	2.2
1	A	209	PRO	2.2
1	A	167	MET	2.2
1	A	43	SER	2.1
1	A	87	SER	2.1
1	A	305	CYS	2.1
1	A	378	LEU	2.1
1	A	470	HIS	2.1
1	A	356	PRO	2.1
1	A	387	ALA	2.1
1	A	495	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	413	TYR	2.1
1	A	317	SER	2.1
1	A	63	ARG	2.1
1	A	504	ILE	2.1
1	A	234	LEU	2.1
1	A	450	TRP	2.1
1	A	341	LYS	2.1
1	A	140	ALA	2.1
1	A	212	ALA	2.1
1	A	249	THR	2.1
1	A	332	ALA	2.1
1	A	198	TYR	2.1
1	A	312	VAL	2.1
1	A	67	GLU	2.1
1	A	419	PHE	2.1
1	A	514	GLU	2.1
1	A	347	ASP	2.1
1	A	441	ARG	2.1
1	A	224	ILE	2.1
1	A	152	ASN	2.1
1	A	182	ASN	2.1
1	A	478	TRP	2.1
1	A	159	VAL	2.1
1	A	172[A]	ARG	2.1
1	A	187	ILE	2.1
1	A	406	THR	2.1
1	A	380	GLY	2.0
1	A	128	SER	2.0
1	A	319	GLN	2.0
1	A	141	ASN	2.0
1	A	83	ALA	2.0
1	A	381	GLU	2.0
1	A	327	TYR	2.0
1	A	193	ASP	2.0
1	A	334	HIS	2.0
1	A	446	GLN	2.0
1	A	409	LEU	2.0
1	A	289	CYS	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)

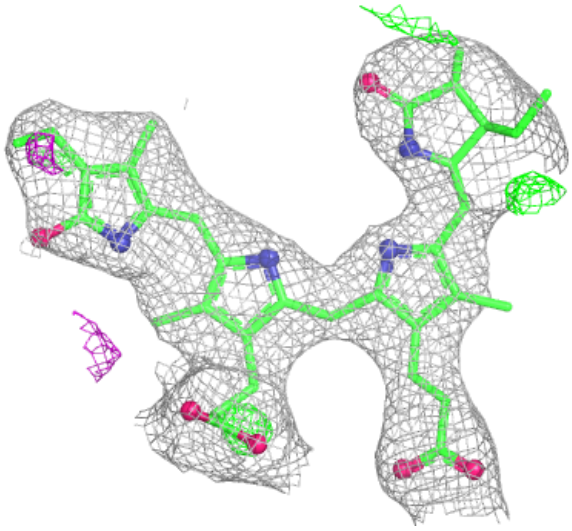
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

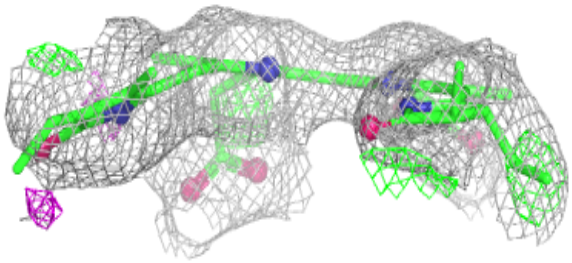
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CYC	A	1521	43/43	0.87	0.16	71,76,78,80	0

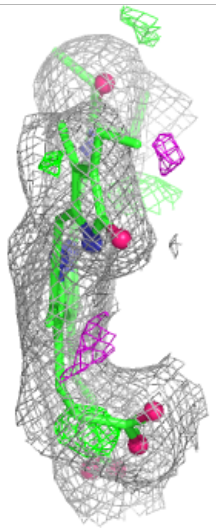
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC A 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)

There are no such residues in this entry.