



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:04 PM UTC

PDB ID : 2VEA / pdb_00002vea
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

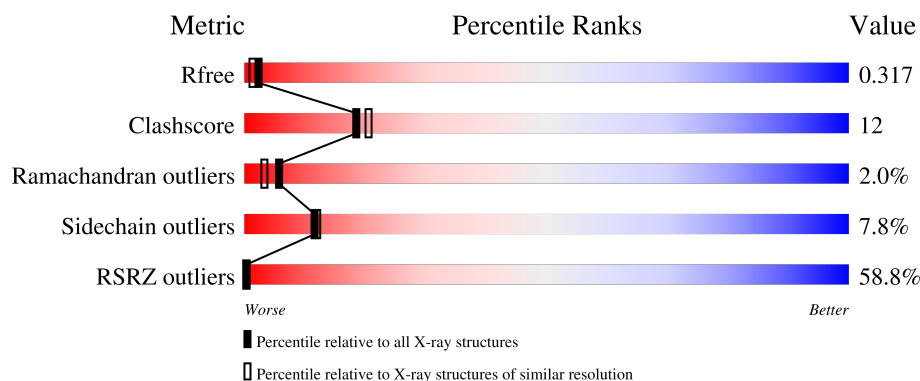
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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 $\leq 5\%$. 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	520	

2 Entry composition [i](#)

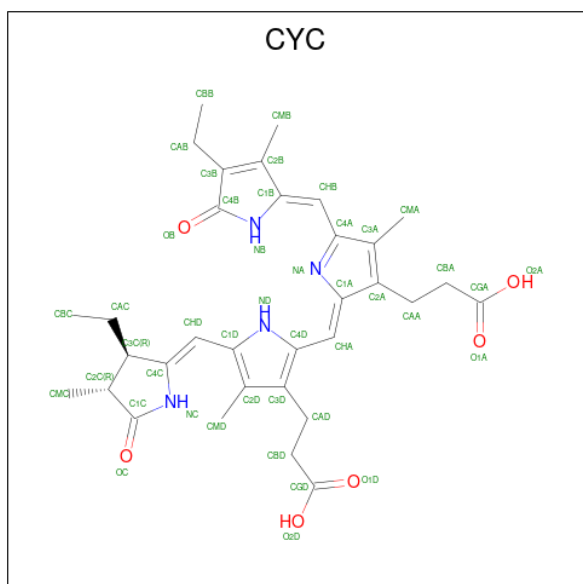
There are 3 unique types of molecules in this entry. The entry contains 4022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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

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

• Molecule 1: PHYTOCHROME-LIKE PROTEIN CPH1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.*

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: 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	0.48	0/4049	0.74	1/5510 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	68	VAL	N-CA-C	-7.55	105.31	111.81

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	90	0
2	A	43	0	36	11	0
3	A	29	0	0	1	0
All	All	4022	0	3909	95	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 12.

All (95) 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:174:MET:CE	2:A:1521:CYC:HBB3	2.18	0.74
1:A:403:VAL:HG21	1:A:498:LEU:HD11	1.74	0.69
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
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:174:MET:HE3	2:A:1521:CYC:HBB3	1.81	0.61
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
2:A:1521:CYC:HMA2	2:A:1521:CYC:HB	1.70	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:O	1:A:509:LEU:HD23	2.10	0.52
1:A:131:LEU:HD22	1:A:136:PHE:CZ	2.46	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:431:ILE:O	1:A:432:ALA:HB3	2.10	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:238:VAL:HG23	1:A:244:ARG:C	2.37	0.49
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:99:MET:N	1:A:99:MET:HE3	2.28	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: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
2:A:1521:CYC:HBA2	2:A:1521:CYC:HMA3	1.96	0.47
1:A:33:VAL:HG12	1:A:45:ILE:HG13	1.96	0.47
1:A:174:MET:HE1	2:A:1521:CYC:CBB	2.45	0.47
1:A:157:TYR:CE1	1:A:187:ILE:HD12	2.50	0.47
1:A:257:TYR:HB3	2:A:1521:CYC:HMD3	1.97	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:353:THR:HG21	1:A:377:ILE:HG21	1.98	0.46
1:A:174:MET:HE3	2:A:1521:CYC:OB	2.16	0.46
1:A:384:ASP:O	1:A:388:VAL:HG12	2.16	0.45
1:A:33:VAL:HG23	1:A:35:LEU:CD2	2.47	0.45
1:A:97:ARG:HB3	1:A:99:MET:HE1	1.99	0.45
1:A:105:ILE:HD12	1:A:105:ILE:N	2.31	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:263:TYR:OH	2:A:1521:CYC:CMB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:C	1:A:26:ILE:HD12	2.43	0.44
1:A:213:ARG:HG2	1:A:283:LEU:HD23	1.99	0.44
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:144:LEU:HD23	1:A:144:LEU:C	2.45	0.41
1:A:481:ILE:HG21	1:A:483:ARG:NH2	2.36	0.41
1:A:130:ASN:CG	1:A:131:LEU:HD23	2.45	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
2:A:1521:CYC:CMA	2:A:1521:CYC:NB	2.84	0.40
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
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 ⓘ

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%)	392 (92%)	33 (8%)	11	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	34	VAL
1	A	39	ASP
1	A	63	ARG
1	A	68	VAL
1	A	102	ASP
1	A	117	LEU
1	A	129	ASP
1	A	131	LEU
1	A	155	ASP
1	A	191	LYS
1	A	205	GLU
1	A	210	GLN
1	A	261	LEU
1	A	266	ASN
1	A	275	ILE
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	319	GLN
1	A	322	THR
1	A	330	GLN
1	A	357	ASP
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	485	GLN
1	A	500	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	85	GLN
1	A	111	HIS
1	A	138	HIS
1	A	145	ASN
1	A	260	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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	46,46,46	3.34	18 (39%)	63,67,67	3.13	31 (49%)

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	-	13/26/74/74	0/4/4/4

All (18) 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	C1C-NC	-8.01	1.27	1.37
2	A	1521	CYC	CBD-CAD	-5.60	1.32	1.51
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	CHA-C1A	4.63	1.47	1.38
2	A	1521	CYC	CHB-C1B	4.40	1.48	1.37
2	A	1521	CYC	CHD-C1D	4.20	1.49	1.40
2	A	1521	CYC	C1B-C2B	-3.72	1.38	1.45
2	A	1521	CYC	CHA-C4D	3.72	1.48	1.40
2	A	1521	CYC	CHB-C4A	3.58	1.48	1.40
2	A	1521	CYC	C3D-C2D	3.32	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1521	CYC	C1D-C2D	3.29	1.49	1.41
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

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	CHA-C4D-C3D	-5.18	116.09	127.22
2	A	1521	CYC	C1D-C2D-C3D	-5.03	101.47	107.76
2	A	1521	CYC	C2D-C1D-ND	4.79	113.96	107.43
2	A	1521	CYC	CHB-C4A-NA	-4.78	114.63	124.95
2	A	1521	CYC	OC-C1C-C2C	-4.31	122.75	126.17
2	A	1521	CYC	C3D-C4D-ND	4.23	112.88	107.57
2	A	1521	CYC	C1A-C2A-C3A	-3.80	102.61	106.73
2	A	1521	CYC	C4D-CHA-C1A	3.58	136.04	128.22
2	A	1521	CYC	C2B-C1B-NB	3.47	112.02	106.97
2	A	1521	CYC	CHD-C1D-C2D	-3.27	119.50	127.53
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	CBD-CAD-C3D	2.81	120.30	112.53
2	A	1521	CYC	CAD-CBD-CGD	2.70	120.83	113.67
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	CHA-C4D-ND	2.53	131.01	125.29
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	C4D-ND-C1D	-2.33	105.70	109.78
2	A	1521	CYC	CAA-CBA-CGA	-2.31	107.55	113.67
2	A	1521	CYC	CMD-C2D-C3D	2.17	130.24	125.62
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:

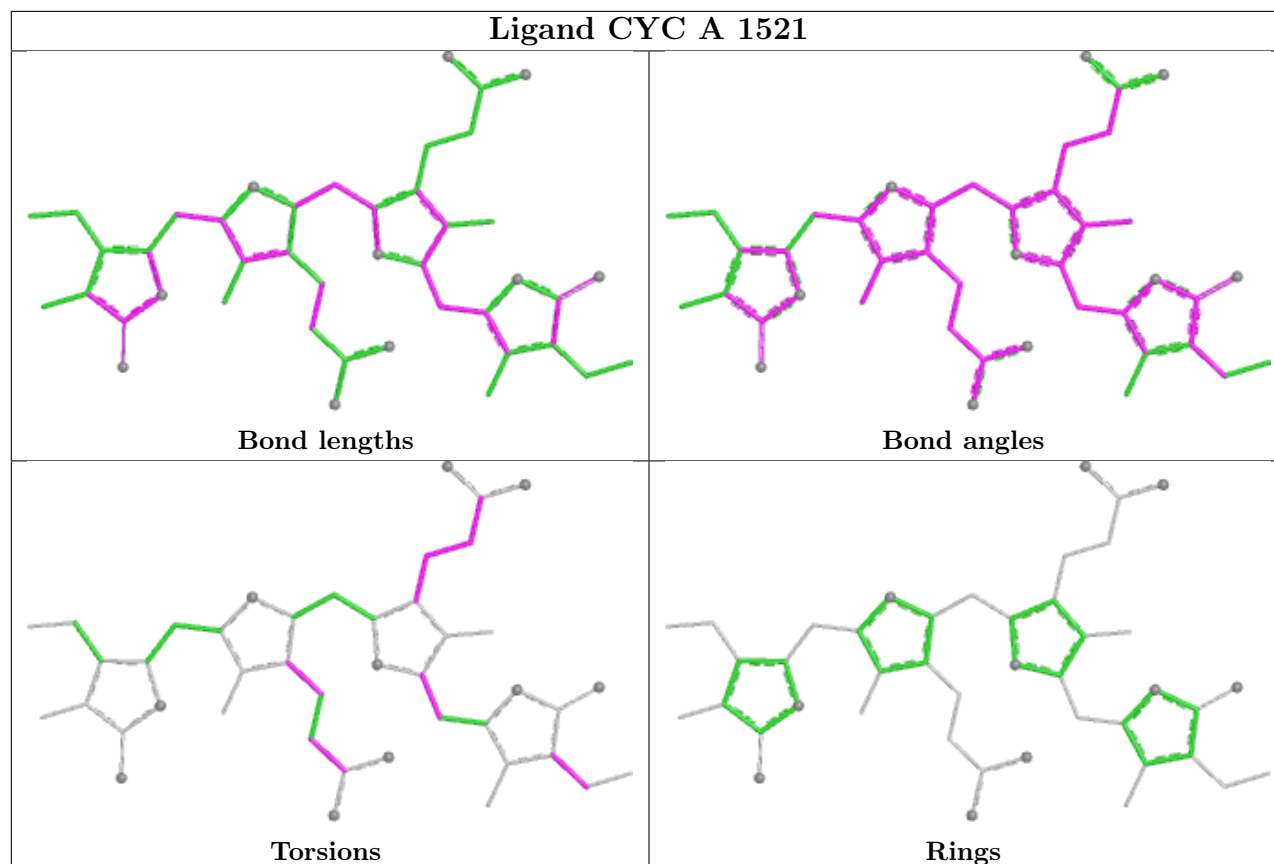
Mol	Chain	Res	Type	Atoms
2	A	1521	CYC	C3A-C2A-CAA-CBA
2	A	1521	CYC	NA-C4A-CHB-C1B
2	A	1521	CYC	C2D-C3D-CAD-CBD
2	A	1521	CYC	C2B-C3B-CAB-CBB
2	A	1521	CYC	C1A-C2A-CAA-CBA
2	A	1521	CYC	C4D-C3D-CAD-CBD
2	A	1521	CYC	C4B-C3B-CAB-CBB
2	A	1521	CYC	C3A-C4A-CHB-C1B
2	A	1521	CYC	C2A-CAA-CBA-CGA
2	A	1521	CYC	CAA-CBA-CGA-O2A
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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	500/520 (96%)	2.35	294 (58%) 0 0	44, 79, 84, 90	2 (0%)

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	6.9
1	A	237	ALA	6.6
1	A	54	GLY	6.6
1	A	195	MET	6.4
1	A	238	VAL	6.2
1	A	351	GLY	6.1
1	A	142	ALA	5.8
1	A	393	GLN	5.5
1	A	245	ALA	5.3
1	A	82	THR	5.1
1	A	242	THR	4.9
1	A	61	LEU	4.8
1	A	353	THR	4.8
1	A	194	ASP	4.7
1	A	81	LEU	4.7
1	A	461	THR	4.7
1	A	186	VAL	4.6
1	A	239	ASN	4.6
1	A	329	VAL	4.6
1	A	98	VAL	4.6
1	A	175	LEU	4.6
1	A	283	LEU	4.5
1	A	144	LEU	4.5
1	A	36	GLN	4.4
1	A	132	PRO	4.4
1	A	232	VAL	4.4
1	A	453	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	4.3
1	A	37	GLU	4.3
1	A	21	HIS	4.2
1	A	50	THR	4.2
1	A	520	HIS	4.2
1	A	424	SER	4.1
1	A	298	PRO	4.1
1	A	143	ALA	4.1
1	A	41	THR	4.1
1	A	161	VAL	3.9
1	A	346	ALA	3.9
1	A	304	ALA	3.9
1	A	64	THR	3.9
1	A	285	GLY	3.8
1	A	395	LEU	3.8
1	A	113	ASN	3.8
1	A	135	GLY	3.8
1	A	199	LEU	3.8
1	A	240	PRO	3.8
1	A	7	LEU	3.8
1	A	214	ARG	3.7
1	A	12	LEU	3.7
1	A	475	PHE	3.7
1	A	131	LEU	3.7
1	A	129	ASP	3.7
1	A	56	SER	3.7
1	A	49	CYS	3.6
1	A	86	ILE	3.6
1	A	307	PHE	3.6
1	A	34	VAL	3.6
1	A	411	GLN	3.6
1	A	310[A]	ARG	3.6
1	A	116	GLY	3.6
1	A	145	ASN	3.6
1	A	418	ASN	3.6
1	A	200	GLY	3.6
1	A	360	LEU	3.5
1	A	170	PHE	3.5
1	A	402	ASP	3.5
1	A	422	VAL	3.5
1	A	188	ALA	3.5
1	A	84	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	426	LEU	3.5
1	A	137	TYR	3.5
1	A	130	ASN	3.5
1	A	513	GLU	3.4
1	A	96	ALA	3.4
1	A	273	LEU	3.4
1	A	396	GLU	3.4
1	A	85	GLN	3.4
1	A	196	GLU	3.4
1	A	284	TRP	3.3
1	A	439	TRP	3.3
1	A	352	LEU	3.3
1	A	427	LEU	3.3
1	A	217	ILE	3.3
1	A	257	TYR	3.3
1	A	246	VAL	3.3
1	A	316	ILE	3.3
1	A	369	ALA	3.2
1	A	282	HIS	3.2
1	A	22	THR	3.2
1	A	505	VAL	3.2
1	A	146	ARG	3.2
1	A	288	ALA	3.2
1	A	349	VAL	3.2
1	A	178	PHE	3.2
1	A	309	GLY	3.2
1	A	350	GLU	3.2
1	A	431	ILE	3.2
1	A	136	PHE	3.1
1	A	348	PHE	3.1
1	A	367	GLY	3.1
1	A	11	SER	3.1
1	A	299	PHE	3.1
1	A	277	LEU	3.1
1	A	339	LEU	3.1
1	A	274	THR	3.1
1	A	173	VAL	3.1
1	A	160	ILE	3.1
1	A	58	GLU	3.1
1	A	400	VAL	3.1
1	A	362	LEU	3.1
1	A	180	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	THR	3.0
1	A	516	HIS	3.0
1	A	139	MET	3.0
1	A	147	LEU	3.0
1	A	33	VAL	3.0
1	A	337	VAL	3.0
1	A	509	LEU	3.0
1	A	158	ASP	3.0
1	A	455	ASN	3.0
1	A	25	LEU	2.9
1	A	4	THR	2.9
1	A	301	LEU	2.9
1	A	368	ALA	2.9
1	A	519	HIS	2.9
1	A	502	LYS	2.9
1	A	71	SER	2.9
1	A	354	ASN	2.9
1	A	438	LEU	2.9
1	A	10	GLN	2.9
1	A	412	ILE	2.9
1	A	169	GLY	2.9
1	A	340	ASP	2.9
1	A	153	LEU	2.9
1	A	432	ALA	2.9
1	A	243	ASN	2.9
1	A	191	LYS	2.8
1	A	390	TYR	2.8
1	A	440	PHE	2.8
1	A	322	THR	2.8
1	A	39	ASP	2.8
1	A	468	GLU	2.8
1	A	296	VAL	2.8
1	A	308	PHE	2.8
1	A	208	ILE	2.8
1	A	407	SER	2.8
1	A	379	VAL	2.8
1	A	59	ASP	2.7
1	A	219	ASN	2.7
1	A	490	GLN	2.7
1	A	57	PRO	2.7
1	A	112	ARG	2.7
1	A	510	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	287	ILE	2.7
1	A	377	ILE	2.7
1	A	365	SER	2.7
1	A	488	PRO	2.7
1	A	507	LEU	2.7
1	A	318	ALA	2.7
1	A	247	ASP	2.7
1	A	363	THR	2.7
1	A	398	ARG	2.7
1	A	291	HIS	2.7
1	A	336	ALA	2.6
1	A	457	ALA	2.6
1	A	295	LYS	2.6
1	A	311	VAL	2.6
1	A	35	LEU	2.6
1	A	47	ALA	2.6
1	A	102	ASP	2.6
1	A	126	TYR	2.6
1	A	117	LEU	2.6
1	A	391	LEU	2.6
1	A	460	ALA	2.6
1	A	90	ASN	2.6
1	A	168	THR	2.6
1	A	220	PRO	2.6
1	A	138	HIS	2.6
1	A	68	VAL	2.6
1	A	403	VAL	2.6
1	A	376	LEU	2.5
1	A	32	VAL	2.5
1	A	223	VAL	2.5
1	A	491	SER	2.5
1	A	157	TYR	2.5
1	A	125	ALA	2.5
1	A	280	ASP	2.5
1	A	392	LEU	2.5
1	A	133	PHE	2.5
1	A	275	ILE	2.5
1	A	60	LEU	2.5
1	A	261	LEU	2.5
1	A	294	PRO	2.5
1	A	269	VAL	2.4
1	A	134	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	190	ASP	2.4
1	A	97	ARG	2.4
1	A	233	PRO	2.4
1	A	302	ARG	2.4
1	A	423	ALA	2.4
1	A	394	TRP	2.4
1	A	359	LEU	2.4
1	A	518	HIS	2.4
1	A	397	ASN	2.4
1	A	241	SER	2.4
1	A	216	PHE	2.4
1	A	297	ILE	2.4
1	A	388	VAL	2.4
1	A	292	GLN	2.4
1	A	55	ARG	2.4
1	A	258	HIS	2.4
1	A	511	GLN	2.4
1	A	345	ALA	2.3
1	A	127	THR	2.3
1	A	106	PHE	2.3
1	A	201	LEU	2.3
1	A	477	LEU	2.3
1	A	95	TRP	2.3
1	A	16	GLU	2.3
1	A	436	PHE	2.3
1	A	120	CYS	2.3
1	A	338	LEU	2.3
1	A	445	LEU	2.3
1	A	278	ILE	2.3
1	A	209	PRO	2.3
1	A	413	TYR	2.3
1	A	387	ALA	2.3
1	A	450	TRP	2.3
1	A	378	LEU	2.2
1	A	305	CYS	2.2
1	A	356	PRO	2.2
1	A	167	MET	2.2
1	A	140	ALA	2.2
1	A	198	TYR	2.2
1	A	212	ALA	2.2
1	A	332	ALA	2.2
1	A	470	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	43	SER	2.2
1	A	87	SER	2.2
1	A	478	TRP	2.2
1	A	504	ILE	2.2
1	A	234	LEU	2.2
1	A	312	VAL	2.2
1	A	419	PHE	2.2
1	A	495	GLN	2.2
1	A	249	THR	2.2
1	A	317	SER	2.2
1	A	224	ILE	2.2
1	A	159	VAL	2.2
1	A	187	ILE	2.2
1	A	63	ARG	2.2
1	A	152	ASN	2.2
1	A	182	ASN	2.2
1	A	347	ASP	2.2
1	A	380	GLY	2.2
1	A	83	ALA	2.2
1	A	406	THR	2.2
1	A	327	TYR	2.1
1	A	441	ARG	2.1
1	A	67	GLU	2.1
1	A	341	LYS	2.1
1	A	514	GLU	2.1
1	A	128	SER	2.1
1	A	172[A]	ARG	2.1
1	A	409	LEU	2.1
1	A	141	ASN	2.1
1	A	319	GLN	2.1
1	A	334	HIS	2.1
1	A	417	VAL	2.1
1	A	364	GLY	2.1
1	A	289	CYS	2.1
1	A	193	ASP	2.1
1	A	446	GLN	2.1
1	A	103	PHE	2.1
1	A	425	GLY	2.1
1	A	259	CYS	2.1
1	A	293	THR	2.1
1	A	381	GLU	2.1
1	A	221	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	PHE	2.1
1	A	452	GLY	2.1
1	A	267	MET	2.0
1	A	162	GLU	2.0
1	A	236	PRO	2.0
1	A	176	TYR	2.0
1	A	244	ARG	2.0
1	A	325	PHE	2.0
1	A	466	LYS	2.0
1	A	324	THR	2.0
1	A	421	SER	2.0
1	A	434	HIS	2.0
1	A	53	LEU	2.0
1	A	467	ILE	2.0
1	A	386	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

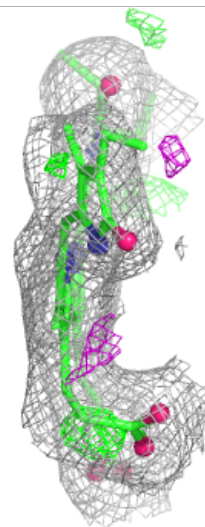
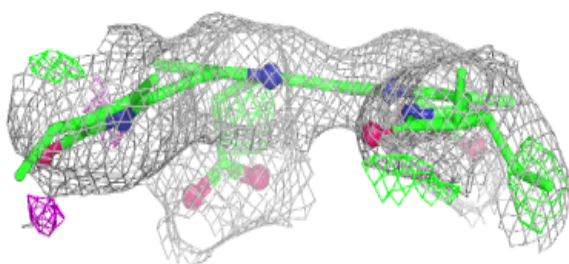
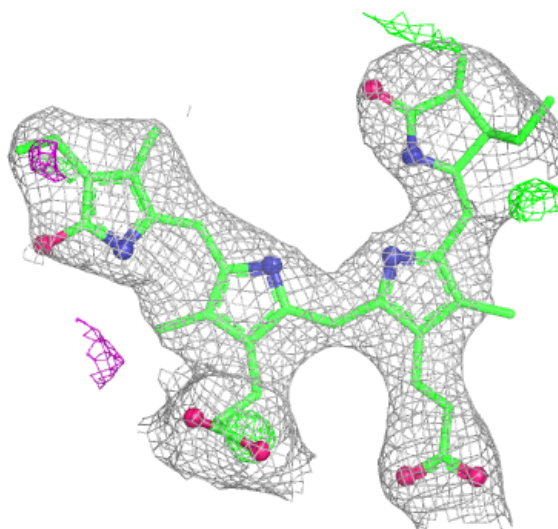
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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 ⓘ

There are no such residues in this entry.