



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:56 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

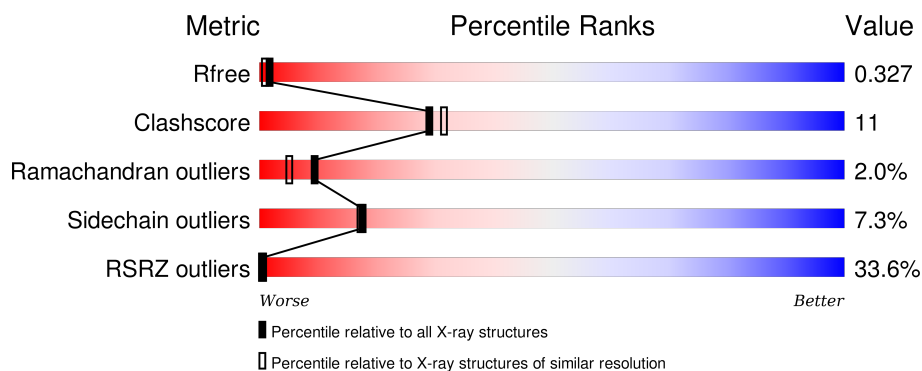
1 Overall quality at a glance

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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (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. 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	<div> <div>32%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>

2 Entry composition [i](#)

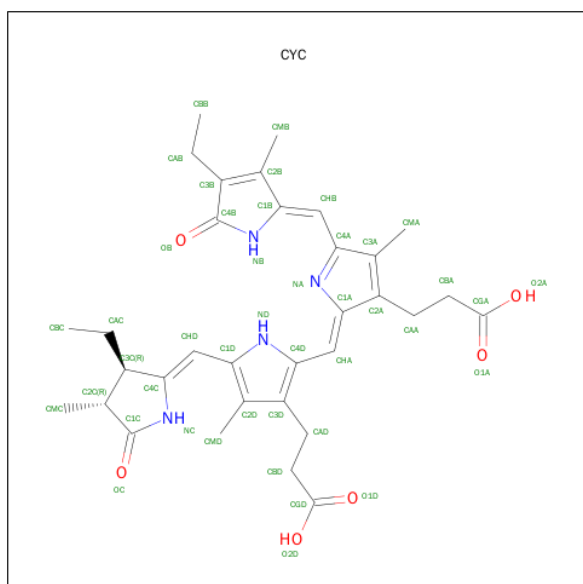
There are 3 unique types of molecules in this entry. The entry contains 4022 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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		

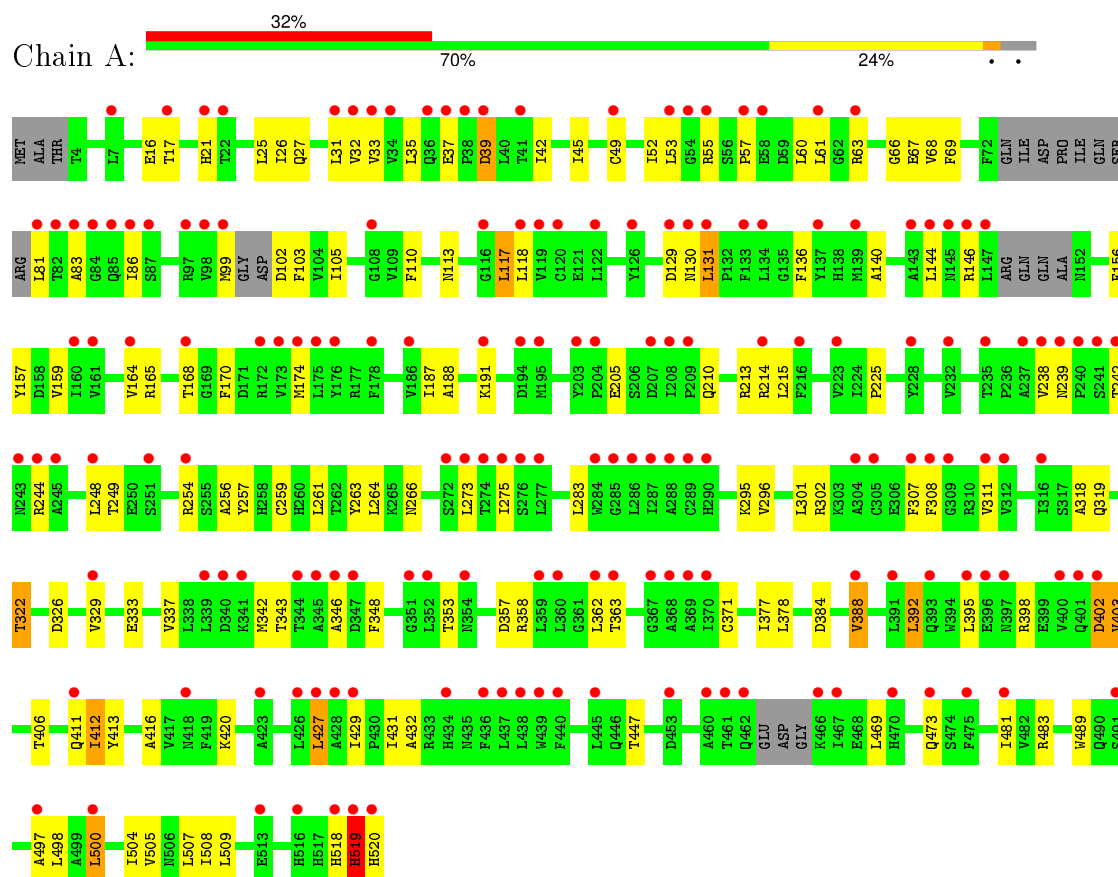
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	77.18 Å 77.18 Å 249.00 Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.22 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.271 0.331 , 0.327	Depositor DCC
R_{free} test set	1097 reflections (4.36%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26251 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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 [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	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: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: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:505:VAL:O	1:A:509:LEU:HD23	2.10	0.52
1:A:342:MET:CG	1:A:348:PHE:HB2	2.39	0.52
1:A:431:ILE:O	1:A:432:ALA:HB3	2.10	0.52
1:A:257:TYR:HD2	2:A:1521:CYC:HMD2	1.76	0.51
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: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
2:A:1521:CYC:HBD2	2:A:1521:CYC:HMD1	1.97	0.45
1:A:105:ILE:HD12	1:A:105:ILE:N	2.31	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

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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:333:GLU:O	1:A:337:VAL:HG23	2.19	0.42
1:A:113:ASN:HB2	1:A:117:LEU:HD22	2.01	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:481:ILE:HG21	1:A:483:ARG:NH2	2.36	0.41
1:A:130:ASN:CB	1:A:131:LEU:HD23	2.51	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%)	9 5

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 ⓘ

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%)	17	17

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

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 ⓘ

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	35,46,46	4.16	16 (45%)	47,67,67	3.80	24 (51%)

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	-	2/21/74/74	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	C1C-NC	-8.22	1.27	1.37
2	A	1521	CYC	C4B-C3B	-4.12	1.39	1.48
2	A	1521	CYC	C1B-C2B	-3.52	1.38	1.45
2	A	1521	CYC	CBD-CAD	-3.04	1.32	1.53
2	A	1521	CYC	C4A-C3A	-2.43	1.40	1.45
2	A	1521	CYC	CAD-C3D	-2.07	1.48	1.52
2	A	1521	CYC	C2C-C1C	-2.04	1.50	1.52
2	A	1521	CYC	C4D-CHA	2.21	1.48	1.40
2	A	1521	CYC	C1D-CHD	2.51	1.49	1.40
2	A	1521	CYC	C3D-C2D	3.33	1.47	1.37
2	A	1521	CYC	CHB-C4A	3.40	1.48	1.40
2	A	1521	CYC	CHB-C1B	4.45	1.48	1.37
2	A	1521	CYC	OC-C1C	5.10	1.33	1.23
2	A	1521	CYC	C2A-C3A	5.45	1.48	1.36
2	A	1521	CYC	OB-C4B	12.94	1.48	1.23
2	A	1521	CYC	CHA-C1A	13.88	1.47	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1521	CYC	C4B-C3B-C2B	-11.48	101.50	108.05
2	A	1521	CYC	C1B-NB-C4B	-6.15	101.73	110.73
2	A	1521	CYC	CHB-C4A-NA	-5.40	114.63	124.91
2	A	1521	CYC	OB-C4B-C3B	-5.16	121.91	128.09
2	A	1521	CYC	OC-C1C-C2C	-4.34	122.75	126.25
2	A	1521	CYC	CAD-C3D-C4D	-4.03	122.64	127.01
2	A	1521	CYC	C1A-C2A-C3A	-3.76	102.61	106.81
2	A	1521	CYC	CAA-CBA-CGA	-2.84	107.55	112.75
2	A	1521	CYC	C4A-C3A-C2A	-2.75	103.22	106.50
2	A	1521	CYC	CHA-C1A-C2A	-2.54	119.59	125.55
2	A	1521	CYC	CHB-C1B-C2B	-2.03	122.67	126.89
2	A	1521	CYC	C2D-C1D-ND	2.24	113.96	110.29
2	A	1521	CYC	CMA-C3A-C4A	2.31	128.81	125.06
2	A	1521	CYC	CMD-C2D-C3D	2.39	130.24	125.24
2	A	1521	CYC	C2A-C1A-NA	2.52	113.77	109.86
2	A	1521	CYC	C3A-C4A-NA	2.58	116.45	110.55
2	A	1521	CYC	CAA-C2A-C3A	3.07	133.37	128.01
2	A	1521	CYC	C3C-C4C-NC	3.37	111.31	107.93
2	A	1521	CYC	C2B-C1B-NB	3.47	112.02	107.00
2	A	1521	CYC	CBD-CAD-C3D	4.34	120.30	112.53
2	A	1521	CYC	CAD-CBD-CGD	4.41	120.83	112.75
2	A	1521	CYC	C2C-C1C-NC	4.95	113.02	108.30
2	A	1521	CYC	C3B-C4B-NB	10.15	115.97	106.74
2	A	1521	CYC	CAB-C3B-C4B	11.64	131.67	121.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1521	CYC	C1B-CHB-C4A-C3A
2	A	1521	CYC	C1B-CHB-C4A-NA

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	500/520 (96%)	1.64	168 (33%) 0 0	71, 79, 84, 90	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	7.8
1	A	439	TRP	7.6
1	A	287	ILE	7.4
1	A	346	ALA	6.8
1	A	175	LEU	6.8
1	A	520	HIS	6.5
1	A	38	PRO	6.0
1	A	98	VAL	5.9
1	A	438	LEU	5.8
1	A	7	LEU	5.8
1	A	99	MET	5.8
1	A	134	LEU	5.7
1	A	85	GLN	5.4
1	A	466	LYS	5.4
1	A	237	ALA	5.3
1	A	146	ARG	5.3
1	A	286	LEU	5.2
1	A	427	LEU	5.2
1	A	160	ILE	5.1
1	A	244	ARG	5.1
1	A	174	MET	5.0
1	A	369	ALA	5.0
1	A	82	THR	4.8
1	A	288	ALA	4.8
1	A	368	ALA	4.8
1	A	274	THR	4.8
1	A	54	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	4.7
1	A	176	TYR	4.7
1	A	359	LEU	4.7
1	A	437	LEU	4.7
1	A	500	LEU	4.6
1	A	305	CYS	4.5
1	A	351	GLY	4.5
1	A	467	ILE	4.4
1	A	144	LEU	4.4
1	A	240	PRO	4.4
1	A	195	MET	4.3
1	A	275	ILE	4.3
1	A	120	CYS	4.3
1	A	273	LEU	4.3
1	A	243	ASN	4.2
1	A	309	GLY	4.1
1	A	312	VAL	4.1
1	A	426	LEU	4.1
1	A	81	LEU	4.0
1	A	131	LEU	4.0
1	A	277	LEU	4.0
1	A	36	GLN	4.0
1	A	214	ARG	3.8
1	A	352	LEU	3.8
1	A	161	VAL	3.7
1	A	143	ALA	3.6
1	A	164	VAL	3.6
1	A	308	PHE	3.6
1	A	139	MET	3.5
1	A	440	PHE	3.5
1	A	473	GLN	3.5
1	A	242	THR	3.5
1	A	232	VAL	3.5
1	A	130	ASN	3.5
1	A	316	ILE	3.5
1	A	34	VAL	3.4
1	A	228	TYR	3.4
1	A	58	GLU	3.4
1	A	285	GLY	3.4
1	A	33	VAL	3.4
1	A	461	THR	3.4
1	A	362	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	133	PHE	3.3
1	A	21	HIS	3.3
1	A	83	ALA	3.3
1	A	429	ILE	3.3
1	A	393	GLN	3.3
1	A	418	ASN	3.2
1	A	248	LEU	3.2
1	A	388	VAL	3.2
1	A	411	GLN	3.2
1	A	37	GLU	3.2
1	A	245	ALA	3.2
1	A	126	TYR	3.2
1	A	32	VAL	3.2
1	A	119	VAL	3.2
1	A	87	SER	3.1
1	A	401	GLN	3.1
1	A	519	HIS	3.1
1	A	289	CYS	3.1
1	A	31	LEU	3.0
1	A	241	SER	3.0
1	A	307	PHE	3.0
1	A	347	ASP	3.0
1	A	462	GLN	3.0
1	A	86	ILE	2.9
1	A	491	SER	2.9
1	A	391	LEU	2.9
1	A	63	ARG	2.9
1	A	137	TYR	2.9
1	A	436	PHE	2.9
1	A	39	ASP	2.9
1	A	428	ALA	2.8
1	A	61	LEU	2.8
1	A	97	ARG	2.8
1	A	173	VAL	2.8
1	A	186	VAL	2.8
1	A	513	GLU	2.8
1	A	208	ILE	2.8
1	A	470	HIS	2.7
1	A	311	VAL	2.7
1	A	209	PRO	2.7
1	A	367	GLY	2.7
1	A	397	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	284	TRP	2.6
1	A	345	ALA	2.6
1	A	518	HIS	2.6
1	A	354	ASN	2.6
1	A	481	ILE	2.6
1	A	272	SER	2.6
1	A	363	THR	2.6
1	A	84	GLY	2.5
1	A	204	PRO	2.5
1	A	207	ASP	2.5
1	A	423	ALA	2.5
1	A	235	THR	2.4
1	A	216	PHE	2.4
1	A	340	ASP	2.4
1	A	168	THR	2.4
1	A	445	LEU	2.4
1	A	339	LEU	2.3
1	A	304	ALA	2.3
1	A	370	ILE	2.3
1	A	17	THR	2.3
1	A	251	SER	2.3
1	A	223	VAL	2.3
1	A	122	LEU	2.3
1	A	145	ASN	2.3
1	A	129	ASP	2.2
1	A	203	TYR	2.2
1	A	147	LEU	2.2
1	A	360	LEU	2.2
1	A	395	LEU	2.2
1	A	194	ASP	2.2
1	A	55	ARG	2.2
1	A	254	ARG	2.2
1	A	172[A]	ARG	2.2
1	A	329	VAL	2.2
1	A	460	ALA	2.2
1	A	108	GLY	2.2
1	A	453	ASP	2.2
1	A	191	LYS	2.2
1	A	49	CYS	2.2
1	A	402	ASP	2.1
1	A	516	HIS	2.1
1	A	396	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	2.1
1	A	475	PHE	2.1
1	A	341	LYS	2.1
1	A	400	VAL	2.1
1	A	497	ALA	2.1
1	A	434	HIS	2.1
1	A	41	THR	2.1
1	A	239	ASN	2.1
1	A	118	LEU	2.0
1	A	116	GLY	2.0
1	A	22	THR	2.0
1	A	53	LEU	2.0
1	A	290	HIS	2.0
1	A	276	SER	2.0
1	A	57	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CYC	A	1521	43/43	0.88	0.34	1.13	71,76,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.