



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 PM UTC

PDB ID : 3O18 / pdb_00003o18
Title : Crystal structure of c-phycoerythrin from *Thermosynechococcus vulcanus* at 1.35 angstroms resolution
Authors : Marx, A.; David, L.; Adir, N.
Deposited on : 2010-07-21
Resolution : 1.35 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

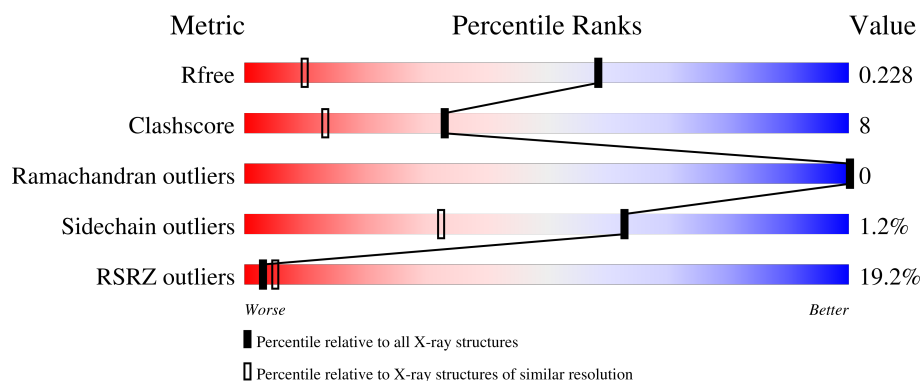
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	162	15% 81% 17% ..
2	B	172	23% 84% 15% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3044 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.

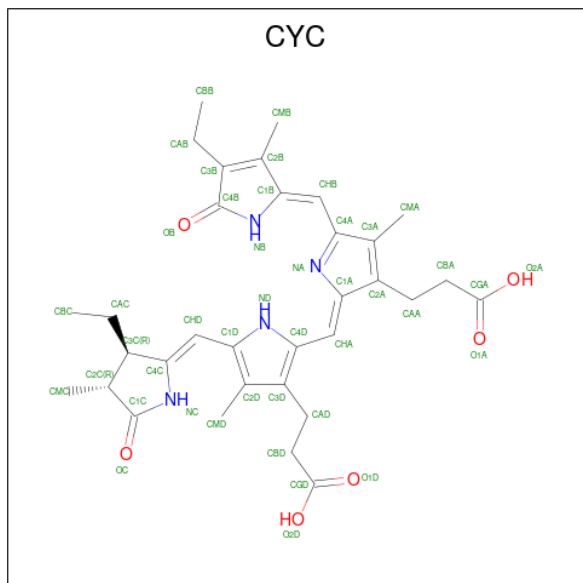
- Molecule 1 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	1	0
			1232	776	206	243	7			

- Molecule 2 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	1	0
			1282	793	230	251	8			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

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

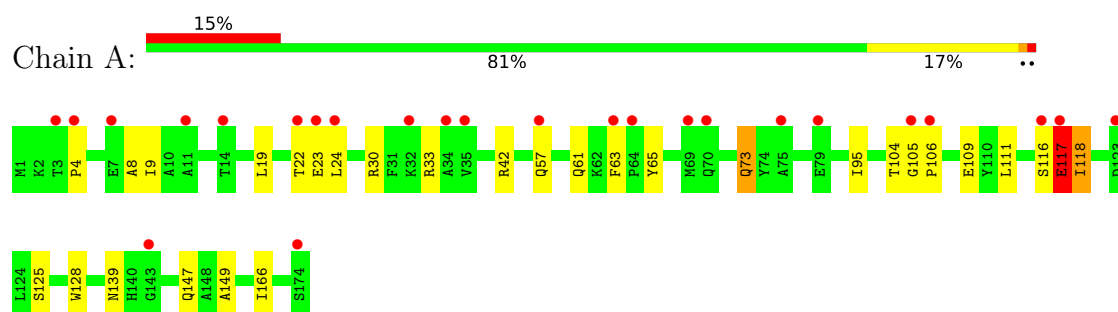
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	177	Total	O	0	0
			177	177		

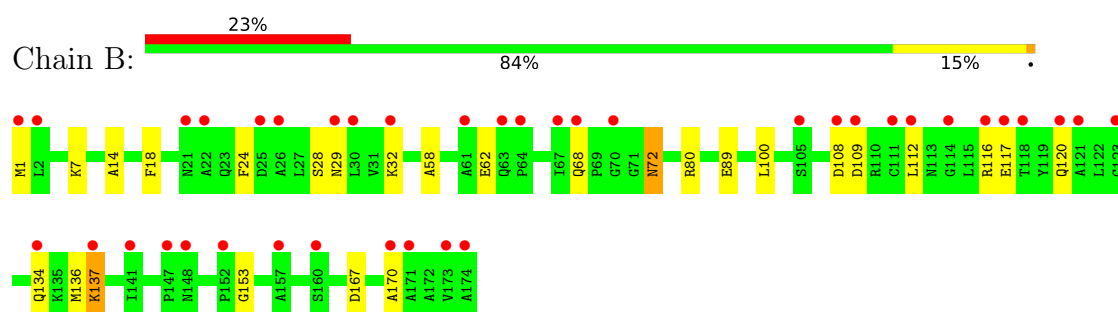
3 Residue-property plots

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: C-phycocyanin alpha subunit



- Molecule 2: C-phycocyanin beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	186.81Å 186.81Å 59.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.23 – 1.35 27.23 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (27.23-1.35) 98.9 (27.23-1.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.35Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.226 0.212 , 0.228	Depositor DCC
R_{free} test set	4325 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, MEN

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	0.98	4/1257 (0.3%)	0.80	3/1704 (0.2%)
2	B	1.03	5/1286 (0.4%)	0.87	3/1740 (0.2%)
All	All	1.00	9/2543 (0.4%)	0.84	6/3444 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	29	ASN	C-N	-9.84	1.21	1.33
1	A	22	THR	C-N	6.93	1.44	1.33
2	B	136	MET	C-N	6.79	1.43	1.33
1	A	109	GLU	C-O	-6.23	1.16	1.24
2	B	14	ALA	C-N	-6.22	1.24	1.33
2	B	7	LYS	C-N	-5.76	1.26	1.33
1	A	73	GLN	C-O	-5.65	1.16	1.24
2	B	68	GLN	C-O	-5.57	1.16	1.23
1	A	149	ALA	C-N	-5.21	1.27	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	137	LYS	O-C-N	5.92	130.47	122.59
2	B	18	PHE	N-CA-C	-5.91	102.58	110.55
2	B	109	ASP	N-CA-C	5.86	117.47	111.14
1	A	117	GLU	N-CA-C	-5.58	105.10	111.07
1	A	118	ILE	N-CA-CB	5.52	117.01	110.55
1	A	139	ASN	N-CA-C	5.08	120.10	112.94

There are no chirality outliers.

There are no planarity outliers.

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	1232	0	1212	26	0
2	B	1282	0	1280	17	0
3	A	43	0	37	1	0
3	B	86	0	74	3	0
4	A	224	0	0	0	0
4	B	177	0	0	1	0
All	All	3044	0	2603	41	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 8.

All (41) 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:117:GLU:H	1:A:117:GLU:CD	1.87	0.82
1:A:117:GLU:CD	1:A:117:GLU:N	2.41	0.78
1:A:117:GLU:N	1:A:117:GLU:OE2	2.29	0.66
1:A:30:ARG:O	1:A:30:ARG:HD3	1.98	0.63
1:A:116:SER:HB2	1:A:117:GLU:OE2	1.98	0.63
2:B:116:ARG:O	2:B:120:GLN:HG3	2.02	0.59
1:A:30:ARG:HD3	1:A:30:ARG:C	2.30	0.57
1:A:33:ARG:HH12	1:A:147:GLN:HE21	1.51	0.56
2:B:134:GLN:OE1	2:B:137:LYS:NZ	2.37	0.56
1:A:30:ARG:C	1:A:30:ARG:CD	2.80	0.55
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.53
1:A:33:ARG:HH12	1:A:147:GLN:NE2	2.08	0.51
2:B:72:MEN:HE22	3:B:584:CYC:HBD2	1.94	0.50
1:A:19:LEU:HD13	2:B:100:LEU:HD22	1.94	0.50
2:B:153:GLY:HA3	3:B:555:CYC:CMD	2.42	0.49
2:B:89:GLU:CD	4:B:205:HOH:O	2.55	0.49
1:A:4:PRO:HG2	1:A:30:ARG:CG	2.46	0.46
2:B:134:GLN:OE1	2:B:137:LYS:HE2	2.16	0.45
2:B:108:ASP:HA	2:B:112:LEU:HB2	2.00	0.43
1:A:9:ILE:HG22	2:B:1:MET:HE1	1.99	0.43
2:B:137:LYS:NZ	2:B:167:ASP:OD1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:SER:HB3	1:A:128:TRP:CE2	2.54	0.43
2:B:134:GLN:HE21	2:B:170:ALA:CB	2.32	0.43
1:A:104:THR:O	1:A:105:GLY:C	2.60	0.43
1:A:95:ILE:HD13	1:A:166:ILE:HG12	2.01	0.42
2:B:72:MEN:O	2:B:80:ARG:HD2	2.19	0.42
1:A:33:ARG:NH1	1:A:147:GLN:HE21	2.15	0.42
1:A:42:ARG:CZ	2:B:24:PHE:HB3	2.49	0.42
2:B:28:SER:O	2:B:32:LYS:HG3	2.19	0.42
1:A:73:GLN:HA	3:A:484:CYC:HBD2	2.01	0.42
1:A:63:PHE:HB3	1:A:65:TYR:CE1	2.55	0.42
2:B:134:GLN:OE1	2:B:137:LYS:CE	2.68	0.42
1:A:8:ALA:HB1	1:A:23:GLU:HB3	2.01	0.41
2:B:117:GLU:OE1	2:B:117:GLU:N	2.47	0.41
1:A:111:LEU:C	1:A:111:LEU:HD23	2.45	0.41
3:B:584:CYC:CMD	3:B:584:CYC:HC	2.33	0.41
1:A:33:ARG:HH22	1:A:147:GLN:NE2	2.19	0.40
1:A:105:GLY:O	1:A:106:PRO:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	161/162 (99%)	158 (98%)	3 (2%)	0	100	100
2	B	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
All	All	331/334 (99%)	324 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	124/123 (101%)	121 (98%)	3 (2%)	43	12
2	B	128/127 (101%)	128 (100%)	0	100	100
All	All	252/250 (101%)	249 (99%)	3 (1%)	63	32

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	117	GLU
1	A	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	46	ASN
1	A	61	GLN
1	A	147	GLN
2	B	35	ASN
2	B	54	ASN
2	B	78	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	MEN	B	72	2	7,8,9	1.19	1 (14%)	4,9,11	0.71	0

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	MEN	B	72	2	-	4/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	CE2-ND2	2.93	1.50	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2
2	B	72	MEN	CB-CG-ND2-CE2
2	B	72	MEN	OD1-CG-ND2-CE2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	A	484	1	46,46,46	2.12	15 (32%)	63,67,67	3.12	24 (38%)
3	CYC	B	584	2	46,46,46	2.21	14 (30%)	63,67,67	3.33	26 (41%)
3	CYC	B	555	2	46,46,46	2.55	17 (36%)	63,67,67	3.48	28 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	A	484	1	-	10/26/74/74	0/4/4/4
3	CYC	B	584	2	-	9/26/74/74	0/4/4/4
3	CYC	B	555	2	-	9/26/74/74	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	484	CYC	OB-C4B	7.04	1.36	1.23
3	B	584	CYC	OB-C4B	6.97	1.36	1.23
3	B	555	CYC	OB-C4B	6.76	1.36	1.23
3	B	555	CYC	O2D-CGD	-6.54	1.09	1.30
3	B	555	CYC	CBD-CGD	-5.90	1.36	1.50
3	B	584	CYC	C1C-NC	-5.16	1.30	1.37
3	B	555	CYC	C1C-NC	-5.12	1.31	1.37
3	B	584	CYC	OC-C1C	4.87	1.32	1.23
3	A	484	CYC	OC-C1C	4.85	1.32	1.23
3	B	555	CYC	OC-C1C	4.75	1.32	1.23
3	A	484	CYC	C1C-NC	-4.68	1.31	1.37
3	B	584	CYC	CHB-C4A	3.91	1.49	1.40
3	B	555	CYC	O1D-CGD	-3.90	1.09	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	555	CYC	CHB-C4A	3.69	1.49	1.40
3	B	584	CYC	CHD-C1D	3.67	1.48	1.40
3	B	584	CYC	C2A-C3A	3.55	1.44	1.36
3	B	555	CYC	CHD-C1D	3.52	1.48	1.40
3	A	484	CYC	CHD-C1D	3.36	1.47	1.40
3	B	555	CYC	C3D-C2D	3.35	1.47	1.38
3	B	584	CYC	C3D-C2D	3.25	1.47	1.38
3	B	555	CYC	C4B-C3B	-3.22	1.42	1.48
3	A	484	CYC	CHB-C4A	3.12	1.47	1.40
3	A	484	CYC	C3D-C2D	3.10	1.47	1.38
3	B	555	CYC	C2A-C3A	3.08	1.43	1.36
3	A	484	CYC	C2A-C3A	3.07	1.43	1.36
3	B	584	CYC	C4B-C3B	-2.91	1.42	1.48
3	A	484	CYC	C4B-C3B	-2.81	1.43	1.48
3	A	484	CYC	C2C-C1C	2.65	1.54	1.52
3	B	584	CYC	C1B-NB	-2.58	1.33	1.37
3	B	584	CYC	CMB-C2B	-2.55	1.45	1.50
3	A	484	CYC	C2C-C3C	-2.54	1.47	1.54
3	B	584	CYC	CBD-CAD	-2.48	1.43	1.51
3	B	555	CYC	C1B-NB	-2.44	1.33	1.37
3	B	584	CYC	C3B-C2B	2.41	1.42	1.36
3	B	584	CYC	CHA-C4D	2.37	1.45	1.40
3	B	555	CYC	CBD-CAD	-2.33	1.43	1.51
3	B	555	CYC	C3B-C2B	2.32	1.41	1.36
3	A	484	CYC	C4B-NB	-2.29	1.32	1.38
3	B	555	CYC	CMB-C2B	-2.28	1.46	1.50
3	A	484	CYC	C3B-C2B	2.27	1.41	1.36
3	A	484	CYC	CBD-CAD	-2.25	1.44	1.51
3	B	584	CYC	C4B-NB	-2.24	1.32	1.38
3	B	555	CYC	C2C-C3C	-2.23	1.48	1.54
3	A	484	CYC	CMB-C2B	-2.18	1.46	1.50
3	A	484	CYC	C1B-NB	-2.00	1.34	1.37
3	B	555	CYC	C4B-NB	-2.00	1.33	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	555	CYC	C3B-C4B-NB	13.01	117.14	106.77
3	B	584	CYC	C3B-C4B-NB	12.72	116.91	106.77
3	A	484	CYC	C3B-C4B-NB	12.37	116.64	106.77
3	B	584	CYC	OC-C1C-C2C	-11.07	117.37	126.17
3	B	555	CYC	OC-C1C-C2C	-10.25	118.03	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	484	CYC	OC-C1C-C2C	-9.36	118.73	126.17
3	B	584	CYC	C2C-C1C-NC	9.17	115.92	108.29
3	B	555	CYC	C2C-C1C-NC	8.91	115.70	108.29
3	B	555	CYC	OB-C4B-C3B	-8.49	119.10	128.03
3	B	584	CYC	OB-C4B-C3B	-8.01	119.61	128.03
3	A	484	CYC	OB-C4B-C3B	-7.79	119.84	128.03
3	A	484	CYC	C2C-C1C-NC	7.65	114.65	108.29
3	B	555	CYC	O1D-CGD-CBD	-6.01	104.04	123.09
3	B	555	CYC	CBC-CAC-C3C	5.96	126.06	113.41
3	A	484	CYC	C1C-NC-C4C	-5.63	106.34	113.41
3	B	555	CYC	CAD-CBD-CGD	5.18	127.40	113.67
3	A	484	CYC	CAB-C3B-C4B	5.15	129.34	121.37
3	B	555	CYC	C1B-NB-C4B	-5.09	104.42	110.66
3	B	555	CYC	C1C-NC-C4C	-5.09	107.03	113.41
3	B	584	CYC	CAB-C3B-C4B	5.04	129.16	121.37
3	B	584	CYC	C1C-NC-C4C	-4.97	107.18	113.41
3	A	484	CYC	C1B-NB-C4B	-4.94	104.60	110.66
3	B	555	CYC	CAB-C3B-C4B	4.66	128.58	121.37
3	B	584	CYC	C1B-NB-C4B	-4.65	104.95	110.66
3	A	484	CYC	CHD-C1D-ND	-3.63	117.10	125.29
3	B	555	CYC	CHA-C4D-C3D	-3.41	119.89	127.22
3	B	584	CYC	CHD-C1D-ND	-3.23	118.00	125.29
3	A	484	CYC	C1A-C2A-C3A	-3.22	103.24	106.73
3	B	555	CYC	CHD-C4C-NC	-3.21	121.62	125.63
3	B	584	CYC	C1A-C2A-C3A	-3.21	103.25	106.73
3	B	584	CYC	C3C-C4C-NC	3.15	112.00	107.94
3	B	584	CYC	O2D-CGD-O1D	-3.08	115.41	123.33
3	B	584	CYC	C1D-CHD-C4C	3.05	132.98	127.76
3	B	555	CYC	C1A-C2A-C3A	-3.02	103.45	106.73
3	B	555	CYC	C3C-C4C-NC	3.02	111.83	107.94
3	B	584	CYC	O1A-CGA-CBA	-2.98	113.65	123.09
3	A	484	CYC	O2D-CGD-CBD	2.95	123.31	114.00
3	B	555	CYC	C4D-C3D-C2D	-2.92	104.22	107.62
3	B	584	CYC	CHA-C4D-C3D	-2.92	120.94	127.22
3	B	584	CYC	CHD-C4C-NC	-2.90	122.01	125.63
3	B	584	CYC	O2D-CGD-CBD	2.89	123.14	114.00
3	A	484	CYC	O2D-CGD-O1D	-2.85	116.00	123.33
3	B	555	CYC	CHB-C4A-C3A	2.83	132.15	124.87
3	B	555	CYC	O2D-CGD-CBD	2.80	122.86	114.00
3	A	484	CYC	O1A-CGA-CBA	-2.77	114.31	123.09
3	A	484	CYC	CHA-C4D-C3D	-2.70	121.42	127.22
3	B	584	CYC	C1A-NA-C4A	2.68	111.44	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	584	CYC	C4A-C3A-C2A	2.65	109.48	106.48
3	B	584	CYC	C4D-C3D-C2D	-2.64	104.55	107.62
3	A	484	CYC	C1A-NA-C4A	2.63	111.34	106.52
3	B	555	CYC	CHD-C1D-ND	-2.60	119.42	125.29
3	B	555	CYC	C1A-NA-C4A	2.59	111.27	106.52
3	B	584	CYC	O2A-CGA-CBA	2.58	122.14	114.00
3	A	484	CYC	C4D-C3D-C2D	-2.57	104.62	107.62
3	B	555	CYC	C3D-C4D-ND	2.51	110.72	107.57
3	A	484	CYC	CHB-C4A-C3A	2.51	131.32	124.87
3	B	584	CYC	CHB-C4A-C3A	2.49	131.28	124.87
3	A	484	CYC	C2B-C1B-NB	2.46	110.55	106.97
3	B	555	CYC	C2B-C1B-NB	2.44	110.52	106.97
3	A	484	CYC	CHD-C1D-C2D	2.43	133.49	127.53
3	A	484	CYC	C4A-C3A-C2A	2.40	109.20	106.48
3	B	555	CYC	O1A-CGA-CBA	-2.39	115.52	123.09
3	A	484	CYC	CHD-C4C-NC	-2.31	122.75	125.63
3	B	584	CYC	C2B-C1B-NB	2.27	110.28	106.97
3	B	555	CYC	C4A-C3A-C2A	2.26	109.04	106.48
3	A	484	CYC	CAA-CBA-CGA	-2.26	107.68	113.67
3	A	484	CYC	O2A-CGA-CBA	2.21	120.99	114.00
3	B	584	CYC	CHA-C1A-NA	2.21	129.23	124.60
3	A	484	CYC	C1D-CHD-C4C	2.18	131.49	127.76
3	A	484	CYC	C3D-C4D-ND	2.18	110.30	107.57
3	B	584	CYC	CAA-CBA-CGA	-2.14	108.00	113.67
3	B	555	CYC	CAB-C3B-C2B	2.12	131.46	127.56
3	B	555	CYC	O2D-CGD-O1D	2.11	128.76	123.33
3	B	584	CYC	CHD-C1D-C2D	2.09	132.64	127.53
3	B	555	CYC	CHA-C1A-NA	2.06	128.93	124.60
3	B	555	CYC	O2A-CGA-CBA	2.05	120.47	114.00
3	B	555	CYC	C3A-C4A-NA	-2.01	106.18	110.58
3	B	584	CYC	C3D-C4D-ND	2.00	110.08	107.57

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	484	CYC	NA-C4A-CHB-C1B
3	A	484	CYC	C3A-C4A-CHB-C1B
3	A	484	CYC	C4C-C3C-CAC-CBC
3	B	584	CYC	NA-C4A-CHB-C1B
3	B	584	CYC	C3A-C4A-CHB-C1B
3	B	555	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
3	B	555	CYC	C3A-C4A-CHB-C1B
3	B	555	CYC	C2C-C3C-CAC-CBC
3	B	555	CYC	C4C-C3C-CAC-CBC
3	A	484	CYC	ND-C1D-CHD-C4C
3	B	555	CYC	C2D-C1D-CHD-C4C
3	B	584	CYC	ND-C1D-CHD-C4C
3	B	555	CYC	ND-C1D-CHD-C4C
3	B	584	CYC	C2B-C3B-CAB-CBB
3	A	484	CYC	C2D-C1D-CHD-C4C
3	B	584	CYC	C2D-C1D-CHD-C4C
3	A	484	CYC	C2B-C3B-CAB-CBB
3	B	584	CYC	C4B-C3B-CAB-CBB
3	A	484	CYC	C2C-C3C-CAC-CBC
3	B	555	CYC	CAA-CBA-CGA-O2A
3	B	555	CYC	CAA-CBA-CGA-O1A
3	A	484	CYC	CAA-CBA-CGA-O2A
3	A	484	CYC	CAA-CBA-CGA-O1A
3	B	555	CYC	CAD-CBD-CGD-O2D
3	B	584	CYC	CAA-CBA-CGA-O1A
3	B	584	CYC	CAA-CBA-CGA-O2A
3	B	584	CYC	CAD-CBD-CGD-O2D
3	A	484	CYC	CAD-CBD-CGD-O2D

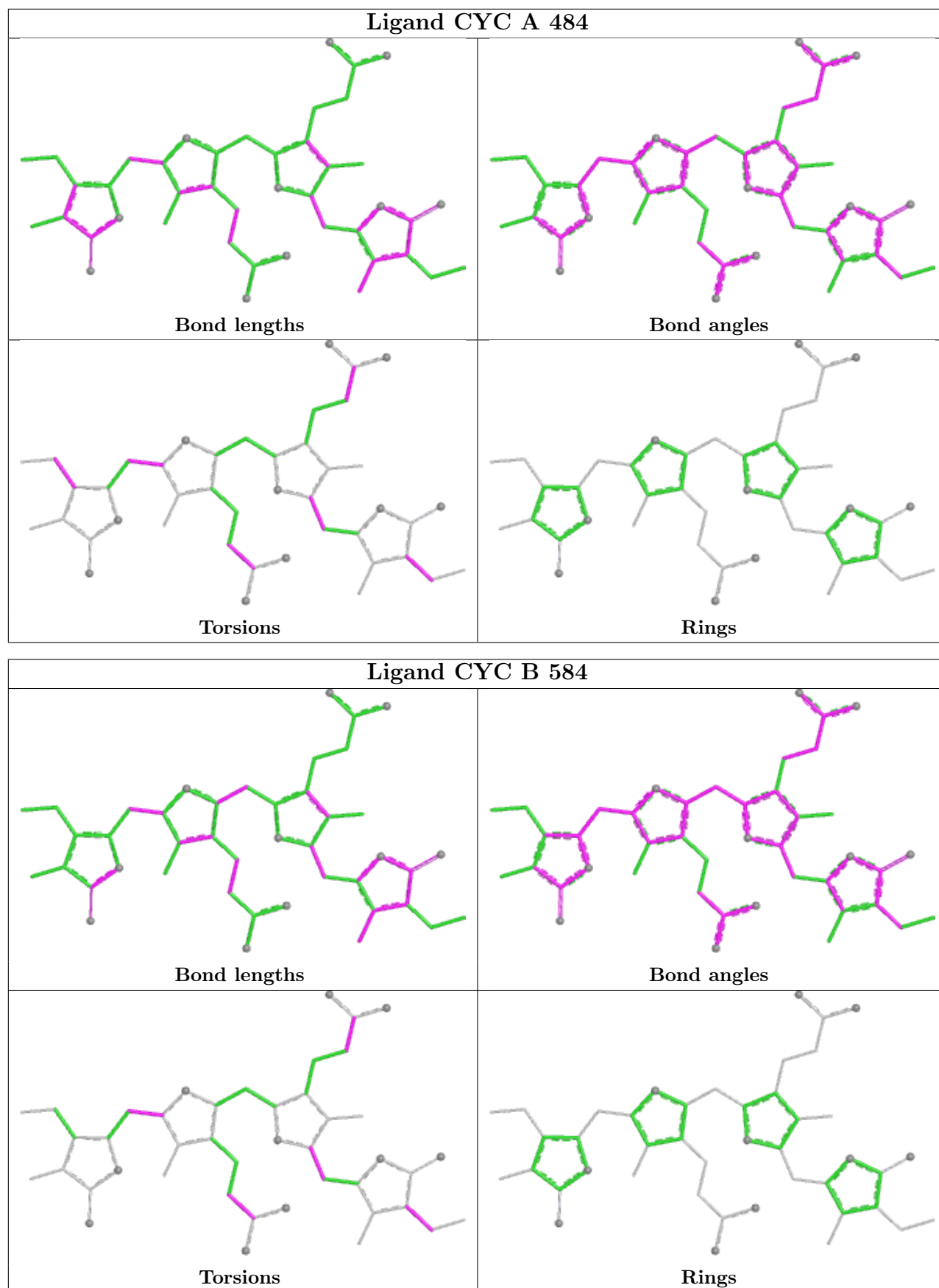
There are no ring outliers.

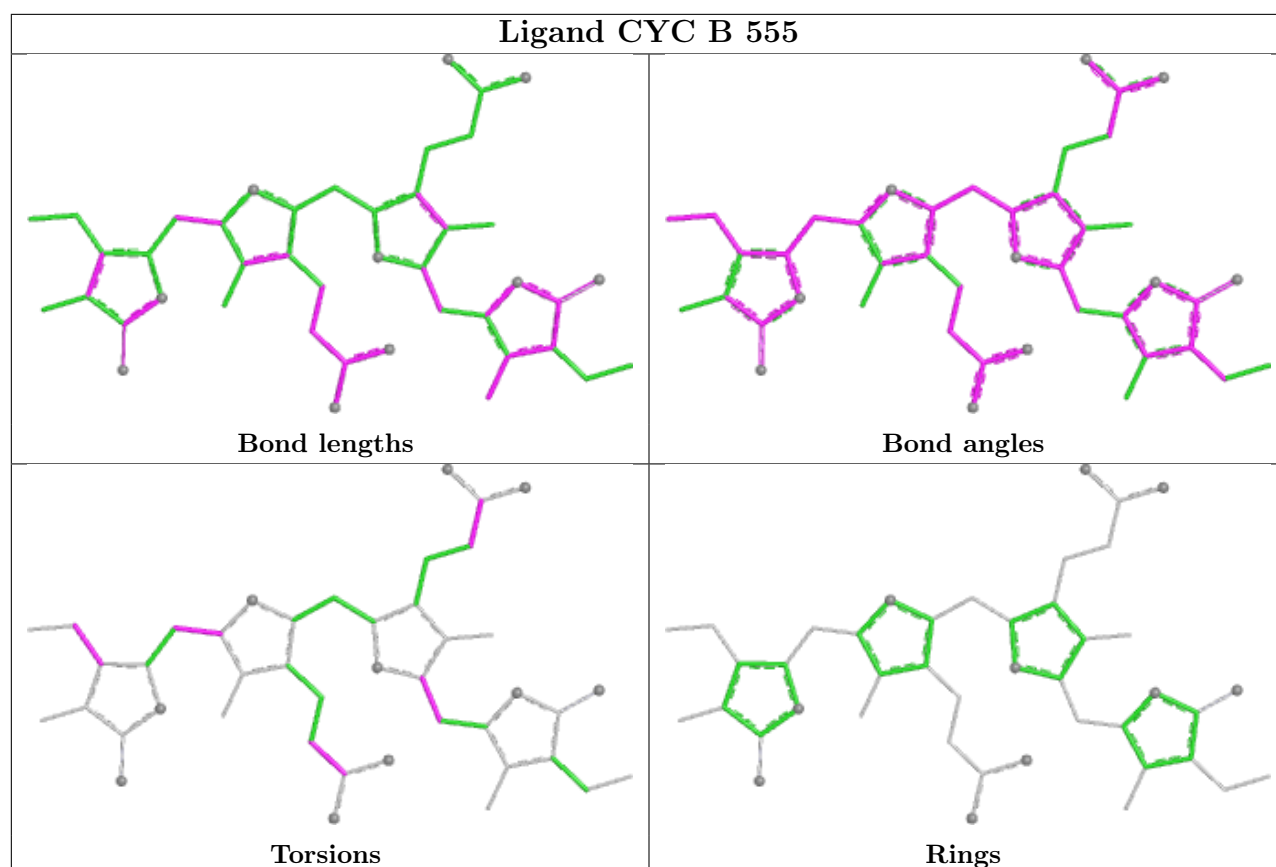
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	484	CYC	1	0
3	B	584	CYC	2	0
3	B	555	CYC	1	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	162/162 (100%)	0.96	25 (15%) 5 9	11, 16, 27, 34	1 (0%)
2	B	171/172 (99%)	1.41	39 (22%) 2 3	14, 20, 28, 36	1 (0%)
All	All	333/334 (99%)	1.19	64 (19%) 3 5	11, 18, 28, 36	2 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	ALA	7.9
1	A	117	GLU	6.0
2	B	22	ALA	5.8
1	A	75	ALA	5.6
2	B	111	CYS	5.4
1	A	57[A]	GLN	4.8
1	A	24	LEU	3.9
2	B	61	ALA	3.8
2	B	148[A]	ASN	3.7
2	B	32	LYS	3.7
1	A	70	GLN	3.6
2	B	112	LEU	3.5
2	B	29	ASN	3.4
1	A	4	PRO	3.3
2	B	30	LEU	3.2
2	B	173	VAL	3.2
2	B	67	ILE	3.2
2	B	2	LEU	3.2
2	B	116	ARG	3.0
2	B	68	GLN	3.0
1	A	22	THR	3.0
1	A	174	SER	3.0
2	B	117	GLU	2.9
1	A	105	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	MET	2.9
2	B	123	GLY	2.9
2	B	134	GLN	2.9
2	B	64	PRO	2.8
2	B	157	ALA	2.7
2	B	1	MET	2.7
1	A	7	GLU	2.7
2	B	114	GLY	2.7
2	B	109	ASP	2.7
2	B	63	GLN	2.6
2	B	160	SER	2.6
2	B	26	ALA	2.6
2	B	21	ASN	2.6
2	B	70	GLY	2.5
1	A	34	ALA	2.5
1	A	123	ASP	2.5
2	B	118	THR	2.5
1	A	35	VAL	2.5
2	B	171	ALA	2.4
1	A	116	SER	2.4
2	B	105	SER	2.4
2	B	120	GLN	2.4
2	B	152	PRO	2.4
1	A	11	ALA	2.4
1	A	63	PHE	2.4
2	B	170	ALA	2.4
2	B	121	ALA	2.3
1	A	14	THR	2.3
1	A	23	GLU	2.3
1	A	3	THR	2.3
2	B	141	ILE	2.3
2	B	147	PRO	2.3
2	B	25	ASP	2.2
2	B	137	LYS	2.1
1	A	79	GLU	2.1
2	B	108	ASP	2.1
1	A	64	PRO	2.1
1	A	106	PRO	2.1
1	A	32	LYS	2.0
1	A	143	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	MEN	B	72	9/10	0.91	0.11	18,20,21,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

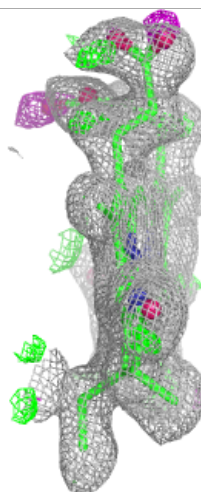
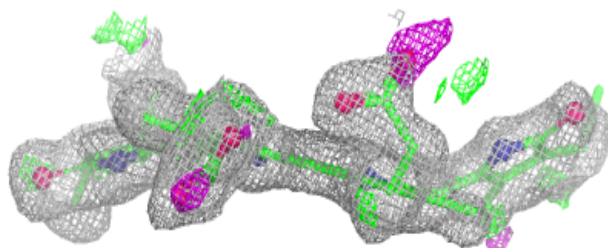
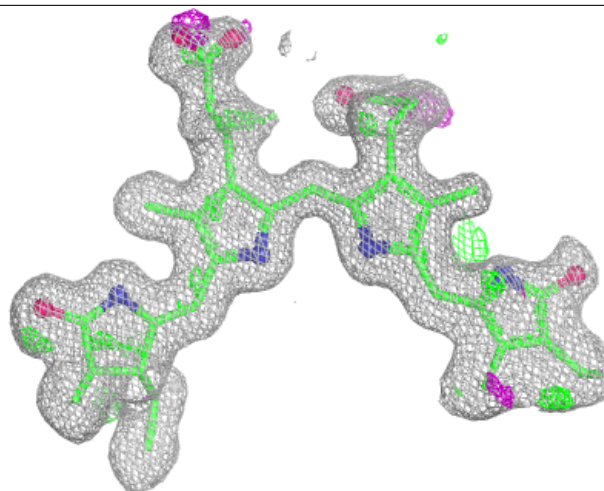
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CYC	B	584	43/43	0.89	0.14	14,24,34,35	0
3	CYC	B	555	43/43	0.89	0.12	16,19,33,41	0
3	CYC	A	484	43/43	0.95	0.07	10,12,16,19	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.

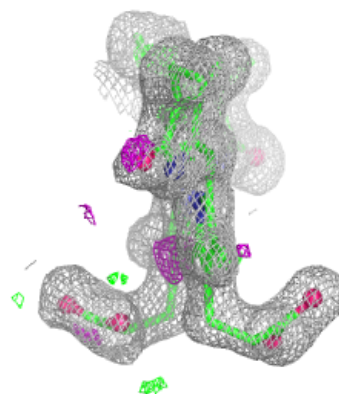
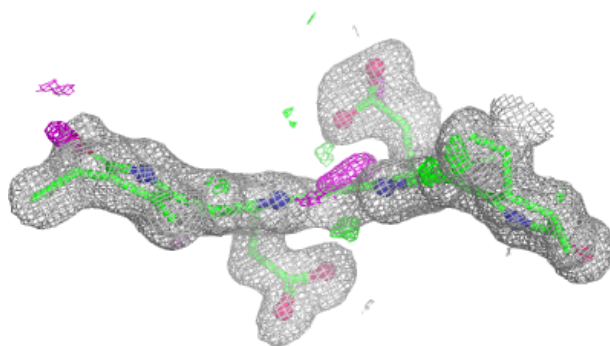
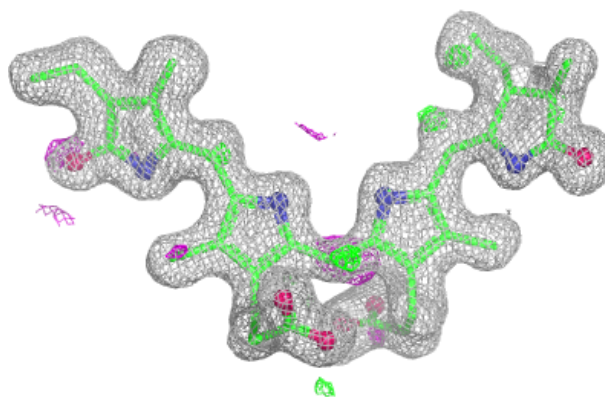
Electron density around CYC B 584:

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



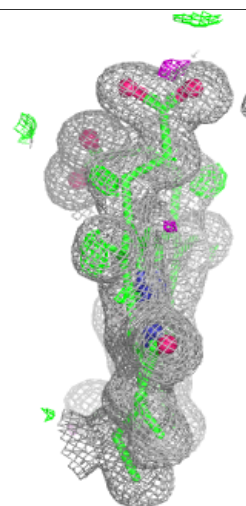
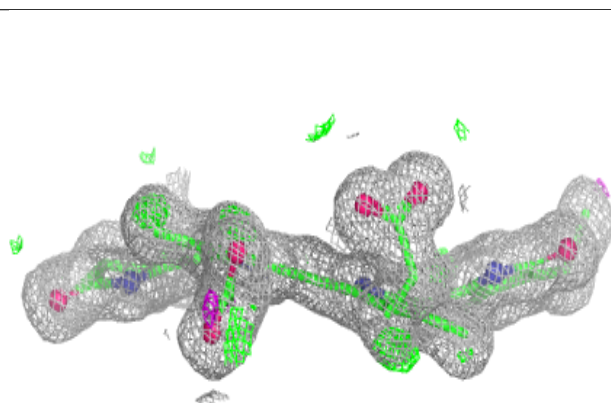
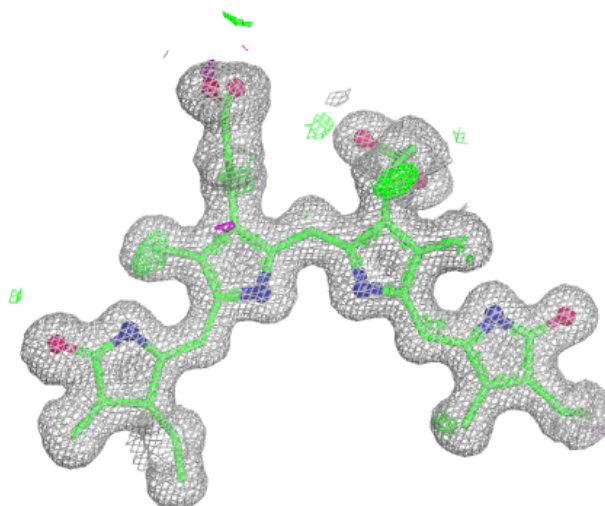
Electron density around CYC B 555:

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



Electron density around CYC A 484:

$2mF_o-DF_c$ (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.