Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:52 AM EDT

PDB ID	:	1JBO
Title	:	The 1.45A Three-Dimensional Structure of c-Phycocyanin from the Thermophylic Cyanobacterium Synechococcus elongatus
Authors	:	Nield, J.; Rizkallah, P.J.; Barber, J.; Chayen, N.E.
Deposited on	:	2002-05-02
Resolution	:	1.45 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 (i) 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 (i)) were used in the production of this report:

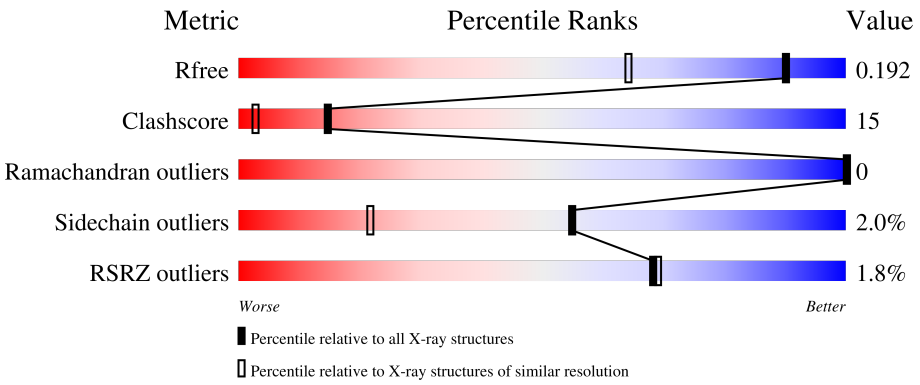
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

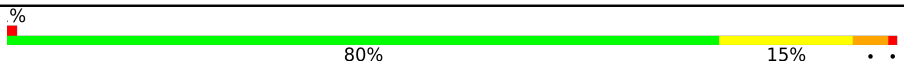
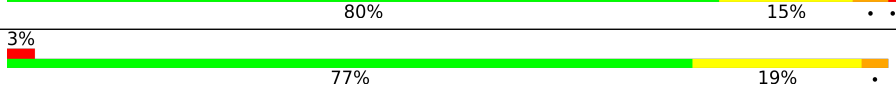
The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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% 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	
2	B	172	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3153 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1244	780	207	249	8	0	7	0

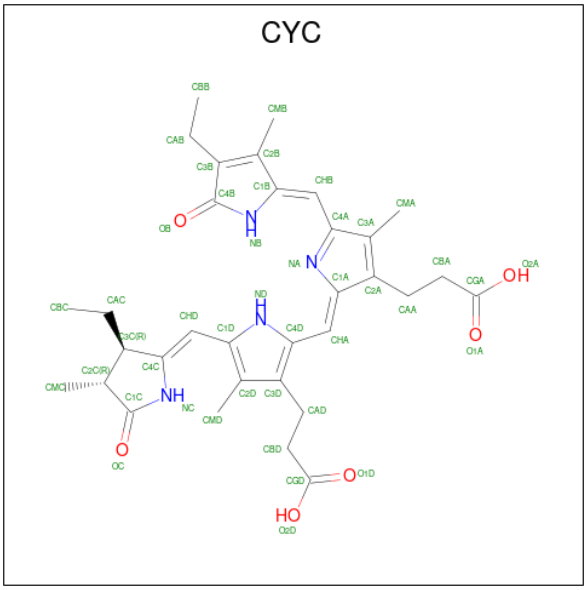
- Molecule 2 is a protein called C-Phycocyanin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1306	803	239	256	8	0	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MEN	ASN	modified residue	UNP P50033

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 4 is water.

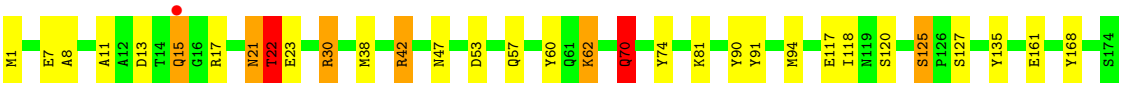
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	257	257	257	0	0
4	B	217	217	217	0	0

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 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.

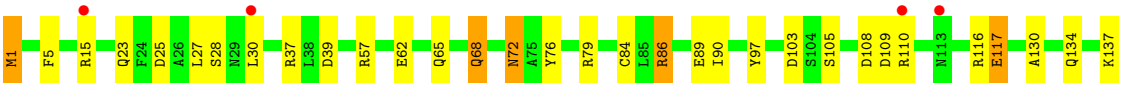
- Molecule 1: C-Phycocyanin alpha chain

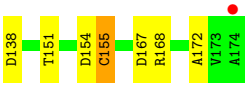
Chain A:



- Molecule 2: C-Phycocyanin beta chain

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	188.00Å 188.00Å 60.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.70 – 1.45 56.75 – 1.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (56.70-1.45) 98.8 (56.75-1.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.188 0.154 , 0.192	Depositor DCC
R_{free} test set	3617 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.6	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	0.97	EDS
Total number of atoms	3153	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 4.31% 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 (i)

5.1 Standard geometry (i)

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	1.82	21/1303 (1.6%)	1.41	13/1765 (0.7%)
2	B	1.61	13/1365 (1.0%)	1.41	16/1842 (0.9%)
All	All	1.72	34/2668 (1.3%)	1.41	29/3607 (0.8%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	LYS	CB-CG	-19.44	1.00	1.52
1	A	70[A]	GLN	CG-CD	9.95	1.74	1.51
1	A	70[B]	GLN	CG-CD	9.95	1.74	1.51
1	A	62	LYS	CG-CD	-7.74	1.26	1.52
2	B	89[A]	GLU	CD-OE2	7.69	1.34	1.25
2	B	89[B]	GLU	CD-OE2	7.69	1.34	1.25
1	A	47	ASN	CG-OD1	-7.25	1.07	1.24
1	A	125[A]	SER	CB-OG	7.24	1.51	1.42
1	A	125[B]	SER	CB-OG	7.24	1.51	1.42
1	A	161	GLU	CD-OE1	7.04	1.33	1.25
1	A	168	TYR	CD2-CE2	-6.77	1.29	1.39
1	A	15	GLN	CB-CG	-6.64	1.34	1.52
1	A	11	ALA	CA-CB	-6.51	1.38	1.52
2	B	172	ALA	CA-CB	6.36	1.65	1.52
1	A	21	ASN	N-CA	-6.22	1.33	1.46
2	B	168	ARG	CB-CG	-5.98	1.36	1.52
2	B	62	GLU	CG-CD	5.96	1.60	1.51
1	A	120[A]	SER	CA-CB	5.71	1.61	1.52
1	A	120[B]	SER	CA-CB	5.71	1.61	1.52
2	B	65	GLN	CG-CD	5.66	1.64	1.51
2	B	155	CYS	CB-SG	-5.65	1.72	1.81
2	B	76	TYR	CE1-CZ	-5.57	1.31	1.38
2	B	28	SER	CB-OG	5.57	1.49	1.42
1	A	42	ARG	NE-CZ	5.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	MET	CB-CG	-5.45	1.33	1.51
1	A	81	LYS	CE-NZ	5.42	1.62	1.49
1	A	135	TYR	CD1-CE1	5.39	1.47	1.39
1	A	127	SER	CB-OG	5.28	1.49	1.42
2	B	68	GLN	CB-CG	-5.23	1.38	1.52
2	B	130	ALA	CA-CB	5.18	1.63	1.52
2	B	105	SER	CB-OG	-5.12	1.35	1.42
1	A	74	TYR	CE2-CZ	-5.05	1.31	1.38
1	A	7[A]	GLU	CD-OE1	5.02	1.31	1.25
1	A	7[B]	GLU	CD-OE1	5.02	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	TYR	CB-CG-CD2	9.77	126.86	121.00
2	B	154	ASP	CB-CG-OD2	8.53	125.98	118.30
2	B	116	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	42	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	53	ASP	CB-CG-OD2	7.53	125.07	118.30
2	B	167	ASP	CB-CG-OD1	7.48	125.03	118.30
2	B	116	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	1	MET	CG-SD-CE	7.20	111.72	100.20
2	B	138	ASP	CB-CG-OD1	6.99	124.59	118.30
2	B	39	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	13	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	108	ASP	CB-CG-OD2	6.54	124.19	118.30
2	B	37	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	B	57	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	B	86	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	B	57	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	B	103	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	22	THR	OG1-CB-CG2	-5.96	96.28	110.00
1	A	135	TYR	CG-CD2-CE2	5.78	125.92	121.30
2	B	25	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	53	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	117	GLU	CG-CD-OE1	5.63	129.56	118.30
1	A	91	TYR	CB-CG-CD1	5.37	124.22	121.00
2	B	97	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	74	TYR	CB-CG-CD1	5.21	124.13	121.00
1	A	30	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	13	ASP	OD1-CG-OD2	-5.10	113.61	123.30
2	B	117[A]	GLU	CA-CB-CG	5.08	124.57	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	117[B]	GLU	CA-CB-CG	5.08	124.57	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1244	0	1218	15	0
2	B	1306	0	1302	46	0
3	A	43	0	35	7	0
3	B	86	0	74	32	0
4	A	257	0	0	8	4
4	B	217	0	0	12	3
All	All	3153	0	2629	82	4

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 15.

All (82) 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)
2:B:155:CYS:SG	3:B:503:CYC:HAC1	1.19	1.70
2:B:84:CYS:SG	3:B:502:CYC:HAC2	1.32	1.64
2:B:155:CYS:SG	3:B:503:CYC:CAC	2.15	1.32
2:B:84:CYS:SG	3:B:502:CYC:CAC	2.19	1.30
1:A:38[B]:MET:CE	1:A:38[B]:MET:SD	2.28	1.21
3:B:502:CYC:HMA1	3:B:502:CYC:HB	0.95	1.05
3:B:502:CYC:HMA1	3:B:502:CYC:NB	1.77	0.99
3:B:503:CYC:HMD2	3:B:503:CYC:HC	1.26	0.98
3:B:502:CYC:HB	3:B:502:CYC:CMA	1.79	0.95
2:B:79[A]:ARG:HD3	4:B:658:HOH:O	1.67	0.94
2:B:90:ILE:HG21	3:B:502:CYC:HBB3	1.55	0.89
3:B:502:CYC:HMD2	3:B:502:CYC:HC	1.38	0.88
3:B:502:CYC:HMA3	4:B:649:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:N	2:B:110[A]:ARG:HH22	1.76	0.84
2:B:151:THR:O	3:B:503:CYC:HMD2	1.78	0.83
2:B:72:MEN:HE22	3:B:502:CYC:HBD2	1.60	0.82
3:A:501:CYC:HC	3:A:501:CYC:HMD2	1.46	0.80
2:B:84:CYS:SG	3:B:502:CYC:CBC	2.69	0.79
3:B:503:CYC:HB	3:B:503:CYC:HMA1	1.46	0.79
3:A:501:CYC:NB	3:A:501:CYC:HMA1	1.98	0.79
1:A:15:GLN:HG3	1:A:17:ARG:HD3	1.64	0.79
2:B:155:CYS:SG	3:B:503:CYC:C3C	2.73	0.76
3:B:503:CYC:HC	3:B:503:CYC:CMD	1.99	0.76
3:B:502:CYC:HC	3:B:502:CYC:CMD	1.99	0.76
3:B:503:CYC:HMA1	3:B:503:CYC:NB	2.02	0.75
1:A:21:ASN:HB2	4:A:642:HOH:O	1.87	0.73
2:B:1:MET:H1	2:B:110[A]:ARG:HH22	1.36	0.73
1:A:125[B]:SER:OG	4:A:595:HOH:O	2.06	0.71
2:B:79[B]:ARG:HD2	4:B:658:HOH:O	1.91	0.68
3:A:501:CYC:HMA1	3:A:501:CYC:HB	1.59	0.67
2:B:30[B]:LEU:HD11	4:B:698:HOH:O	1.95	0.67
2:B:72:MEN:OD1	3:B:502:CYC:HMD2	1.95	0.65
2:B:134:GLN:NE2	2:B:137:LYS:HE2	2.10	0.65
2:B:134:GLN:HE22	2:B:137:LYS:NZ	1.95	0.65
3:B:503:CYC:HMD2	3:B:503:CYC:NC	2.06	0.65
2:B:84:CYS:CB	3:B:502:CYC:HAC2	2.29	0.61
1:A:42:ARG:NH2	4:A:757:HOH:O	1.91	0.61
2:B:30[B]:LEU:CD1	4:B:698:HOH:O	2.47	0.60
2:B:155:CYS:SG	3:B:503:CYC:CBC	2.88	0.60
1:A:15:GLN:CG	1:A:17:ARG:HD3	2.32	0.59
2:B:117[B]:GLU:OE1	4:B:671:HOH:O	2.17	0.59
2:B:151:THR:O	3:B:503:CYC:CMD	2.50	0.59
2:B:90:ILE:CG2	3:B:502:CYC:HBB3	2.31	0.58
2:B:117[B]:GLU:OE2	4:B:696:HOH:O	2.17	0.58
2:B:86:ARG:HH22	3:B:502:CYC:C1A	2.18	0.57
2:B:86:ARG:NH2	3:B:502:CYC:C1A	2.69	0.56
2:B:110[A]:ARG:NH2	4:B:715:HOH:O	2.02	0.56
1:A:57:GLN:NE2	4:A:580:HOH:O	2.36	0.55
1:A:42:ARG:NE	4:A:757:HOH:O	2.39	0.55
3:A:501:CYC:HB	3:A:501:CYC:CMA	2.19	0.54
3:B:503:CYC:CMD	3:B:503:CYC:NC	2.68	0.54
1:A:22:THR:HB	4:A:636:HOH:O	2.08	0.53
2:B:30[B]:LEU:HD12	4:B:620:HOH:O	2.09	0.53
2:B:155:CYS:CB	3:B:503:CYC:HAC1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:N	2:B:110[A]:ARG:NH2	2.53	0.52
3:B:502:CYC:CMD	3:B:502:CYC:NC	2.72	0.50
2:B:134:GLN:HE22	2:B:137:LYS:CE	2.25	0.50
2:B:134:GLN:NE2	2:B:137:LYS:CE	2.75	0.50
2:B:117[B]:GLU:HG3	4:B:648:HOH:O	2.13	0.48
3:B:502:CYC:CMA	4:B:649:HOH:O	2.48	0.48
3:A:501:CYC:HMD2	3:A:501:CYC:NC	2.21	0.48
2:B:84:CYS:SG	3:B:502:CYC:C3C	2.95	0.45
2:B:109:ASP:HB2	2:B:110[A]:ARG:HD2	1.98	0.45
1:A:57:GLN:HE21	1:A:57:GLN:HB3	1.42	0.43
2:B:68:GLN:NE2	4:B:535:HOH:O	2.50	0.43
2:B:1:MET:H3	2:B:110[A]:ARG:HH22	1.61	0.43
1:A:22:THR:CB	4:A:636:HOH:O	2.65	0.43
1:A:90:TYR:O	1:A:94:MET:HG2	2.19	0.42
2:B:5:PHE:CD1	2:B:27:LEU:HD22	2.55	0.42
3:A:501:CYC:HC	3:A:501:CYC:CMD	2.25	0.41
1:A:8:ALA:HB1	1:A:23:GLU:HB3	2.02	0.41
3:A:501:CYC:HMA3	4:A:510:HOH:O	2.20	0.41
2:B:1:MET:H3	2:B:110[A]:ARG:NH2	2.17	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:735:HOH:O	4:A:735:HOH:O[6_556]	1.59	0.61
4:A:561:HOH:O	4:B:607:HOH:O[3_555]	1.85	0.35
4:A:661:HOH:O	4:B:617:HOH:O[5_556]	1.92	0.28
4:A:628:HOH:O	4:B:692:HOH:O[5_556]	2.19	0.01

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	167/162 (103%)	164 (98%)	3 (2%)	0	100	100
2	B	179/172 (104%)	176 (98%)	3 (2%)	0	100	100
All	All	346/334 (104%)	340 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	130/123 (106%)	124 (95%)	6 (5%)	27	2
2	B	137/127 (108%)	137 (100%)	0	100	100
All	All	267/250 (107%)	261 (98%)	6 (2%)	55	18

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	30	ARG
1	A	62	LYS
1	A	70[A]	GLN
1	A	70[B]	GLN
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	15	GLN
1	A	57	GLN
2	B	35	ASN
2	B	63	GLN
2	B	68	GLN
2	B	78	ASN
2	B	134	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.57	1 (14%)	6,9,11	0.55	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	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	CE2-ND2	6.28	1.56	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (2) 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

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	501	1	42,46,46	2.11	12 (28%)	50,67,67	3.52	21 (42%)
3	CYC	B	502	-	42,46,46	3.92	18 (42%)	50,67,67	4.82	30 (60%)
3	CYC	B	503	-	42,46,46	4.20	22 (52%)	50,67,67	4.53	23 (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
3	CYC	A	501	1	-	11/25/74/74	0/4/4/4
3	CYC	B	502	-	-	8/25/74/74	0/4/4/4
3	CYC	B	503	-	-	9/25/74/74	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	CYC	CHA-C1A	14.92	1.47	1.35
3	B	503	CYC	C2C-C1C	-13.63	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CYC	CHA-C1A	11.68	1.44	1.35
3	B	503	CYC	OC-C1C	9.94	1.43	1.23
3	B	502	CYC	C1B-NB	-9.28	1.22	1.37
3	B	503	CYC	CAC-C3C	-7.86	1.38	1.54
3	B	502	CYC	C2C-C1C	-7.74	1.45	1.52
3	B	502	CYC	OC-C1C	7.10	1.37	1.23
3	A	501	CYC	OB-C4B	6.73	1.36	1.23
3	B	502	CYC	CAC-C3C	-6.15	1.41	1.54
3	B	503	CYC	C4C-NC	-5.59	1.25	1.37
3	B	502	CYC	CMC-C2C	-5.27	1.41	1.53
3	B	503	CYC	C4B-C3B	-5.22	1.38	1.48
3	B	503	CYC	OB-C4B	4.89	1.32	1.23
3	B	502	CYC	C2A-C3A	4.73	1.46	1.36
3	B	503	CYC	CHB-C4A	4.56	1.51	1.40
3	B	502	CYC	C1C-NC	-4.51	1.31	1.37
3	A	501	CYC	OC-C1C	4.40	1.32	1.23
3	B	503	CYC	C3C-C4C	-4.38	1.44	1.50
3	B	502	CYC	C3C-C4C	-4.31	1.44	1.50
3	A	501	CYC	C1C-NC	-4.25	1.32	1.37
3	B	503	CYC	CMA-C3A	-4.12	1.42	1.50
3	B	502	CYC	C2C-C3C	-3.95	1.43	1.54
3	B	503	CYC	C2C-C3C	-3.59	1.44	1.54
3	A	501	CYC	C3D-C2D	3.52	1.48	1.37
3	B	502	CYC	CBA-CAA	-3.47	1.41	1.52
3	B	503	CYC	C2A-C3A	3.31	1.43	1.36
3	B	503	CYC	CBD-CGD	3.25	1.58	1.50
3	A	501	CYC	C2A-C3A	3.23	1.43	1.36
3	B	503	CYC	C3B-C2B	3.22	1.43	1.36
3	A	501	CYC	CHB-C4A	3.22	1.48	1.40
3	B	502	CYC	C3D-C2D	3.20	1.47	1.37
3	B	503	CYC	C1B-NB	-3.17	1.32	1.37
3	A	501	CYC	C4B-C3B	-3.06	1.42	1.48
3	A	501	CYC	CMB-C2B	-2.81	1.44	1.50
3	A	501	CYC	C1B-NB	-2.80	1.33	1.37
3	B	502	CYC	CHB-C4A	2.74	1.46	1.40
3	B	502	CYC	OB-C4B	2.64	1.28	1.23
3	B	503	CYC	C1B-C2B	-2.59	1.40	1.45
3	B	503	CYC	O2A-CGA	2.56	1.39	1.30
3	A	501	CYC	CBA-CAA	-2.56	1.43	1.52
3	B	503	CYC	C3D-C2D	2.41	1.44	1.37
3	B	502	CYC	CMB-C2B	-2.40	1.45	1.50
3	B	503	CYC	C1A-C2A	-2.28	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CYC	CAD-CBD	2.22	1.63	1.52
3	A	501	CYC	C4B-NB	-2.14	1.33	1.38
3	B	502	CYC	C1B-C2B	2.14	1.49	1.45
3	B	503	CYC	C1D-CHD	2.13	1.49	1.41
3	B	502	CYC	O2A-CGA	2.06	1.37	1.30
3	A	501	CYC	C2C-C1C	2.05	1.53	1.52
3	B	503	CYC	CMD-C2D	-2.04	1.47	1.51
3	B	502	CYC	C1A-NA	-2.03	1.34	1.38

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	CYC	OC-C1C-C2C	-14.46	114.67	126.17
3	B	502	CYC	C2C-C1C-NC	12.92	119.41	108.27
3	B	503	CYC	CHD-C4C-NC	-12.89	109.88	125.20
3	B	503	CYC	C2C-C1C-NC	12.88	119.38	108.27
3	B	502	CYC	CAA-CBA-CGA	-12.88	85.89	113.60
3	B	502	CYC	C3B-C4B-NB	12.83	117.14	106.78
3	A	501	CYC	OC-C1C-C2C	-11.36	117.14	126.17
3	A	501	CYC	C3B-C4B-NB	11.10	115.75	106.78
3	B	503	CYC	C3B-C4B-NB	10.10	114.94	106.78
3	A	501	CYC	OB-C4B-C3B	-10.05	117.14	128.04
3	B	503	CYC	OC-C1C-C2C	-9.54	118.59	126.17
3	B	502	CYC	CAB-C3B-C4B	9.00	135.60	121.38
3	B	503	CYC	CBC-CAC-C3C	8.58	132.57	113.47
3	B	503	CYC	CAB-C3B-C4B	8.01	134.03	121.38
3	B	503	CYC	OC-C1C-NC	-7.95	115.31	124.94
3	B	503	CYC	OB-C4B-C3B	-7.82	119.55	128.04
3	A	501	CYC	C2C-C1C-NC	7.75	114.95	108.27
3	B	503	CYC	CMC-C2C-C1C	6.59	126.61	112.40
3	B	503	CYC	CBD-CAD-C3D	-5.68	102.92	112.62
3	B	502	CYC	C1B-NB-C4B	-5.57	103.57	110.67
3	B	502	CYC	CBB-CAB-C3B	-5.49	97.29	112.43
3	B	502	CYC	C2B-C1B-NB	5.40	114.89	106.99
3	A	501	CYC	C1B-NB-C4B	-5.34	103.87	110.67
3	B	503	CYC	C1B-NB-C4B	-5.18	104.07	110.67
3	B	502	CYC	O1A-CGA-CBA	-5.01	106.98	123.08
3	B	502	CYC	CBA-CAA-C2A	4.81	125.98	112.63
3	B	503	CYC	CAC-C3C-C4C	4.52	124.28	112.67
3	B	502	CYC	CBD-CAD-C3D	4.42	120.16	112.62
3	A	501	CYC	CAB-C3B-C4B	4.39	128.31	121.38
3	B	503	CYC	CMA-C3A-C4A	4.37	131.79	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	CYC	CBC-CAC-C3C	4.32	123.08	113.47
3	A	501	CYC	CAA-CBA-CGA	-4.15	104.66	113.60
3	B	502	CYC	CMA-C3A-C4A	4.12	131.41	125.06
3	A	501	CYC	CAC-C3C-C2C	3.98	124.21	114.26
3	B	502	CYC	CMC-C2C-C1C	3.85	120.71	112.40
3	B	502	CYC	O2A-CGA-CBA	3.81	126.26	114.03
3	B	502	CYC	CMB-C2B-C1B	3.62	128.68	124.17
3	B	502	CYC	C1A-C2A-C3A	-3.30	103.13	106.78
3	B	502	CYC	CHB-C4A-NA	-3.27	118.09	124.93
3	B	502	CYC	OB-C4B-NB	-3.16	117.72	125.08
3	A	501	CYC	C1A-C2A-C3A	-3.14	103.31	106.78
3	B	502	CYC	CHA-C1A-C2A	-3.13	118.09	125.32
3	A	501	CYC	O2D-CGD-O1D	-3.06	115.67	123.30
3	B	502	CYC	O1D-CGD-CBD	-3.02	113.37	123.08
3	B	502	CYC	CHB-C4A-C3A	2.98	132.56	124.90
3	B	503	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
3	B	502	CYC	CAC-C3C-C4C	2.94	120.22	112.67
3	A	501	CYC	CBD-CAD-C3D	2.89	117.55	112.62
3	A	501	CYC	CMC-C2C-C1C	2.87	118.59	112.40
3	B	503	CYC	CMC-C2C-C3C	2.86	125.38	113.83
3	B	503	CYC	CAA-C2A-C1A	2.84	130.04	125.01
3	A	501	CYC	O1A-CGA-CBA	-2.74	114.28	123.08
3	B	503	CYC	CAA-CBA-CGA	2.70	119.41	113.60
3	A	501	CYC	C4A-C3A-C2A	2.69	109.60	106.51
3	B	502	CYC	OB-C4B-C3B	-2.69	125.12	128.04
3	B	503	CYC	CHB-C1B-C2B	-2.64	121.73	126.95
3	A	501	CYC	O2D-CGD-CBD	2.56	122.26	114.03
3	B	502	CYC	CMC-C2C-C3C	2.56	124.15	113.83
3	A	501	CYC	CAC-C3C-C4C	2.55	119.23	112.67
3	A	501	CYC	CMC-C2C-C3C	2.55	124.11	113.83
3	A	501	CYC	C1A-NA-C4A	2.52	111.27	106.51
3	B	503	CYC	C4D-CHA-C1A	-2.50	125.82	128.81
3	B	502	CYC	C4D-CHA-C1A	-2.48	125.84	128.81
3	A	501	CYC	C2B-C1B-NB	2.40	110.51	106.99
3	B	503	CYC	CHA-C1A-C2A	-2.40	119.78	125.32
3	B	503	CYC	CAC-C3C-C2C	2.37	120.17	114.26
3	A	501	CYC	CHB-C4A-C3A	2.22	130.61	124.90
3	B	503	CYC	CAD-CBD-CGD	2.20	119.93	113.76
3	B	503	CYC	CBA-CAA-C2A	-2.18	106.57	112.63
3	B	502	CYC	CHB-C1B-NB	-2.15	121.45	126.06
3	A	501	CYC	O2A-CGA-CBA	2.10	120.79	114.03
3	B	502	CYC	CAA-C2A-C1A	2.10	128.72	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	CYC	C2C-C3C-C4C	2.05	104.41	101.34
3	B	502	CYC	OC-C1C-NC	-2.03	122.49	124.94

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CYC	NA-C4A-CHB-C1B
3	A	501	CYC	C3A-C4A-CHB-C1B
3	A	501	CYC	C4C-C3C-CAC-CBC
3	A	501	CYC	ND-C1D-CHD-C4C
3	A	501	CYC	C2D-C1D-CHD-C4C
3	B	502	CYC	C3A-C4A-CHB-C1B
3	B	502	CYC	ND-C1D-CHD-C4C
3	B	502	CYC	C2D-C1D-CHD-C4C
3	B	503	CYC	C3A-C4A-CHB-C1B
3	B	503	CYC	ND-C1D-CHD-C4C
3	B	503	CYC	C2D-C1D-CHD-C4C
3	B	502	CYC	C3A-C2A-CAA-CBA
3	B	502	CYC	C1A-C2A-CAA-CBA
3	B	503	CYC	C2B-C3B-CAB-CBB
3	B	502	CYC	NA-C4A-CHB-C1B
3	B	503	CYC	NA-C4A-CHB-C1B
3	A	501	CYC	C1A-C2A-CAA-CBA
3	A	501	CYC	C3A-C2A-CAA-CBA
3	B	502	CYC	CAA-CBA-CGA-O1A
3	A	501	CYC	CAA-CBA-CGA-O1A
3	A	501	CYC	CAA-CBA-CGA-O2A
3	B	502	CYC	CAA-CBA-CGA-O2A
3	B	503	CYC	CAA-CBA-CGA-O2A
3	B	503	CYC	CAD-CBD-CGD-O2D
3	B	503	CYC	CAA-CBA-CGA-O1A
3	A	501	CYC	CAD-CBD-CGD-O1D
3	B	503	CYC	CAD-CBD-CGD-O1D
3	A	501	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

3 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CYC	7	0

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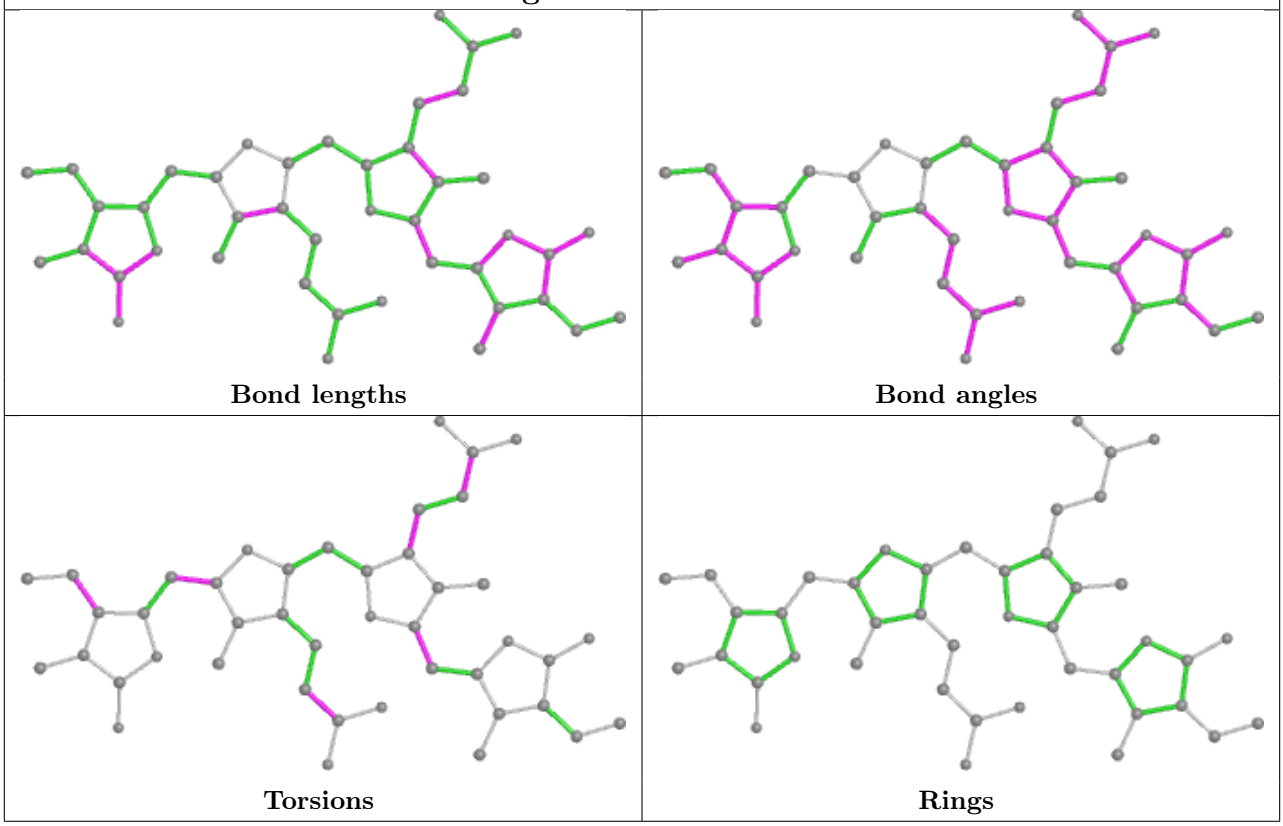
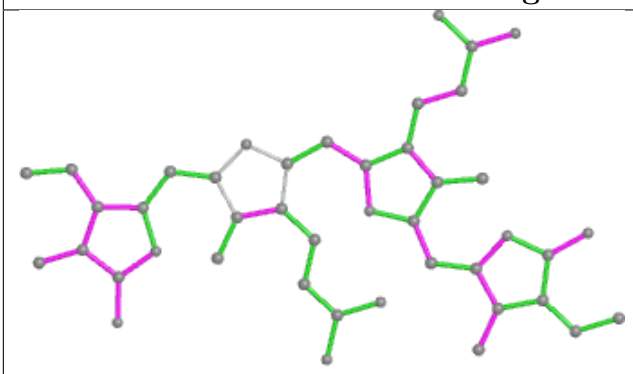
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	CYC	19	0
3	B	503	CYC	13	0

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.

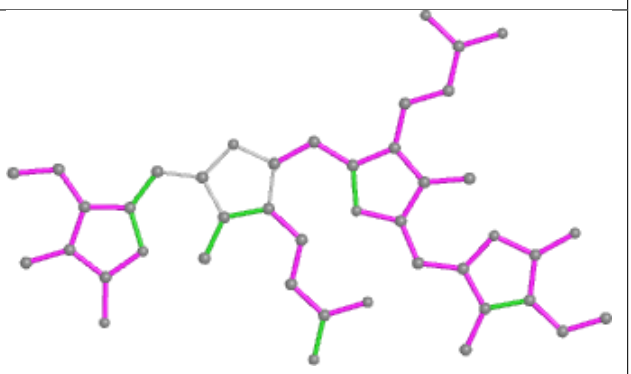
Ligand CYC A 501



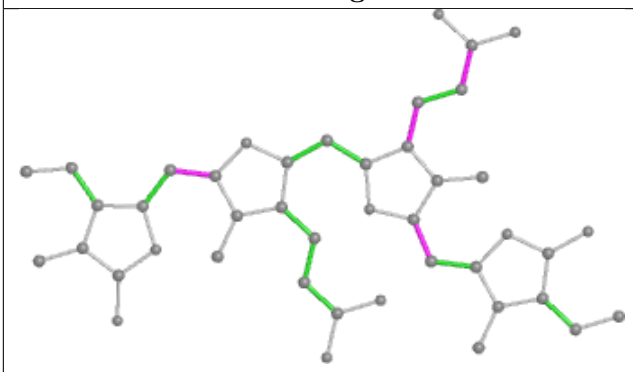
Ligand CYC B 502



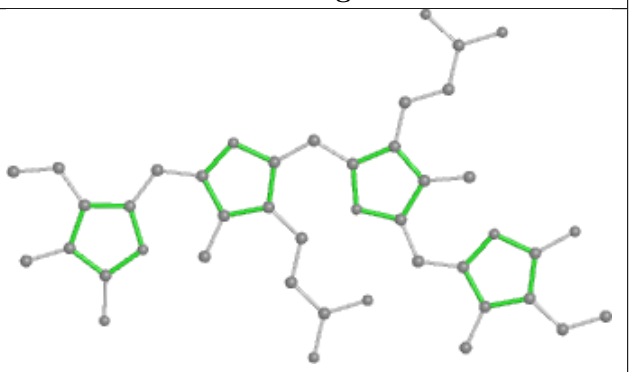
Bond lengths



Bond angles

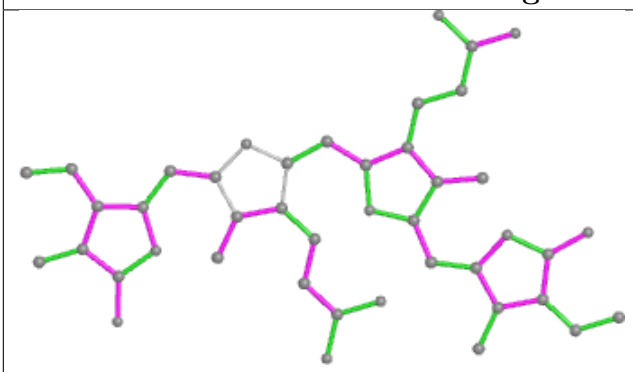


Torsions

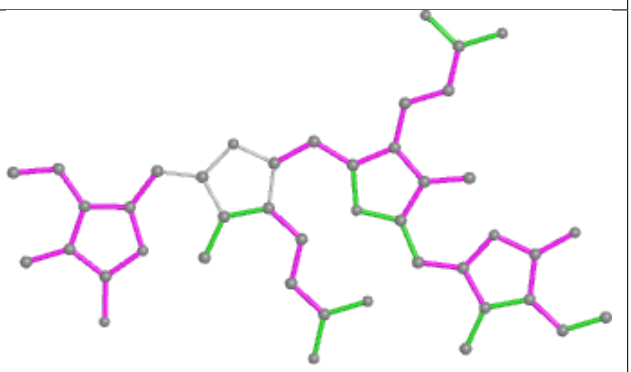


Rings

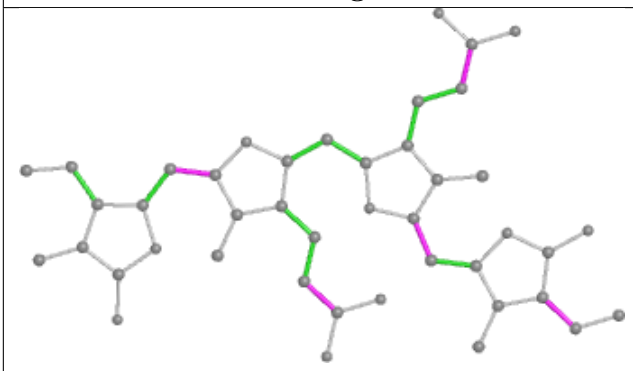
Ligand CYC B 503



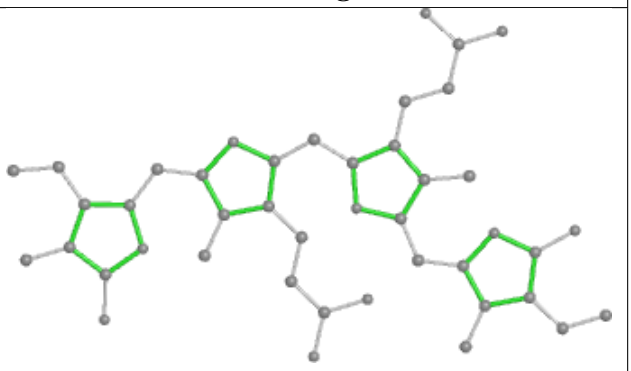
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.01	1 (0%)	89	91	11, 15, 25, 32	0
2	B	171/172 (99%)	-0.03	5 (2%)	51	53	13, 19, 28, 39	0
All	All	333/334 (99%)	-0.01	6 (1%)	68	69	11, 17, 27, 39	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	ALA	3.4
2	B	113	ASN	2.2
2	B	15[A]	ARG	2.1
2	B	110[A]	ARG	2.1
2	B	30[A]	LEU	2.1
1	A	15	GLN	2.1

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	0.97	0.07	15,18,21,24	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

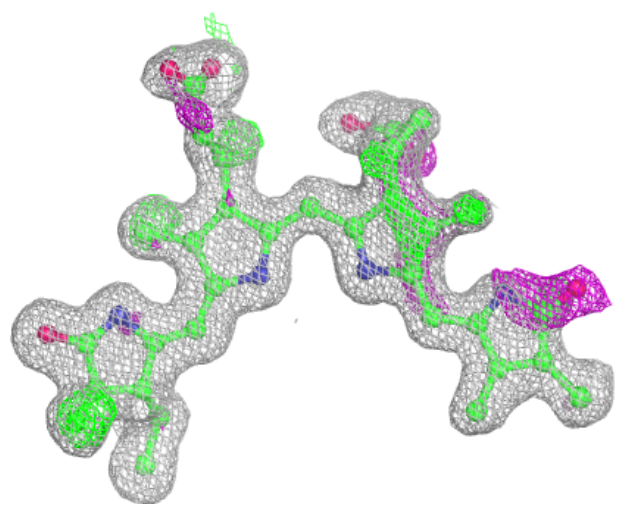
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

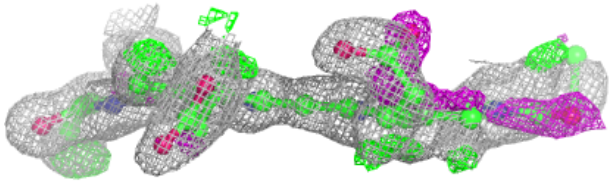
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CYC	B	502	43/43	0.87	0.16	13,22,39,48	0
3	CYC	B	503	43/43	0.88	0.13	16,20,27,31	0
3	CYC	A	501	43/43	0.95	0.10	9,12,16,18	0

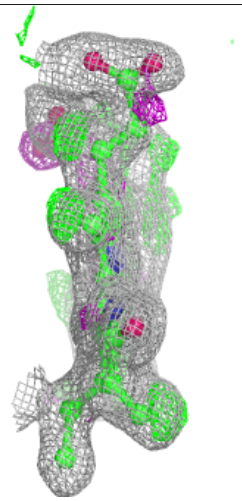
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC B 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

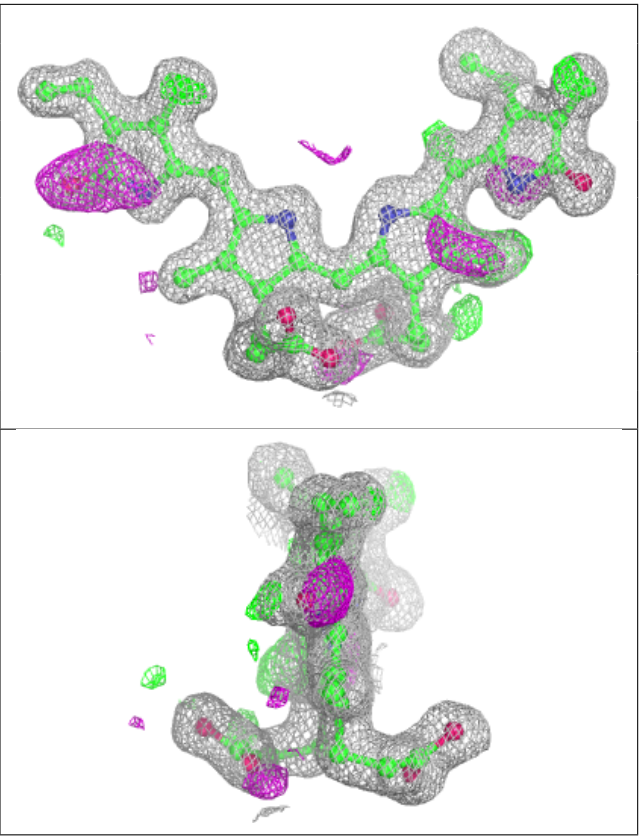






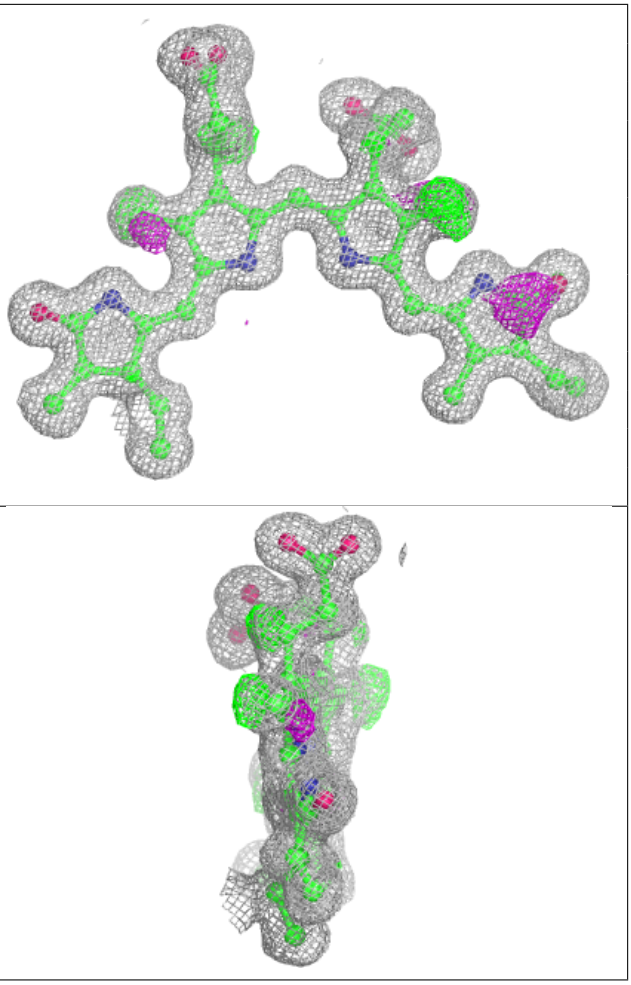
Electron density around CYC B 503:

$2mF_o$-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 501:

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.