Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:48 PM EDT

PDB ID	:	3MWN
Title	:	Structure of the Novel 14 kDa Fragment of alpha-Subunit of Phycoerythrin from the Starving Cyanobacterium Phormidium Tenue
Authors	:	Soni, B.R.; Hasan, M.I.; Parmar, A.; Ethayathulla, A.S.; Kumar, R.P.; Singh, N.K.; Sinha, M.; Kaur, P.; Yadav, S.; Sharma, S.; Madamwar, D.; Singh, T.P.
Deposited on	:	2010-05-06
Resolution	:	2.60 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:

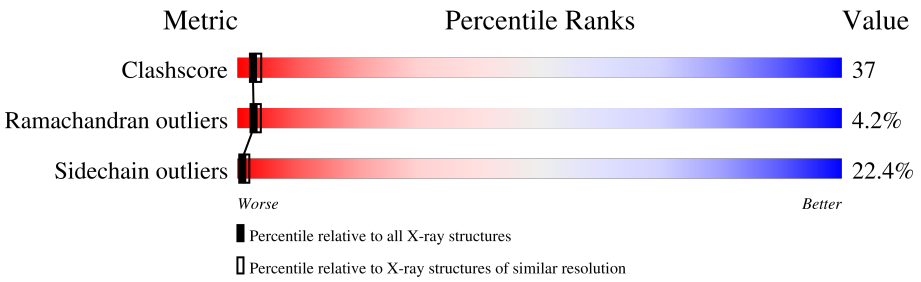
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	133	53% 35% 10% •
1	B	133	45% 39% 14% •

2 Entry composition (i)

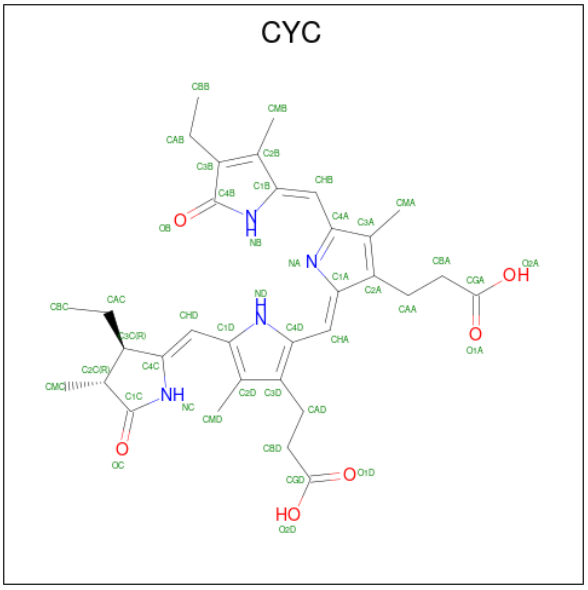
There are 3 unique types of molecules in this entry. The entry contains 2242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1008	630	179	193	6	0	0	0
1	B	133	1008	630	179	193	6	0	0	0

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 3 is water.

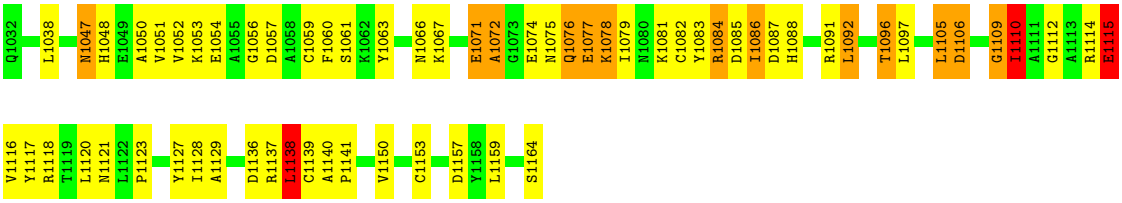
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	33	33	33	0	0
			Total	O		
3	B	21	21	21	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

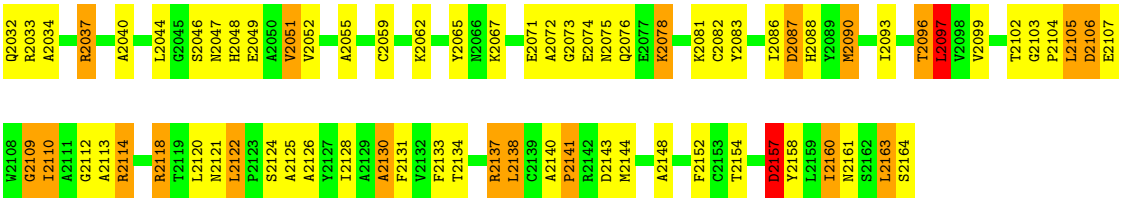
• Molecule 1: PHYCOERYTHRIN

Chain A:



• Molecule 1: PHYCOERYTHRIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.36Å 83.79Å 62.48Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 9.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.6 (10.00-2.60) 84.8 (9.96-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.60Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.238 , 0.286 0.354 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
Reported twinning fraction	0.400 for h,-k,-l	Depositor
Outliers	0 of 15225 reflections	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	2242	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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

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	0.77	0/1027	0.97	4/1391 (0.3%)
1	B	0.80	0/1027	1.02	9/1391 (0.6%)
All	All	0.79	0/2054	0.99	13/2782 (0.5%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2118	ARG	CD-NE-CZ	6.74	133.04	123.60
1	B	2137	ARG	CD-NE-CZ	6.34	132.48	123.60
1	A	1115	GLU	CB-CA-C	6.11	122.61	110.40
1	B	2081	LYS	CD-CE-NZ	5.83	125.10	111.70
1	B	2065	TYR	CA-CB-CG	5.77	124.36	113.40
1	B	2051	VAL	O-C-N	5.68	131.79	122.70
1	B	2097	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	1138	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	2076	GLN	CB-CG-CD	5.33	125.46	111.60
1	A	1136	ASP	CA-CB-CG	5.31	125.08	113.40
1	B	2075	ASN	CA-CB-CG	5.28	125.02	113.40
1	A	1105	LEU	CA-CB-CG	5.22	127.32	115.30
1	B	2157	ASP	CA-CB-CG	5.12	124.66	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	1008	0	958	53	0
1	B	1008	0	957	88	0
2	A	86	0	77	24	0
2	B	86	0	76	22	0
3	A	33	0	0	2	0
3	B	21	0	0	0	0
All	All	2242	0	2068	156	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 37.

All (156) 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:1139:CYS:SG	2:A:3002:CYC:HAC1	1.22	1.73
2:B:3003:CYC:CAA	2:B:3003:CYC:CBA	1.84	1.51
1:B:2128:ILE:CG1	1:B:2163:LEU:HG	1.73	1.16
1:B:2128:ILE:HG12	1:B:2163:LEU:CG	1.82	1.09
1:A:1096:THR:HG22	1:A:1097:LEU:HD12	1.33	1.05
1:B:2128:ILE:HG12	1:B:2163:LEU:HG	1.34	1.01
1:A:1078:LYS:O	2:A:3001:CYC:HMD3	1.62	0.99
1:B:2090:MET:HE3	1:B:2090:MET:HA	1.45	0.96
1:B:2128:ILE:HG12	1:B:2163:LEU:CB	1.99	0.94
1:A:1138:LEU:O	2:A:3002:CYC:HBC1	1.68	0.93
1:A:1139:CYS:HG	2:A:3002:CYC:HAC1	1.23	0.92
2:B:3003:CYC:NB	2:B:3003:CYC:HMA1	1.84	0.90
1:B:2128:ILE:HG12	1:B:2163:LEU:HB3	1.53	0.88
1:A:1115:GLU:HG3	1:A:1118:ARG:HG3	1.55	0.88
1:A:1114:ARG:HD2	3:A:3137:HOH:O	1.74	0.87
1:B:2120:LEU:HD13	2:B:3003:CYC:HBD1	1.59	0.83
1:B:2067:LYS:HA	1:B:2073:GLY:O	1.79	0.83
2:A:3001:CYC:NB	2:A:3001:CYC:HMA1	1.95	0.82
1:A:1052:VAL:HG21	1:A:1087:ASP:HA	1.63	0.80
1:A:1138:LEU:O	2:A:3002:CYC:CBC	2.29	0.80
1:B:2051:VAL:HG12	2:B:3004:CYC:HMA1	1.63	0.80
1:A:1052:VAL:HG11	1:A:1087:ASP:OD1	1.84	0.76
1:B:2143:ASP:OD2	2:B:3004:CYC:HMB2	1.86	0.76
1:A:1139:CYS:SG	2:A:3002:CYC:CBC	2.73	0.75
1:B:2140:ALA:HB3	1:B:2141:PRO:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2128:ILE:CG1	1:B:2163:LEU:CG	2.51	0.74
2:A:3001:CYC:NB	2:A:3001:CYC:CMA	2.50	0.74
1:B:2090:MET:HA	1:B:2090:MET:CE	2.18	0.74
1:B:2128:ILE:CD1	1:B:2163:LEU:HG	2.19	0.72
1:B:2154:THR:HA	1:B:2157:ASP:HB2	1.71	0.72
1:B:2044:LEU:HG	2:B:3004:CYC:HBB1	1.71	0.72
1:A:1087:ASP:O	1:A:1091:ARG:HB2	1.88	0.71
1:A:1067:LYS:O	1:A:1074:GLU:HA	1.91	0.71
2:B:3003:CYC:CMA	2:B:3003:CYC:HB	2.05	0.70
1:A:1078:LYS:O	2:A:3001:CYC:CMD	2.37	0.70
1:B:2126:ALA:HB3	2:B:3003:CYC:HMC1	1.73	0.69
1:B:2154:THR:O	1:B:2157:ASP:HB2	1.93	0.69
1:B:2044:LEU:HD13	1:B:2093:ILE:HG22	1.75	0.68
2:B:3003:CYC:HMA1	2:B:3003:CYC:HB	1.56	0.68
1:B:2138:LEU:CD1	1:B:2152:PHE:CD2	2.77	0.67
1:A:1063:TYR:HE2	1:A:1129:ALA:HB2	1.60	0.66
1:A:1076:GLN:HA	1:A:1079:ILE:HG22	1.78	0.66
1:B:2106:ASP:HA	1:B:2110:ILE:HB	1.77	0.66
1:B:2088:HIS:HB2	2:B:3003:CYC:CMB	2.26	0.65
1:B:2128:ILE:HG13	1:B:2163:LEU:HG	1.76	0.65
1:B:2048:HIS:O	1:B:2052:VAL:HB	1.95	0.65
1:B:2160:ILE:HG13	1:B:2163:LEU:O	1.96	0.65
2:B:3003:CYC:NB	2:B:3003:CYC:CMA	2.59	0.64
1:B:2131:PHE:HA	1:B:2134:THR:HB	1.81	0.63
1:A:1096:THR:HG22	1:A:1097:LEU:CD1	2.20	0.63
1:B:2140:ALA:HB3	1:B:2141:PRO:HD3	1.78	0.63
1:B:2072:ALA:HB1	2:B:3003:CYC:C1C	2.29	0.63
1:A:1140:ALA:HB3	1:A:1141:PRO:HD3	1.81	0.62
1:B:2138:LEU:HD12	1:B:2152:PHE:CD2	2.34	0.62
1:B:2071:GLU:O	1:B:2074:GLU:HG2	2.00	0.61
1:B:2138:LEU:HD21	1:B:2144:MET:HG2	1.83	0.61
1:A:1048:HIS:HA	1:A:1051:VAL:HG12	1.83	0.61
1:B:2037:ARG:HD3	1:B:2097:LEU:O	2.02	0.60
1:A:1078:LYS:HE3	2:A:3001:CYC:O1D	2.02	0.60
1:B:2055:ALA:HB1	1:B:2130:ALA:HB1	1.84	0.60
1:B:2163:LEU:CD1	1:B:2163:LEU:N	2.65	0.59
1:B:2082:CYS:HA	2:B:3003:CYC:CHD	2.33	0.58
1:A:1096:THR:CG2	1:A:1097:LEU:HD12	2.22	0.58
1:B:2044:LEU:HD13	1:B:2093:ILE:CG2	2.34	0.58
1:B:2040:ALA:HB2	1:B:2148:ALA:HB1	1.85	0.57
1:B:2125:ALA:HA	1:B:2128:ILE:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:ALA:HB1	2:A:3001:CYC:C1C	2.34	0.57
1:B:2032:GLN:C	1:B:2034:ALA:H	2.08	0.57
1:B:2138:LEU:HD13	1:B:2152:PHE:CD2	2.39	0.56
1:B:2033:ARG:O	1:B:2037:ARG:HG3	2.05	0.56
1:A:1047:ASN:O	1:A:1047:ASN:ND2	2.28	0.56
1:B:2160:ILE:HG23	1:B:2160:ILE:O	2.04	0.56
1:B:2044:LEU:HD21	1:B:2152:PHE:HE1	1.71	0.55
1:B:2096:THR:OG1	1:B:2102:THR:HA	2.07	0.55
1:B:2154:THR:CA	1:B:2157:ASP:HB2	2.37	0.55
1:A:1050:ALA:O	1:A:1054:GLU:HB2	2.05	0.55
1:A:1052:VAL:HG12	1:A:1053:LYS:N	2.22	0.55
1:B:2088:HIS:HB2	2:B:3003:CYC:HMB2	1.89	0.55
1:B:2158:TYR:O	1:B:2161:ASN:HB2	2.06	0.55
1:A:1082:CYS:HB2	2:A:3001:CYC:C4C	2.37	0.55
1:A:1096:THR:HG22	1:A:1097:LEU:N	2.22	0.54
1:A:1081:LYS:O	1:A:1084:ARG:HB3	2.07	0.54
1:B:2128:ILE:HD11	1:B:2163:LEU:HG	1.88	0.54
1:B:2088:HIS:HB2	2:B:3003:CYC:HMB1	1.87	0.54
1:B:2126:ALA:CB	2:B:3003:CYC:HMC1	2.38	0.54
1:B:2109:GLY:O	1:B:2113:ALA:HB2	2.07	0.54
1:A:1056:GLY:O	1:A:1059:CYS:HB3	2.09	0.53
1:B:2072:ALA:HB1	2:B:3003:CYC:NC	2.24	0.53
1:A:1052:VAL:HG21	1:A:1087:ASP:CA	2.35	0.52
1:B:2105:LEU:O	1:B:2110:ILE:HB	2.08	0.52
2:B:3004:CYC:O2A	2:B:3004:CYC:HHA	2.09	0.52
1:A:1066:ASN:O	1:A:1071:GLU:HB3	2.11	0.51
1:B:2032:GLN:C	1:B:2034:ALA:N	2.62	0.51
1:B:2140:ALA:CB	1:B:2141:PRO:CD	2.84	0.51
1:B:2106:ASP:OD2	1:B:2106:ASP:N	2.43	0.50
1:B:2140:ALA:HB3	1:B:2141:PRO:HD2	1.93	0.50
1:A:1082:CYS:CB	2:A:3001:CYC:C4C	2.90	0.50
1:A:1071:GLU:H	1:A:1074:GLU:HB3	1.76	0.50
1:A:1115:GLU:HG3	1:A:1118:ARG:CG	2.35	0.50
2:A:3001:CYC:HMA1	2:A:3001:CYC:C1B	2.41	0.49
1:A:1083:TYR:O	1:A:1086:ILE:HG13	2.12	0.49
2:A:3002:CYC:HMD2	2:A:3002:CYC:HC	1.78	0.49
1:B:2163:LEU:N	1:B:2163:LEU:HD12	2.28	0.49
1:B:2082:CYS:HB2	2:B:3003:CYC:C4C	2.43	0.48
2:B:3004:CYC:HMD2	2:B:3004:CYC:HC	1.78	0.48
1:B:2160:ILE:O	1:B:2160:ILE:CG2	2.62	0.48
2:A:3001:CYC:HMA1	2:A:3001:CYC:C4B	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2120:LEU:HB2	1:B:2122:LEU:HD21	1.96	0.47
1:B:2154:THR:C	1:B:2157:ASP:HB2	2.34	0.47
1:A:1128:ILE:HG22	1:A:1128:ILE:O	2.14	0.47
1:B:2072:ALA:O	1:B:2078:LYS:HB3	2.15	0.47
1:B:2160:ILE:HG23	1:B:2163:LEU:O	2.14	0.47
1:A:1060:PHE:HZ	1:A:1082:CYS:SG	2.39	0.47
2:B:3003:CYC:HMD2	2:B:3003:CYC:HC	1.80	0.46
1:B:2090:MET:CE	1:B:2090:MET:CA	2.88	0.46
1:A:1138:LEU:HD12	1:A:1153:CYS:SG	2.55	0.46
2:A:3001:CYC:NB	2:A:3001:CYC:C3A	2.76	0.46
1:A:1084:ARG:NH2	3:A:3119:HOH:O	2.48	0.46
1:B:2096:THR:O	1:B:2096:THR:HG23	2.16	0.46
2:A:3001:CYC:HMD2	2:A:3001:CYC:HC	1.80	0.46
1:A:1117:TYR:O	1:A:1121:ASN:N	2.48	0.46
1:B:2032:GLN:O	1:B:2034:ALA:N	2.49	0.45
1:A:1072:ALA:HB1	2:A:3001:CYC:OC	2.15	0.45
1:A:1074:GLU:HG2	1:A:1075:ASN:N	2.32	0.45
1:B:2138:LEU:HD12	1:B:2152:PHE:CE2	2.51	0.45
1:B:2124:SER:O	1:B:2128:ILE:N	2.51	0.44
1:B:2157:ASP:O	1:B:2161:ASN:N	2.51	0.44
1:B:2034:ALA:HA	1:B:2037:ARG:NE	2.32	0.44
1:B:2082:CYS:O	1:B:2086:ILE:HG13	2.17	0.44
1:A:1138:LEU:HD23	2:A:3002:CYC:CMB	2.48	0.43
1:A:1112:GLY:O	1:A:1116:VAL:HG13	2.19	0.43
1:A:1123:PRO:O	1:A:1127:TYR:HD1	2.02	0.43
1:B:2120:LEU:HB2	1:B:2122:LEU:CD2	2.49	0.43
1:A:1106:ASP:O	1:A:1109:GLY:N	2.43	0.43
1:A:1092:LEU:HB3	1:A:1105:LEU:HA	2.00	0.43
1:A:1078:LYS:CE	2:A:3001:CYC:O1D	2.66	0.43
1:B:2126:ALA:CB	2:B:3003:CYC:CMC	2.96	0.42
1:B:2160:ILE:O	1:B:2163:LEU:O	2.37	0.42
1:B:2154:THR:O	1:B:2157:ASP:CB	2.65	0.42
1:A:1078:LYS:HE3	2:A:3001:CYC:CGD	2.48	0.42
1:B:2083:TYR:O	1:B:2087:ASP:N	2.53	0.42
1:B:2103:GLY:O	1:B:2104:PRO:C	2.56	0.41
1:B:2105:LEU:HD13	1:B:2105:LEU:HA	1.83	0.41
1:B:2160:ILE:HA	1:B:2163:LEU:HB2	2.02	0.41
1:B:2037:ARG:O	1:B:2097:LEU:HB3	2.20	0.41
1:A:1118:ARG:HH22	1:B:2046:SER:HA	1.84	0.41
1:B:2121:ASN:C	1:B:2122:LEU:HD13	2.41	0.41
1:A:1105:LEU:HD21	1:A:1159:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1138:LEU:O	2:A:3002:CYC:HBC3	2.15	0.41
1:B:2114:ARG:O	1:B:2118:ARG:HG3	2.21	0.41
2:A:3001:CYC:CMA	2:A:3001:CYC:HB	2.29	0.41
1:B:2122:LEU:HD13	1:B:2122:LEU:N	2.36	0.41
1:B:2138:LEU:HG	1:B:2143:ASP:OD2	2.21	0.40
1:B:2044:LEU:HD21	1:B:2152:PHE:CE1	2.52	0.40
1:A:1106:ASP:HA	1:A:1110:ILE:HB	2.03	0.40
1:B:2140:ALA:CB	1:B:2141:PRO:HD3	2.47	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	131/133 (98%)	107 (82%)	17 (13%)	7 (5%)	2	2
1	B	131/133 (98%)	105 (80%)	22 (17%)	4 (3%)	4	6
All	All	262/266 (98%)	212 (81%)	39 (15%)	11 (4%)	3	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1077	GLU
1	A	1106	ASP
1	A	1076	GLN
1	A	1109	GLY
1	A	1138	LEU
1	B	2109	GLY
1	A	1072	ALA
1	A	1110	ILE
1	B	2130	ALA
1	B	2141	PRO

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Mol	Chain	Res	Type
1	B	2112	GLY

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	98/103 (95%)	78 (80%)	20 (20%)	1 2
1	B	98/103 (95%)	74 (76%)	24 (24%)	0 1
All	All	196/206 (95%)	152 (78%)	44 (22%)	1 1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1038	LEU
1	A	1047	ASN
1	A	1057	ASP
1	A	1061	SER
1	A	1071	GLU
1	A	1077	GLU
1	A	1078	LYS
1	A	1084	ARG
1	A	1085	ASP
1	A	1086	ILE
1	A	1088	HIS
1	A	1092	LEU
1	A	1096	THR
1	A	1110	ILE
1	A	1115	GLU
1	A	1120	LEU
1	A	1137	ARG
1	A	1150	VAL
1	A	1157	ASP
1	A	1164	SER
1	B	2037	ARG
1	B	2047	ASN

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Mol	Chain	Res	Type
1	B	2049	GLU
1	B	2059	CYS
1	B	2062	LYS
1	B	2078	LYS
1	B	2087	ASP
1	B	2090	MET
1	B	2096	THR
1	B	2097	LEU
1	B	2099	VAL
1	B	2105	LEU
1	B	2106	ASP
1	B	2107	GLU
1	B	2110	ILE
1	B	2114	ARG
1	B	2122	LEU
1	B	2133	PHE
1	B	2137	ARG
1	B	2138	LEU
1	B	2157	ASP
1	B	2160	ILE
1	B	2163	LEU
1	B	2164	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	CYC	B	3004	1	42,46,46	2.83	13 (30%)	50,67,67	2.35	17 (34%)
2	CYC	A	3001	1	42,46,46	3.03	15 (35%)	50,67,67	3.54	22 (44%)
2	CYC	A	3002	1	42,46,46	2.83	13 (30%)	50,67,67	2.24	16 (32%)
2	CYC	B	3003	1	42,46,46	3.40	16 (38%)	50,67,67	3.18	19 (38%)

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	B	3004	1	-	13/25/74/74	0/4/4/4
2	CYC	A	3001	1	-	11/25/74/74	0/4/4/4
2	CYC	A	3002	1	-	13/25/74/74	0/4/4/4
2	CYC	B	3003	1	-	13/25/74/74	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	CYC	C2C-C1C	-13.42	1.40	1.52
2	B	3003	CYC	C2C-C1C	-13.35	1.40	1.52
2	B	3004	CYC	C2C-C1C	-11.87	1.41	1.52
2	A	3002	CYC	C2C-C1C	-11.82	1.41	1.52
2	B	3003	CYC	CBA-CAA	10.23	1.84	1.52
2	A	3001	CYC	CHA-C1A	7.38	1.41	1.35
2	B	3003	CYC	CHA-C1A	7.33	1.41	1.35
2	A	3002	CYC	CHA-C1A	6.46	1.40	1.35
2	B	3004	CYC	CHA-C1A	6.41	1.40	1.35
2	B	3004	CYC	O2A-CGA	4.73	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3002	CYC	O2A-CGA	4.70	1.46	1.30
2	B	3003	CYC	O2A-CGA	4.47	1.45	1.30
2	A	3001	CYC	O2A-CGA	4.46	1.45	1.30
2	B	3003	CYC	O2D-CGD	4.23	1.45	1.30
2	A	3001	CYC	O2D-CGD	4.22	1.44	1.30
2	A	3002	CYC	C4B-C3B	-4.11	1.40	1.48
2	B	3004	CYC	C4B-C3B	-4.09	1.40	1.48
2	A	3002	CYC	O2D-CGD	3.84	1.43	1.30
2	A	3001	CYC	C2A-C3A	3.84	1.44	1.36
2	B	3004	CYC	O2D-CGD	3.82	1.43	1.30
2	B	3003	CYC	C2A-C3A	3.79	1.44	1.36
2	A	3002	CYC	C1B-NB	3.60	1.43	1.37
2	B	3004	CYC	C1B-NB	3.55	1.43	1.37
2	B	3003	CYC	C4B-C3B	-3.47	1.41	1.48
2	A	3001	CYC	C4B-C3B	-3.46	1.41	1.48
2	B	3003	CYC	CAC-C3C	3.23	1.60	1.54
2	A	3001	CYC	CAC-C3C	3.22	1.60	1.54
2	B	3004	CYC	C4C-NC	3.21	1.44	1.37
2	B	3003	CYC	C3B-C2B	3.20	1.43	1.36
2	A	3002	CYC	C4C-NC	3.20	1.44	1.37
2	A	3001	CYC	C3B-C2B	3.19	1.43	1.36
2	A	3002	CYC	C3B-C2B	3.14	1.43	1.36
2	B	3004	CYC	C3B-C2B	3.14	1.43	1.36
2	B	3004	CYC	CHB-C1B	3.00	1.45	1.38
2	A	3002	CYC	CHB-C1B	2.97	1.45	1.38
2	B	3003	CYC	C4C-NC	2.82	1.43	1.37
2	A	3001	CYC	C4C-NC	2.82	1.43	1.37
2	B	3004	CYC	C2A-C3A	2.77	1.42	1.36
2	A	3002	CYC	C2A-C3A	2.76	1.42	1.36
2	A	3001	CYC	CHD-C4C	2.40	1.44	1.38
2	B	3003	CYC	CHD-C4C	2.38	1.44	1.38
2	B	3003	CYC	C3C-C4C	2.37	1.54	1.50
2	A	3001	CYC	C3C-C4C	2.34	1.54	1.50
2	A	3001	CYC	C4B-NB	-2.32	1.33	1.38
2	A	3001	CYC	C4A-NA	2.30	1.41	1.36
2	B	3003	CYC	C4A-NA	2.29	1.41	1.36
2	B	3004	CYC	CHD-C4C	2.29	1.43	1.38
2	A	3002	CYC	CHD-C4C	2.28	1.43	1.38
2	B	3003	CYC	C4B-NB	-2.27	1.33	1.38
2	A	3001	CYC	C1B-NB	2.25	1.41	1.37
2	B	3003	CYC	C1B-NB	2.24	1.41	1.37
2	A	3001	CYC	C1C-NC	-2.17	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3003	CYC	C1C-NC	-2.16	1.34	1.37
2	B	3004	CYC	CAD-C3D	2.11	1.55	1.52
2	A	3002	CYC	C1A-C2A	-2.09	1.42	1.45
2	A	3002	CYC	CAD-C3D	2.05	1.55	1.52
2	B	3004	CYC	C1A-C2A	-2.03	1.42	1.45

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3003	CYC	CAA-CBA-CGA	14.26	144.28	113.60
2	A	3001	CYC	CBA-CAA-C2A	12.04	146.07	112.63
2	A	3001	CYC	CBD-CAD-C3D	11.45	132.16	112.62
2	A	3001	CYC	CAD-CBD-CGD	8.16	136.62	113.76
2	B	3003	CYC	CBA-CAA-C2A	7.23	132.72	112.63
2	A	3002	CYC	CBC-CAC-C3C	-6.36	99.30	113.47
2	B	3004	CYC	CBC-CAC-C3C	-6.34	99.36	113.47
2	A	3002	CYC	CMC-C2C-C1C	6.33	126.05	112.40
2	B	3004	CYC	CMC-C2C-C1C	6.33	126.05	112.40
2	A	3001	CYC	C1B-CHB-C4A	-6.02	113.38	128.08
2	A	3001	CYC	CMC-C2C-C1C	5.94	125.22	112.40
2	B	3003	CYC	CMC-C2C-C1C	5.92	125.17	112.40
2	B	3004	CYC	CAD-CBD-CGD	5.27	128.53	113.76
2	B	3003	CYC	C1B-C2B-C3B	-5.17	102.48	107.87
2	A	3001	CYC	C1B-C2B-C3B	-5.14	102.50	107.87
2	B	3003	CYC	C3B-C4B-NB	4.48	110.39	106.78
2	A	3002	CYC	C1B-C2B-C3B	-4.41	103.27	107.87
2	B	3004	CYC	C1B-C2B-C3B	-4.39	103.29	107.87
2	A	3001	CYC	C3B-C4B-NB	4.38	110.31	106.78
2	A	3002	CYC	CHD-C4C-NC	4.24	130.24	125.20
2	B	3004	CYC	CHD-C4C-NC	4.23	130.24	125.20
2	B	3003	CYC	CAC-C3C-C2C	-4.18	103.83	114.26
2	A	3001	CYC	CAC-C3C-C2C	-4.17	103.84	114.26
2	A	3001	CYC	CAC-C3C-C4C	3.93	122.76	112.67
2	B	3003	CYC	CAC-C3C-C4C	3.92	122.74	112.67
2	B	3004	CYC	C4D-CHA-C1A	-3.81	124.25	128.81
2	A	3002	CYC	C4D-CHA-C1A	-3.80	124.27	128.81
2	A	3001	CYC	CBC-CAC-C3C	-3.58	105.50	113.47
2	B	3003	CYC	CBC-CAC-C3C	-3.56	105.54	113.47
2	B	3003	CYC	CMB-C2B-C1B	3.39	128.40	124.17
2	A	3001	CYC	CMB-C2B-C1B	3.39	128.40	124.17
2	A	3001	CYC	O2A-CGA-O1A	-3.38	114.87	123.30
2	B	3003	CYC	O2A-CGA-O1A	-3.38	114.88	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3002	CYC	OC-C1C-C2C	3.31	128.80	126.17
2	B	3004	CYC	OC-C1C-C2C	3.29	128.79	126.17
2	A	3001	CYC	C4D-CHA-C1A	-3.22	124.97	128.81
2	B	3003	CYC	C1B-NB-C4B	-3.21	106.59	110.67
2	A	3001	CYC	O2A-CGA-CBA	3.16	124.19	114.03
2	B	3003	CYC	C4D-CHA-C1A	-3.16	125.04	128.81
2	A	3001	CYC	C1B-NB-C4B	-3.15	106.65	110.67
2	B	3003	CYC	O2A-CGA-CBA	3.15	124.16	114.03
2	B	3004	CYC	O2D-CGD-CBD	2.98	123.59	114.03
2	A	3002	CYC	O2D-CGD-CBD	2.96	123.53	114.03
2	B	3003	CYC	CMC-C2C-C3C	2.87	125.39	113.83
2	A	3001	CYC	CMC-C2C-C3C	2.86	125.37	113.83
2	A	3002	CYC	C1A-NA-C4A	-2.86	101.12	106.51
2	B	3004	CYC	C1A-NA-C4A	-2.85	101.13	106.51
2	B	3004	CYC	CBB-CAB-C3B	2.81	120.19	112.43
2	B	3003	CYC	O2D-CGD-CBD	2.81	123.06	114.03
2	A	3001	CYC	O2D-CGD-CBD	2.81	123.06	114.03
2	A	3002	CYC	CBB-CAB-C3B	2.81	120.18	112.43
2	A	3002	CYC	O2A-CGA-CBA	2.76	122.91	114.03
2	B	3004	CYC	O2A-CGA-CBA	2.76	122.89	114.03
2	A	3002	CYC	CMA-C3A-C4A	2.58	129.04	125.06
2	B	3004	CYC	CMA-C3A-C4A	2.58	129.03	125.06
2	A	3002	CYC	CAA-C2A-C1A	2.53	129.49	125.01
2	B	3004	CYC	CAA-C2A-C1A	2.52	129.47	125.01
2	A	3001	CYC	CAA-CBA-CGA	2.49	118.96	113.60
2	B	3003	CYC	CBB-CAB-C3B	2.43	119.13	112.43
2	A	3001	CYC	CBB-CAB-C3B	2.41	119.06	112.43
2	A	3001	CYC	CHB-C4A-NA	-2.35	120.01	124.93
2	B	3003	CYC	CHB-C4A-NA	-2.33	120.05	124.93
2	B	3003	CYC	O1D-CGD-CBD	-2.32	115.63	123.08
2	A	3001	CYC	O1D-CGD-CBD	-2.32	115.64	123.08
2	B	3003	CYC	CHA-C1A-NA	-2.27	125.68	128.83
2	B	3004	CYC	CBD-CAD-C3D	2.26	116.48	112.62
2	A	3002	CYC	CMB-C2B-C1B	2.26	126.98	124.17
2	A	3002	CYC	CBD-CAD-C3D	2.25	116.46	112.62
2	B	3004	CYC	CMB-C2B-C1B	2.25	126.97	124.17
2	A	3001	CYC	CHA-C1A-NA	-2.23	125.74	128.83
2	B	3004	CYC	O2A-CGA-O1A	-2.18	117.86	123.30
2	A	3002	CYC	O2A-CGA-O1A	-2.17	117.89	123.30
2	A	3002	CYC	CMC-C2C-C3C	2.17	122.56	113.83
2	B	3004	CYC	CMC-C2C-C3C	2.15	122.51	113.83

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	CYC	C3A-C4A-CHB-C1B
2	A	3001	CYC	C4C-C3C-CAC-CBC
2	A	3001	CYC	ND-C1D-CHD-C4C
2	A	3001	CYC	C2D-C1D-CHD-C4C
2	A	3002	CYC	C3D-C4D-CHA-C1A
2	A	3002	CYC	NA-C4A-CHB-C1B
2	A	3002	CYC	C3A-C4A-CHB-C1B
2	A	3002	CYC	C4C-C3C-CAC-CBC
2	A	3002	CYC	ND-C1D-CHD-C4C
2	A	3002	CYC	C2D-C1D-CHD-C4C
2	B	3003	CYC	C3A-C4A-CHB-C1B
2	B	3003	CYC	C4C-C3C-CAC-CBC
2	B	3003	CYC	ND-C1D-CHD-C4C
2	B	3003	CYC	C2D-C1D-CHD-C4C
2	B	3004	CYC	C3D-C4D-CHA-C1A
2	B	3004	CYC	NA-C4A-CHB-C1B
2	B	3004	CYC	C3A-C4A-CHB-C1B
2	B	3004	CYC	C4C-C3C-CAC-CBC
2	B	3004	CYC	ND-C1D-CHD-C4C
2	B	3004	CYC	C2D-C1D-CHD-C4C
2	B	3004	CYC	C3D-CAD-CBD-CGD
2	A	3001	CYC	C2B-C3B-CAB-CBB
2	B	3003	CYC	C2B-C3B-CAB-CBB
2	B	3003	CYC	C2A-CAA-CBA-CGA
2	A	3001	CYC	NA-C4A-CHB-C1B
2	B	3003	CYC	NA-C4A-CHB-C1B
2	A	3001	CYC	C2A-CAA-CBA-CGA
2	A	3001	CYC	C2C-C3C-CAC-CBC
2	A	3002	CYC	C2C-C3C-CAC-CBC
2	B	3003	CYC	C2C-C3C-CAC-CBC
2	B	3004	CYC	C2C-C3C-CAC-CBC
2	A	3002	CYC	C4B-C3B-CAB-CBB
2	B	3004	CYC	C4B-C3B-CAB-CBB
2	A	3001	CYC	C3D-CAD-CBD-CGD
2	B	3003	CYC	C3D-CAD-CBD-CGD
2	B	3004	CYC	C2B-C3B-CAB-CBB
2	A	3002	CYC	C2B-C3B-CAB-CBB
2	B	3003	CYC	CAA-CBA-CGA-O2A
2	A	3002	CYC	CAA-CBA-CGA-O1A
2	A	3002	CYC	CAA-CBA-CGA-O2A
2	A	3002	CYC	CAD-CBD-CGD-O1D
2	B	3003	CYC	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	3003	CYC	CAD-CBD-CGD-O1D
2	B	3004	CYC	CAA-CBA-CGA-O1A
2	B	3003	CYC	CAD-CBD-CGD-O2D
2	A	3002	CYC	CAD-CBD-CGD-O2D
2	A	3001	CYC	CAA-CBA-CGA-O1A
2	A	3001	CYC	CAA-CBA-CGA-O2A
2	B	3004	CYC	CAA-CBA-CGA-O2A
2	B	3004	CYC	CAD-CBD-CGD-O1D

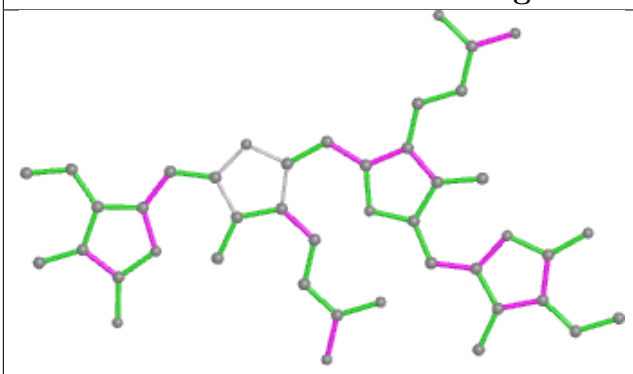
There are no ring outliers.

4 monomers are involved in 46 short contacts:

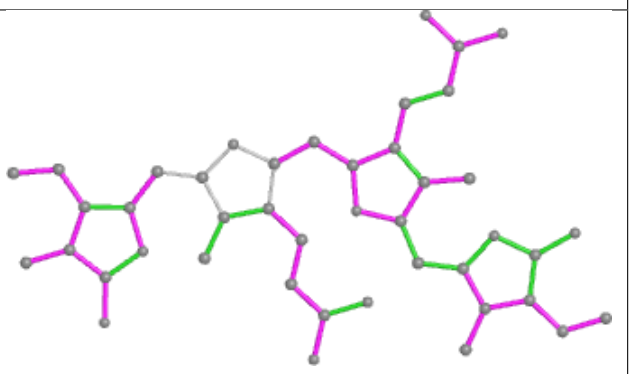
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3004	CYC	5	0
2	A	3001	CYC	16	0
2	A	3002	CYC	8	0
2	B	3003	CYC	17	0

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.

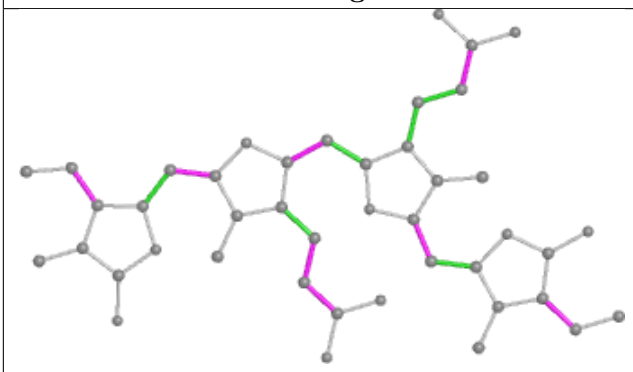
Ligand CYC B 3004



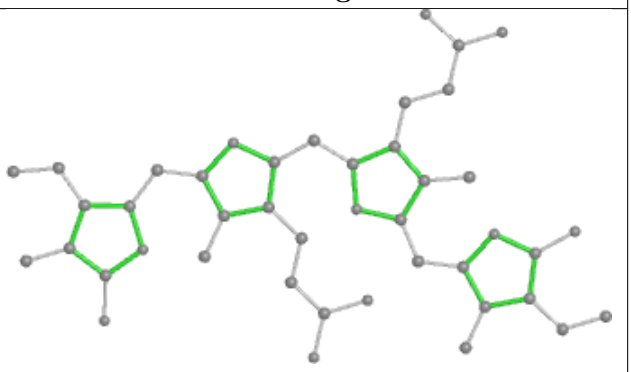
Bond lengths



Bond angles

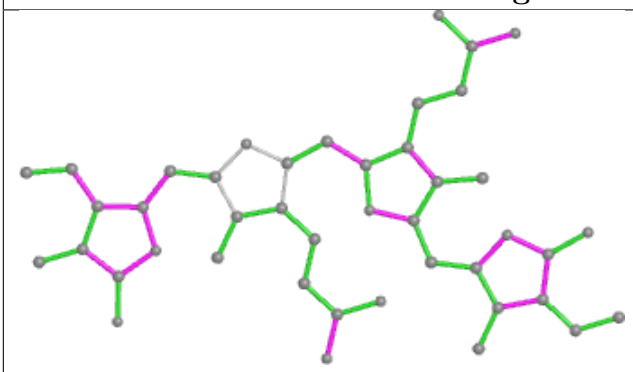


Torsions

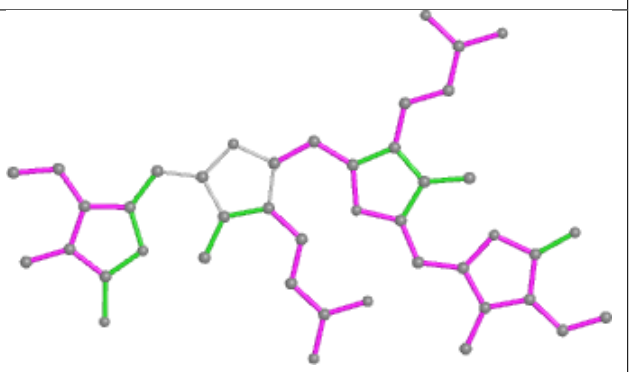


Rings

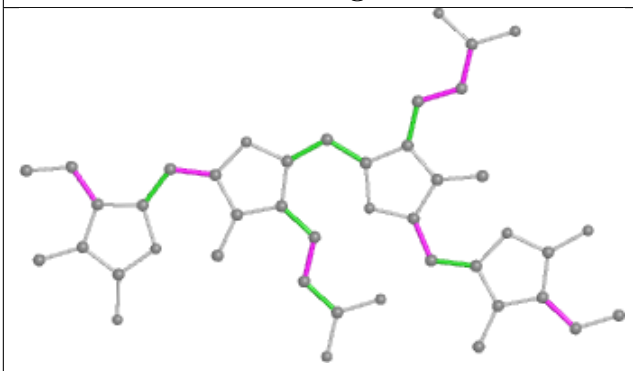
Ligand CYC A 3001



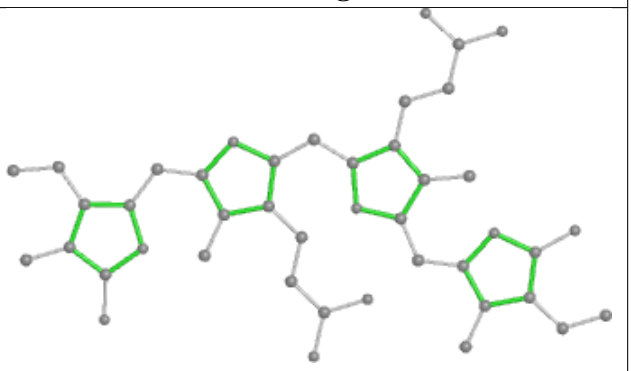
Bond lengths



Bond angles

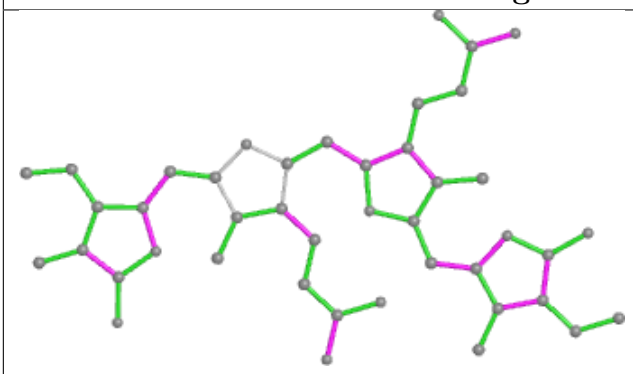


Torsions

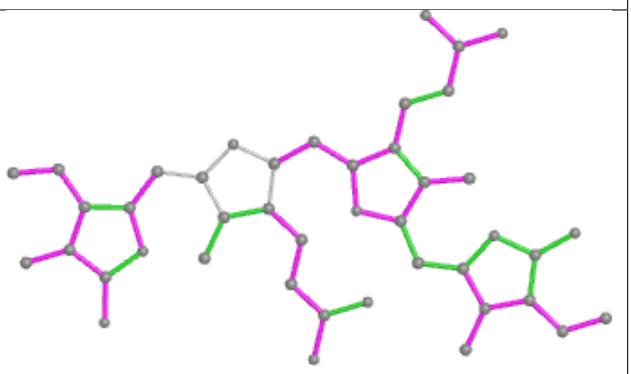


Rings

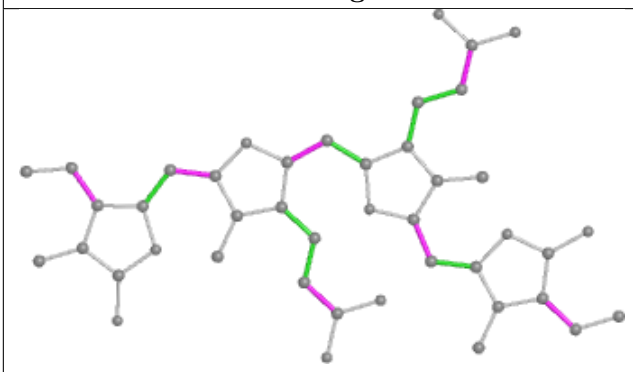
Ligand CYC A 3002



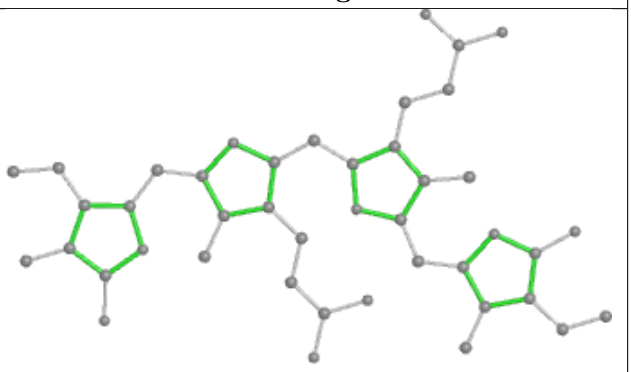
Bond lengths



Bond angles

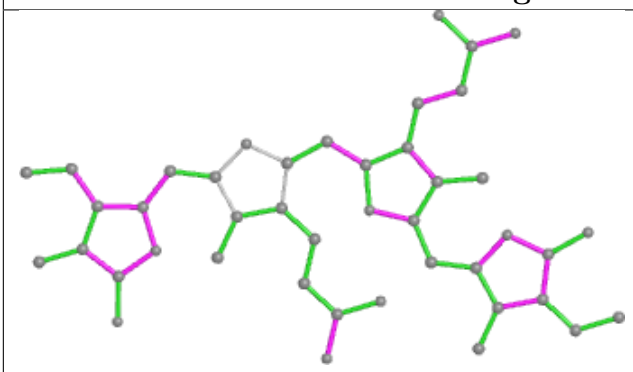


Torsions

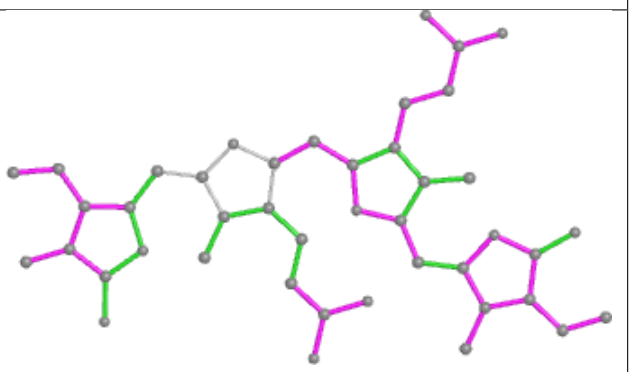


Rings

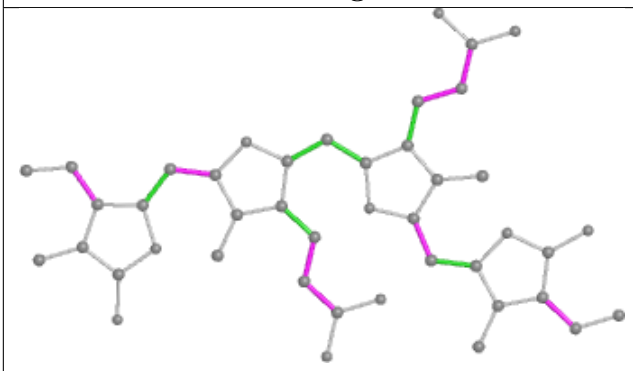
Ligand CYC B 3003



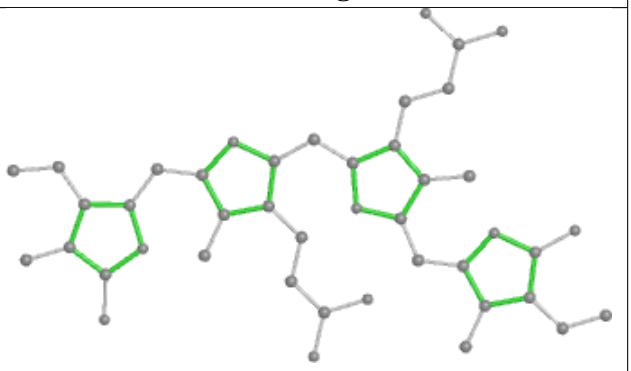
Bond lengths



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

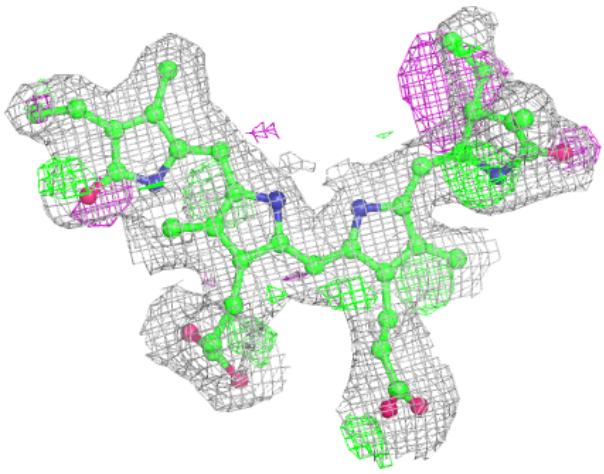
6.4 Ligands (i)

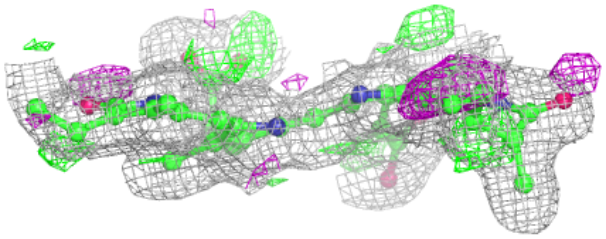
Unable to reproduce the depositors R factor - this section is therefore empty.

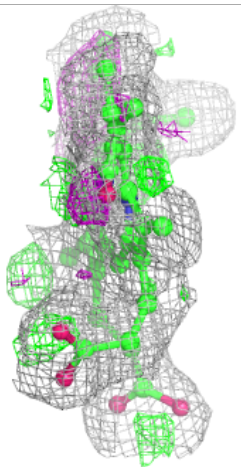
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC A 3001:

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

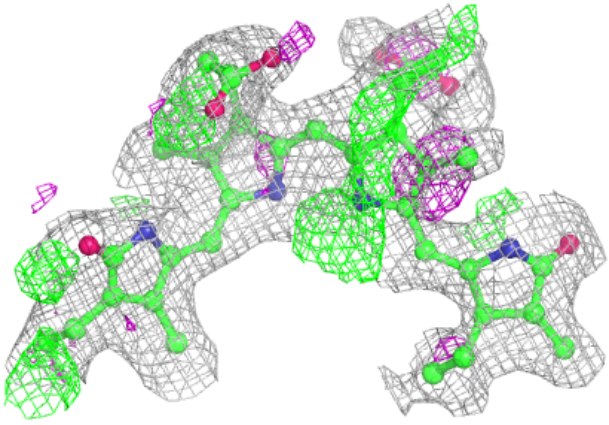


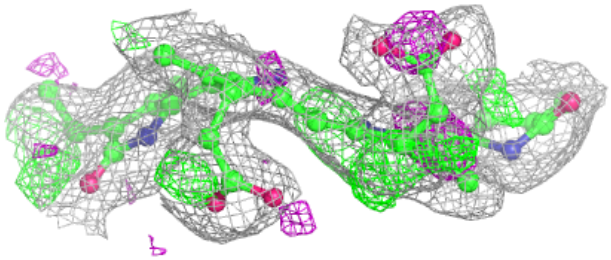


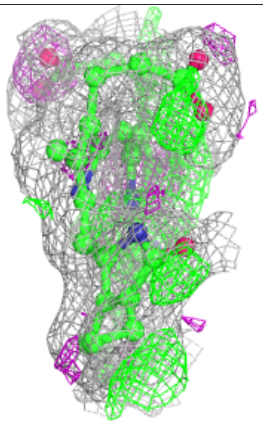


Electron density around CYC A 3002:

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

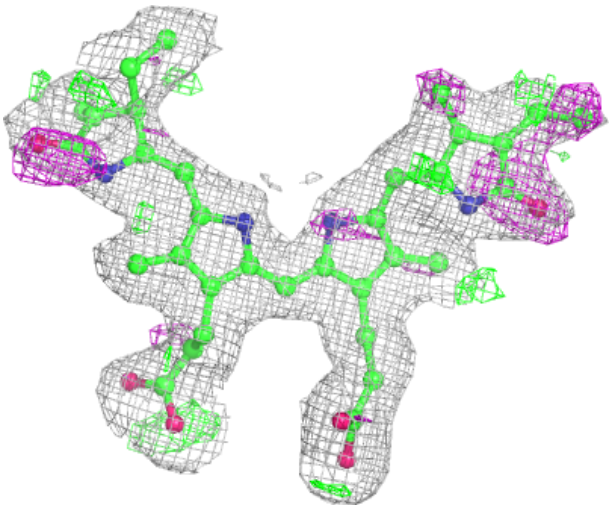


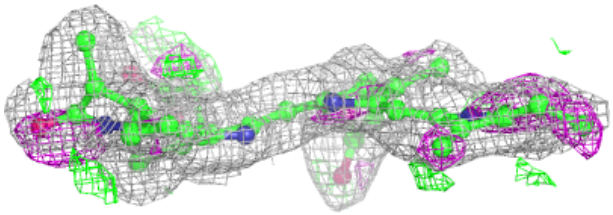


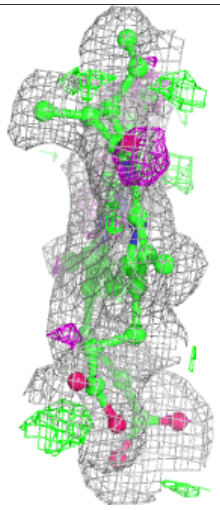


Electron density around CYC B 3003:

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

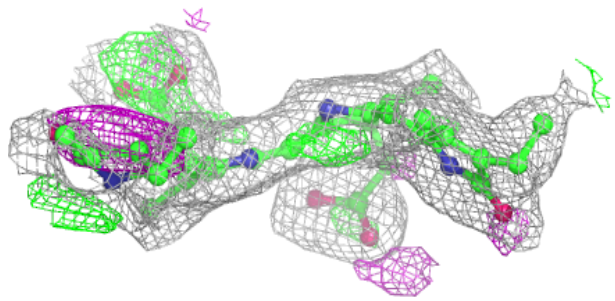


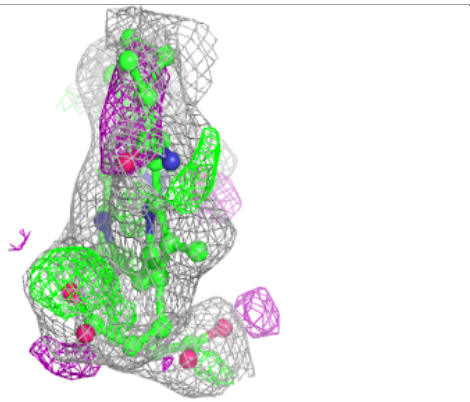




Electron density around CYC B 3004:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.