



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:06 PM UTC

PDB ID : 3MWN / pdb_00003mwn
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

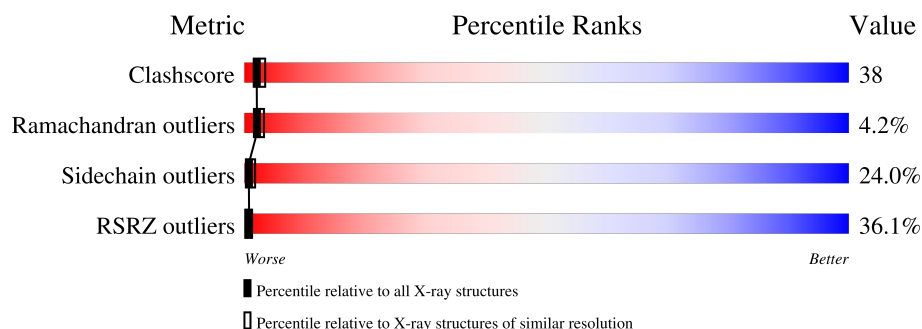
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	133	29% 47% 39% 11% .
1	B	133	43% 42% 36% 19% .

2 Entry composition [i](#)

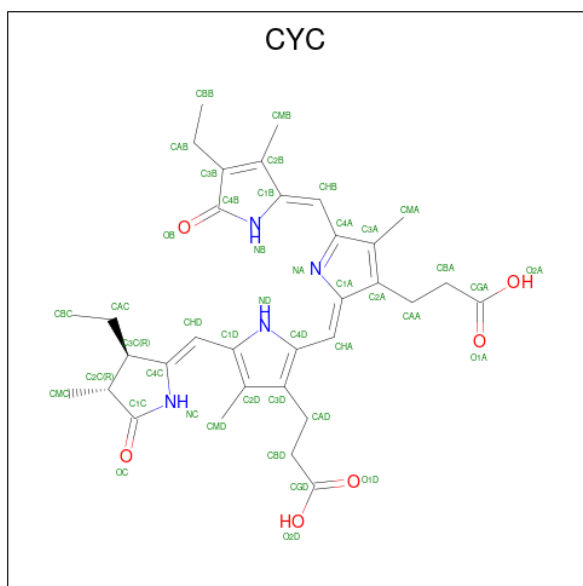
There are 3 unique types of molecules in this entry. The entry contains 2242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	133	Total	C	N	O	S	0	0	0
			1008	630	179	193	6			
1	B	133	Total	C	N	O	S	0	0	0
			1008	630	179	193	6			

- Molecule 2 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

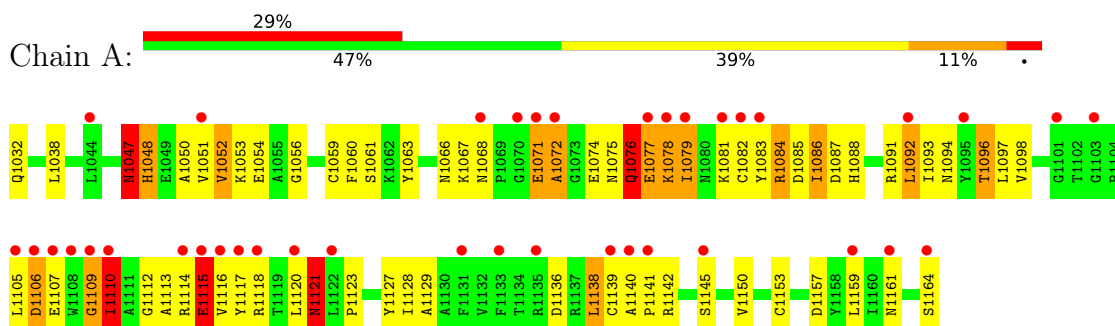
- Molecule 3 is water.

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

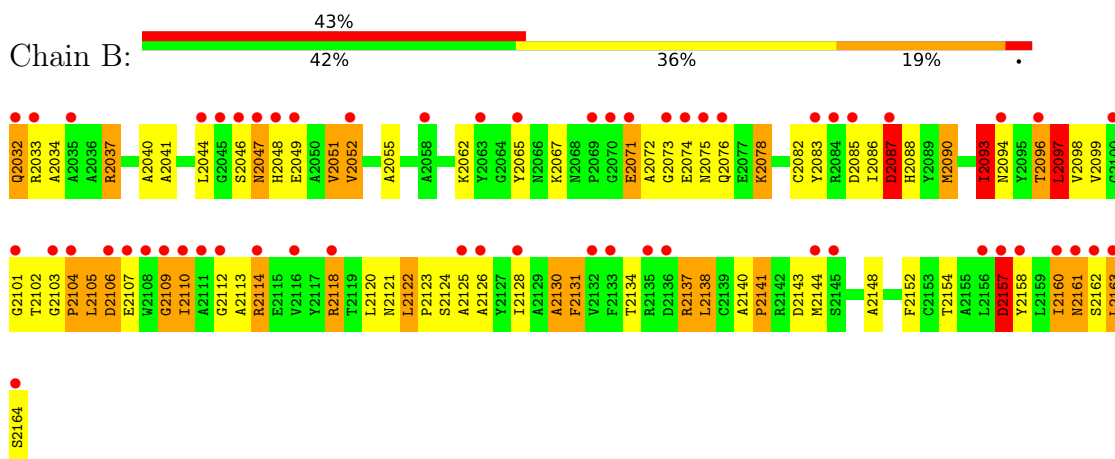
3 Residue-property plots [i](#)

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 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: PHYCOERYTHRIN



• Molecule 1: PHYCOERYTHRIN



4 Data and refinement statistics

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 10.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.6 (10.00-2.60) 83.3 (10.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.60Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.238 , 0.286 0.352 , (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)	0.29 , 136.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	6/1027 (0.6%)	1.52	17/1391 (1.2%)
1	B	1.05	6/1027 (0.6%)	1.48	17/1391 (1.2%)
All	All	1.02	12/2054 (0.6%)	1.50	34/2782 (1.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2093	ILE	CA-CB	7.82	1.64	1.54
1	A	1098	VAL	CA-CB	-7.39	1.47	1.55
1	A	1115	GLU	C-N	6.74	1.41	1.33
1	A	1110	ILE	C-N	-6.17	1.25	1.33
1	B	2098	VAL	N-CA	5.99	1.51	1.46
1	A	1094	ASN	CG-OD1	5.75	1.34	1.23
1	B	2076	GLN	CD-OE1	5.64	1.34	1.23
1	B	2097	LEU	CA-C	5.48	1.60	1.52
1	B	2161	ASN	CG-OD1	5.34	1.33	1.23
1	A	1161	ASN	CG-OD1	5.09	1.33	1.23
1	A	1048	HIS	CB-CG	5.08	1.57	1.50
1	B	2161	ASN	CG-ND2	-5.01	1.22	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1136	ASP	CA-CB-CG	12.47	125.08	112.60
1	B	2075	ASN	CA-CB-CG	12.42	125.02	112.60
1	B	2157	ASP	CA-CB-CG	12.06	124.66	112.60
1	A	1121	ASN	CA-CB-CG	10.77	123.37	112.60
1	A	1032	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	B	2032	GLN	OE1-CD-NE2	-10.20	112.40	122.60
1	A	1085	ASP	CA-CB-CG	9.91	122.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1076	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	1113	ALA	CA-C-N	9.00	132.68	120.44
1	A	1113	ALA	C-N-CA	9.00	132.68	120.44
1	B	2076	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	B	2087	ASP	CA-CB-CG	8.57	121.17	112.60
1	B	2047	ASN	CA-CB-CG	8.24	120.84	112.60
1	A	1047	ASN	CA-CB-CG	7.94	120.54	112.60
1	B	2076	GLN	CB-CG-CD	7.57	125.46	112.60
1	A	1115	GLU	CB-CG-CD	7.20	124.83	112.60
1	A	1048	HIS	CA-CB-CG	7.17	120.97	113.80
1	B	2051	VAL	O-C-N	7.01	131.79	122.12
1	A	1076	GLN	CG-CD-NE2	7.01	126.91	116.40
1	A	1115	GLU	CB-CA-C	7.00	122.61	110.01
1	A	1032	GLN	CG-CD-NE2	6.88	126.73	116.40
1	B	2131	PHE	CA-CB-CG	-6.87	106.93	113.80
1	B	2032	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	1161	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	1145	SER	N-CA-C	6.23	117.65	108.86
1	B	2118	ARG	CD-NE-CZ	6.17	133.04	124.40
1	B	2065	TYR	CA-CB-CG	5.81	124.36	113.90
1	B	2137	ARG	CD-NE-CZ	5.77	132.48	124.40
1	B	2041	ALA	O-C-N	-5.76	115.81	122.03
1	B	2094	ASN	N-CA-C	-5.69	105.60	112.54
1	B	2071	GLU	CB-CG-CD	5.68	122.25	112.60
1	A	1079	ILE	CB-CA-C	-5.07	105.35	110.88
1	B	2104	PRO	CB-CA-C	5.05	119.90	111.56
1	A	1079	ILE	N-CA-C	-5.03	107.54	113.42

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	1008	0	958	55	0
1	B	1008	0	957	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	86	0	77	24	0
2	B	86	0	76	23	0
3	A	33	0	0	2	0
3	B	21	0	0	0	0
All	All	2242	0	2068	161	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 38.

All (161) 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:A:1139:CYS:HG	2:A:3002:CYC:HAC1	1.22	0.94
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
2:B:3003:CYC:NB	2:B:3003:CYC:HMA1	1.84	0.90
1:B:2090:MET:HE3	1:B:2090:MET:HA	1.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2032:GLN:C	1:B:2034:ALA:H	2.08	0.60
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
1:A:1072:ALA:HB1	2:A:3001:CYC:C1C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:ASN:O	1:A:1047:ASN:ND2	2.28	0.56
1:B:2032:GLN:C	1:B:2034:ALA:N	2.62	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: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:A:1052:VAL:HG12	1:A:1053:LYS:N	2.22	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:B:2154:THR:C	1:B:2157:ASP:HB2	2.34	0.53
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: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
1:B:2120:LEU:HB2	1:B:2122:LEU:HD21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2103:GLY:O	1:B:2104:PRO:C	2.56	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
1:B:2121:ASN:C	1:B:2122:LEU:HD13	2.41	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:A:1052:VAL:HG11	1:A:1087:ASP:CG	2.42	0.45
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:2085:ASP:CG	2:B:3003:CYC:HD	2.25	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:B:2162:SER:C	1:B:2163:LEU:HD12	2.44	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:2101:GLY:C	1:B:2103:GLY:H	2.28	0.42
1:B:2083:TYR:O	1:B:2087:ASP:N	2.53	0.42
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: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
1:A:1067:LYS:O	1:A:1068:ASN:C	2.64	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%)	1	1
1	B	131/133 (98%)	105 (80%)	22 (17%)	4 (3%)	3	5
All	All	262/266 (98%)	212 (81%)	39 (15%)	11 (4%)	2	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

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Mol	Chain	Res	Type
1	B	2141	PRO
1	B	2112	GLY

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	98/103 (95%)	76 (78%)	22 (22%)	1	1
1	B	98/103 (95%)	73 (74%)	25 (26%)	0	1
All	All	196/206 (95%)	149 (76%)	47 (24%)	1	1

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1038	LEU
1	A	1047	ASN
1	A	1052	VAL
1	A	1061	SER
1	A	1071	GLU
1	A	1077	GLU
1	A	1078	LYS
1	A	1084	ARG
1	A	1086	ILE
1	A	1088	HIS
1	A	1092	LEU
1	A	1093	ILE
1	A	1096	THR
1	A	1107	GLU
1	A	1110	ILE
1	A	1115	GLU
1	A	1120	LEU
1	A	1121	ASN
1	A	1142	ARG
1	A	1150	VAL
1	A	1157	ASP

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Mol	Chain	Res	Type
1	A	1164	SER
1	B	2037	ARG
1	B	2047	ASN
1	B	2049	GLU
1	B	2052	VAL
1	B	2062	LYS
1	B	2078	LYS
1	B	2087	ASP
1	B	2090	MET
1	B	2093	ILE
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	2123	PRO
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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1080	ASN
1	B	2032	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	3002	1	46,46,46	2.66	13 (28%)	63,67,67	2.31	23 (36%)
2	CYC	B	3004	1	46,46,46	2.66	13 (28%)	63,67,67	2.41	24 (38%)
2	CYC	B	3003	1	46,46,46	3.10	15 (32%)	63,67,67	2.79	23 (36%)
2	CYC	A	3001	1	46,46,46	2.79	14 (30%)	63,67,67	3.11	25 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYC	A	3002	1	-	13/26/74/74	0/4/4/4
2	CYC	B	3004	1	-	12/26/74/74	0/4/4/4
2	CYC	B	3003	1	-	14/26/74/74	0/4/4/4
2	CYC	A	3001	1	-	13/26/74/74	0/4/4/4

All (55) 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	9.40	1.84	1.51
2	B	3004	CYC	O2A-CGA	4.79	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3002	CYC	O2A-CGA	4.76	1.46	1.30
2	A	3001	CYC	CHD-C4C	4.61	1.44	1.36
2	B	3003	CYC	CHD-C4C	4.57	1.44	1.36
2	B	3003	CYC	O2A-CGA	4.52	1.45	1.30
2	A	3001	CYC	O2A-CGA	4.51	1.45	1.30
2	B	3004	CYC	CHD-C4C	4.44	1.43	1.36
2	A	3002	CYC	CHD-C4C	4.42	1.43	1.36
2	B	3003	CYC	O2D-CGD	4.28	1.45	1.30
2	A	3001	CYC	O2D-CGD	4.28	1.44	1.30
2	A	3002	CYC	C4B-C3B	-4.25	1.40	1.48
2	B	3004	CYC	C4B-C3B	-4.23	1.40	1.48
2	A	3002	CYC	O2D-CGD	3.89	1.43	1.30
2	B	3004	CYC	O2D-CGD	3.86	1.43	1.30
2	A	3001	CYC	C2A-C3A	3.76	1.44	1.36
2	B	3003	CYC	C2A-C3A	3.71	1.44	1.36
2	B	3003	CYC	C4B-C3B	-3.59	1.41	1.48
2	A	3001	CYC	C4B-C3B	-3.58	1.41	1.48
2	A	3002	CYC	C1B-NB	3.52	1.43	1.37
2	B	3004	CYC	C4C-NC	3.49	1.44	1.37
2	B	3004	CYC	C1B-NB	3.48	1.43	1.37
2	A	3002	CYC	C4C-NC	3.48	1.44	1.37
2	B	3003	CYC	CAC-C3C	3.31	1.60	1.54
2	A	3001	CYC	CAC-C3C	3.31	1.60	1.54
2	B	3003	CYC	C3B-C2B	3.13	1.43	1.36
2	A	3001	CYC	C3B-C2B	3.12	1.43	1.36
2	B	3003	CYC	C4C-NC	3.07	1.43	1.37
2	A	3002	CYC	C3B-C2B	3.07	1.43	1.36
2	B	3004	CYC	C3B-C2B	3.07	1.43	1.36
2	A	3001	CYC	C4C-NC	3.07	1.43	1.37
2	B	3004	CYC	CHB-C1B	3.03	1.45	1.37
2	A	3002	CYC	CHB-C1B	3.00	1.45	1.37
2	A	3002	CYC	C4D-ND	2.94	1.42	1.37
2	B	3004	CYC	C4D-ND	2.93	1.42	1.37
2	B	3004	CYC	C2A-C3A	2.70	1.42	1.36
2	A	3002	CYC	C2A-C3A	2.70	1.42	1.36
2	B	3004	CYC	C1D-ND	2.46	1.42	1.37
2	A	3002	CYC	C1D-ND	2.42	1.41	1.37
2	A	3001	CYC	C4A-NA	2.33	1.41	1.36
2	B	3003	CYC	C4A-NA	2.32	1.41	1.36
2	A	3001	CYC	C1C-NC	-2.23	1.34	1.37
2	B	3003	CYC	C1C-NC	-2.22	1.34	1.37
2	A	3001	CYC	C1B-NB	2.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3003	CYC	C1B-NB	2.19	1.41	1.37
2	A	3001	CYC	CHD-C1D	2.19	1.45	1.40
2	B	3003	CYC	CHD-C1D	2.18	1.45	1.40
2	A	3001	CYC	C4B-NB	-2.14	1.33	1.38
2	A	3002	CYC	C1A-C2A	-2.14	1.42	1.45
2	B	3003	CYC	C4B-NB	-2.10	1.33	1.38
2	B	3004	CYC	C1A-C2A	-2.08	1.42	1.45

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	CYC	CBA-CAA-C2A	12.13	146.07	112.53
2	B	3003	CYC	CAA-CBA-CGA	11.54	144.28	113.67
2	A	3001	CYC	CAD-CBD-CGD	8.66	136.62	113.67
2	B	3003	CYC	CBA-CAA-C2A	7.30	132.72	112.53
2	A	3001	CYC	CBD-CAD-C3D	7.10	132.16	112.53
2	A	3002	CYC	CBC-CAC-C3C	-6.65	99.30	113.41
2	B	3004	CYC	CBC-CAC-C3C	-6.63	99.36	113.41
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	-5.98	113.38	128.06
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	5.60	128.53	113.67
2	B	3004	CYC	C1C-NC-C4C	-5.26	106.81	113.41
2	B	3003	CYC	C1B-C2B-C3B	-5.24	102.48	107.86
2	A	3002	CYC	C1C-NC-C4C	-5.23	106.85	113.41
2	A	3001	CYC	C1B-C2B-C3B	-5.21	102.50	107.86
2	B	3003	CYC	C1D-CHD-C4C	5.01	136.31	127.76
2	A	3001	CYC	C1D-CHD-C4C	4.99	136.28	127.76
2	B	3003	CYC	C3B-C4B-NB	4.55	110.39	106.77
2	A	3002	CYC	C1B-C2B-C3B	-4.47	103.27	107.86
2	A	3001	CYC	C3B-C4B-NB	4.45	110.31	106.77
2	B	3004	CYC	C1B-C2B-C3B	-4.45	103.29	107.86
2	A	3001	CYC	C1C-NC-C4C	-3.93	108.48	113.41
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	A	3002	CYC	C1D-CHD-C4C	3.91	134.43	127.76
2	B	3004	CYC	C1D-CHD-C4C	3.90	134.42	127.76
2	B	3003	CYC	C1C-NC-C4C	-3.90	108.52	113.41
2	A	3001	CYC	CBC-CAC-C3C	-3.73	105.50	113.41
2	B	3003	CYC	CBC-CAC-C3C	-3.71	105.54	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3002	CYC	CHD-C4C-NC	3.69	130.24	125.63
2	B	3004	CYC	CHD-C4C-NC	3.69	130.24	125.63
2	A	3002	CYC	C3C-C4C-NC	-3.53	103.40	107.94
2	B	3004	CYC	C3C-C4C-NC	-3.51	103.42	107.94
2	B	3003	CYC	CMB-C2B-C1B	3.49	128.40	124.16
2	A	3001	CYC	CMB-C2B-C1B	3.49	128.40	124.16
2	B	3003	CYC	C1B-NB-C4B	-3.32	106.59	110.66
2	A	3002	CYC	OC-C1C-C2C	3.31	128.80	126.17
2	A	3001	CYC	O2A-CGA-O1A	-3.29	114.87	123.33
2	B	3004	CYC	OC-C1C-C2C	3.29	128.79	126.17
2	B	3003	CYC	O2A-CGA-O1A	-3.29	114.88	123.33
2	A	3001	CYC	C1B-NB-C4B	-3.27	106.65	110.66
2	A	3001	CYC	O2A-CGA-CBA	3.23	124.19	114.00
2	B	3003	CYC	O2A-CGA-CBA	3.22	124.16	114.00
2	B	3004	CYC	O2D-CGD-CBD	3.04	123.59	114.00
2	A	3002	CYC	O2D-CGD-CBD	3.02	123.53	114.00
2	B	3004	CYC	C4D-ND-C1D	-3.01	104.50	109.78
2	A	3002	CYC	C4D-ND-C1D	-2.99	104.54	109.78
2	B	3003	CYC	CMD-C2D-C1D	2.97	129.94	125.62
2	A	3001	CYC	CMD-C2D-C1D	2.97	129.93	125.62
2	B	3003	CYC	CMC-C2C-C3C	2.95	125.39	113.98
2	A	3001	CYC	CMC-C2C-C3C	2.95	125.37	113.98
2	A	3002	CYC	C1A-NA-C4A	-2.94	101.12	106.52
2	B	3004	CYC	C1A-NA-C4A	-2.93	101.13	106.52
2	B	3004	CYC	CHD-C1D-ND	-2.88	118.78	125.29
2	B	3003	CYC	O2D-CGD-CBD	2.87	123.06	114.00
2	A	3001	CYC	O2D-CGD-CBD	2.87	123.06	114.00
2	A	3002	CYC	CHD-C1D-ND	-2.87	118.81	125.29
2	B	3004	CYC	CBB-CAB-C3B	2.87	120.19	112.42
2	A	3002	CYC	CBB-CAB-C3B	2.86	120.18	112.42
2	A	3002	CYC	O2A-CGA-CBA	2.82	122.91	114.00
2	B	3004	CYC	O2A-CGA-CBA	2.81	122.89	114.00
2	B	3004	CYC	C3D-C4D-ND	2.76	111.03	107.57
2	A	3002	CYC	C3D-C4D-ND	2.75	111.01	107.57
2	A	3001	CYC	CHD-C1D-ND	-2.72	119.14	125.29
2	B	3003	CYC	CHD-C1D-ND	-2.68	119.23	125.29
2	A	3002	CYC	CAA-C2A-C1A	2.54	129.49	125.02
2	A	3002	CYC	CMA-C3A-C4A	2.54	129.04	125.10
2	B	3004	CYC	CAA-C2A-C1A	2.54	129.47	125.02
2	B	3004	CYC	CMA-C3A-C4A	2.53	129.03	125.10
2	A	3002	CYC	CHA-C4D-C3D	-2.50	121.84	127.22
2	B	3004	CYC	CHA-C4D-C3D	-2.50	121.85	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3003	CYC	CBB-CAB-C3B	2.47	119.13	112.42
2	A	3002	CYC	CMD-C2D-C1D	2.47	129.21	125.62
2	A	3001	CYC	CHD-C1D-C2D	2.45	133.54	127.53
2	A	3001	CYC	CBB-CAB-C3B	2.45	119.06	112.42
2	B	3004	CYC	CMD-C2D-C1D	2.45	129.18	125.62
2	B	3003	CYC	CHD-C1D-C2D	2.43	133.49	127.53
2	B	3003	CYC	O1D-CGD-CBD	-2.35	115.63	123.09
2	A	3001	CYC	O1D-CGD-CBD	-2.35	115.64	123.09
2	A	3002	CYC	CMB-C2B-C1B	2.32	126.98	124.16
2	A	3001	CYC	C4D-ND-C1D	-2.32	105.71	109.78
2	B	3004	CYC	CMB-C2B-C1B	2.31	126.97	124.16
2	B	3003	CYC	C4D-ND-C1D	-2.30	105.74	109.78
2	A	3001	CYC	CHB-C4A-NA	-2.29	120.01	124.95
2	B	3003	CYC	CHB-C4A-NA	-2.27	120.05	124.95
2	A	3002	CYC	CMC-C2C-C3C	2.22	122.56	113.98
2	B	3004	CYC	CMC-C2C-C3C	2.20	122.51	113.98
2	B	3003	CYC	C3C-C4C-NC	-2.18	105.14	107.94
2	A	3001	CYC	C3C-C4C-NC	-2.14	105.19	107.94
2	B	3004	CYC	O2A-CGA-O1A	-2.13	117.86	123.33
2	A	3002	CYC	O2A-CGA-O1A	-2.12	117.89	123.33
2	B	3004	CYC	C2C-C1C-NC	-2.05	106.58	108.29
2	A	3002	CYC	C2C-C1C-NC	-2.04	106.59	108.29

There are no chirality outliers.

All (52) 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	C3C-C4C-CHD-C1D
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	C3C-C4C-CHD-C1D
2	A	3002	CYC	ND-C1D-CHD-C4C
2	B	3003	CYC	C3A-C4A-CHB-C1B
2	B	3003	CYC	C4C-C3C-CAC-CBC
2	B	3003	CYC	C3C-C4C-CHD-C1D
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	C3C-C4C-CHD-C1D

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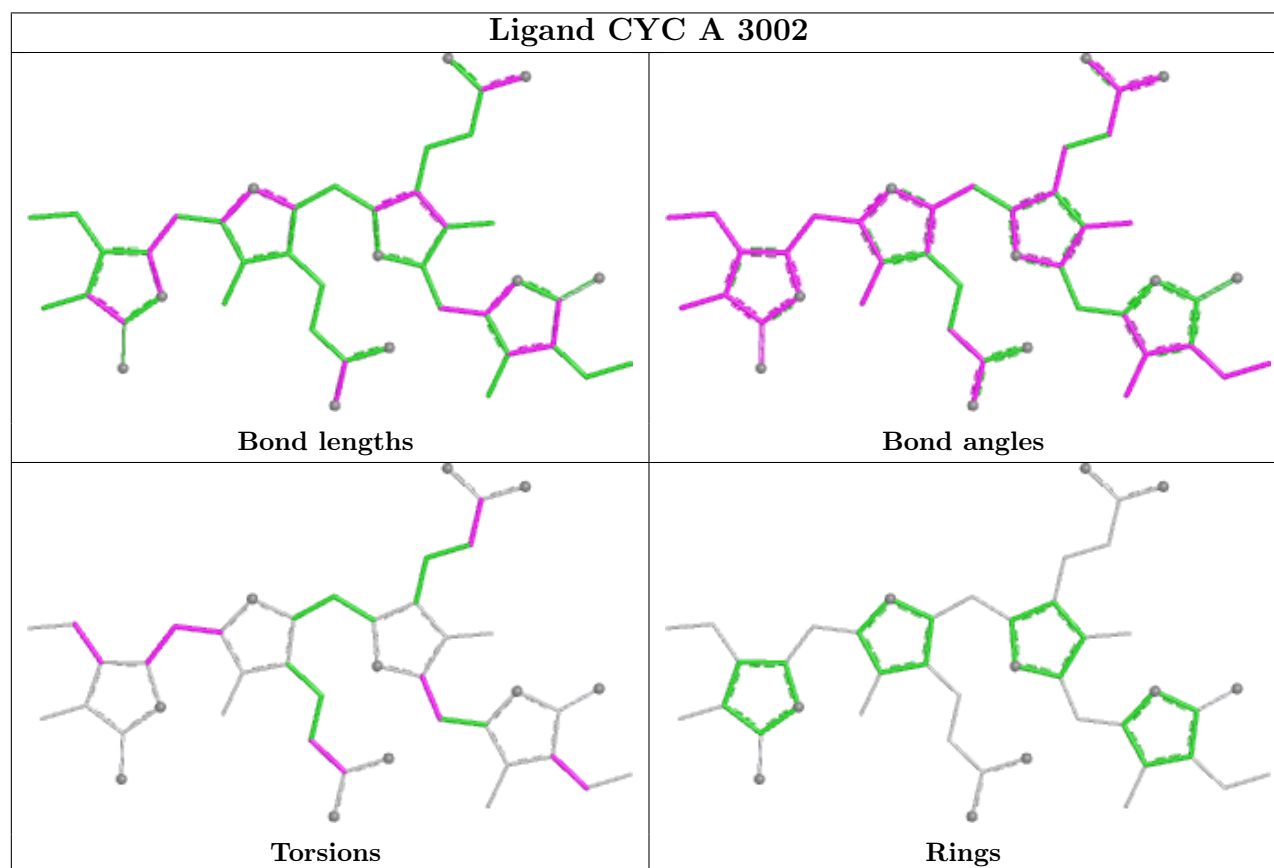
Mol	Chain	Res	Type	Atoms
2	B	3004	CYC	ND-C1D-CHD-C4C
2	A	3001	CYC	ND-C1D-CHD-C4C
2	B	3003	CYC	ND-C1D-CHD-C4C
2	A	3002	CYC	C2D-C1D-CHD-C4C
2	B	3004	CYC	C2D-C1D-CHD-C4C
2	A	3001	CYC	C2B-C3B-CAB-CBB
2	B	3003	CYC	C2B-C3B-CAB-CBB
2	B	3004	CYC	C3D-CAD-CBD-CGD
2	A	3001	CYC	C2D-C1D-CHD-C4C
2	B	3003	CYC	C2D-C1D-CHD-C4C
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	3002	CYC	C4B-C3B-CAB-CBB
2	B	3004	CYC	C4B-C3B-CAB-CBB
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	B	3004	CYC	C2B-C3B-CAB-CBB
2	A	3001	CYC	C4D-C3D-CAD-CBD
2	A	3002	CYC	C2B-C3B-CAB-CBB
2	A	3001	CYC	C3D-CAD-CBD-CGD
2	B	3003	CYC	C3D-CAD-CBD-CGD
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	B	3003	CYC	CAA-CBA-CGA-O1A
2	A	3002	CYC	CAD-CBD-CGD-O1D
2	B	3003	CYC	CAD-CBD-CGD-O1D
2	A	3001	CYC	CAA-CBA-CGA-O1A
2	A	3001	CYC	CAA-CBA-CGA-O2A
2	B	3003	CYC	CAD-CBD-CGD-O2D
2	A	3002	CYC	CAD-CBD-CGD-O2D
2	B	3004	CYC	CAA-CBA-CGA-O1A
2	B	3004	CYC	CAA-CBA-CGA-O2A

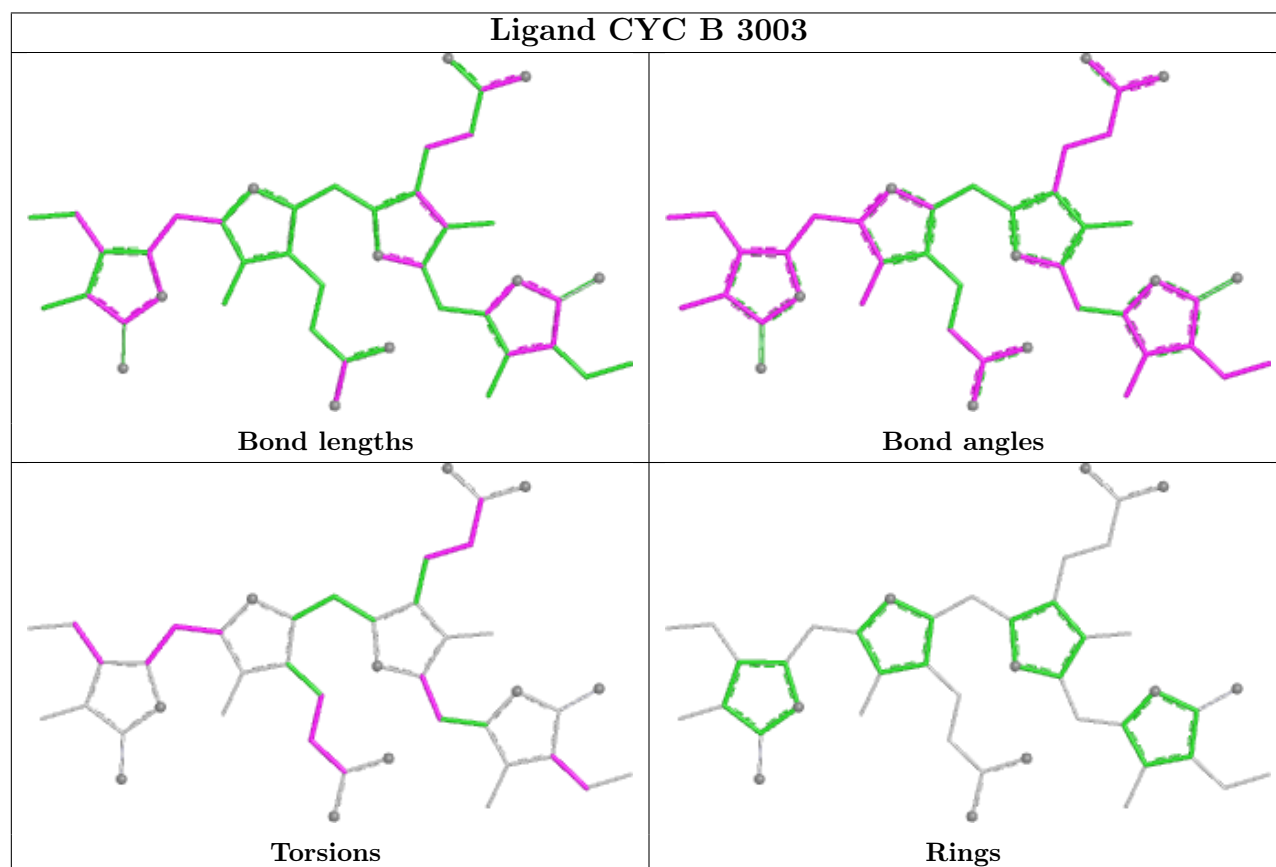
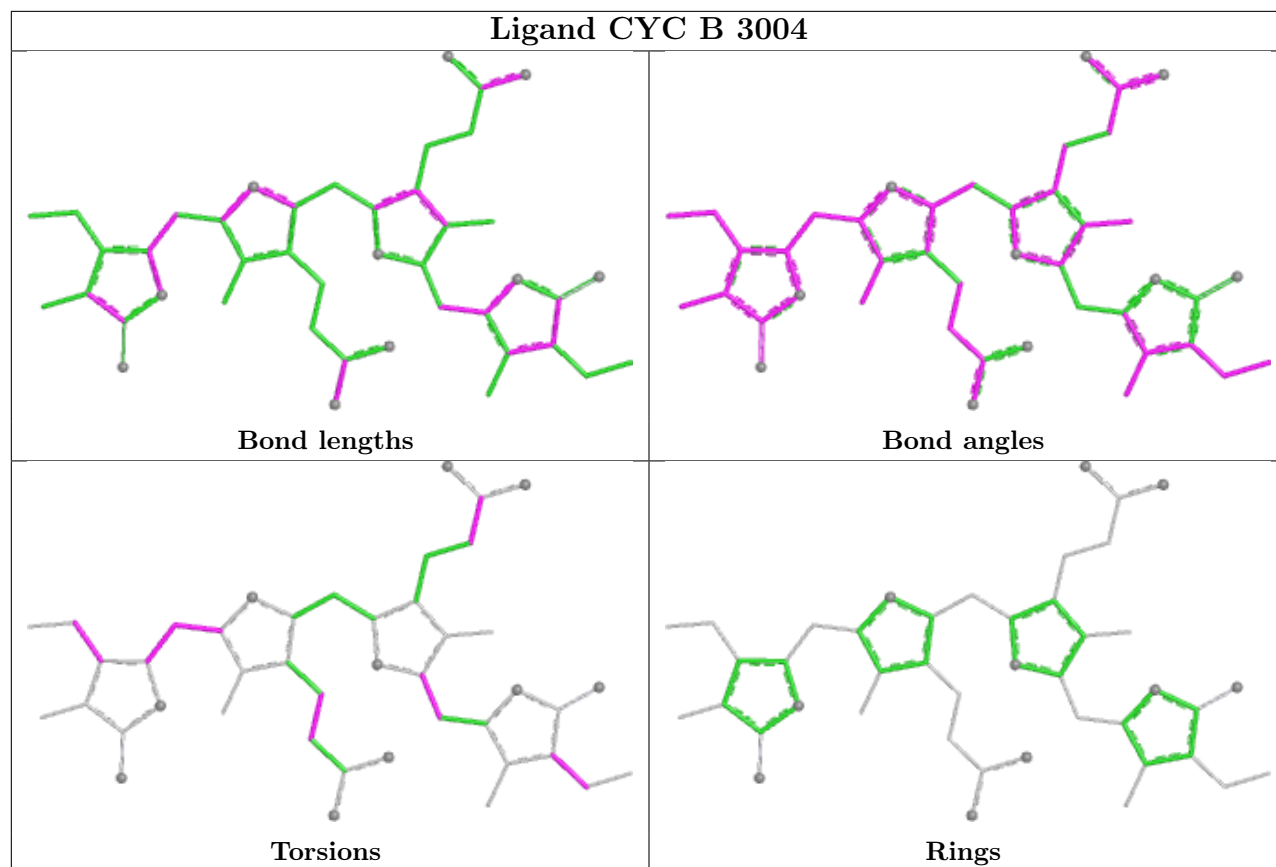
There are no ring outliers.

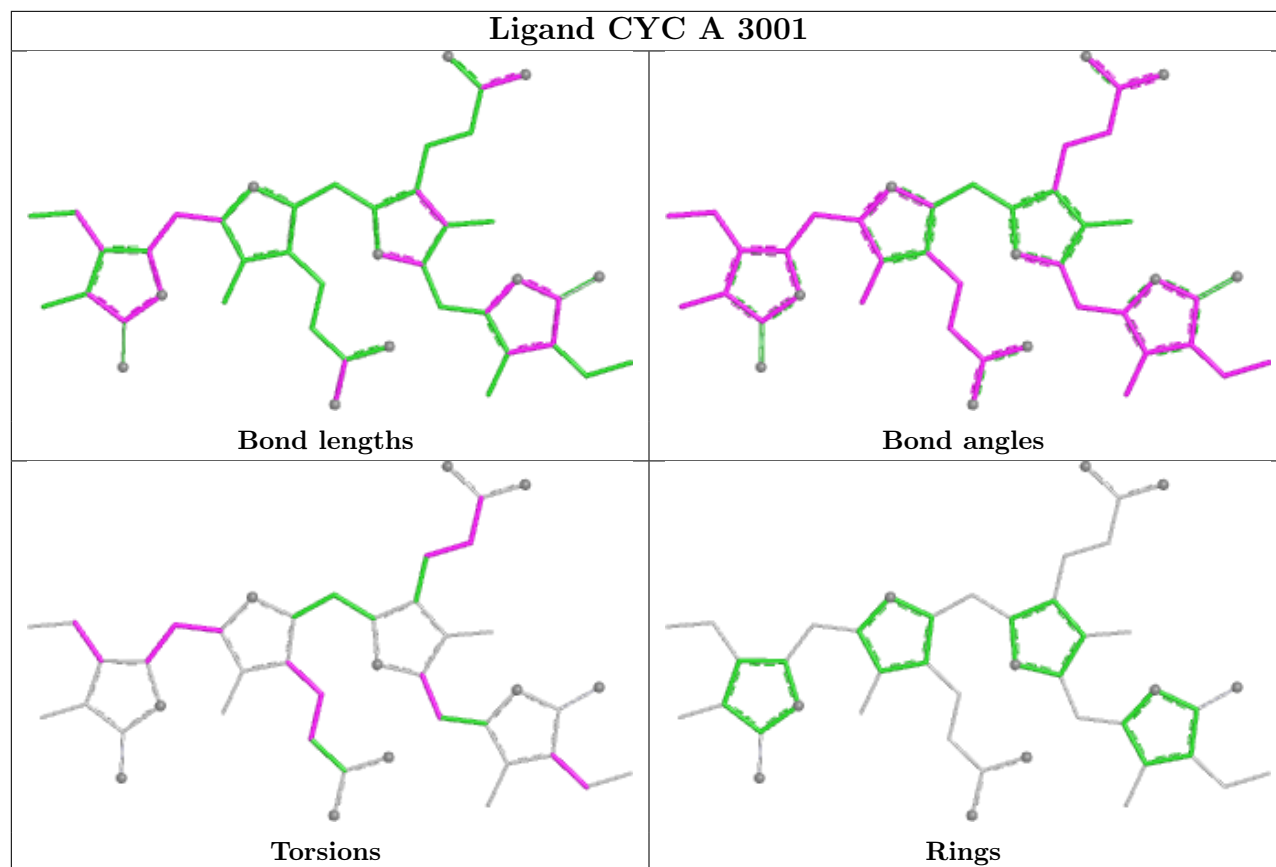
4 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	CYC	8	0
2	B	3004	CYC	5	0
2	B	3003	CYC	18	0
2	A	3001	CYC	16	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	133/133 (100%)	1.71	39 (29%) 1 1	11, 33, 65, 78	0
1	B	133/133 (100%)	2.15	57 (42%) 0 0	4, 39, 76, 99	0
All	All	266/266 (100%)	1.93	96 (36%) 1 0	4, 36, 72, 99	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1115	GLU	8.8
1	B	2164	SER	7.6
1	B	2108	TRP	6.7
1	B	2162	SER	6.6
1	B	2087	ASP	6.1
1	A	1140	ALA	5.8
1	B	2126	ALA	5.4
1	B	2065	TYR	5.3
1	B	2163	LEU	5.2
1	B	2048	HIS	5.1
1	A	1082	CYS	4.9
1	A	1071	GLU	4.8
1	B	2076	GLN	4.8
1	B	2110	ILE	4.8
1	B	2107	GLU	4.5
1	B	2161	ASN	4.4
1	A	1159	LEU	4.4
1	B	2111	ALA	4.4
1	A	1108	TRP	4.3
1	B	2074	GLU	4.2
1	A	1114	ARG	4.2
1	B	2075	ASN	4.1
1	A	1095	TYR	4.0
1	B	2046	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	2132	VAL	3.8
1	B	2104	PRO	3.8
1	A	1122	LEU	3.8
1	A	1109	GLY	3.7
1	A	1078	LYS	3.7
1	B	2096	THR	3.7
1	A	1116	VAL	3.7
1	A	1145	SER	3.6
1	A	1070	GLY	3.6
1	B	2157	ASP	3.5
1	A	1107	GLU	3.5
1	B	2047	ASN	3.4
1	B	2071	GLU	3.4
1	B	2106	ASP	3.4
1	B	2160	ILE	3.4
1	B	2085	ASP	3.4
1	B	2063	TYR	3.3
1	B	2083	TYR	3.3
1	A	1068	ASN	3.2
1	A	1135	ARG	3.2
1	B	2128	ILE	3.2
1	B	2094	ASN	3.1
1	A	1141	PRO	3.1
1	A	1079	ILE	3.1
1	A	1106	ASP	3.0
1	B	2058	ALA	3.0
1	A	1103	GLY	3.0
1	A	1072	ALA	3.0
1	B	2035	ALA	3.0
1	B	2145	SER	2.9
1	B	2136	ASP	2.9
1	A	1110	ILE	2.9
1	B	2044	LEU	2.9
1	B	2033	ARG	2.9
1	B	2073	GLY	2.8
1	A	1139	CYS	2.8
1	B	2114	ARG	2.8
1	A	1117	TYR	2.8
1	B	2103	GLY	2.7
1	B	2112	GLY	2.7
1	A	1092	LEU	2.7
1	B	2032	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1077	GLU	2.7
1	A	1081	LYS	2.7
1	B	2135	ARG	2.6
1	B	2101	GLY	2.6
1	A	1083	TYR	2.6
1	A	1164	SER	2.5
1	A	1118	ARG	2.5
1	B	2118	ARG	2.5
1	B	2158	TYR	2.5
1	B	2069	PRO	2.5
1	A	1161	ASN	2.4
1	B	2109	GLY	2.4
1	B	2156	LEU	2.3
1	A	1133	PHE	2.3
1	A	1105	LEU	2.3
1	B	2049	GLU	2.3
1	B	2133	PHE	2.3
1	A	1051	VAL	2.3
1	A	1131	PHE	2.3
1	B	2144	MET	2.2
1	B	2100	GLY	2.2
1	B	2116	VAL	2.2
1	B	2070	GLY	2.2
1	A	1044	LEU	2.2
1	B	2125	ALA	2.2
1	A	1120	LEU	2.1
1	B	2045	GLY	2.1
1	B	2052	VAL	2.1
1	B	2084	ARG	2.0
1	A	1101	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

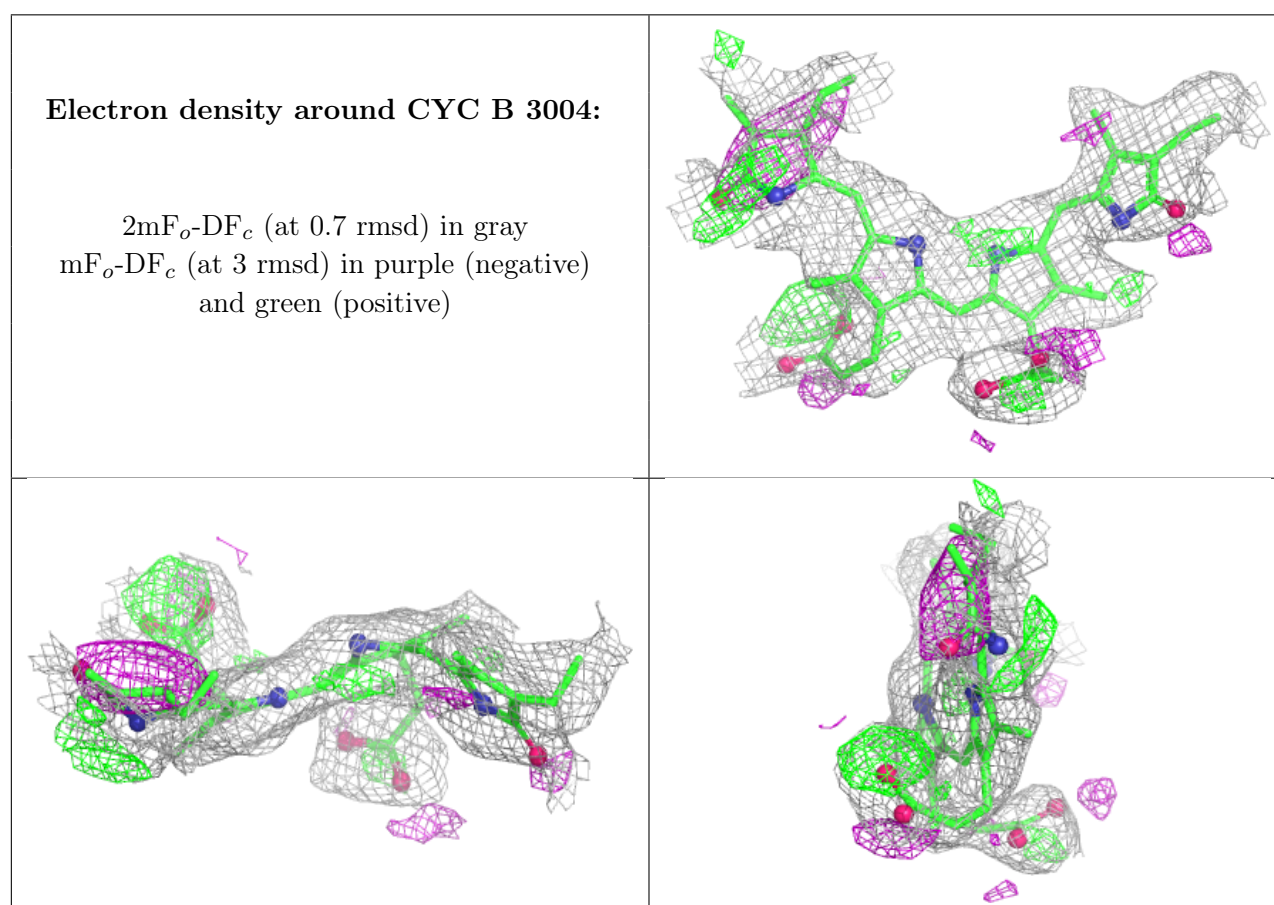
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

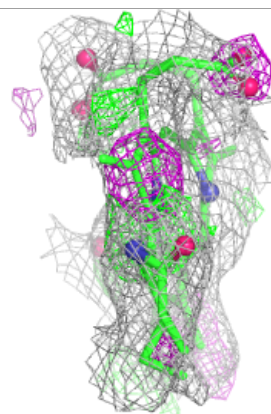
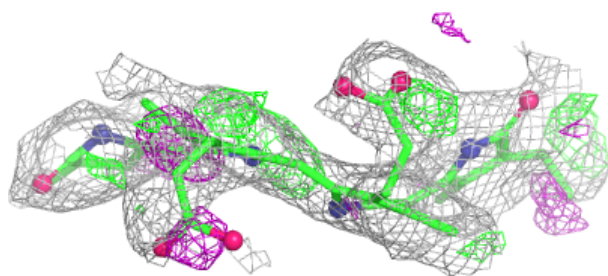
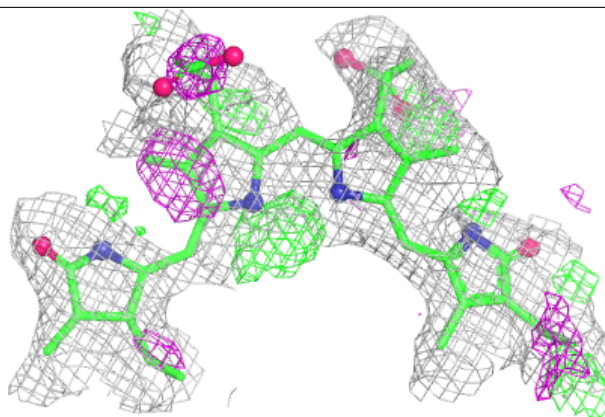
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CYC	B	3004	43/43	0.56	0.23	15,23,31,34	0
2	CYC	A	3002	43/43	0.62	0.21	15,23,31,34	0
2	CYC	B	3003	43/43	0.70	0.15	6,9,19,32	0
2	CYC	A	3001	43/43	0.72	0.16	6,9,19,32	0

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



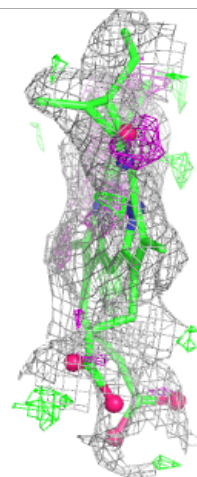
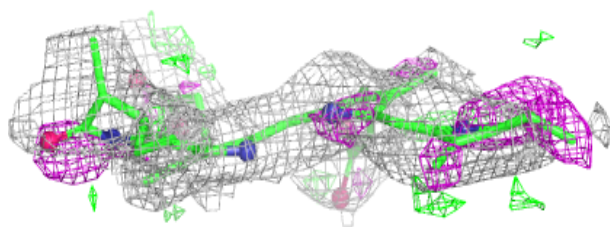
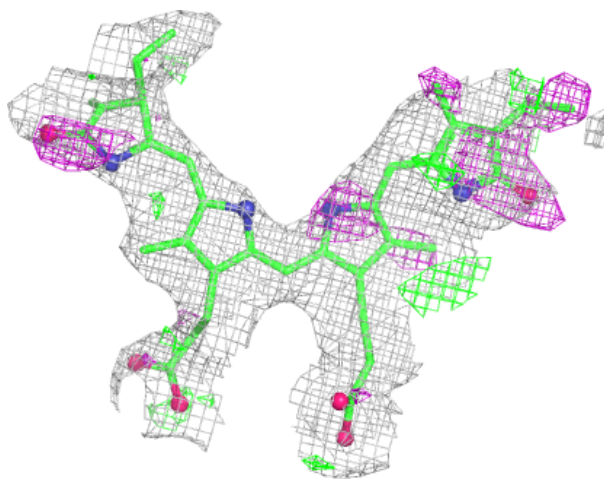
Electron density around CYC A 3002:

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



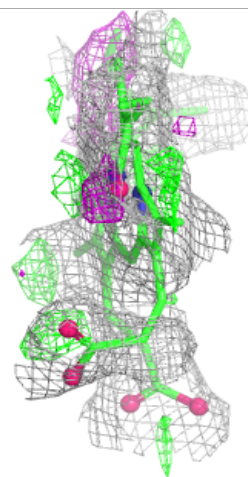
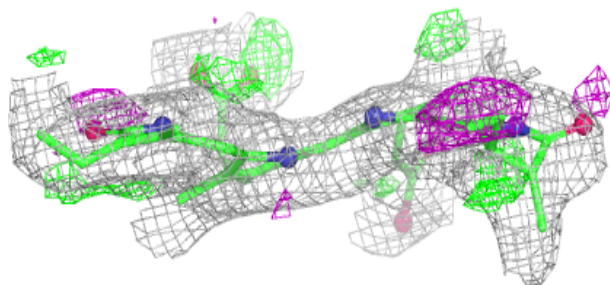
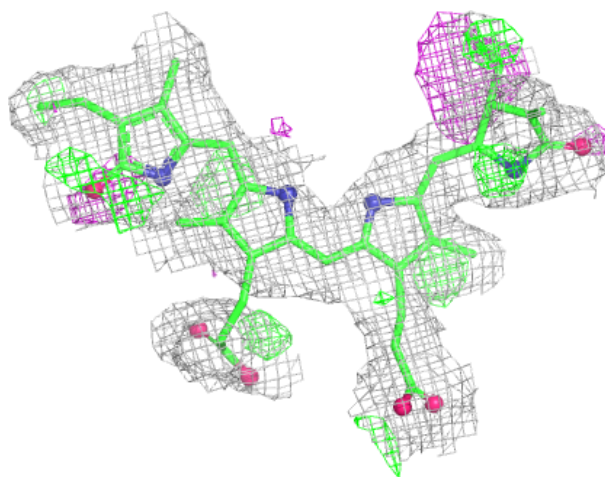
Electron density around CYC B 3003:

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



Electron density around CYC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.