



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:07 AM GMT

PDB ID : 4F0T
Title : X-Ray Crystal Structure of Phycocyanin from Synechocystis sp. PCC 6803
Authors : Marx, A.; Adir, N.
Deposited on : 2012-05-05
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

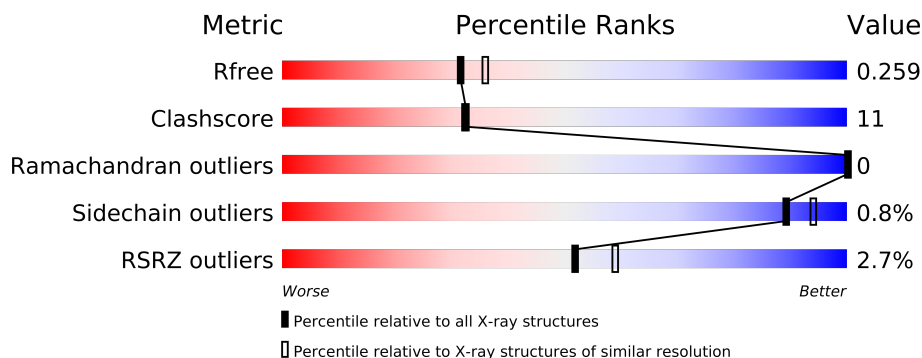
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.25 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 2857 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

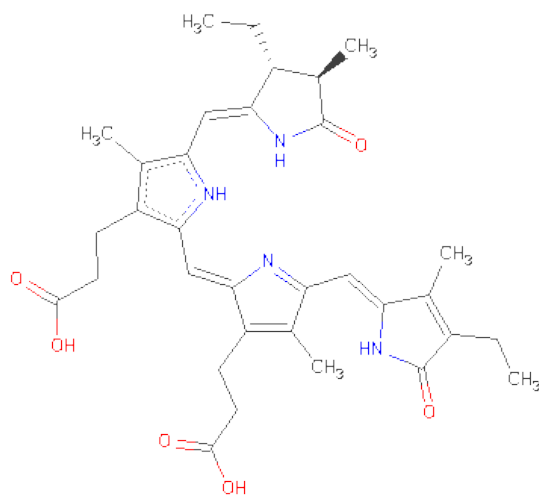
- Molecule 1 is a protein called C-phycocyanin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1240	775	215	247	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1271	785	228	251	7			

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



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

Continued on next page...

Continued from previous page...

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

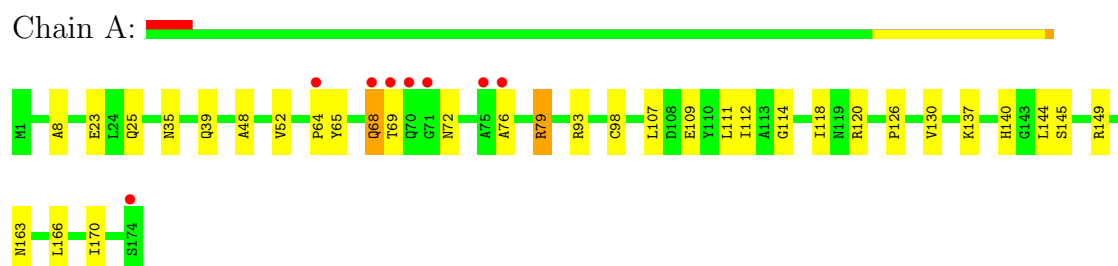
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	143	Total	O	0	0
			143	143		

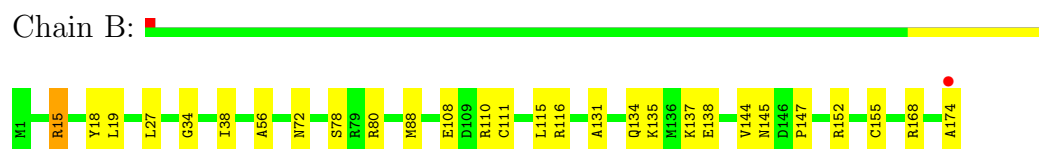
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: C-phycocyanin alpha chain



• Molecule 2: C-phycocyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	153.02Å 153.02Å 40.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.25 38.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.25) 99.9 (38.35-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.250 0.217 , 0.259	Depositor DCC
R_{free} test set	1316 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.8	EDS
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25909 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2857	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/1261	0.53	1/1709 (0.1%)
2	B	0.71	2/1275 (0.2%)	0.63	1/1725 (0.1%)
All	All	0.63	2/2536 (0.1%)	0.59	2/3434 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	155	CYS	CB-SG	-8.16	1.68	1.82
2	B	111	CYS	CB-SG	-5.23	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLN	CB-CA-C	-5.24	99.92	110.40
2	B	15	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1240	0	1206	25	0
2	B	1271	0	1262	26	0
3	A	43	0	37	4	0
3	B	86	0	71	9	0
4	A	74	0	0	3	0
4	B	143	0	0	3	0
All	All	2857	0	2576	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:134:GLN:NE2	2:B:137:LYS:HE2	1.73	1.03
2:B:134:GLN:HE22	2:B:137:LYS:CE	1.75	0.98
2:B:134:GLN:HE22	2:B:137:LYS:HE2	1.33	0.88
2:B:147:PRO:CB	2:B:152:ARG:HH12	1.87	0.88
2:B:147:PRO:HB2	2:B:152:ARG:HH12	1.36	0.88
1:A:144:LEU:O	1:A:149:ARG:HD3	1.89	0.73
1:A:64:PRO:O	1:A:68:GLN:HG2	1.89	0.72
2:B:78:SER:HB2	4:B:409:HOH:O	1.89	0.71
2:B:108:GLU:OE2	2:B:168:ARG:HD3	1.91	0.71
2:B:134:GLN:HE22	2:B:137:LYS:NZ	1.91	0.69
1:A:65:TYR:O	1:A:69:THR:HG22	1.93	0.68
1:A:8:ALA:HB1	1:A:23:GLU:HG2	1.75	0.68
3:B:202:CYC:HMA1	3:B:202:CYC:HB	1.59	0.67
2:B:72:MEN:O	2:B:80:ARG:HD2	1.96	0.66
3:B:201:CYC:HMD2	3:B:201:CYC:HC	1.61	0.65
1:A:166:LEU:O	1:A:170:ILE:HG13	1.97	0.64
3:A:201:CYC:HC	3:A:201:CYC:HMD2	1.64	0.62
3:B:202:CYC:HMA1	3:B:202:CYC:NB	2.15	0.61
2:B:147:PRO:HB2	2:B:152:ARG:NH1	2.12	0.60
2:B:147:PRO:CB	2:B:152:ARG:NH1	2.62	0.59
1:A:114:GLY:O	1:A:118:ILE:HG12	2.02	0.59
2:B:134:GLN:NE2	2:B:137:LYS:CE	2.43	0.58
1:A:35:ASN:O	1:A:39:GLN:HG3	2.05	0.57
1:A:25:GLN:HG3	4:A:301:HOH:O	2.05	0.56
1:A:48:ALA:O	1:A:52:VAL:HG23	2.05	0.56
3:A:201:CYC:NB	3:A:201:CYC:HMA1	2.25	0.52
2:B:115:LEU:HD13	3:B:201:CYC:HMB3	1.91	0.51
2:B:144:VAL:O	3:B:202:CYC:HBC2	2.10	0.51
1:A:107:LEU:O	1:A:112:ILE:HG12	2.12	0.49
1:A:130:VAL:HG13	1:A:170:ILE:HG23	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:ASN:HA	1:A:79:ARG:NH2	2.29	0.48
2:B:15:ARG:NH2	4:B:362:HOH:O	2.46	0.47
1:A:126:PRO:O	1:A:130:VAL:HG23	2.16	0.46
3:A:201:CYC:HC	3:A:201:CYC:CMD	2.29	0.46
1:A:145:SER:N	1:A:149:ARG:HB2	2.31	0.46
1:A:111:LEU:HD23	1:A:111:LEU:C	2.35	0.46
2:B:34:GLY:O	2:B:38:ILE:HG12	2.14	0.46
1:A:109:GLU:HB2	4:A:355:HOH:O	2.17	0.45
1:A:76:ALA:HB3	4:A:374:HOH:O	2.16	0.45
2:B:131:ALA:O	2:B:135:LYS:HG2	2.17	0.45
2:B:56:ALA:HB2	2:B:88:MET:HE2	1.97	0.45
3:A:201:CYC:HMA1	3:A:201:CYC:HB	1.81	0.45
1:A:137:LYS:HG3	1:A:163:ASN:OD1	2.17	0.44
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.82	0.44
2:B:134:GLN:NE2	4:B:402:HOH:O	2.49	0.44
1:A:72:ASN:HA	1:A:79:ARG:HH22	1.83	0.44
1:A:93:ARG:HA	2:B:18:TYR:CE1	2.52	0.44
1:A:140:HIS:CE1	1:A:144:LEU:HB2	2.54	0.43
2:B:145:ASN:HA	3:B:202:CYC:HMC1	2.00	0.43
1:A:145:SER:CA	1:A:149:ARG:HB2	2.48	0.42
2:B:110:ARG:O	3:B:201:CYC:HBB1	2.19	0.42
3:B:201:CYC:HMA1	3:B:201:CYC:NB	2.35	0.42
2:B:116:ARG:NH1	2:B:174:ALA:O	2.52	0.42
2:B:72:MEN:O	2:B:80:ARG:CD	2.67	0.42
1:A:98:CYS:SG	1:A:107:LEU:HG	2.60	0.42
2:B:134:GLN:O	2:B:138:GLU:HG3	2.21	0.41
1:A:69:THR:O	1:A:76:ALA:HB2	2.21	0.40
3:B:202:CYC:HB	3:B:202:CYC:CMA	2.30	0.40
2:B:27:LEU:HD23	2:B:27:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	B	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	329/334 (98%)	323 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/126 (100%)	125 (99%)	1 (1%)	89	94
2	B	127/127 (100%)	126 (99%)	1 (1%)	89	94
All	All	253/253 (100%)	251 (99%)	2 (1%)	89	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
2	B	19	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	139	ASN
2	B	134	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	B	72	2	8,8,9	6.84	3 (37%)	7,9,11	0.45	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	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	O-C	17.68	1.23	1.11
2	B	72	MEN	CE2-ND2	-7.48	1.32	1.45
2	B	72	MEN	CA-C	2.41	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CYC	A	201	1	46,46,46	2.25	16 (34%)	65,67,67	3.79	27 (41%)
3	CYC	B	201	2	46,46,46	2.24	14 (30%)	65,67,67	3.79	25 (38%)
3	CYC	B	202	2	46,46,46	3.71	17 (36%)	65,67,67	4.12	25 (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
3	CYC	A	201	1	-	3/25/74/74	0/4/4/4
3	CYC	B	201	2	-	3/25/74/74	0/4/4/4
3	CYC	B	202	2	-	3/25/74/74	0/4/4/4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	CYC	CBD-CGD	-20.13	0.98	1.50
3	B	201	CYC	OB-C4B	6.89	1.37	1.23
3	A	201	CYC	OB-C4B	6.83	1.36	1.23
3	B	202	CYC	C1C-NC	-6.63	1.29	1.37
3	B	202	CYC	OB-C4B	6.42	1.36	1.23
3	B	201	CYC	C1C-NC	-5.22	1.30	1.37
3	A	201	CYC	C1C-NC	-4.90	1.31	1.37
3	A	201	CYC	OC-C1C	4.52	1.32	1.23
3	B	201	CYC	OC-C1C	4.41	1.32	1.23
3	A	201	CYC	C1D-ND	4.35	1.41	1.36
3	B	201	CYC	CHA-C1A	4.03	1.37	1.35
3	B	201	CYC	CHB-C4A	4.02	1.50	1.40
3	B	202	CYC	OC-C1C	3.88	1.31	1.23
3	B	201	CYC	C1D-ND	3.69	1.40	1.36
3	A	201	CYC	C3D-C2D	3.68	1.48	1.37
3	B	202	CYC	C1D-ND	3.68	1.40	1.36
3	B	202	CYC	C2A-C3A	3.65	1.44	1.36
3	B	201	CYC	C2A-C3A	3.58	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	CYC	C3C-C4C	3.52	1.54	1.51
3	A	201	CYC	C2A-C3A	3.50	1.44	1.36
3	A	201	CYC	CHB-C4A	3.46	1.48	1.40
3	B	201	CYC	C3D-C2D	3.42	1.47	1.37
3	B	202	CYC	CAC-C3C	3.21	1.60	1.54
3	B	202	CYC	C3D-C2D	3.21	1.47	1.37
3	B	202	CYC	CHB-C4A	3.05	1.47	1.40
3	A	201	CYC	CHA-C1A	2.89	1.37	1.35
3	B	201	CYC	C4B-C3B	-2.89	1.42	1.48
3	B	202	CYC	C2C-C1C	2.83	1.54	1.52
3	B	201	CYC	CMB-C2B	-2.74	1.45	1.51
3	A	201	CYC	C3B-C2B	2.62	1.42	1.36
3	B	202	CYC	C4B-C3B	-2.59	1.42	1.48
3	B	201	CYC	C4B-NB	-2.57	1.32	1.37
3	B	202	CYC	C4D-ND	2.56	1.39	1.36
3	B	202	CYC	CHA-C1A	2.53	1.36	1.35
3	B	202	CYC	C1B-NB	-2.52	1.33	1.37
3	B	201	CYC	C1B-NB	-2.51	1.33	1.37
3	A	201	CYC	C4D-ND	2.44	1.39	1.36
3	A	201	CYC	C1B-NB	-2.39	1.33	1.37
3	B	202	CYC	C4B-NB	-2.39	1.32	1.37
3	B	202	CYC	CMB-C2B	-2.39	1.45	1.51
3	A	201	CYC	C4B-NB	-2.32	1.32	1.37
3	A	201	CYC	CMB-C2B	-2.32	1.46	1.51
3	A	201	CYC	C4B-C3B	-2.29	1.43	1.48
3	B	201	CYC	C3B-C2B	2.08	1.41	1.36
3	B	201	CYC	CBA-CAA	-2.04	1.46	1.52
3	B	202	CYC	C3C-C4C	2.03	1.53	1.51
3	A	201	CYC	CBA-CAA	-2.00	1.46	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CYC	C4B-C3B-C2B	-13.61	99.81	108.04
3	B	202	CYC	C2C-C1C-NC	13.35	116.00	108.19
3	B	201	CYC	C2C-C1C-NC	13.26	115.95	108.19
3	A	201	CYC	C2C-C1C-NC	12.96	115.77	108.19
3	B	202	CYC	C4B-C3B-C2B	-12.96	100.20	108.04
3	B	201	CYC	C4B-C3B-C2B	-12.86	100.26	108.04
3	B	202	CYC	CAD-CBD-CGD	12.62	154.01	113.47
3	B	201	CYC	C3B-C4B-NB	11.32	116.80	106.69
3	B	202	CYC	C3B-C4B-NB	11.29	116.77	106.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CYC	C3B-C4B-NB	11.24	116.72	106.69
3	B	201	CYC	OC-C1C-C2C	-10.80	117.32	126.25
3	A	201	CYC	OC-C1C-C2C	-10.23	117.79	126.25
3	B	202	CYC	OC-C1C-C2C	-9.38	118.49	126.25
3	B	202	CYC	CAB-C3B-C4B	8.81	128.83	121.49
3	A	201	CYC	CAB-C3B-C4B	8.80	128.82	121.49
3	B	201	CYC	CAB-C3B-C4B	8.27	128.37	121.49
3	B	202	CYC	OB-C4B-C3B	-8.00	119.18	128.20
3	B	201	CYC	OB-C4B-C3B	-7.80	119.42	128.20
3	A	201	CYC	OB-C4B-C3B	-7.43	119.83	128.20
3	B	202	CYC	C3C-C4C-NC	5.20	112.84	107.83
3	B	201	CYC	C3C-C4C-NC	4.67	112.34	107.83
3	B	202	CYC	C1B-NB-C4B	-4.61	104.23	110.74
3	A	201	CYC	C1B-NB-C4B	-4.11	104.93	110.74
3	A	201	CYC	C3C-C2C-C1C	-4.09	99.91	103.43
3	B	201	CYC	C1B-NB-C4B	-4.06	105.00	110.74
3	B	201	CYC	C1C-NC-C4C	-3.86	107.08	112.96
3	B	202	CYC	O2D-CGD-CBD	3.85	127.83	114.22
3	B	202	CYC	C3C-C2C-C1C	-3.84	100.13	103.43
3	A	201	CYC	C1C-NC-C4C	-3.82	107.14	112.96
3	B	202	CYC	C1C-NC-C4C	-3.77	107.21	112.96
3	A	201	CYC	C1D-CHD-C4C	3.75	133.71	128.81
3	B	201	CYC	C1D-CHD-C4C	3.75	133.71	128.81
3	B	202	CYC	O2D-CGD-O1D	-3.62	114.08	123.30
3	B	202	CYC	CHD-C4C-NC	-3.54	120.24	126.09
3	B	202	CYC	C1A-C2A-C3A	-3.41	102.90	106.86
3	A	201	CYC	CAA-CBA-CGA	-3.36	107.29	113.53
3	B	202	CYC	CAC-C3C-C2C	3.27	121.41	113.89
3	B	201	CYC	C1A-C2A-C3A	-3.25	103.09	106.86
3	A	201	CYC	C3C-C4C-NC	3.23	110.95	107.83
3	B	202	CYC	O1D-CGD-CBD	-3.23	111.92	123.03
3	A	201	CYC	C1A-C2A-C3A	-3.20	103.14	106.86
3	B	201	CYC	CAA-CBA-CGA	-3.14	107.70	113.53
3	B	201	CYC	O2D-CGD-O1D	-3.07	115.48	123.30
3	A	201	CYC	O2D-CGD-O1D	-3.02	115.62	123.30
3	B	201	CYC	C3C-C2C-C1C	-2.91	100.92	103.43
3	A	201	CYC	C2D-C1D-CHD	2.84	133.79	125.72
3	A	201	CYC	O1A-CGA-CBA	-2.67	113.86	123.03
3	B	201	CYC	O1A-CGA-CBA	-2.66	113.87	123.03
3	B	202	CYC	CHB-C4A-C3A	2.62	131.63	125.10
3	B	202	CYC	C4D-C3D-C2D	-2.58	104.24	106.92
3	A	201	CYC	C1A-NA-C4A	2.57	111.56	106.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CYC	O2D-CGD-CBD	2.57	123.32	114.22
3	B	202	CYC	C1A-NA-C4A	2.57	111.54	106.55
3	B	201	CYC	C1A-NA-C4A	2.56	111.53	106.55
3	B	201	CYC	O2D-CGD-CBD	2.55	123.22	114.22
3	A	201	CYC	CHB-C4A-C3A	2.54	131.44	125.10
3	B	201	CYC	C2D-C1D-CHD	2.53	132.92	125.72
3	B	201	CYC	C4A-C3A-C2A	2.51	109.75	106.64
3	A	201	CYC	CHD-C4C-NC	-2.45	122.04	126.09
3	B	202	CYC	C2B-C1B-NB	2.44	110.99	107.14
3	B	202	CYC	CAA-CBA-CGA	-2.40	109.07	113.53
3	B	201	CYC	CHD-C4C-NC	-2.39	122.14	126.09
3	A	201	CYC	CAC-C3C-C2C	2.36	119.31	113.89
3	B	202	CYC	C3D-C4D-ND	2.31	110.60	106.79
3	B	201	CYC	CBD-CAD-C3D	2.24	116.63	112.69
3	B	202	CYC	O1A-CGA-CBA	-2.23	115.37	123.03
3	B	201	CYC	C4D-C3D-C2D	-2.20	104.65	106.92
3	A	201	CYC	C2B-C1B-NB	2.17	110.57	107.14
3	A	201	CYC	C4D-C3D-C2D	-2.14	104.70	106.92
3	A	201	CYC	CAB-C3B-C2B	2.13	131.37	127.50
3	B	201	CYC	CAB-C3B-C2B	2.13	131.36	127.50
3	A	201	CYC	C4A-C3A-C2A	2.12	109.27	106.64
3	B	201	CYC	O2A-CGA-CBA	2.10	121.64	114.22
3	B	202	CYC	C4A-C3A-C2A	2.09	109.24	106.64
3	A	201	CYC	C3D-C4D-ND	2.08	110.21	106.79
3	B	201	CYC	CHB-C4A-C3A	2.06	130.24	125.10
3	A	201	CYC	O2A-CGA-CBA	2.01	121.34	114.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	CYC	C4C-CHD-C1D-ND
3	B	201	CYC	C4C-CHD-C1D-ND
3	B	202	CYC	C1B-CHB-C4A-NA
3	B	202	CYC	C1B-CHB-C4A-C3A
3	B	202	CYC	C4C-CHD-C1D-ND
3	A	201	CYC	C1B-CHB-C4A-NA
3	A	201	CYC	C1B-CHB-C4A-C3A
3	B	201	CYC	C1B-CHB-C4A-NA
3	B	201	CYC	C1B-CHB-C4A-C3A

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/162 (100%)	-0.03	8 (4%) 28 32	14, 38, 69, 84	0
2	B	172/172 (100%)	-0.55	1 (0%) 86 91	12, 21, 33, 39	0
All	All	334/334 (100%)	-0.30	9 (2%) 52 59	12, 26, 61, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	4.5
1	A	76	ALA	4.2
2	B	174	ALA	3.7
1	A	174	SER	3.6
1	A	70	GLN	3.5
1	A	68	GLN	3.1
1	A	64	PRO	2.8
1	A	69	THR	2.6
1	A	75	ALA	2.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MEN	B	72	9/10	0.14	1.37	24,26,28,29	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CYC	B	202	43/43	0.12	0.71	13,17,37,52	0
3	CYC	A	201	43/43	0.15	0.17	30,40,46,48	0
3	CYC	B	201	43/43	0.10	-0.03	20,28,38,45	0

6.5 Other polymers

There are no such residues in this entry.