



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:26 PM GMT

PDB ID : 2C7L
Title : LOW TEMPERATURE STRUCTURE OF PHYCOERYTHROCYANIN
FROM MASTIGOCLADUS LAMINOSUS
Authors : Schmidt, M.; Krasselt, A.; Reuter, W.
Deposited on : 2005-11-25
Resolution : 2.85 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>

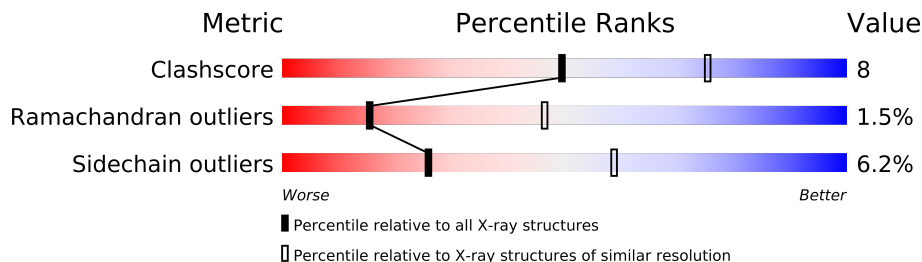
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.85 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	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	
2	B	172	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3055 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.

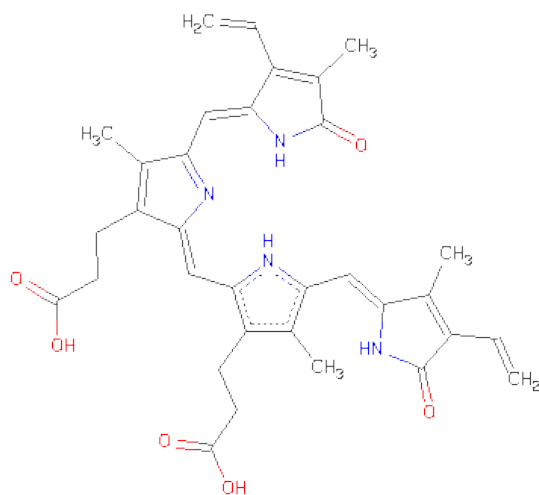
- Molecule 1 is a protein called PHYCOERYTHROCYANIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1239	782	216	236	5			

- Molecule 2 is a protein called PHYCOERYTHROCYANIN BETA CHAIN.

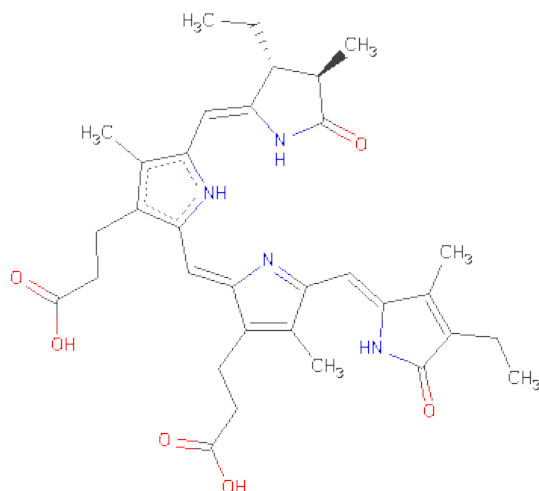
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1295	801	234	252	8			

- Molecule 3 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

- Molecule 4 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	197	Total	O	0	0
			197	197		

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.

Note EDS was not executed.

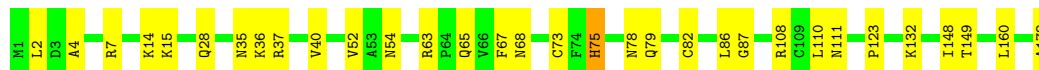
• Molecule 1: PHYCOERYTHROCYANIN ALPHA CHAIN

Chain A: 



• Molecule 2: PHYCOERYTHROCYANIN BETA CHAIN

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	155.00Å 155.00Å 39.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.50 – 2.85	Depositor
% Data completeness (in resolution range)	88.0 (39.50-2.85)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3055	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.68	0/1267	0.73	1/1720 (0.1%)
2	B	0.59	0/1312	0.76	1/1773 (0.1%)
All	All	0.63	0/2579	0.74	2/3493 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	160	LEU	CA-CB-CG	6.18	129.50	115.30
1	A	115	LEU	CA-CB-CG	5.58	128.13	115.30

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	1239	0	1199	13	0
2	B	1295	0	1288	17	0
3	A	43	0	31	3	0
4	B	86	0	74	12	0
5	A	195	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	197	0	0	9	0
All	All	3055	0	2592	40	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 8.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1163:BLA:HMA1	3:A:1163:BLA:HB	1.36	0.89
4:B:1173:CYC:HC	4:B:1173:CYC:HMD2	1.39	0.88
4:B:1174:CYC:HC	4:B:1174:CYC:HMD2	1.51	0.76
4:B:1173:CYC:HC	4:B:1173:CYC:CMD	1.98	0.76
4:B:1174:CYC:HMA1	4:B:1174:CYC:HMB3	1.72	0.72
3:A:1163:BLA:HC	3:A:1163:BLA:HMD2	1.62	0.64
3:A:1163:BLA:HMA1	3:A:1163:BLA:NB	2.11	0.64
2:B:172:ALA:HB1	5:B:2190:HOH:O	1.97	0.64
1:A:49:LYS:HB2	5:A:2117:HOH:O	2.01	0.61
2:B:149:THR:O	4:B:1174:CYC:HMD2	2.03	0.59
2:B:67:PHE:HD2	2:B:79:GLN:HE22	1.51	0.58
2:B:35:ASN:HB2	5:B:2197:HOH:O	2.05	0.57
4:B:1174:CYC:CMD	4:B:1174:CYC:HC	2.16	0.55
1:A:90:HIS:HE1	5:A:2151:HOH:O	1.89	0.54
2:B:63:ARG:HG2	5:B:2128:HOH:O	2.07	0.53
2:B:78:ASN:ND2	4:B:1173:CYC:HAD1	2.25	0.52
2:B:148:ILE:HG21	4:B:1174:CYC:HMC3	1.92	0.50
2:B:28:GLN:HG2	5:B:2077:HOH:O	2.12	0.49
2:B:73:CYS:HB2	4:B:1173:CYC:OC	2.13	0.49
1:A:61:GLN:HB3	5:A:2139:HOH:O	2.13	0.49
1:A:108:ASP:HB3	5:A:2155:HOH:O	2.13	0.48
4:B:1173:CYC:NC	4:B:1173:CYC:CMD	2.74	0.48
2:B:15:LYS:HD2	5:B:2071:HOH:O	2.13	0.47
2:B:52:VAL:HG11	2:B:87:GLY:HA2	1.96	0.47
1:A:64:PRO:HG2	5:A:2084:HOH:O	2.15	0.46
2:B:4:ALA:HA	5:B:2138:HOH:O	2.16	0.46
1:A:114:GLY:HA2	5:A:2159:HOH:O	2.15	0.46
2:B:54:ASN:HB3	5:B:2112:HOH:O	2.16	0.46
2:B:75:HIS:O	2:B:79:GLN:HG2	2.16	0.46
1:A:4:PRO:HG2	1:A:30:ARG:HG3	1.98	0.45
1:A:15:ARG:NH1	1:A:23:GLU:OE1	2.47	0.45
2:B:82:CYS:HA	4:B:1173:CYC:HAC1	1.88	0.44
2:B:36:LYS:O	2:B:40:VAL:HG23	2.17	0.43
1:A:116:LYS:HD2	5:A:2163:HOH:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ALA:HB1	1:A:132:ALA:HB1	2.01	0.43
2:B:14:LYS:HE3	5:B:2042:HOH:O	2.19	0.41
1:A:46:ASN:HB3	5:A:2114:HOH:O	2.21	0.41
4:B:1173:CYC:HBA1	5:B:2194:HOH:O	2.20	0.41
1:A:65:TYR:HE2	1:A:128:TRP:HE1	1.69	0.40
1:A:157:ALA:O	1:A:161:LEU:HD13	2.22	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%)	155 (97%)	3 (2%)	2 (1%)	18	51
2	B	170/172 (99%)	162 (95%)	5 (3%)	3 (2%)	13	41
All	All	330/334 (99%)	317 (96%)	8 (2%)	5 (2%)	15	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	A	144	GLY
2	B	123	PRO
2	B	75	HIS
2	B	111	ASN

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	123/123 (100%)	116 (94%)	7 (6%)	29	64
2	B	135/135 (100%)	126 (93%)	9 (7%)	23	54
All	All	258/258 (100%)	242 (94%)	16 (6%)	26	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	30	ARG
1	A	67	THR
1	A	70	GLN
1	A	115	LEU
1	A	140	HIS
1	A	145	ASP
2	B	2	LEU
2	B	7	ARG
2	B	37	ARG
2	B	65	GLN
2	B	68	ASN
2	B	86	LEU
2	B	108	ARG
2	B	110	LEU
2	B	132	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	57	ASN
1	A	119	ASN
1	A	155	ASN
2	B	54	ASN
2	B	68	ASN
2	B	78	ASN
2	B	79	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	BLA	A	1163	1	46,46,46	3.00	14 (30%)	65,67,67	2.00	16 (24%)
4	CYC	B	1173	2	46,46,46	2.71	9 (19%)	65,67,67	2.46	18 (27%)
4	CYC	B	1174	2	46,46,46	2.56	8 (17%)	65,67,67	2.55	17 (26%)

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	BLA	A	1163	1	-	3/26/74/74	0/4/4/4
4	CYC	B	1173	2	-	3/25/74/74	0/4/4/4
4	CYC	B	1174	2	-	3/25/74/74	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1173	CYC	CHA-C1A	13.35	1.44	1.35
4	B	1174	CYC	CHA-C1A	12.19	1.43	1.35
3	A	1163	BLA	CHA-C4D	11.23	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1173	CYC	CHD-C4C	6.86	1.54	1.36
4	B	1174	CYC	CHD-C4C	6.71	1.53	1.36
3	A	1163	BLA	CHD-C4C	6.68	1.54	1.37
3	A	1163	BLA	C4C-NC	6.65	1.49	1.37
3	A	1163	BLA	CBB-CAB	5.28	1.56	1.29
3	A	1163	BLA	CBC-CAC	5.15	1.55	1.29
3	A	1163	BLA	CHD-C1D	4.98	1.52	1.40
3	A	1163	BLA	C1A-NA	4.80	1.41	1.36
4	B	1173	CYC	C1C-NC	-4.09	1.32	1.37
3	A	1163	BLA	C3C-C2C	3.84	1.44	1.36
4	B	1174	CYC	C4C-NC	3.47	1.46	1.37
4	B	1173	CYC	C4C-NC	3.46	1.45	1.37
4	B	1174	CYC	C2C-C3C	-3.38	1.44	1.54
3	A	1163	BLA	C3D-C2D	3.37	1.43	1.36
4	B	1174	CYC	C3C-C4C	-3.31	1.47	1.51
4	B	1173	CYC	C2C-C3C	-3.25	1.44	1.54
3	A	1163	BLA	C4B-NB	-3.03	1.31	1.37
4	B	1174	CYC	C1C-NC	-3.01	1.33	1.37
4	B	1174	CYC	CMD-C2D	-2.98	1.45	1.51
4	B	1173	CYC	C4D-ND	2.82	1.39	1.36
4	B	1173	CYC	C3C-C4C	-2.74	1.48	1.51
3	A	1163	BLA	C4A-NA	2.48	1.39	1.36
4	B	1173	CYC	C4B-NB	-2.43	1.32	1.37
4	B	1173	CYC	C2A-C3A	2.26	1.41	1.36
3	A	1163	BLA	C1B-C2B	-2.25	1.40	1.45
4	B	1174	CYC	C4B-NB	-2.22	1.32	1.37
3	A	1163	BLA	O1D-CGD	2.14	1.29	1.22
3	A	1163	BLA	CBD-CAD	2.05	1.58	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1174	CYC	C2C-C1C-NC	11.25	114.77	108.19
4	B	1173	CYC	C2C-C1C-NC	11.16	114.72	108.19
4	B	1174	CYC	C1C-NC-C4C	-6.60	102.90	112.96
3	A	1163	BLA	CHD-C4C-NC	-6.42	112.26	126.19
4	B	1173	CYC	CAB-C3B-C4B	6.23	126.68	121.49
4	B	1174	CYC	C3C-C4C-NC	5.96	113.58	107.83
4	B	1174	CYC	CAB-C3B-C4B	5.93	126.42	121.49
4	B	1173	CYC	C1C-NC-C4C	-5.88	104.00	112.96
4	B	1174	CYC	C3B-C4B-NB	5.50	111.60	106.69
3	A	1163	BLA	C3B-C4B-NB	5.29	111.44	106.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1173	CYC	C3B-C4B-NB	5.00	111.15	106.69
4	B	1173	CYC	C3C-C4C-NC	4.89	112.54	107.83
3	A	1163	BLA	C1A-CHA-C4D	-4.83	120.51	129.92
4	B	1174	CYC	C4B-C3B-C2B	-4.44	105.36	108.04
3	A	1163	BLA	CHD-C4C-C3C	-4.36	112.92	127.48
4	B	1173	CYC	C4B-C3B-C2B	-4.35	105.41	108.04
4	B	1174	CYC	OC-C1C-C2C	-4.05	122.90	126.25
4	B	1174	CYC	C1B-NB-C4B	-3.82	105.34	110.74
3	A	1163	BLA	CMD-C2D-C1D	3.71	131.16	125.02
3	A	1163	BLA	C1B-NB-C4B	-3.71	105.50	110.74
3	A	1163	BLA	C4C-CHD-C1D	-3.63	119.08	128.13
4	B	1174	CYC	OB-C4B-C3B	-3.55	124.20	128.20
3	A	1163	BLA	CBB-CAB-C3B	-3.49	109.73	127.09
4	B	1173	CYC	C1B-NB-C4B	-3.49	105.81	110.74
3	A	1163	BLA	C2B-C1B-NB	3.09	112.03	107.14
4	B	1173	CYC	OB-C4B-C3B	-3.09	124.72	128.20
3	A	1163	BLA	CBC-CAC-C3C	-3.00	112.16	127.09
4	B	1173	CYC	OC-C1C-C2C	-2.99	123.78	126.25
4	B	1174	CYC	C2B-C1B-NB	2.83	111.61	107.14
3	A	1163	BLA	CHD-C1D-C2D	2.77	132.01	125.10
3	A	1163	BLA	CAD-C3D-C4D	2.76	129.95	124.85
4	B	1174	CYC	CAD-C3D-C4D	2.75	130.62	124.73
3	A	1163	BLA	CHD-C1D-ND	-2.73	119.78	124.99
4	B	1173	CYC	C2B-C1B-NB	2.71	111.42	107.14
4	B	1173	CYC	C1B-CHB-C4A	-2.68	121.45	128.13
4	B	1173	CYC	OC-C1C-NC	-2.67	121.50	124.80
4	B	1173	CYC	CAD-C3D-C4D	2.60	130.30	124.73
4	B	1173	CYC	CBC-CAC-C3C	-2.57	107.28	113.61
4	B	1174	CYC	CAC-C3C-C4C	-2.57	106.08	112.67
4	B	1174	CYC	CMB-C2B-C1B	2.42	127.53	124.23
3	A	1163	BLA	CAD-C3D-C2D	-2.39	123.72	128.00
4	B	1173	CYC	C2C-C3C-C4C	2.37	104.43	101.08
4	B	1174	CYC	CBC-CAC-C3C	-2.32	107.91	113.61
4	B	1173	CYC	CMB-C2B-C1B	2.26	127.31	124.23
4	B	1174	CYC	CAD-C3D-C2D	-2.25	122.58	129.00
4	B	1174	CYC	C2C-C3C-C4C	2.16	104.13	101.08
4	B	1173	CYC	C4D-CHA-C1A	-2.16	125.72	129.92
3	A	1163	BLA	C4B-C3B-C2B	-2.15	105.21	107.97
4	B	1173	CYC	CAD-C3D-C2D	-2.12	122.94	129.00
3	A	1163	BLA	CHA-C4D-ND	-2.10	124.72	128.59
4	B	1174	CYC	C3C-C4C-CHD	-2.08	121.23	127.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1173	CYC	C4C-CHD-C1D-ND
4	B	1174	CYC	C4C-CHD-C1D-ND
3	A	1163	BLA	C4C-CHD-C1D-ND
3	A	1163	BLA	C4C-CHD-C1D-C2D
3	A	1163	BLA	C1B-CHB-C4A-NA
4	B	1173	CYC	C1B-CHB-C4A-C3A
4	B	1173	CYC	C1B-CHB-C4A-NA
4	B	1174	CYC	C1B-CHB-C4A-NA
4	B	1174	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.