



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:12 PM GMT

PDB ID : 3O2C  
Title : Crystal structure of a rod form of c-phycocyanin from *Themosynechococcus vulcanus* at 1.5 angstroms  
Authors : David, L.; Marx, A.; Adir, N.  
Deposited on : 2010-07-22  
Resolution : 1.50 Å(reported)

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

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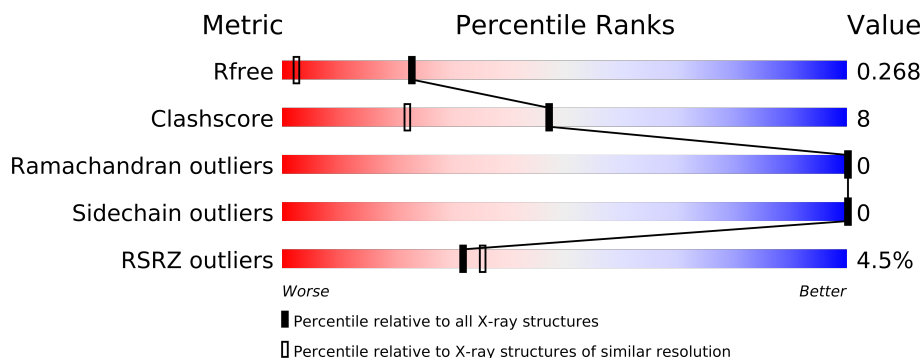
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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  $\geq 3$ , 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 3093 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.

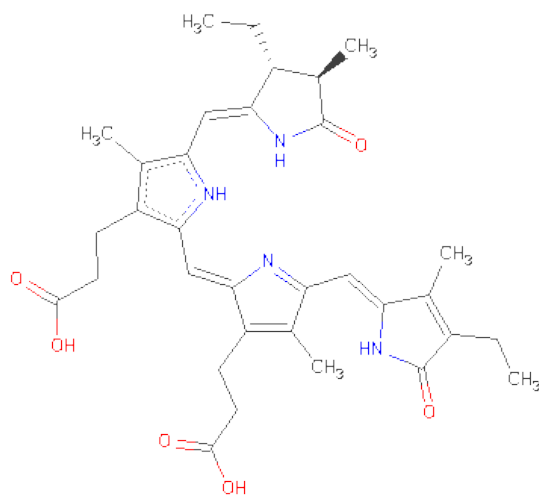
- Molecule 1 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1226	772	205	242	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	1	0
			1279	792	229	250	8			

- 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		

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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	245	Total	O	0	0
			245	245		
4	B	214	Total	O	0	0
			214	214		

### 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.

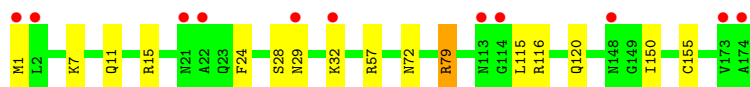
- Molecule 1: C-phycocyanin alpha subunit

Chain A: 



- Molecule 2: C-phycocyanin beta subunit

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.47Å 187.47Å 60.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.00 – 1.50 26.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.00-1.50) 98.0 (26.00-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.02	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.46 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.239 , 0.263 0.241 , 0.268	Depositor DCC
$R_{free}$ test set	3194 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 63026 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.77	2/1248 (0.2%)	0.60	0/1692
2	B	0.71	0/1286	0.66	2/1740 (0.1%)
All	All	0.74	2/2534 (0.1%)	0.63	2/3432 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	TYR	CE2-CZ	-5.58	1.31	1.38
1	A	32	LYS	CE-NZ	-5.51	1.35	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	ARG	NE-CZ-NH2	8.71	124.65	120.30
2	B	79	ARG	NE-CZ-NH1	-8.58	116.01	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	1226	0	1204	20	0
2	B	1279	0	1282	16	0
3	A	43	0	37	4	0
3	B	86	0	76	11	0
4	A	245	0	0	2	0
4	B	214	0	0	2	0
All	All	3093	0	2599	41	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 (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:155:CYS:SG	3:B:555:CYC:HAC1	1.27	1.68
1:A:65:TYR:HD2	1:A:69:MET:SD	1.95	0.89
2:B:79:ARG:NH2	3:B:584:CYC:O2D	2.11	0.83
2:B:155:CYS:SG	3:B:555:CYC:HAC2	2.18	0.82
1:A:65:TYR:CD2	1:A:69:MET:SD	2.73	0.81
3:B:555:CYC:O2D	3:B:555:CYC:HHA	1.82	0.78
1:A:38:MET:O	1:A:42:ARG:HG3	1.95	0.67
3:B:584:CYC:HC	3:B:584:CYC:HMD2	1.59	0.67
2:B:72:MEN:HE22	3:B:584:CYC:HBD2	1.76	0.66
1:A:33:ARG:HH12	1:A:147:GLN:HE21	1.42	0.66
1:A:10:ALA:O	1:A:14:THR:HG23	1.96	0.65
3:A:484:CYC:HMD2	3:A:484:CYC:HC	1.65	0.62
1:A:21:ASN:HB2	4:A:359:HOH:O	2.01	0.61
2:B:7:LYS:O	2:B:11:GLN:HG3	2.04	0.57
2:B:115:LEU:HD13	3:B:584:CYC:HMB3	1.86	0.56
1:A:73:GLN:NE2	1:A:74:TYR:CE2	2.74	0.55
2:B:116:ARG:O	2:B:120:GLN:HG3	2.09	0.53
3:A:484:CYC:NB	3:A:484:CYC:HMA1	2.25	0.52
1:A:73:GLN:HA	3:A:484:CYC:HBD2	1.92	0.51
2:B:29:ASN:HA	2:B:32:LYS:HE2	1.93	0.51
1:A:42:ARG:NH1	2:B:24:PHE:HB3	2.27	0.49
3:B:555:CYC:O2D	3:B:555:CYC:CHA	2.59	0.47
2:B:57:ARG:HD2	4:B:213:HOH:O	2.14	0.47
2:B:150:ILE:HG21	3:B:555:CYC:HMC3	1.96	0.47
1:A:28:ASP:OD2	1:A:32:LYS:HE2	2.15	0.47
2:B:72:MEN:CE2	3:B:584:CYC:HBD2	2.43	0.47
2:B:28:SER:O	2:B:32:LYS:HG3	2.15	0.47
1:A:33:ARG:HH12	1:A:147:GLN:NE2	2.12	0.46
1:A:65:TYR:HB2	1:A:69:MET:SD	2.56	0.46
2:B:1:MET:HB3	4:B:412:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:484:CYC:HB	3:A:484:CYC:HMA1	1.83	0.43
1:A:33:ARG:NH1	1:A:147:GLN:HE21	2.14	0.42
2:B:155:CYS:SG	3:B:555:CYC:C3C	2.99	0.42
1:A:57:GLN:O	1:A:61:GLN:HG3	2.19	0.42
1:A:11:ALA:O	1:A:15:GLN:HG3	2.20	0.42
1:A:77:THR:O	1:A:78:PRO:C	2.58	0.41
1:A:15:GLN:HB2	1:A:17:ARG:HG2	2.02	0.41
1:A:171:ASN:ND2	4:A:441:HOH:O	2.53	0.41
1:A:30:ARG:O	1:A:30:ARG:HD2	2.21	0.41
1:A:77:THR:O	1:A:80:GLY:N	2.54	0.41
2:B:15:ARG:HE	2:B:15:ARG:HB2	1.46	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	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
All	All	330/334 (99%)	324 (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	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	128/127 (101%)	128 (100%)	0	100	100
All	All	251/250 (100%)	251 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	ASN
1	A	57	GLN
1	A	147	GLN
1	A	171	ASN
2	B	35	ASN
2	B	54	ASN
2	B	78	ASN
2	B	145	ASN

### 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	6.24	6 (75%)	7,9,11	10.44	4 (57%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	O-C	13.42	1.20	1.11
2	B	72	MEN	OD1-CG	8.97	1.43	1.23
2	B	72	MEN	CG-ND2	4.93	1.60	1.34
2	B	72	MEN	CE2-ND2	3.85	1.52	1.45
2	B	72	MEN	CB-CA	2.35	1.59	1.53
2	B	72	MEN	CA-C	2.32	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	MEN	OD1-CG-CB	-25.17	85.27	121.24
2	B	72	MEN	CB-CG-ND2	10.31	131.66	115.87
2	B	72	MEN	OD1-CG-ND2	3.51	143.02	122.26
2	B	72	MEN	CE2-ND2-CG	-2.63	98.99	121.79

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	484	1	46,46,46	2.06	14 (30%)	65,67,67	3.72	25 (38%)
3	CYC	B	555	2	46,46,46	3.14	15 (32%)	65,67,67	4.27	29 (44%)
3	CYC	B	584	2	46,46,46	2.23	15 (32%)	65,67,67	3.86	26 (40%)

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	484	1	-	3/25/74/74	0/4/4/4
3	CYC	B	555	2	-	3/25/74/74	0/4/4/4
3	CYC	B	584	2	-	3/25/74/74	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	555	CYC	CBD-CGD	-9.95	1.25	1.50
3	B	555	CYC	O1D-CGD	-9.73	0.87	1.22
3	B	555	CYC	O2D-CGD	8.14	1.60	1.30
3	A	484	CYC	OB-C4B	6.96	1.37	1.23
3	B	584	CYC	OB-C4B	6.87	1.37	1.23
3	B	555	CYC	OB-C4B	6.54	1.36	1.23
3	B	555	CYC	C1C-NC	-5.17	1.30	1.37
3	B	555	CYC	OC-C1C	4.76	1.32	1.23
3	B	584	CYC	C1C-NC	-4.71	1.31	1.37
3	B	584	CYC	OC-C1C	4.70	1.32	1.23
3	A	484	CYC	C1C-NC	-4.58	1.31	1.37
3	A	484	CYC	OC-C1C	4.53	1.32	1.23
3	B	584	CYC	C1D-ND	4.05	1.40	1.36
3	B	584	CYC	C2A-C3A	3.89	1.45	1.36
3	B	584	CYC	CHB-C4A	3.86	1.49	1.40
3	B	555	CYC	C1D-ND	3.43	1.40	1.36
3	A	484	CYC	C3D-C2D	3.39	1.47	1.37
3	B	584	CYC	C3D-C2D	3.38	1.47	1.37
3	B	555	CYC	CHB-C4A	3.37	1.48	1.40
3	B	555	CYC	C2A-C3A	3.34	1.43	1.36
3	A	484	CYC	C2A-C3A	3.32	1.43	1.36
3	A	484	CYC	CHB-C4A	3.27	1.48	1.40
3	B	584	CYC	CHA-C1A	3.26	1.37	1.35
3	B	555	CYC	C3D-C2D	3.23	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	484	CYC	C1D-ND	3.17	1.39	1.36
3	B	584	CYC	C4D-ND	2.67	1.39	1.36
3	B	555	CYC	C4D-ND	2.62	1.39	1.36
3	B	584	CYC	C3B-C2B	2.61	1.42	1.36
3	B	584	CYC	CMB-C2B	-2.61	1.45	1.51
3	B	584	CYC	C1B-NB	-2.53	1.33	1.37
3	B	555	CYC	C3B-C2B	2.47	1.41	1.36
3	B	555	CYC	C4B-C3B	-2.47	1.42	1.48
3	A	484	CYC	C3C-C4C	2.45	1.53	1.51
3	A	484	CYC	C2C-C1C	2.39	1.54	1.52
3	B	555	CYC	CMB-C2B	-2.33	1.46	1.51
3	A	484	CYC	C2C-C3C	-2.27	1.47	1.54
3	B	584	CYC	C4B-C3B	-2.26	1.43	1.48
3	A	484	CYC	CMB-C2B	-2.24	1.46	1.51
3	A	484	CYC	C3B-C2B	2.15	1.41	1.36
3	B	584	CYC	CBA-CAA	-2.12	1.45	1.52
3	B	584	CYC	C4B-NB	-2.10	1.33	1.37
3	B	555	CYC	C1B-NB	-2.09	1.34	1.37
3	A	484	CYC	C4B-C3B	-2.07	1.43	1.48
3	A	484	CYC	C4B-NB	-2.05	1.33	1.37

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	555	CYC	O2D-CGD-O1D	-14.42	86.62	123.30
3	B	584	CYC	C4B-C3B-C2B	-13.85	99.66	108.04
3	B	555	CYC	C4B-C3B-C2B	-13.42	99.92	108.04
3	A	484	CYC	C4B-C3B-C2B	-13.36	99.96	108.04
3	B	584	CYC	C2C-C1C-NC	12.96	115.77	108.19
3	B	555	CYC	C2C-C1C-NC	12.54	115.53	108.19
3	A	484	CYC	C2C-C1C-NC	11.66	115.01	108.19
3	B	555	CYC	C3B-C4B-NB	11.51	116.97	106.69
3	B	584	CYC	C3B-C4B-NB	11.42	116.89	106.69
3	A	484	CYC	C3B-C4B-NB	11.07	116.57	106.69
3	B	584	CYC	OC-C1C-C2C	-10.76	117.35	126.25
3	B	555	CYC	OC-C1C-C2C	-9.97	118.00	126.25
3	A	484	CYC	CAB-C3B-C4B	9.80	129.65	121.49
3	A	484	CYC	OC-C1C-C2C	-9.77	118.17	126.25
3	B	584	CYC	CAB-C3B-C4B	9.59	129.47	121.49
3	B	555	CYC	CAB-C3B-C4B	8.57	128.62	121.49
3	B	555	CYC	OB-C4B-C3B	-8.00	119.18	128.20
3	B	584	CYC	OB-C4B-C3B	-7.68	119.55	128.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	484	CYC	OB-C4B-C3B	-7.42	119.84	128.20
3	B	555	CYC	CBC-CAC-C3C	5.32	126.69	113.61
3	A	484	CYC	C3C-C2C-C1C	-5.31	98.86	103.43
3	B	555	CYC	O2D-CGD-CBD	-5.11	96.15	114.22
3	B	555	CYC	C3C-C4C-NC	5.02	112.67	107.83
3	B	555	CYC	C1B-NB-C4B	-4.55	104.31	110.74
3	A	484	CYC	C1B-NB-C4B	-4.52	104.36	110.74
3	A	484	CYC	C1C-NC-C4C	-4.32	106.38	112.96
3	B	584	CYC	C3C-C4C-NC	4.20	111.88	107.83
3	B	584	CYC	C1B-NB-C4B	-4.09	104.96	110.74
3	B	555	CYC	C1C-NC-C4C	-3.85	107.09	112.96
3	B	584	CYC	C1C-NC-C4C	-3.77	107.21	112.96
3	B	555	CYC	O1D-CGD-CBD	3.76	135.98	123.03
3	B	584	CYC	C1D-CHD-C4C	3.51	133.39	128.81
3	B	584	CYC	O2D-CGD-O1D	-3.19	115.18	123.30
3	A	484	CYC	CAA-CBA-CGA	-3.18	107.62	113.53
3	A	484	CYC	C1A-C2A-C3A	-3.18	103.17	106.86
3	B	555	CYC	C1A-C2A-C3A	-3.14	103.21	106.86
3	B	584	CYC	C1A-C2A-C3A	-3.08	103.28	106.86
3	B	555	CYC	C3C-C2C-C1C	-3.01	100.84	103.43
3	A	484	CYC	O2D-CGD-O1D	-2.87	116.00	123.30
3	A	484	CYC	CAC-C3C-C2C	2.83	120.39	113.89
3	B	584	CYC	CBD-CAD-C3D	2.83	117.67	112.69
3	B	555	CYC	C1D-CHD-C4C	2.82	132.49	128.81
3	B	584	CYC	O1A-CGA-CBA	-2.82	113.34	123.03
3	B	555	CYC	CHB-C4A-C3A	2.79	132.05	125.10
3	B	584	CYC	C3C-C2C-C1C	-2.71	101.09	103.43
3	A	484	CYC	C2D-C1D-CHD	2.69	133.36	125.72
3	A	484	CYC	C3C-C4C-NC	2.68	110.42	107.83
3	B	555	CYC	C4D-C3D-C2D	-2.65	104.17	106.92
3	B	584	CYC	C1A-NA-C4A	2.65	111.70	106.55
3	B	555	CYC	CAD-CBD-CGD	-2.63	105.03	113.47
3	A	484	CYC	O1A-CGA-CBA	-2.62	114.01	123.03
3	A	484	CYC	O2D-CGD-CBD	2.58	123.35	114.22
3	B	584	CYC	CAA-CBA-CGA	-2.57	108.77	113.53
3	B	584	CYC	O2D-CGD-CBD	2.55	123.24	114.22
3	B	584	CYC	CHB-C4A-C3A	2.49	131.31	125.10
3	B	555	CYC	CHD-C4C-NC	-2.46	122.01	126.09
3	B	555	CYC	C1A-NA-C4A	2.46	111.33	106.55
3	B	584	CYC	CHD-C4C-NC	-2.39	122.13	126.09
3	B	584	CYC	C2D-C1D-CHD	2.38	132.47	125.72
3	A	484	CYC	C1A-NA-C4A	2.38	111.17	106.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	584	CYC	O2A-CGA-CBA	2.37	122.60	114.22
3	A	484	CYC	CHB-C4A-C3A	2.36	130.99	125.10
3	B	555	CYC	O1A-CGA-CBA	-2.31	115.09	123.03
3	B	584	CYC	C4D-C3D-C2D	-2.25	104.59	106.92
3	A	484	CYC	C3D-C4D-ND	2.25	110.50	106.79
3	B	555	CYC	CAA-CBA-CGA	-2.25	109.36	113.53
3	B	555	CYC	C2B-C1B-NB	2.25	110.69	107.14
3	A	484	CYC	C1D-CHD-C4C	2.25	131.74	128.81
3	B	555	CYC	C3D-C4D-ND	2.25	110.50	106.79
3	A	484	CYC	CHD-C4C-NC	-2.23	122.39	126.09
3	A	484	CYC	C4D-C3D-C2D	-2.20	104.64	106.92
3	B	584	CYC	C4A-C3A-C2A	2.20	109.37	106.64
3	B	555	CYC	CAB-C3B-C2B	2.18	131.45	127.50
3	A	484	CYC	C2B-C1B-NB	2.18	110.58	107.14
3	B	555	CYC	CBD-CAD-C3D	-2.15	108.91	112.69
3	B	555	CYC	C3D-C4D-CHA	-2.11	119.75	125.72
3	B	584	CYC	C2C-C3C-C4C	2.09	104.03	101.08
3	B	584	CYC	C2B-C1B-NB	2.05	110.38	107.14
3	B	555	CYC	C4A-C3A-C2A	2.01	109.14	106.64
3	A	484	CYC	C4A-C3A-C2A	2.01	109.13	106.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	584	CYC	C4C-CHD-C1D-ND
3	A	484	CYC	C4C-CHD-C1D-ND
3	A	484	CYC	C1B-CHB-C4A-NA
3	A	484	CYC	C1B-CHB-C4A-C3A
3	B	555	CYC	C4C-CHD-C1D-ND
3	B	555	CYC	C1B-CHB-C4A-C3A
3	B	555	CYC	C1B-CHB-C4A-NA
3	B	584	CYC	C1B-CHB-C4A-C3A
3	B	584	CYC	C1B-CHB-C4A-NA

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	162/162 (100%)	0.30	4 (2%) 54 61	10, 15, 24, 33	0
2	B	172/172 (100%)	0.57	11 (6%) 19 20	12, 20, 32, 44	0
All	All	334/334 (100%)	0.44	15 (4%) 32 35	10, 17, 30, 44	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	ALA	4.3
2	B	114	GLY	3.3
2	B	21	ASN	3.1
1	A	77	THR	3.0
2	B	113[A]	ASN	3.0
2	B	32	LYS	2.7
1	A	69	MET	2.6
2	B	148	ASN	2.5
1	A	70	GLN	2.3
2	B	173	VAL	2.2
2	B	1	MET	2.2
2	B	29	ASN	2.2
2	B	2	LEU	2.1
1	A	15	GLN	2.1
2	B	22	ALA	2.0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MEN	B	72	9/10	0.12	0.88	19,19,31,31	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CYC	B	584	43/43	0.17	1.77	13,25,33,35	0
3	CYC	B	555	43/43	0.18	1.74	16,20,36,44	0
3	CYC	A	484	43/43	0.11	0.16	8,12,16,17	0

### 6.5 Other polymers

There are no such residues in this entry.