



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2017 – 08:53 PM EST

PDB ID : 5MJP
Title : Multi-bunch pink beam serial crystallography: Phycocyanin (One chip)
Authors : Meents, A.; Oberthuer, D.; Lieske, J.; Srajer, V.; Sarrou, I.
Deposited on : unknown
Resolution : 2.11 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

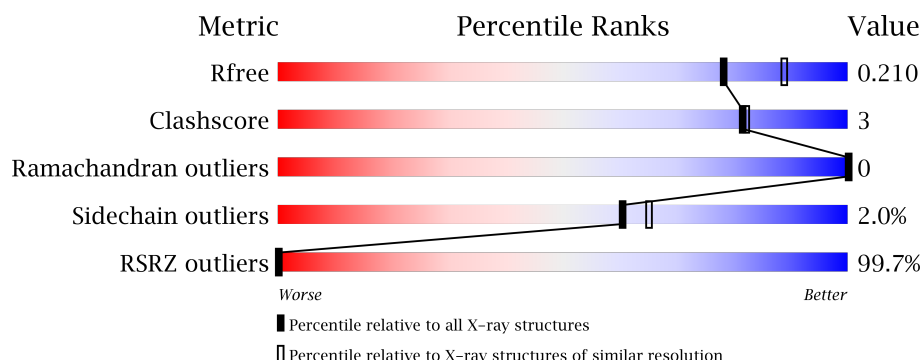
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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. 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	162	<div> <div>100%</div> <div> <div></div> <div>94%</div> <div>6%</div> <div>.</div> </div> <div>99%</div> </div>
2	B	172	<div> <div></div> <div>95%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

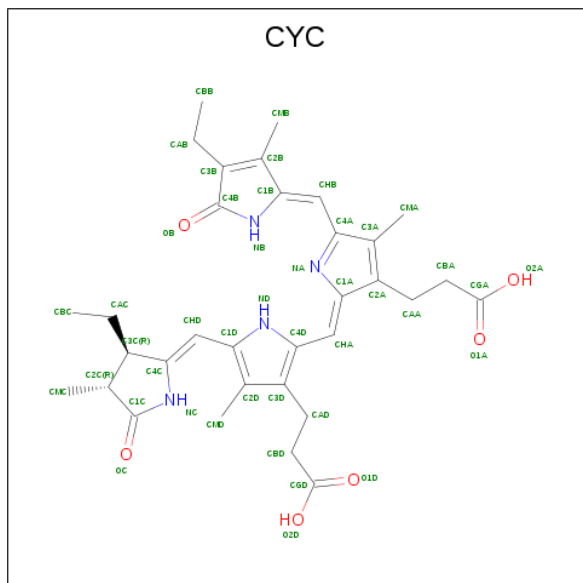
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYC	A	501	-	-	-	X
3	CYC	B	201	-	-	-	X
3	CYC	B	202	-	-	-	X

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 2 is a protein called C-phycocyanin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	172	Total	C	H	N	O	S	0	2	0
			2559	794	1277	229	251	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 80	C 33	H 37	N 4	O 6	0	0
3	B	1	Total 80	C 33	H 37	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

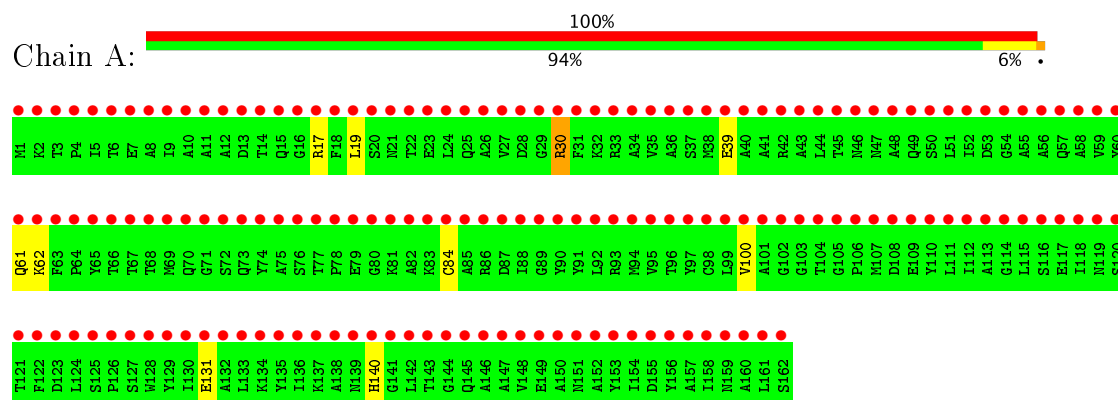
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	89	Total	O	0	0
			89	89		

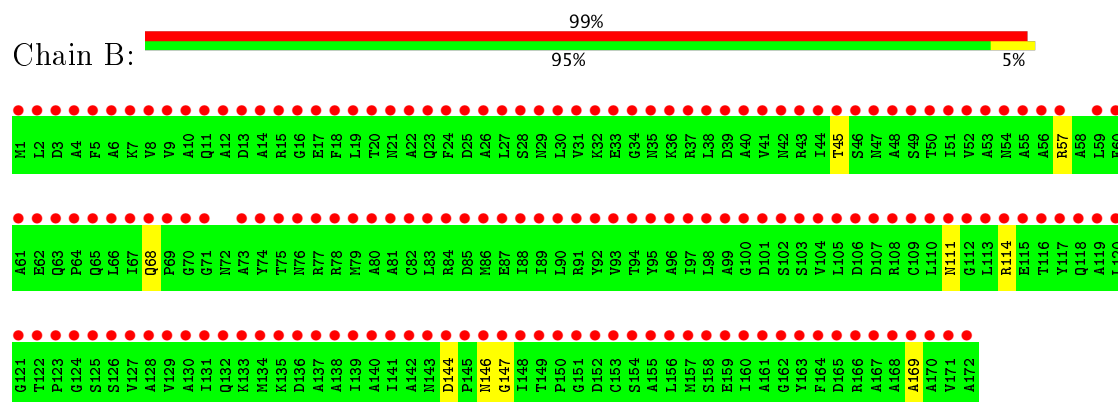
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: C-phycocyanin alpha chain



• Molecule 2: C-phycocyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	187.80Å 187.80Å 60.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.90 – 2.11 36.21 – 2.11	Depositor EDS
% Data completeness (in resolution range)	65.3 (14.90-2.11) 65.4 (36.21-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.98 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.169 , 0.200 0.170 , 0.210	Depositor DCC
R_{free} test set	1519 reflections (9.90%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.35	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 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	0.28	0/1270	0.41	0/1721
2	B	0.26	0/1292	0.40	0/1748
All	All	0.27	0/2562	0.41	0/3469

There are no bond length outliers.

There are no bond angle outliers.

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	1236	1216	1206	7	0
2	B	1282	1277	1282	6	0
3	A	43	37	37	3	0
3	B	86	74	73	2	0
4	A	91	0	0	3	2
4	B	89	0	0	4	1
All	All	2827	2604	2598	16	2

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 3.

All (16) 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:61:GLN:NE2	4:A:601:HOH:O	2.06	0.87
2:B:68[B]:GLN:OE1	4:B:601:HOH:O	2.05	0.74
1:A:39:GLU:OE1	4:A:602:HOH:O	2.12	0.67
2:B:144:ASP:OD1	4:B:602:HOH:O	2.14	0.66
1:A:131:GLU:OE1	4:A:603:HOH:O	2.18	0.56
3:A:501:CYC:HBC2	3:A:501:CYC:HMC1	1.89	0.55
1:A:84:CYS:HA	3:A:501:CYC:HHD	1.88	0.54
3:B:202:CYC:NC	3:B:202:CYC:HMD2	2.24	0.53
3:A:501:CYC:NB	3:A:501:CYC:HMA1	2.24	0.52
2:B:57:ARG:NH1	4:B:610:HOH:O	2.46	0.48
2:B:114:ARG:NH2	2:B:169:ALA:O	2.47	0.48
1:A:30:ARG:NH2	1:A:100:VAL:O	2.50	0.44
3:B:201:CYC:NB	3:B:201:CYC:HMA1	2.32	0.44
1:A:19:LEU:O	2:B:45:THR:HG21	2.18	0.43
1:A:17[B]:ARG:HB3	1:A:17[B]:ARG:CZ	2.49	0.42
2:B:147:GLY:O	4:B:603:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:677:HOH:O	4:A:677:HOH:O[6_556]	1.77	0.43
4:A:647:HOH:O	4:B:672:HOH:O[5_556]	2.04	0.16

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	162/162 (100%)	160 (99%)	2 (1%)	0	100	100
2	B	171/172 (99%)	169 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	333/334 (100%)	329 (99%)	4 (1%)	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	125/123 (102%)	122 (98%)	3 (2%)	54	58
2	B	129/127 (102%)	127 (98%)	2 (2%)	68	73
All	All	254/250 (102%)	249 (98%)	5 (2%)	60	65

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	62	LYS
1	A	140	HIS
2	B	111	ASN
2	B	146	ASN

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

5.3.3 RNA ⓘ

There are no RNA molecules 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	1.12	1 (12%)	8,9,11	1.02	1 (12%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	CA-C	2.13	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	MEN	CB-CA-C	-2.24	107.10	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	501	1	38,46,46	3.64	18 (47%)	46,67,67	1.81	10 (21%)
3	CYC	B	201	2	38,46,46	3.68	18 (47%)	46,67,67	1.80	12 (26%)
3	CYC	B	202	2	38,46,46	3.62	19 (50%)	46,67,67	1.66	10 (21%)

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	501	1	-	3/21/74/74	0/4/4/4
3	CYC	B	201	2	-	3/21/74/74	0/4/4/4
3	CYC	B	202	2	-	3/21/74/74	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CYC	CHA-C1A	-4.64	1.31	1.35
3	B	201	CYC	C2C-C1C	-4.40	1.47	1.52
3	A	501	CYC	C2C-C1C	-4.24	1.48	1.52
3	B	202	CYC	CHA-C1A	-3.71	1.31	1.35
3	B	202	CYC	C2C-C1C	-3.51	1.48	1.52
3	B	201	CYC	CHA-C1A	-3.36	1.32	1.35
3	B	202	CYC	OB-C4B	-2.66	1.18	1.23
3	A	501	CYC	OB-C4B	-2.64	1.18	1.23
3	A	501	CYC	CHB-C1B	-2.62	1.31	1.37
3	A	501	CYC	OC-C1C	-2.61	1.18	1.23
3	B	202	CYC	CHB-C1B	-2.55	1.31	1.37
3	B	201	CYC	OC-C1C	-2.48	1.18	1.23
3	B	201	CYC	OB-C4B	-2.43	1.19	1.23
3	B	202	CYC	CHD-C4C	-2.24	1.32	1.38
3	B	202	CYC	OC-C1C	-2.23	1.19	1.23
3	B	201	CYC	CHB-C1B	-2.21	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CYC	C1B-C2B	2.40	1.49	1.45
3	B	202	CYC	C1B-C2B	2.49	1.49	1.45
3	A	501	CYC	C3B-C2B	2.51	1.42	1.36
3	A	501	CYC	C4D-CHA	2.55	1.52	1.45
3	B	201	CYC	C1B-C2B	2.62	1.49	1.45
3	B	202	CYC	C3B-C2B	2.65	1.42	1.36
3	B	202	CYC	C1D-CHD	2.65	1.53	1.45
3	B	201	CYC	C3B-C2B	2.70	1.42	1.36
3	B	201	CYC	C4D-CHA	2.80	1.53	1.45
3	B	202	CYC	C4D-CHA	2.83	1.53	1.45
3	A	501	CYC	C1D-CHD	2.92	1.53	1.45
3	B	201	CYC	C1D-CHD	2.94	1.54	1.45
3	A	501	CYC	C1A-C2A	4.16	1.52	1.45
3	B	201	CYC	C1A-C2A	4.45	1.53	1.45
3	B	202	CYC	C1A-C2A	4.58	1.53	1.45
3	A	501	CYC	C2A-C3A	4.69	1.46	1.36
3	B	202	CYC	C2A-C3A	4.80	1.47	1.36
3	B	201	CYC	C2A-C3A	4.84	1.47	1.36
3	B	202	CYC	CHB-C4A	5.17	1.52	1.40
3	B	202	CYC	C4A-NA	5.30	1.48	1.36
3	A	501	CYC	CHB-C4A	5.30	1.53	1.40
3	A	501	CYC	C4A-NA	5.33	1.48	1.36
3	B	201	CYC	C4A-NA	5.56	1.49	1.36
3	B	201	CYC	CHB-C4A	5.70	1.54	1.40
3	B	202	CYC	C1A-NA	5.76	1.51	1.38
3	A	501	CYC	C1A-NA	5.90	1.51	1.38
3	B	201	CYC	C1A-NA	6.13	1.52	1.38
3	B	201	CYC	C4C-NC	6.74	1.52	1.37
3	B	202	CYC	C4C-NC	6.76	1.52	1.37
3	A	501	CYC	C4C-NC	6.87	1.52	1.37
3	A	501	CYC	C4B-NB	7.38	1.53	1.37
3	B	202	CYC	C4B-NB	7.56	1.53	1.37
3	B	201	CYC	C4B-NB	7.64	1.54	1.37
3	A	501	CYC	C1B-NB	9.11	1.53	1.37
3	B	202	CYC	C1B-NB	9.18	1.53	1.37
3	B	201	CYC	C1B-NB	9.28	1.53	1.37
3	A	501	CYC	C1C-NC	9.31	1.49	1.37
3	B	201	CYC	C1C-NC	9.34	1.49	1.37
3	B	202	CYC	C1C-NC	9.48	1.49	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CYC	C3C-C4C-NC	-6.03	102.28	107.97
3	B	202	CYC	C2A-C1A-NA	-3.04	105.29	109.93
3	B	201	CYC	C2A-C1A-NA	-3.03	105.30	109.93
3	B	202	CYC	C1B-NB-C4B	-2.94	106.79	110.70
3	A	501	CYC	C1B-NB-C4B	-2.84	106.92	110.70
3	A	501	CYC	CBD-CAD-C3D	-2.72	107.28	112.48
3	A	501	CYC	C2A-C1A-NA	-2.54	106.05	109.93
3	A	501	CYC	C1B-CHB-C4A	-2.39	122.06	128.08
3	B	201	CYC	CMC-C2C-C1C	-2.37	107.45	112.43
3	B	201	CYC	C1B-NB-C4B	-2.34	107.59	110.70
3	B	201	CYC	C3C-C4C-NC	-2.14	105.94	107.97
3	B	202	CYC	C3C-C4C-NC	-2.13	105.96	107.97
3	B	201	CYC	C1B-CHB-C4A	-2.08	122.84	128.08
3	B	202	CYC	C1B-CHB-C4A	-2.05	122.90	128.08
3	B	201	CYC	OC-C1C-C2C	-2.03	124.61	126.25
3	B	201	CYC	CAC-C3C-C2C	-2.03	109.14	114.24
3	B	202	CYC	CAA-CBA-CGA	-2.02	109.22	112.66
3	B	202	CYC	C1B-C2B-C3B	2.50	110.57	107.83
3	A	501	CYC	C1A-C2A-C3A	2.52	109.63	106.81
3	A	501	CYC	C1B-C2B-C3B	2.55	110.61	107.83
3	B	201	CYC	C1A-C2A-C3A	2.61	109.73	106.81
3	B	202	CYC	C1A-C2A-C3A	2.74	109.88	106.81
3	A	501	CYC	CMA-C3A-C4A	2.84	129.47	125.04
3	B	201	CYC	C1B-C2B-C3B	3.10	111.23	107.83
3	B	202	CYC	C2C-C3C-C4C	3.68	106.86	101.34
3	B	202	CYC	CAB-C3B-C4B	3.81	124.74	121.53
3	A	501	CYC	CAB-C3B-C4B	3.91	124.82	121.53
3	B	201	CYC	CAB-C3B-C4B	3.91	124.82	121.53
3	B	201	CYC	C4B-C3B-C2B	3.94	110.28	108.01
3	A	501	CYC	C4B-C3B-C2B	4.07	110.35	108.01
3	B	202	CYC	C4B-C3B-C2B	4.11	110.37	108.01
3	B	201	CYC	C2C-C3C-C4C	4.52	108.12	101.34

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	CYC	C1B-CHB-C4A-C3A
3	B	201	CYC	C1B-CHB-C4A-C3A
3	A	501	CYC	C4C-CHD-C1D-ND
3	A	501	CYC	C1B-CHB-C4A-C3A
3	B	202	CYC	C1B-CHB-C4A-NA
3	B	201	CYC	C1B-CHB-C4A-NA

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Mol	Chain	Res	Type	Atoms
3	A	501	CYC	C1B-CHB-C4A-NA
3	B	202	CYC	C4C-CHD-C1D-ND
3	B	201	CYC	C4C-CHD-C1D-ND

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CYC	3	0
3	B	201	CYC	1	0
3	B	202	CYC	1	0

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	162/162 (100%)	9.32	162 (100%) 0 0	12, 19, 35, 53	0
2	B	171/172 (99%)	9.97	170 (99%) 0 0	13, 25, 42, 57	0
All	All	333/334 (99%)	9.66	332 (99%) 0 0	12, 22, 40, 57	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ALA	34.3
2	B	110	LEU	26.5
2	B	81	ALA	25.5
2	B	2	LEU	25.4
1	A	11	ALA	23.9
1	A	34	ALA	22.3
2	B	67	ILE	22.3
2	B	26	ALA	22.2
2	B	131	ILE	21.6
2	B	150	PRO	21.5
2	B	142	ALA	19.3
2	B	172	ALA	18.4
2	B	116	THR	18.3
1	A	89	GLY	18.2
2	B	125	SER	17.9
1	A	45	THR	17.7
2	B	29	ASN	17.6
1	A	5	ILE	17.5
2	B	24	PHE	17.0
2	B	154	SER	16.9
1	A	58	ALA	16.7
2	B	68[A]	GLN	16.7
2	B	50	THR	16.6
2	B	151	GLY	16.5

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Mol	Chain	Res	Type	RSRZ
2	B	144	ASP	16.3
2	B	8	VAL	16.1
2	B	21	ASN	16.0
2	B	112	GLY	15.7
1	A	22	THR	15.6
2	B	97	ILE	15.5
1	A	111	LEU	15.5
1	A	83	LYS	15.2
2	B	127	VAL	15.0
1	A	70	GLN	15.0
1	A	31	PHE	15.0
2	B	93	VAL	14.9
1	A	74	TYR	14.8
1	A	93	ARG	14.8
1	A	133	LEU	14.7
1	A	140	HIS	14.5
1	A	64	PRO	14.4
2	B	111	ASN	14.3
2	B	160	ILE	14.3
2	B	120	LEU	14.3
1	A	40	ALA	14.2
1	A	27	VAL	14.2
1	A	136	ILE	14.2
2	B	74	TYR	14.0
1	A	41	ALA	13.8
2	B	5	PHE	13.7
2	B	170	ALA	13.7
2	B	99	ALA	13.6
1	A	57	GLN	13.6
2	B	100	GLY	13.5
2	B	161	ALA	13.4
1	A	52	ILE	13.3
1	A	66	THR	13.3
2	B	89	ILE	13.2
2	B	141	ILE	13.2
2	B	54	ASN	13.1
2	B	30	LEU	13.1
1	A	148	VAL	13.0
1	A	81	LYS	12.9
1	A	44	LEU	12.9
2	B	59	LEU	12.9
2	B	136	ASP	12.9

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Mol	Chain	Res	Type	RSRZ
2	B	10	ALA	12.9
1	A	79	GLU	12.8
1	A	29	GLY	12.8
1	A	128	TRP	12.7
1	A	150	ALA	12.7
1	A	125	SER	12.6
2	B	41	VAL	12.6
2	B	138	ALA	12.6
2	B	1	MET	12.6
2	B	55	ALA	12.5
1	A	12	ALA	12.5
1	A	20	SER	12.5
2	B	104	VAL	12.5
2	B	46	SER	12.5
1	A	94	MET	12.3
2	B	139	ILE	12.3
1	A	43	ALA	12.2
2	B	105	LEU	12.1
1	A	90	TYR	12.0
1	A	72	SER	11.9
2	B	82	CYS	11.9
2	B	7	LYS	11.8
1	A	9	ILE	11.7
2	B	52	VAL	11.6
2	B	171	VAL	11.5
1	A	142	LEU	11.4
2	B	11	GLN	11.3
2	B	69	PRO	11.2
1	A	37	SER	11.1
1	A	96	THR	11.1
2	B	64	PRO	11.0
1	A	67	THR	10.9
1	A	42	ARG	10.9
1	A	118	ILE	10.9
1	A	110	TYR	10.8
1	A	156	TYR	10.8
2	B	95	TYR	10.8
1	A	18[A]	PHE	10.8
2	B	159	GLU	10.8
1	A	3	THR	10.8
1	A	63	PHE	10.8
1	A	25	GLN	10.7

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	10.7
2	B	114	ARG	10.6
2	B	92	TYR	10.6
1	A	158	ILE	10.6
1	A	65	TYR	10.5
2	B	119	ALA	10.5
2	B	9	VAL	10.5
1	A	129	TYR	10.5
1	A	68	THR	10.4
2	B	146	ASN	10.4
1	A	15	GLN	10.4
1	A	46	ASN	10.3
1	A	98	CYS	10.3
1	A	114	GLY	10.1
1	A	116	SER	10.0
1	A	105	GLY	10.0
2	B	134	MET	10.0
1	A	87	ASP	10.0
1	A	139	ASN	10.0
2	B	51	ILE	9.9
2	B	149	THR	9.9
2	B	61	ALA	9.9
2	B	83	LEU	9.9
1	A	14	THR	9.9
2	B	22	ALA	9.8
1	A	30	ARG	9.8
1	A	76	SER	9.7
2	B	31	VAL	9.7
2	B	75	THR	9.7
1	A	113	ALA	9.6
1	A	161	LEU	9.5
1	A	1	MET	9.4
1	A	24	LEU	9.4
2	B	113	LEU	9.4
1	A	17[A]	ARG	9.4
1	A	26	ALA	9.3
1	A	47	ASN	9.3
2	B	87	GLU	9.2
1	A	117	GLU	9.2
2	B	62	GLU	9.2
2	B	96	ALA	9.1
2	B	84	ARG	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	77	ARG	9.1
1	A	97	TYR	9.1
1	A	112	ILE	9.1
1	A	130	ILE	9.1
2	B	164	PHE	9.0
2	B	42	ASN	9.0
2	B	12	ALA	9.0
2	B	73	ALA	9.0
2	B	117	TYR	8.9
1	A	95	VAL	8.8
2	B	108	ARG	8.8
1	A	28	ASP	8.8
2	B	121	GLY	8.7
2	B	39	ASP	8.7
2	B	53	ALA	8.7
2	B	25	ASP	8.7
2	B	57	ARG	8.7
1	A	54	GLY	8.7
2	B	65	GLN	8.6
1	A	21	ASN	8.6
1	A	60	TYR	8.6
2	B	27	LEU	8.6
2	B	130	ALA	8.6
1	A	69	MET	8.5
2	B	137	ALA	8.5
2	B	145	PRO	8.5
1	A	124	LEU	8.5
1	A	35	VAL	8.5
2	B	103	SER	8.5
1	A	106	PRO	8.4
2	B	32	LYS	8.4
2	B	56	ALA	8.4
2	B	36	LYS	8.4
1	A	73	GLN	8.4
2	B	94	THR	8.3
1	A	19	LEU	8.3
1	A	78	PRO	8.2
2	B	18	PHE	8.2
2	B	132	GLN	8.2
2	B	16	GLY	8.2
1	A	91	TYR	8.1
2	B	109	CYS	8.1

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Mol	Chain	Res	Type	RSRZ
2	B	152	ASP	8.1
2	B	162	GLY	8.1
1	A	135	TYR	8.1
2	B	45	THR	8.0
1	A	77	THR	8.0
2	B	71	GLY	8.0
2	B	107	ASP	8.0
2	B	168	ALA	7.9
2	B	102	SER	7.9
2	B	163	TYR	7.9
2	B	86	MET	7.9
1	A	85	ALA	7.8
1	A	157	ALA	7.8
2	B	98	LEU	7.8
1	A	104	THR	7.8
2	B	28	SER	7.7
2	B	135	LYS	7.7
2	B	156	LEU	7.7
1	A	153	TYR	7.7
1	A	92	LEU	7.6
1	A	123	ASP	7.6
1	A	159	ASN	7.6
2	B	153	CYS	7.6
1	A	100	VAL	7.5
1	A	50	SER	7.5
2	B	118	GLN	7.5
2	B	38	LEU	7.5
2	B	122	THR	7.5
1	A	59	VAL	7.4
2	B	60	PHE	7.4
2	B	20[A]	THR	7.3
2	B	40	ALA	7.3
2	B	63	GLN	7.3
1	A	56	ALA	7.3
2	B	126	SER	7.3
1	A	127	SER	7.3
2	B	147	GLY	7.3
1	A	122	PHE	7.2
1	A	51	LEU	7.2
1	A	120	SER	7.2
2	B	66	LEU	7.1
2	B	128	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	7.1
1	A	84	CYS	7.1
2	B	148	ILE	7.1
2	B	14	ALA	7.0
2	B	78	ARG	7.0
1	A	8	ALA	7.0
2	B	155	ALA	6.9
2	B	17	GLU	6.9
1	A	162	SER	6.9
1	A	132	ALA	6.9
1	A	49	GLN	6.9
1	A	109	GLU	6.8
2	B	44	ILE	6.8
1	A	138	ALA	6.7
2	B	49	SER	6.7
2	B	91	ARG	6.7
2	B	35	ASN	6.6
1	A	115	LEU	6.6
2	B	167	ALA	6.5
1	A	82	ALA	6.5
1	A	99	LEU	6.5
2	B	165	ASP	6.5
2	B	3	ASP	6.4
2	B	6	ALA	6.4
2	B	157	MET	6.4
1	A	39	GLU	6.4
2	B	158	SER	6.3
1	A	101	ALA	6.3
1	A	6	THR	6.3
1	A	107	MET	6.2
2	B	88	ILE	6.1
1	A	126	PRO	6.1
1	A	146	ALA	6.1
1	A	10	ALA	6.1
2	B	48	ALA	6.1
1	A	32	LYS	6.1
2	B	76	ASN	6.0
1	A	137	LYS	6.0
1	A	134	LYS	6.0
1	A	143	THR	6.0
1	A	62	LYS	6.0
1	A	121	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	6.0
1	A	71	GLY	5.9
2	B	19	LEU	5.9
2	B	33	GLU	5.9
2	B	15	ARG	5.8
1	A	119	ASN	5.8
2	B	123	PRO	5.8
2	B	133	LYS	5.6
1	A	147	ALA	5.6
1	A	4	PRO	5.6
2	B	166	ARG	5.6
2	B	23	GLN	5.5
2	B	4	ALA	5.5
2	B	85	ASP	5.5
1	A	55	ALA	5.4
2	B	70	GLY	5.3
1	A	154	ILE	5.3
2	B	90	LEU	5.3
2	B	143	ASN	5.2
1	A	38	MET	5.1
1	A	103	GLY	5.0
1	A	33	ARG	5.0
1	A	13	ASP	4.9
2	B	43	ARG	4.9
2	B	101	ASP	4.9
2	B	124	GLY	4.9
1	A	53	ASP	4.8
2	B	47	ASN	4.8
1	A	152	ALA	4.7
1	A	141	GLY	4.6
1	A	149	GLU	4.5
2	B	13	ASP	4.5
2	B	129	VAL	4.4
1	A	2	LYS	4.4
1	A	7	GLU	4.4
1	A	86	ARG	4.4
1	A	75	ALA	4.4
2	B	140	ALA	4.3
1	A	108	ASP	4.1
1	A	80	GLY	4.1
1	A	145	GLN	4.0
1	A	155	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	48	ALA	3.9
2	B	106	ASP	3.9
2	B	115	GLU	3.9
2	B	79	MET	3.8
2	B	169	ALA	3.7
1	A	160	ALA	3.6
2	B	80	ALA	3.6
2	B	34	GLY	3.6
1	A	131	GLU	3.5
1	A	61	GLN	3.5
1	A	102	GLY	3.3
1	A	151	ASN	3.3
1	A	23	GLU	3.1
2	B	37	ARG	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MEN	B	72	9/10	0.29	0.98	-	26,42,59,59	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CYC	B	201	43/43	0.18	0.81	0.50	25,34,63,64	0
3	CYC	B	202	43/43	0.28	0.74	0.27	21,29,39,40	0
3	CYC	A	501	43/43	0.23	0.62	-0.18	12,17,24,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.