Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID	:	1CPC
Title	:	ISOLATION, CRYSTALLIZATION, CRYSTAL STRUCTURE ANALYSIS AND REFINEMENT OF CONSTITUTIVE C-PHYCOCYANIN FROM THE CHROMATICALLY ADAPTING CYANOBACTERIUM FREMYELLA DIPLOSIPHON AT 1.66 ANGSTROMS RESOLUTION
Authors	:	Duerring, M.; Schmidt, G.B.; Huber, R.
Deposited on	:	1990-10-11
Resolution	:	1.66 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:

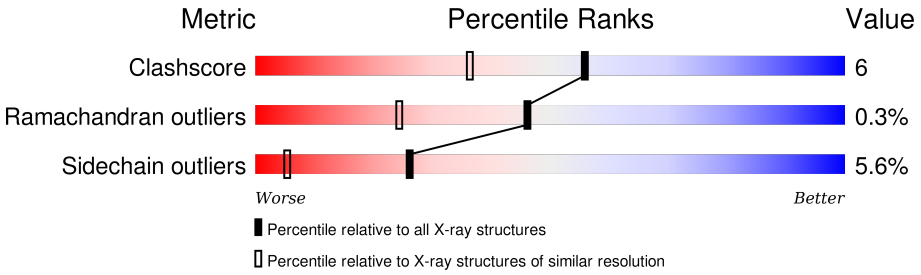
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	83% 14%
1	K	162	81% 17%
2	B	172	84% 13%
2	L	172	78% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5434 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C-PHYCOCYANIN (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	11	0	0
			1214	766	203	241	4			
1	K	162	Total	C	N	O	S	14	0	0
			1214	766	203	241	4			

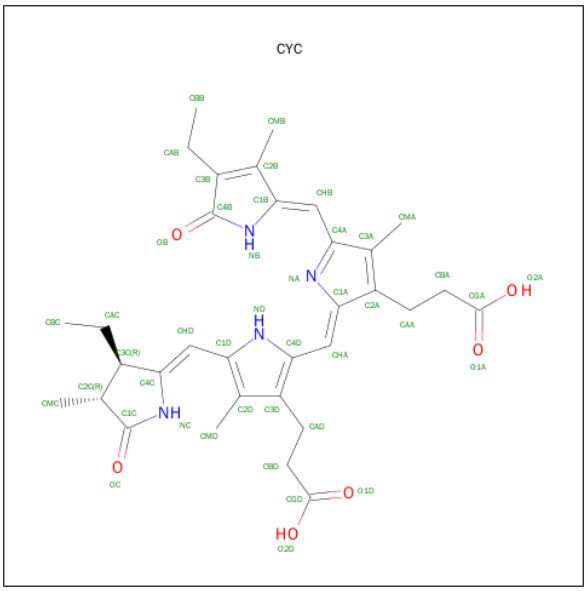
- Molecule 2 is a protein called C-PHYCOCYANIN (BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	23	0	0
			1253	775	220	249	9			
2	L	172	Total	C	N	O	S	26	0	0
			1252	775	220	248	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	171	SER	SER	CONFLICT	UNP P07119

- 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 43 33 4 6	0	0
3	B	1	Total C N O 43 33 4 6	0	0
3	B	1	Total C N O 43 33 4 6	0	0
3	K	1	Total C N O 43 33 4 6	0	0
3	L	1	Total C N O 43 33 4 6	0	0
3	L	1	Total C N O 43 33 4 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	58	Total O 58 58	0	0
4	K	57	Total O 57 57	0	0
4	L	53	Total O 53 53	0	0

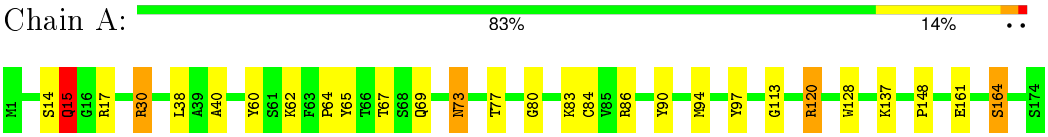
3 Residue-property plots (i)

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.

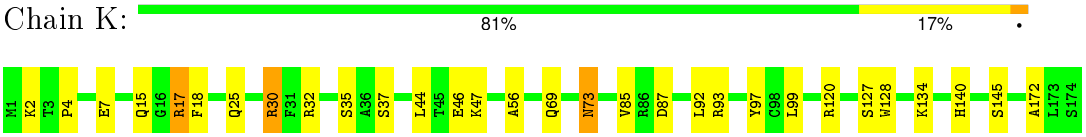
- Molecule 1: C-PHYCOCYANIN (ALPHA SUBUNIT)

Chain A:



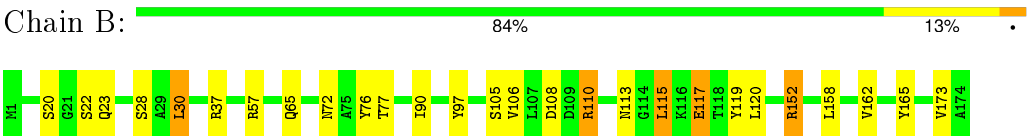
- Molecule 1: C-PHYCOCYANIN (ALPHA SUBUNIT)

Chain K:



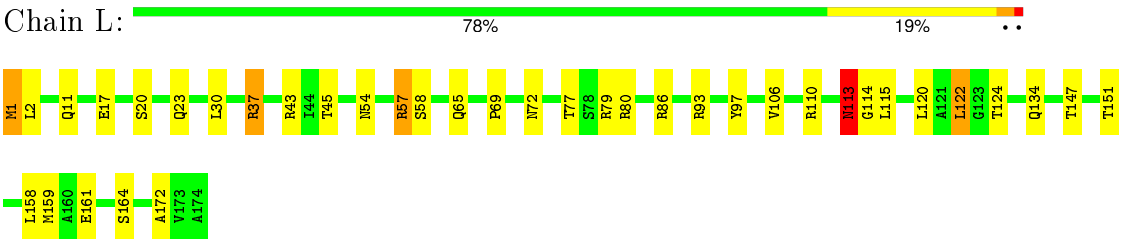
- Molecule 2: C-PHYCOCYANIN (BETA SUBUNIT)

Chain B:



- Molecule 2: C-PHYCOCYANIN (BETA SUBUNIT)

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	180.26Å 180.26Å 61.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.66	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.66)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5434	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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, 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	1.08	2/1238 (0.2%)	1.46	13/1680 (0.8%)
1	K	1.03	2/1238 (0.2%)	1.37	11/1680 (0.7%)
2	B	1.01	0/1255	1.54	12/1694 (0.7%)
2	L	0.99	0/1254	1.41	11/1693 (0.6%)
All	All	1.03	4/4985 (0.1%)	1.45	47/6747 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	K	0	2
2	L	1	8
All	All	1	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	SER	CB-OG	-6.12	1.34	1.42
1	K	128	TRP	NE1-CE2	-5.82	1.29	1.37
1	A	128	TRP	NE1-CE2	-5.69	1.30	1.37
1	K	120	ARG	CZ-NH1	5.49	1.40	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ARG	NE-CZ-NH1	14.71	127.65	120.30
2	B	110	ARG	NE-CZ-NH1	14.35	127.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	120	ARG	NE-CZ-NH2	-13.31	113.64	120.30
2	B	152	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	120	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	K	30	ARG	NE-CZ-NH1	11.73	126.17	120.30
2	B	110	ARG	NE-CZ-NH2	-10.46	115.07	120.30
2	B	37	ARG	NE-CZ-NH1	10.39	125.49	120.30
2	L	110	ARG	NE-CZ-NH1	9.65	125.12	120.30
2	L	43	ARG	NE-CZ-NH2	-9.27	115.67	120.30
2	L	93	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	164	SER	N-CA-CB	-8.44	97.84	110.50
1	K	17	ARG	NE-CZ-NH1	-7.65	116.47	120.30
2	B	105	SER	CB-CA-C	-7.55	95.76	110.10
1	A	30	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	120	ARG	NH1-CZ-NH2	-7.48	111.17	119.40
2	L	57	ARG	NE-CZ-NH1	-7.39	116.60	120.30
1	A	97	TYR	CB-CG-CD2	-7.35	116.59	121.00
2	B	152	ARG	CD-NE-CZ	7.33	133.86	123.60
2	L	110	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	L	80	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	K	134	LYS	CA-CB-CG	-6.74	98.57	113.40
2	B	97	TYR	CB-CG-CD2	-6.42	117.15	121.00
2	B	28	SER	N-CA-CB	6.32	119.98	110.50
1	A	137	LYS	N-CA-CB	-6.17	99.49	110.60
1	K	30	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	B	37	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	L	93	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	38	LEU	CB-CG-CD2	5.84	120.93	111.00
2	L	97	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	L	37	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	K	97	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	83	LYS	CA-CB-CG	-5.68	100.89	113.40
2	B	76	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	K	145	SER	N-CA-CB	-5.62	102.06	110.50
2	B	119	TYR	CB-CG-CD2	-5.56	117.66	121.00
2	L	86	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	38	LEU	CB-CG-CD1	5.41	120.19	111.00
2	L	113	ASN	CA-CB-CG	-5.39	101.53	113.40
1	K	172	ALA	N-CA-CB	5.37	117.62	110.10
2	B	165	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	K	17	ARG	CD-NE-CZ	-5.17	116.36	123.60
1	K	87	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	K	17	ARG	NE-CZ-NH2	5.10	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	62	LYS	N-CA-CB	-5.07	101.48	110.60
1	A	86	ARG	NE-CZ-NH2	5.01	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	124	THR	CB

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLY	Mainchain
1	A	120	ARG	Sidechain
1	A	15	GLN	Mainchain
1	K	35	SER	Mainchain
1	K	93	ARG	Mainchain
2	L	114	GLY	Mainchain,Peptide
2	L	151	THR	Mainchain
2	L	17	GLU	Mainchain
2	L	172	ALA	Mainchain
2	L	2	LEU	Mainchain
2	L	58	SER	Mainchain
2	L	69	PRO	Mainchain

5.2 Too-close contacts (i)

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	1214	0	1190	19	0
1	K	1214	0	1190	18	0
2	B	1253	0	1257	15	1
2	L	1252	0	1254	12	1
3	A	43	0	37	1	0
3	B	86	0	74	5	0
3	K	43	0	37	1	0
3	L	86	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	75	0	0	1	1
4	B	58	0	0	0	0
4	K	57	0	0	0	1
4	L	53	0	0	0	0
All	All	5434	0	5113	63	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 6.

All (63) 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:15:GLN:HG3	1:A:17:ARG:HD3	1.24	1.19
1:K:73:ASN:HD22	1:K:73:ASN:H	1.17	0.88
2:B:20:SER:H	2:B:23:GLN:HE21	1.24	0.85
1:A:73:ASN:HD22	1:A:73:ASN:H	1.22	0.84
2:L:20:SER:H	2:L:23:GLN:HE21	1.38	0.71
2:B:106:VAL:HG23	2:B:110:ARG:HD2	1.76	0.67
2:L:122:LEU:HB3	2:L:124:THR:HG23	1.77	0.67
2:L:30:LEU:HD11	2:L:37:ARG:HH21	1.59	0.66
1:K:73:ASN:ND2	1:K:73:ASN:H	1.93	0.66
1:A:30:ARG:HH11	1:K:25:GLN:HE22	1.44	0.64
2:L:72:MEN:OD1	2:L:124:THR:HG22	1.98	0.63
1:K:4:PRO:HG2	1:K:30:ARG:HD3	1.81	0.63
1:A:15:GLN:CG	1:A:17:ARG:HD3	2.16	0.62
1:A:73:ASN:ND2	1:A:73:ASN:H	1.96	0.62
3:L:176:CYC:HMD2	3:L:176:CYC:HC	1.67	0.60
2:L:30:LEU:HD11	2:L:37:ARG:NH2	2.18	0.57
1:A:77:THR:HG23	1:A:80:GLY:H	1.69	0.57
1:K:73:ASN:HA	3:K:175:CYC:HBD2	1.86	0.57
1:A:30:ARG:HD2	1:K:25:GLN:HE22	1.70	0.57
1:A:77:THR:HG22	4:A:229:HOH:O	2.06	0.56
2:L:54:ASN:ND2	2:L:57:ARG:HH12	2.03	0.56
1:A:30:ARG:HD2	1:K:25:GLN:NE2	2.21	0.56
2:B:115:LEU:HD13	2:B:173:VAL:CG1	2.37	0.54
1:A:84:CYS:HA	3:A:175:CYC:HHD	1.91	0.53
2:L:54:ASN:HD22	2:L:57:ARG:HH12	1.56	0.52
2:B:90:ILE:HG21	3:B:176:CYC:HAB1	1.90	0.52
1:A:161:GLU:O	1:A:164:SER:HB3	2.09	0.52
2:B:115:LEU:HD13	2:B:173:VAL:HG12	1.91	0.52
1:A:65:TYR:HB2	1:A:69:GLN:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HA	1:K:25:GLN:HE21	1.76	0.50
1:A:30:ARG:HH11	1:K:25:GLN:NE2	2.10	0.49
1:K:56:ALA:HB2	1:K:85:VAL:HG12	1.94	0.49
2:B:20:SER:N	2:B:23:GLN:HE21	2.03	0.49
2:L:1:MET:HG3	2:L:106:VAL:HB	1.94	0.49
1:A:64:PRO:O	1:A:67:THR:HG22	2.12	0.48
2:B:72:MEN:HE22	3:B:176:CYC:HBD2	1.94	0.48
3:L:177:CYC:HHA	3:L:177:CYC:O2D	2.14	0.47
3:B:176:CYC:HMD2	3:B:176:CYC:HC	1.78	0.47
2:B:158:LEU:O	2:B:162:VAL:HG23	2.15	0.47
1:K:2:LYS:HE3	1:K:7:GLU:OE1	2.15	0.47
1:K:69:GLN:HB3	1:K:69:GLN:HE21	1.43	0.47
1:K:18:PHE:HB3	2:L:45:THR:HG23	1.97	0.47
2:B:20:SER:H	2:B:23:GLN:NE2	2.01	0.46
1:K:56:ALA:CB	1:K:85:VAL:HG12	2.45	0.46
2:B:117:GLU:H	2:B:117:GLU:HG2	1.42	0.46
2:L:161:GLU:O	2:L:164:SER:HB3	2.16	0.46
1:A:90:TYR:O	1:A:94:MET:HG2	2.17	0.45
1:K:17:ARG:HD2	1:K:17:ARG:HH11	1.52	0.44
2:B:115:LEU:HD21	3:B:176:CYC:HMB3	2.00	0.44
1:A:40:ALA:HB2	1:A:148:PRO:HB3	2.00	0.44
2:B:65:GLN:H	2:B:65:GLN:CD	2.20	0.43
2:B:30:LEU:HA	2:B:30:LEU:HD12	1.73	0.43
1:K:44:LEU:HD21	1:K:140:HIS:HB2	2.00	0.43
1:A:73:ASN:HD22	1:A:73:ASN:N	2.02	0.43
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.80	0.43
2:L:113:ASN:HA	2:L:113:ASN:HD22	1.17	0.43
2:B:108:ASP:O	2:B:113:ASN:HB2	2.19	0.42
1:K:30:ARG:HA	1:K:30:ARG:HD2	1.98	0.41
1:K:37:SER:HB3	1:K:99:LEU:O	2.20	0.41
3:B:177:CYC:NB	3:B:177:CYC:HMA1	2.35	0.41
2:L:54:ASN:HD22	2:L:57:ARG:NH1	2.18	0.40
3:L:177:CYC:HAA1	3:L:177:CYC:HHA	1.94	0.40
1:A:17:ARG:HD2	1:A:17:ARG:HH11	1.55	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)
2:B:57:ARG:NH1	4:A:216:HOH:O[3_555]	2.05	0.15
2:L:57:ARG:NH2	4:K:221:HOH:O[2_555]	2.15	0.05

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%)	159 (99%)	1 (1%)	0	100 100
1	K	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
2	B	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	30 9
2	L	169/172 (98%)	167 (99%)	1 (1%)	1 (1%)	30 9
All	All	658/668 (98%)	648 (98%)	8 (1%)	2 (0%)	46 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77	THR
2	L	77	THR

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	125/125 (100%)	122 (98%)	3 (2%)	57 28
1	K	125/125 (100%)	118 (94%)	7 (6%)	26 5
2	B	126/126 (100%)	120 (95%)	6 (5%)	31 7
2	L	125/126 (99%)	113 (90%)	12 (10%)	10 2
All	All	501/502 (100%)	473 (94%)	28 (6%)	26 5

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	15	GLN
1	A	73	ASN
2	B	22	SER
2	B	30	LEU
2	B	115	LEU
2	B	117	GLU
2	B	120	LEU
2	B	152	ARG
1	K	15	GLN
1	K	32	ARG
1	K	46	GLU
1	K	47	LYS
1	K	73	ASN
1	K	92	LEU
1	K	127	SER
2	L	1	MET
2	L	11	GLN
2	L	65	GLN
2	L	79	ARG
2	L	113	ASN
2	L	115	LEU
2	L	120	LEU
2	L	122	LEU
2	L	134	GLN
2	L	147	THR
2	L	158	LEU
2	L	159	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	57	ASN
1	A	73	ASN
2	B	23	GLN
2	B	35	ASN
2	B	134	GLN
1	K	15	GLN
1	K	25	GLN
1	K	33	GLN
1	K	57	ASN
1	K	69	GLN

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Mol	Chain	Res	Type
1	K	73	ASN
1	K	119	ASN
2	L	23	GLN
2	L	35	ASN
2	L	47	ASN
2	L	54	ASN
2	L	63	GLN
2	L	65	GLN
2	L	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MEN	B	72	2	7,8,9	1.07	1 (14%)	5,9,11	0.78	0
2	MEN	L	72	2	7,8,9	0.92	0	5,9,11	2.08	3 (60%)

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
2	MEN	L	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	CB-CA	2.13	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	72	MEN	OD1-CG-CB	-2.88	117.10	121.30
2	L	72	MEN	O-C-CA	-2.57	118.81	125.49
2	L	72	MEN	CB-CG-ND2	2.42	119.42	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	1	0
2	L	72	MEN	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	175	1	35,46,46	1.91	7 (20%)	47,67,67	2.24	8 (17%)
3	CYC	B	176	2	35,46,46	2.01	6 (17%)	47,67,67	2.54	11 (23%)
3	CYC	B	177	2	35,46,46	1.83	9 (25%)	47,67,67	1.97	10 (21%)
3	CYC	K	175	1	35,46,46	1.87	7 (20%)	47,67,67	2.21	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CYC	L	176	2	35,46,46	1.78	7 (20%)	47,67,67	2.26	9 (19%)
3	CYC	L	177	2	35,46,46	2.11	10 (28%)	47,67,67	1.99	8 (17%)

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	175	1	-	2/21/74/74	0/4/4/4
3	CYC	B	176	2	-	2/21/74/74	0/4/4/4
3	CYC	B	177	2	-	2/21/74/74	0/4/4/4
3	CYC	K	175	1	-	2/21/74/74	0/4/4/4
3	CYC	L	176	2	-	2/21/74/74	0/4/4/4
3	CYC	L	177	2	-	2/21/74/74	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	176	CYC	C1C-NC	-5.56	1.30	1.37
3	B	177	CYC	C1A-C2A	-3.76	1.39	1.45
3	A	175	CYC	C1C-NC	-3.71	1.32	1.37
3	L	176	CYC	C1C-NC	-3.14	1.33	1.37
3	L	177	CYC	C1A-C2A	-2.68	1.41	1.45
3	B	176	CYC	C1A-C2A	-2.62	1.41	1.45
3	B	177	CYC	C1C-NC	-2.58	1.34	1.37
3	K	175	CYC	C4B-NB	-2.54	1.32	1.37
3	L	177	CYC	C1C-NC	-2.40	1.34	1.37
3	A	175	CYC	C1A-C2A	-2.36	1.41	1.45
3	L	177	CYC	CAD-C3D	-2.33	1.48	1.52
3	B	176	CYC	C4A-C3A	-2.25	1.40	1.45
3	L	177	CYC	C4B-NB	-2.22	1.32	1.37
3	B	177	CYC	C4B-NB	-2.19	1.32	1.37
3	B	177	CYC	CAD-C3D	-2.19	1.48	1.52
3	B	177	CYC	CMC-C2C	2.02	1.57	1.53
3	K	175	CYC	CHD-C4C	2.03	1.43	1.38
3	L	177	CYC	CHB-C1B	2.09	1.42	1.37
3	K	175	CYC	C4C-NC	2.17	1.42	1.37
3	A	175	CYC	C4C-NC	2.18	1.42	1.37
3	B	177	CYC	C2A-C3A	2.22	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	175	CYC	CHB-C1B	2.33	1.43	1.37
3	L	176	CYC	C4C-NC	2.40	1.42	1.37
3	L	176	CYC	CHB-C1B	2.41	1.43	1.37
3	B	177	CYC	C4C-NC	2.49	1.43	1.37
3	L	177	CYC	C4C-NC	2.53	1.43	1.37
3	L	176	CYC	C2A-C3A	2.58	1.42	1.36
3	L	176	CYC	C3B-C2B	2.66	1.42	1.36
3	L	177	CYC	C2A-C3A	2.67	1.42	1.36
3	A	175	CYC	C3B-C2B	2.85	1.42	1.36
3	B	176	CYC	C4C-NC	2.87	1.43	1.37
3	K	175	CYC	C3B-C2B	2.93	1.43	1.36
3	L	177	CYC	C1B-NB	3.08	1.43	1.37
3	L	177	CYC	C3B-C2B	3.21	1.43	1.36
3	B	176	CYC	C3B-C2B	3.30	1.43	1.36
3	A	175	CYC	CAC-C3C	3.37	1.60	1.54
3	A	175	CYC	C2A-C3A	3.39	1.44	1.36
3	L	176	CYC	C1B-NB	3.45	1.43	1.37
3	K	175	CYC	C1B-NB	3.53	1.44	1.37
3	B	177	CYC	C3B-C2B	3.97	1.45	1.36
3	B	177	CYC	CHA-C1A	5.70	1.40	1.35
3	L	176	CYC	CHA-C1A	5.98	1.40	1.35
3	K	175	CYC	CHA-C1A	6.88	1.41	1.35
3	A	175	CYC	CHA-C1A	6.90	1.41	1.35
3	B	176	CYC	CHA-C1A	7.10	1.41	1.35
3	L	177	CYC	CHA-C1A	8.30	1.42	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	176	CYC	C4B-C3B-C2B	-7.94	103.52	108.05
3	A	175	CYC	C4B-C3B-C2B	-7.13	103.98	108.05
3	L	177	CYC	C4B-C3B-C2B	-7.12	103.98	108.05
3	K	175	CYC	C3C-C2C-C1C	-6.56	97.91	103.41
3	L	176	CYC	OC-C1C-C2C	-6.55	120.96	126.25
3	B	176	CYC	OC-C1C-C2C	-6.27	121.19	126.25
3	A	175	CYC	C3C-C2C-C1C	-5.49	98.81	103.41
3	B	177	CYC	C4B-C3B-C2B	-5.11	105.13	108.05
3	B	176	CYC	CAD-CBD-CGD	-4.43	104.63	112.75
3	B	177	CYC	OC-C1C-C2C	-4.01	123.01	126.25
3	L	176	CYC	C3C-C2C-C1C	-3.81	100.21	103.41
3	L	177	CYC	CAA-CBA-CGA	-3.58	106.18	112.75
3	B	176	CYC	C3C-C2C-C1C	-3.42	100.54	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	175	CYC	C3C-C4C-NC	-3.35	104.58	107.93
3	K	175	CYC	CAA-CBA-CGA	-3.22	106.84	112.75
3	A	175	CYC	CAD-C3D-C4D	-3.16	123.57	127.01
3	K	175	CYC	OC-C1C-C2C	-3.04	123.80	126.25
3	B	177	CYC	C3C-C2C-C1C	-2.90	100.98	103.41
3	K	175	CYC	CHA-C1A-NA	-2.85	123.58	128.67
3	B	177	CYC	CAA-CBA-CGA	-2.83	107.56	112.75
3	A	175	CYC	C1B-NB-C4B	-2.73	106.73	110.73
3	L	177	CYC	OC-C1C-C2C	-2.68	124.09	126.25
3	K	175	CYC	C1B-C2B-C3B	-2.66	104.97	107.81
3	K	175	CYC	CAA-C2A-C3A	-2.56	123.54	128.01
3	L	176	CYC	CMC-C2C-C1C	-2.54	107.08	112.43
3	K	175	CYC	C4B-C3B-C2B	-2.43	106.66	108.05
3	L	177	CYC	CAC-C3C-C2C	-2.22	108.55	114.13
3	L	176	CYC	CAB-C3B-C2B	-2.15	123.73	127.51
3	B	176	CYC	CAA-C2A-C3A	-2.10	124.34	128.01
3	L	176	CYC	CAD-CBD-CGD	-2.04	109.01	112.75
3	B	177	CYC	CAD-C3D-C2D	-2.02	123.24	129.00
3	K	175	CYC	C2B-C1B-NB	2.11	110.05	107.00
3	B	176	CYC	C1D-CHD-C4C	2.13	134.96	127.23
3	K	175	CYC	CAA-C2A-C1A	2.13	128.87	125.06
3	L	177	CYC	C1A-C2A-C3A	2.35	109.44	106.81
3	B	176	CYC	CMA-C3A-C4A	2.47	129.08	125.06
3	K	175	CYC	C2C-C1C-NC	2.51	110.70	108.30
3	A	175	CYC	C2B-C1B-NB	2.66	110.85	107.00
3	K	175	CYC	C3B-C4B-NB	2.67	109.16	106.74
3	K	175	CYC	CMB-C2B-C1B	2.77	127.88	124.20
3	B	177	CYC	CMA-C3A-C4A	2.80	129.61	125.06
3	B	176	CYC	C3B-C4B-NB	2.96	109.43	106.74
3	K	175	CYC	CMA-C3A-C4A	3.12	130.13	125.06
3	B	177	CYC	C3B-C4B-NB	3.12	109.58	106.74
3	A	175	CYC	C2C-C1C-NC	3.14	111.30	108.30
3	L	176	CYC	CMB-C2B-C1B	3.23	128.49	124.20
3	B	176	CYC	C2C-C3C-C4C	3.29	107.08	101.50
3	B	177	CYC	C2C-C3C-C4C	3.38	107.22	101.50
3	L	177	CYC	C2C-C1C-NC	3.39	111.54	108.30
3	L	177	CYC	C3B-C4B-NB	3.84	110.23	106.74
3	L	176	CYC	C2C-C3C-C4C	3.85	108.02	101.50
3	A	175	CYC	C3B-C4B-NB	4.43	110.76	106.74
3	B	177	CYC	C2C-C1C-NC	4.62	112.71	108.30
3	B	177	CYC	CAB-C3B-C4B	4.83	125.72	121.51
3	L	176	CYC	C2C-C1C-NC	5.26	113.33	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	176	CYC	C2C-C1C-NC	5.85	113.89	108.30
3	L	177	CYC	CAB-C3B-C4B	6.30	127.02	121.51
3	K	175	CYC	CAB-C3B-C4B	7.02	127.64	121.51
3	A	175	CYC	CAB-C3B-C4B	7.43	128.00	121.51
3	B	176	CYC	CAB-C3B-C4B	8.39	128.84	121.51
3	L	176	CYC	CAB-C3B-C4B	8.67	129.08	121.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	175	CYC	C1B-CHB-C4A-C3A
3	L	177	CYC	C1B-CHB-C4A-C3A
3	L	176	CYC	C1B-CHB-C4A-C3A
3	B	176	CYC	C1B-CHB-C4A-C3A
3	K	175	CYC	C1B-CHB-C4A-C3A
3	B	177	CYC	C1B-CHB-C4A-C3A
3	L	176	CYC	C1B-CHB-C4A-NA
3	K	175	CYC	C1B-CHB-C4A-NA
3	L	177	CYC	C1B-CHB-C4A-NA
3	A	175	CYC	C1B-CHB-C4A-NA
3	B	176	CYC	C1B-CHB-C4A-NA
3	B	177	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	175	CYC	1	0
3	B	176	CYC	4	0
3	B	177	CYC	1	0
3	K	175	CYC	1	0
3	L	176	CYC	1	0
3	L	177	CYC	2	0

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.