



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:57 am GMT

PDB ID : 2UUN
Title : CRYSTAL STRUCTURE OF C-PHYCOCYANIN FROM PHORMIDIUM, LYNGBYA SPP. (MARINE) AND SPIRULINA SP. (FRESH WATER) SHOWS TWO DIFFERENT WAYS OF ENERGY TRANSFER BETWEEN TWO HEXAMERS.
Authors : Satyanarayana, L.; Patel, A.; Mishra, S.; K Ghosh, P.; Suresh, C.G.
Deposited on : 2007-03-05
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	trunk28620
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)	:	recalc28949

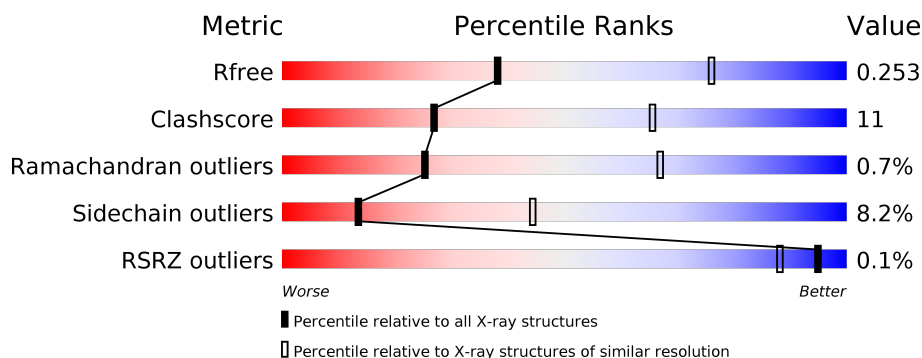
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




















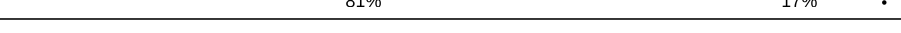
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	
1	C	162	
1	E	162	
1	G	162	
1	I	162	
1	K	162	

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Mol	Chain	Length	Quality of chain
1	M	162	 79% 19% ..
1	O	162	 81% 15% .
1	Q	162	 79% 17% .
1	S	162	 79% 17% .
1	U	162	 81% 18% ..
1	W	162	 83% 12% .
2	B	172	 76% 21% ..
2	F	172	 80% 19% .
2	H	172	 79% 17% .
2	J	172	 82% 16% .
2	L	172	 82% 16% .
2	N	172	 81% 17% .
2	P	172	 78% 19% .
2	R	172	 75% 23% .
2	T	172	 80% 18% .
2	V	172	 80% 18% .
2	X	172	 81% 17% .
3	D	172	 72% 24% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31361 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	C	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	E	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	G	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	I	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	K	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	M	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	O	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	Q	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	S	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	U	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			
1	W	162	Total	C	N	O	S	0	0	0
			1211	761	203	240	7			

- Molecule 2 is a protein called C-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	F	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			

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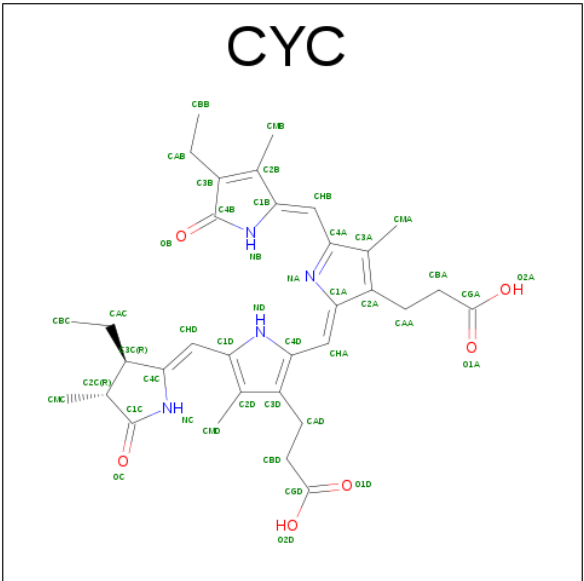
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	J	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	L	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	N	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	P	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	R	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	T	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	V	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			
2	X	172	Total	C	N	O	S	0	0	0
			1242	768	218	247	9			

- Molecule 3 is a protein called C-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	172	Total	C	N	O	S	0	0	0
			1244	770	218	247	9			

- Molecule 4 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: C₃₃H₄₀N₄O₆).



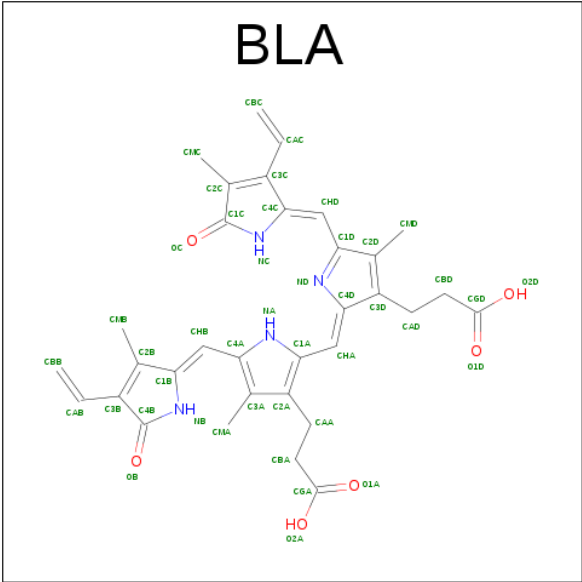
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 43	C 33	N 4	O 6	0	0
4	B	1	Total 43	C 33	N 4	O 6	0	0
4	C	1	Total 43	C 33	N 4	O 6	0	0
4	D	1	Total 43	C 33	N 4	O 6	0	0
4	D	1	Total 43	C 33	N 4	O 6	0	0
4	E	1	Total 43	C 33	N 4	O 6	0	0
4	F	1	Total 43	C 33	N 4	O 6	0	0
4	F	1	Total 43	C 33	N 4	O 6	0	0
4	G	1	Total 43	C 33	N 4	O 6	0	0
4	H	1	Total 43	C 33	N 4	O 6	0	0
4	H	1	Total 43	C 33	N 4	O 6	0	0
4	I	1	Total 43	C 33	N 4	O 6	0	0
4	J	1	Total 43	C 33	N 4	O 6	0	0
4	J	1	Total 43	C 33	N 4	O 6	0	0
4	K	1	Total 43	C 33	N 4	O 6	0	0
4	L	1	Total 43	C 33	N 4	O 6	0	0
4	L	1	Total 43	C 33	N 4	O 6	0	0
4	M	1	Total 43	C 33	N 4	O 6	0	0
4	N	1	Total 43	C 33	N 4	O 6	0	0
4	N	1	Total 43	C 33	N 4	O 6	0	0
4	O	1	Total 43	C 33	N 4	O 6	0	0
4	P	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			43	33	4	6		
4	Q	1	Total	C	N	O	0	0
			43	33	4	6		
4	R	1	Total	C	N	O	0	0
			43	33	4	6		
4	R	1	Total	C	N	O	0	0
			43	33	4	6		
4	S	1	Total	C	N	O	0	0
			43	33	4	6		
4	T	1	Total	C	N	O	0	0
			43	33	4	6		
4	T	1	Total	C	N	O	0	0
			43	33	4	6		
4	U	1	Total	C	N	O	0	0
			43	33	4	6		
4	V	1	Total	C	N	O	0	0
			43	33	4	6		
4	V	1	Total	C	N	O	0	0
			43	33	4	6		
4	W	1	Total	C	N	O	0	0
			43	33	4	6		
4	X	1	Total	C	N	O	0	0
			43	33	4	6		
4	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	31	Total	O	0	0
			31	31		
6	D	13	Total	O	0	0
			13	13		
6	E	8	Total	O	0	0
			8	8		
6	F	39	Total	O	0	0
			39	39		
6	I	40	Total	O	0	0
			40	40		
6	J	15	Total	O	0	0
			15	15		
6	K	9	Total	O	0	0
			9	9		
6	L	31	Total	O	0	0
			31	31		
6	M	40	Total	O	0	0
			40	40		
6	N	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	13	Total 13	O 13	0	0
6	P	27	Total 27	O 27	0	0
6	Q	2	Total 2	O 2	0	0
6	R	3	Total 3	O 3	0	0
6	S	6	Total 6	O 6	0	0
6	T	30	Total 30	O 30	0	0
6	W	34	Total 34	O 34	0	0
6	X	19	Total 19	O 19	0	0

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.

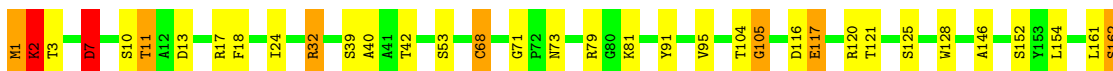
• Molecule 1: C-PHYCOCYANIN

Chain A: 




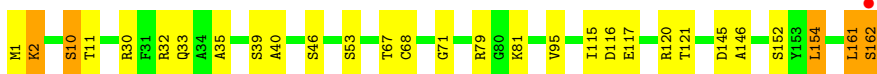
• Molecule 1: C-PHYCOCYANIN

Chain C: 




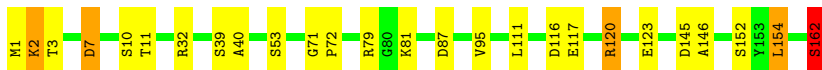
• Molecule 1: C-PHYCOCYANIN

Chain E: 



• Molecule 1: C-PHYCOCYANIN

Chain G: 




• Molecule 1: C-PHYCOCYANIN

Chain I: 

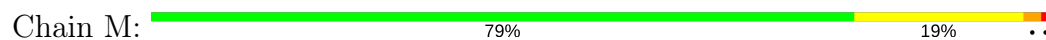


• Molecule 1: C-PHYCOCYANIN

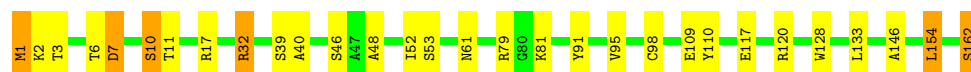
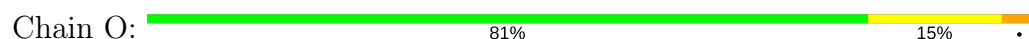
Chain K: 



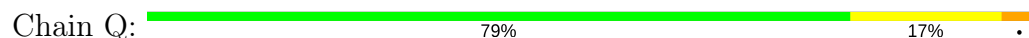
• Molecule 1: C-PHYCOCYANIN



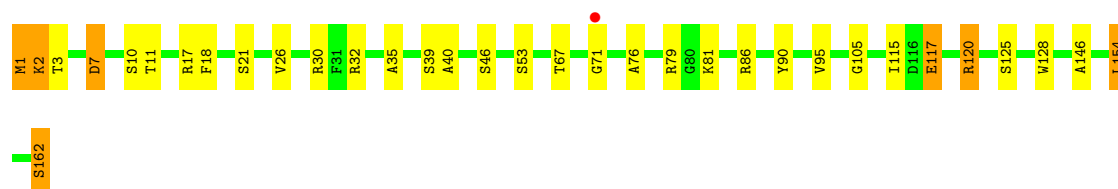
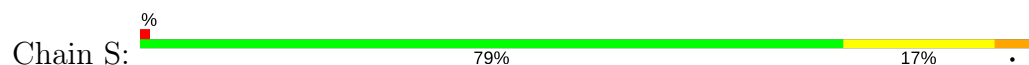
• Molecule 1: C-PHYCOCYANIN



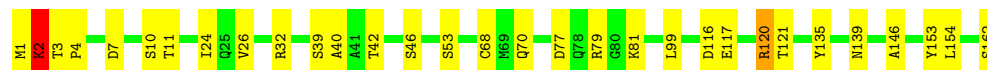
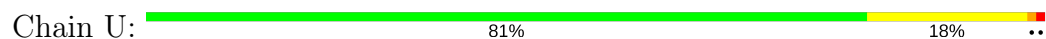
• Molecule 1: C-PHYCOCYANIN



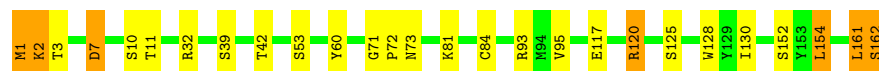
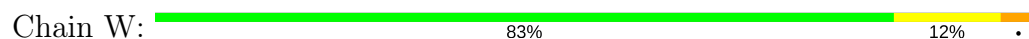
• Molecule 1: C-PHYCOCYANIN



• Molecule 1: C-PHYCOCYANIN

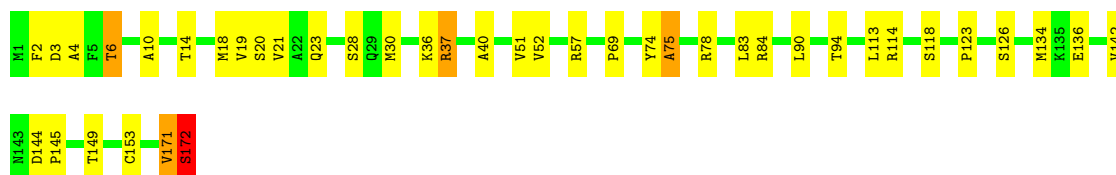


• Molecule 1: C-PHYCOCYANIN



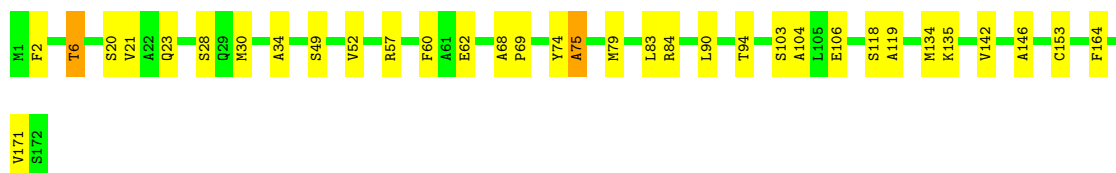
• Molecule 2: C-PHYCOCYANIN





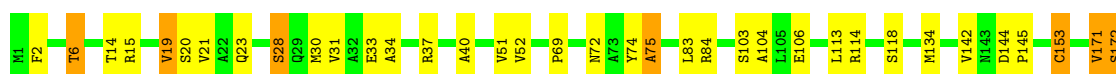
- Molecule 2: C-PHYCOCYANIN

Chain F: 80% 19%



- Molecule 2: C-PHYCOCYANIN

Chain H: 79% 17%



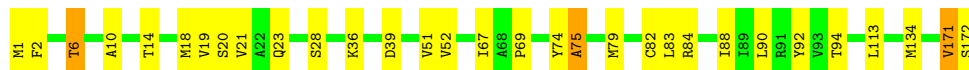
- Molecule 2: C-PHYCOCYANIN

Chain J: 82% 16%



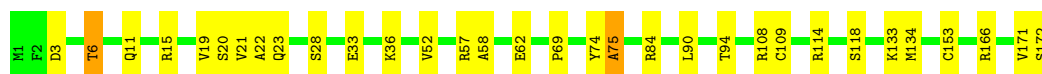
- Molecule 2: C-PHYCOCYANIN

Chain L: 82% 16%



- Molecule 2: C-PHYCOCYANIN

Chain N: 81% 17%

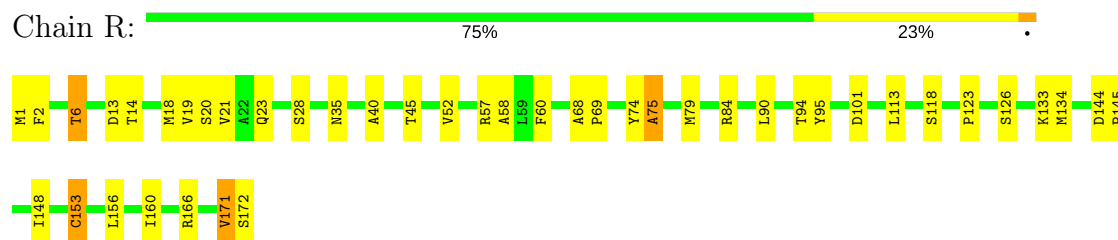


- Molecule 2: C-PHYCOCYANIN

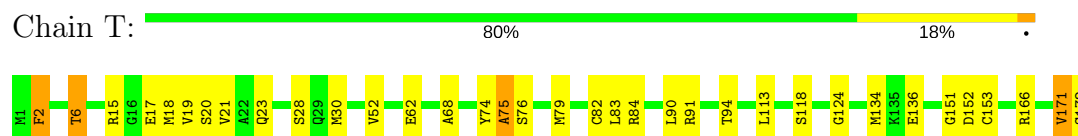
Chain P: 78% 19%



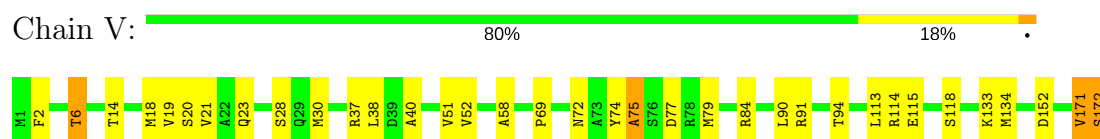
- Molecule 2: C-PHYCOCYANIN



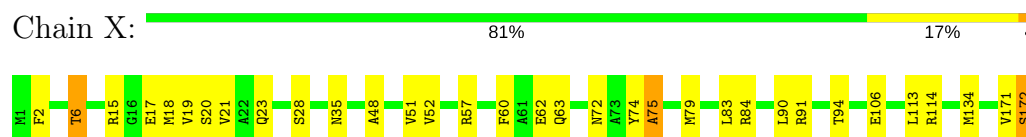
- Molecule 2: C-PHYCOCYANIN



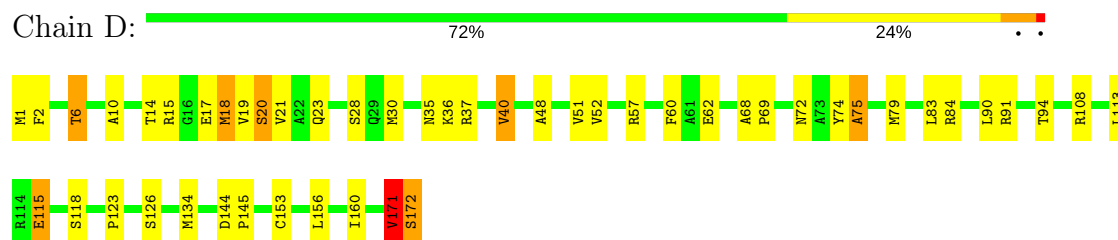
- Molecule 2: C-PHYCOCYANIN



- Molecule 2: C-PHYCOCYANIN



- Molecule 3: C-PHYCOCYANIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.46Å 115.33Å 183.37Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	182.57 – 3.00 24.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (182.57-3.00) 96.2 (24.86-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.262 0.208 , 0.253	Depositor DCC
R_{free} test set	4349 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31361	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.14	3/1234 (0.2%)	0.93	3/1676 (0.2%)
1	C	1.13	6/1234 (0.5%)	0.99	6/1676 (0.4%)
1	E	1.24	3/1234 (0.2%)	1.06	9/1676 (0.5%)
1	G	1.13	4/1234 (0.3%)	0.95	5/1676 (0.3%)
1	I	1.05	0/1234	0.90	0/1676
1	K	1.17	6/1234 (0.5%)	0.98	6/1676 (0.4%)
1	M	1.05	2/1234 (0.2%)	0.88	2/1676 (0.1%)
1	O	1.13	6/1234 (0.5%)	0.96	1/1676 (0.1%)
1	Q	1.14	4/1234 (0.3%)	0.94	2/1676 (0.1%)
1	S	1.16	7/1234 (0.6%)	0.99	3/1676 (0.2%)
1	U	1.12	4/1234 (0.3%)	0.93	4/1676 (0.2%)
1	W	1.14	3/1234 (0.2%)	0.96	3/1676 (0.2%)
2	B	1.08	2/1256 (0.2%)	0.97	5/1704 (0.3%)
2	F	1.14	3/1256 (0.2%)	0.96	2/1704 (0.1%)
2	H	1.12	4/1256 (0.3%)	0.96	3/1704 (0.2%)
2	J	1.07	1/1256 (0.1%)	0.95	3/1704 (0.2%)
2	L	1.07	0/1256	0.99	1/1704 (0.1%)
2	N	1.13	1/1256 (0.1%)	0.95	0/1704
2	P	1.07	2/1256 (0.2%)	0.98	2/1704 (0.1%)
2	R	1.13	2/1256 (0.2%)	1.01	4/1704 (0.2%)
2	T	1.09	3/1256 (0.2%)	0.96	0/1704
2	V	1.09	1/1256 (0.1%)	0.97	5/1704 (0.3%)
2	X	1.06	2/1256 (0.2%)	0.94	2/1704 (0.1%)
3	D	1.13	4/1258 (0.3%)	0.96	2/1707 (0.1%)
All	All	1.12	73/29882 (0.2%)	0.96	73/40563 (0.2%)

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	1
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	S	0	1
1	W	0	1
All	All	0	8

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	68	CYS	CB-SG	-15.62	1.55	1.82
1	E	161	LEU	C-O	-13.97	0.96	1.23
2	F	171	VAL	C-O	-11.88	1.00	1.23
2	R	171	VAL	C-O	-9.22	1.05	1.23
2	J	153	CYS	CB-SG	-8.24	1.68	1.82

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	LEU	CA-C-N	8.91	136.80	117.20
1	E	161	LEU	O-C-N	-8.31	109.41	122.70
1	O	120	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	K	30	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	E	162	SER	N-CA-C	-7.46	90.86	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	GLY	Peptide
1	C	71	GLY	Peptide
1	E	71	GLY	Peptide
1	G	71	GLY	Peptide
1	I	71	GLY	Peptide

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	1211	0	1172	13	0
1	C	1211	0	1172	22	0
1	E	1211	0	1172	18	1
1	G	1211	0	1172	12	0
1	I	1211	0	1172	18	0
1	K	1211	0	1172	16	0
1	M	1211	0	1172	25	0
1	O	1211	0	1172	15	1
1	Q	1211	0	1172	23	0
1	S	1211	0	1172	19	0
1	U	1211	0	1172	12	0
1	W	1211	0	1172	13	0
2	B	1242	0	1234	35	0
2	F	1242	0	1233	22	0
2	H	1242	0	1234	28	1
2	J	1242	0	1234	24	0
2	L	1242	0	1234	37	0
2	N	1242	0	1233	33	1
2	P	1242	0	1233	26	0
2	R	1242	0	1234	41	0
2	T	1242	0	1235	37	1
2	V	1242	0	1233	18	0
2	X	1242	0	1233	25	0
3	D	1244	0	1237	38	1
4	A	43	0	37	6	0
4	B	43	0	37	10	0
4	C	43	0	37	5	0
4	D	86	0	72	16	0
4	E	43	0	37	6	0
4	F	86	0	73	9	0
4	G	43	0	37	6	0
4	H	86	0	75	18	0
4	I	43	0	37	4	0
4	J	86	0	74	20	0
4	K	43	0	36	5	0
4	L	86	0	75	27	0
4	M	43	0	36	3	0
4	N	86	0	74	18	0
4	O	43	0	37	6	0
4	P	86	0	73	24	0
4	Q	43	0	37	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	86	0	74	20	0
4	S	43	0	37	11	0
4	T	86	0	76	27	0
4	U	43	0	37	5	0
4	V	86	0	74	13	0
4	W	43	0	37	5	0
4	X	86	0	72	9	0
5	B	43	0	32	16	0
6	A	2	0	0	1	0
6	C	31	0	0	3	0
6	D	13	0	0	2	0
6	E	8	0	0	2	0
6	F	39	0	0	5	0
6	I	40	0	0	3	0
6	J	15	0	0	1	0
6	K	9	0	0	3	0
6	L	31	0	0	2	0
6	M	40	0	0	5	0
6	N	13	0	0	6	0
6	O	13	0	0	3	0
6	P	27	0	0	4	0
6	Q	2	0	0	1	0
6	R	3	0	0	0	0
6	S	6	0	0	0	0
6	T	30	0	0	4	0
6	W	34	0	0	3	0
6	X	19	0	0	4	0
All	All	31361	0	30194	699	3

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 11.

The worst 5 of 699 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)
2:R:153:CYS:SG	4:R:255:CYC:HAC1	1.18	1.71
2:J:82:CYS:SG	4:J:184:CYC:HAC2	1.15	1.66
2:H:153:CYS:SG	4:H:255:CYC:HAC1	1.15	1.64
2:T:153:CYS:SG	4:T:255:CYC:HAC1	1.41	1.58
2:T:82:CYS:SG	4:T:184:CYC:HAC2	1.42	1.58

All (3) 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)
3:D:62:GLU:OE1	2:H:23:GLN:CG[2_746]	2.05	0.15
1:E:67:THR:O	1:O:61:ASN:CG[1_554]	2.07	0.13
2:N:114:ARG:NH1	2:T:15:ARG:NH2[2_547]	2.19	0.01

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%)	156 (98%)	3 (2%)	1 (1%)	28	70
1	C	160/162 (99%)	152 (95%)	6 (4%)	2 (1%)	14	51
1	E	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	28	70
1	G	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	28	70
1	I	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	28	70
1	K	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	28	70
1	M	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	28	70
1	O	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	28	70
1	Q	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	28	70
1	S	160/162 (99%)	154 (96%)	4 (2%)	2 (1%)	14	51
1	U	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	28	70
1	W	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	28	70
2	B	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	28	70
2	F	170/172 (99%)	164 (96%)	4 (2%)	2 (1%)	15	53
2	H	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	28	70
2	J	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	28	70
2	L	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	28	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	28	70
2	P	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	28	70
2	R	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	28	70
2	T	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	15	53
2	V	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	28	70
2	X	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	28	70
3	D	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	15	53
All	All	3960/4008 (99%)	3813 (96%)	118 (3%)	29 (1%)	25	67

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	LYS
1	G	2	LYS
1	M	2	LYS
1	O	2	LYS
1	Q	2	LYS

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	120/120 (100%)	108 (90%)	12 (10%)	9	33
1	C	120/120 (100%)	107 (89%)	13 (11%)	7	29
1	E	120/120 (100%)	108 (90%)	12 (10%)	9	33
1	G	120/120 (100%)	107 (89%)	13 (11%)	7	29
1	I	120/120 (100%)	107 (89%)	13 (11%)	7	29
1	K	120/120 (100%)	109 (91%)	11 (9%)	11	38
1	M	120/120 (100%)	109 (91%)	11 (9%)	11	38
1	O	120/120 (100%)	109 (91%)	11 (9%)	11	38
1	Q	120/120 (100%)	109 (91%)	11 (9%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	120/120 (100%)	108 (90%)	12 (10%)	9	33
1	U	120/120 (100%)	107 (89%)	13 (11%)	7	29
1	W	120/120 (100%)	108 (90%)	12 (10%)	9	33
2	B	123/123 (100%)	114 (93%)	9 (7%)	16	50
2	F	123/123 (100%)	116 (94%)	7 (6%)	24	62
2	H	123/123 (100%)	113 (92%)	10 (8%)	14	45
2	J	123/123 (100%)	118 (96%)	5 (4%)	35	73
2	L	123/123 (100%)	118 (96%)	5 (4%)	35	73
2	N	123/123 (100%)	117 (95%)	6 (5%)	29	68
2	P	123/123 (100%)	114 (93%)	9 (7%)	16	50
2	R	123/123 (100%)	114 (93%)	9 (7%)	16	50
2	T	123/123 (100%)	115 (94%)	8 (6%)	20	56
2	V	123/123 (100%)	113 (92%)	10 (8%)	14	45
2	X	123/123 (100%)	117 (95%)	6 (5%)	29	68
3	D	124/124 (100%)	114 (92%)	10 (8%)	14	45
All	All	2917/2917 (100%)	2679 (92%)	238 (8%)	13	44

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	11	THR
2	N	28	SER
2	V	172	SER
1	K	46	SER
1	M	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	139	ASN
2	N	35	ASN
1	W	139	ASN
2	L	35	ASN
1	O	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

36 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	$\# Z > 2$
4	CYC	A	184	1	36,46,46	3.85	11 (30%)	44,67,67	3.41	20 (45%)
4	CYC	B	184	2	36,46,46	3.82	11 (30%)	44,67,67	3.44	17 (38%)
5	BLA	B	255	-	36,46,46	4.72	14 (38%)	46,67,67	2.79	19 (41%)
4	CYC	C	184	1	36,46,46	3.52	12 (33%)	44,67,67	3.35	19 (43%)
4	CYC	D	184	3	36,46,46	4.04	12 (33%)	44,67,67	3.51	22 (50%)
4	CYC	D	255	3	36,46,46	3.66	13 (36%)	44,67,67	3.64	20 (45%)
4	CYC	E	184	1	36,46,46	3.32	13 (36%)	44,67,67	3.48	14 (31%)
4	CYC	F	184	2	36,46,46	4.04	13 (36%)	44,67,67	3.04	18 (40%)
4	CYC	F	255	2	36,46,46	4.20	13 (36%)	44,67,67	2.92	17 (38%)
4	CYC	G	184	1	36,46,46	3.39	13 (36%)	44,67,67	3.06	15 (34%)
4	CYC	H	184	2	36,46,46	4.25	12 (33%)	44,67,67	3.67	12 (27%)
4	CYC	H	255	-	36,46,46	3.53	13 (36%)	44,67,67	3.39	18 (40%)
4	CYC	I	184	1	36,46,46	3.78	12 (33%)	44,67,67	3.21	20 (45%)
4	CYC	J	184	2	36,46,46	3.35	13 (36%)	44,67,67	4.14	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CYC	J	255	2	36,46,46	3.73	15 (41%)	44,67,67	3.45	23 (52%)
4	CYC	K	184	1	36,46,46	3.87	12 (33%)	44,67,67	2.92	15 (34%)
4	CYC	L	184	-	36,46,46	3.86	13 (36%)	44,67,67	3.40	18 (40%)
4	CYC	L	255	2	36,46,46	3.94	12 (33%)	44,67,67	2.99	17 (38%)
4	CYC	M	184	1	36,46,46	3.89	13 (36%)	44,67,67	3.40	20 (45%)
4	CYC	N	184	2	36,46,46	3.74	14 (38%)	44,67,67	2.90	15 (34%)
4	CYC	N	255	2	36,46,46	3.82	13 (36%)	44,67,67	2.80	16 (36%)
4	CYC	O	184	1	36,46,46	3.42	12 (33%)	44,67,67	3.31	15 (34%)
4	CYC	P	184	2	36,46,46	4.35	12 (33%)	44,67,67	3.35	21 (47%)
4	CYC	P	255	2	36,46,46	3.31	13 (36%)	44,67,67	3.48	19 (43%)
4	CYC	Q	184	1	36,46,46	3.45	15 (41%)	44,67,67	3.14	14 (31%)
4	CYC	R	184	2	36,46,46	4.07	12 (33%)	44,67,67	3.90	21 (47%)
4	CYC	R	255	-	36,46,46	4.01	10 (27%)	44,67,67	4.04	20 (45%)
4	CYC	S	184	1	36,46,46	3.88	14 (38%)	44,67,67	3.69	19 (43%)
4	CYC	T	184	-	36,46,46	3.49	14 (38%)	44,67,67	3.54	18 (40%)
4	CYC	T	255	-	36,46,46	3.38	14 (38%)	44,67,67	2.46	14 (31%)
4	CYC	U	184	1	36,46,46	3.66	15 (41%)	44,67,67	3.70	22 (50%)
4	CYC	V	184	2	36,46,46	3.53	13 (36%)	44,67,67	3.47	15 (34%)
4	CYC	V	255	2	36,46,46	3.94	16 (44%)	44,67,67	3.61	15 (34%)
4	CYC	W	184	1	36,46,46	3.67	14 (38%)	44,67,67	3.10	14 (31%)
4	CYC	X	184	2	36,46,46	4.54	13 (36%)	44,67,67	2.83	17 (38%)
4	CYC	X	255	2	36,46,46	3.47	12 (33%)	44,67,67	2.97	16 (36%)

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
4	CYC	A	184	1	-	2/21/74/74	0/4/4/4
4	CYC	B	184	2	-	2/21/74/74	0/4/4/4
5	BLA	B	255	-	-	2/22/74/74	0/4/4/4
4	CYC	C	184	1	-	2/21/74/74	0/4/4/4
4	CYC	D	184	3	-	2/21/74/74	0/4/4/4
4	CYC	D	255	3	-	2/21/74/74	0/4/4/4
4	CYC	E	184	1	-	2/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYC	F	184	2	-	2/21/74/74	0/4/4/4
4	CYC	F	255	2	-	2/21/74/74	0/4/4/4
4	CYC	G	184	1	-	2/21/74/74	0/4/4/4
4	CYC	H	184	2	-	2/21/74/74	0/4/4/4
4	CYC	H	255	-	-	2/21/74/74	0/4/4/4
4	CYC	I	184	1	-	2/21/74/74	0/4/4/4
4	CYC	J	184	2	-	2/21/74/74	0/4/4/4
4	CYC	J	255	2	-	2/21/74/74	0/4/4/4
4	CYC	K	184	1	-	2/21/74/74	0/4/4/4
4	CYC	L	184	-	-	2/21/74/74	0/4/4/4
4	CYC	L	255	2	-	2/21/74/74	0/4/4/4
4	CYC	M	184	1	-	2/21/74/74	0/4/4/4
4	CYC	N	184	2	-	2/21/74/74	0/4/4/4
4	CYC	N	255	2	-	2/21/74/74	0/4/4/4
4	CYC	O	184	1	-	2/21/74/74	0/4/4/4
4	CYC	P	184	2	-	2/21/74/74	0/4/4/4
4	CYC	P	255	2	-	2/21/74/74	0/4/4/4
4	CYC	Q	184	1	-	2/21/74/74	0/4/4/4
4	CYC	R	184	2	-	2/21/74/74	0/4/4/4
4	CYC	R	255	-	-	2/21/74/74	0/4/4/4
4	CYC	S	184	1	-	2/21/74/74	0/4/4/4
4	CYC	T	184	-	-	2/21/74/74	0/4/4/4
4	CYC	T	255	-	-	2/21/74/74	0/4/4/4
4	CYC	U	184	1	-	2/21/74/74	0/4/4/4
4	CYC	V	184	2	-	2/21/74/74	0/4/4/4
4	CYC	V	255	2	-	2/21/74/74	0/4/4/4
4	CYC	W	184	1	-	2/21/74/74	0/4/4/4
4	CYC	X	184	2	-	2/21/74/74	0/4/4/4
4	CYC	X	255	2	-	2/21/74/74	0/4/4/4

The worst 5 of 466 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	184	CYC	C4B-C3B	-7.41	1.33	1.48
4	F	255	CYC	C4B-C3B	-6.20	1.35	1.48
4	J	255	CYC	C4B-C3B	-6.13	1.35	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	184	CYC	C4B-C3B	-6.10	1.36	1.48
4	I	184	CYC	C4B-C3B	-6.03	1.36	1.48

The worst 5 of 630 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	184	CYC	C4B-C3B-C2B	-13.36	100.33	108.01
4	S	184	CYC	OB-C4B-C3B	-12.16	114.55	128.11
4	D	255	CYC	C4B-C3B-C2B	-12.12	101.05	108.01
4	R	255	CYC	C4B-C3B-C2B	-11.78	101.24	108.01
4	M	184	CYC	OC-C1C-C2C	-10.87	117.47	126.25

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	184	CYC	C1B-CHB-C4A-C3A
5	B	255	BLA	C4C-CHD-C1D-C2D
4	X	184	CYC	C1B-CHB-C4A-C3A
4	H	184	CYC	C1B-CHB-C4A-C3A
4	F	184	CYC	C1B-CHB-C4A-C3A

There are no ring outliers.

35 monomers are involved in 295 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	184	CYC	6	0
4	B	184	CYC	10	0
5	B	255	BLA	16	0
4	C	184	CYC	5	0
4	D	184	CYC	8	0
4	D	255	CYC	8	0
4	E	184	CYC	6	0
4	F	184	CYC	4	0
4	F	255	CYC	5	0
4	G	184	CYC	6	0
4	H	184	CYC	5	0
4	H	255	CYC	13	0
4	I	184	CYC	4	0
4	J	184	CYC	5	0
4	J	255	CYC	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	184	CYC	5	0
4	L	184	CYC	15	0
4	L	255	CYC	12	0
4	M	184	CYC	3	0
4	N	184	CYC	5	0
4	N	255	CYC	13	0
4	O	184	CYC	6	0
4	P	184	CYC	12	0
4	P	255	CYC	12	0
4	Q	184	CYC	6	0
4	R	184	CYC	5	0
4	R	255	CYC	15	0
4	S	184	CYC	11	0
4	T	184	CYC	14	0
4	T	255	CYC	13	0
4	U	184	CYC	5	0
4	V	184	CYC	6	0
4	V	255	CYC	7	0
4	W	184	CYC	5	0
4	X	184	CYC	9	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%)	-0.51	0 100 100	2, 2, 2, 10	0
1	C	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	E	162/162 (100%)	-0.62	1 (0%) 89 71	2, 2, 2, 10	0
1	G	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	I	162/162 (100%)	-0.60	0 100 100	2, 2, 2, 10	0
1	K	162/162 (100%)	-0.55	1 (0%) 89 71	2, 2, 2, 10	0
1	M	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	O	162/162 (100%)	-0.58	0 100 100	2, 2, 2, 10	0
1	Q	162/162 (100%)	-0.47	0 100 100	2, 2, 2, 10	0
1	S	162/162 (100%)	-0.43	1 (0%) 89 71	2, 2, 2, 10	0
1	U	162/162 (100%)	-0.56	0 100 100	2, 2, 2, 10	0
1	W	162/162 (100%)	-0.60	0 100 100	2, 2, 2, 10	0
2	B	172/172 (100%)	-0.42	0 100 100	2, 2, 2, 11	0
2	F	172/172 (100%)	-0.59	0 100 100	2, 2, 2, 11	0
2	H	172/172 (100%)	-0.54	0 100 100	2, 2, 2, 11	0
2	J	172/172 (100%)	-0.54	0 100 100	2, 2, 2, 11	0
2	L	172/172 (100%)	-0.59	0 100 100	2, 2, 2, 11	0
2	N	172/172 (100%)	-0.43	0 100 100	2, 2, 2, 11	0
2	P	172/172 (100%)	-0.47	0 100 100	2, 2, 2, 11	0
2	R	172/172 (100%)	-0.48	0 100 100	2, 2, 2, 11	0
2	T	172/172 (100%)	-0.51	0 100 100	2, 2, 2, 11	0
2	V	172/172 (100%)	-0.39	0 100 100	2, 2, 2, 11	0
2	X	172/172 (100%)	-0.51	0 100 100	2, 2, 2, 11	0
3	D	172/172 (100%)	-0.43	0 100 100	2, 2, 2, 11	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4008/4008 (100%)	-0.53	3 (0%) 95 88	2, 2, 2, 11	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	162	SER	2.3
1	E	162	SER	2.1
1	S	71	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
4	CYC	X	184	43/43	0.91	0.20	1.16	2,2,7,10	0
4	CYC	D	184	43/43	0.91	0.21	1.02	2,11,23,26	0
4	CYC	R	184	43/43	0.90	0.20	0.99	2,4,19,24	0
4	CYC	V	184	43/43	0.90	0.23	0.87	7,16,24,29	0
4	CYC	H	184	43/43	0.93	0.19	0.77	2,6,19,28	0
4	CYC	F	184	43/43	0.92	0.19	0.77	2,2,13,15	0
4	CYC	N	255	43/43	0.92	0.22	0.69	2,10,23,28	0
4	CYC	T	184	43/43	0.91	0.19	0.63	2,3,10,15	0
4	CYC	C	184	43/43	0.95	0.17	0.62	2,2,3,4	0
4	CYC	J	184	43/43	0.94	0.18	0.60	2,2,9,10	0
4	CYC	I	184	43/43	0.95	0.17	0.53	2,2,2,3	0
4	CYC	P	184	43/43	0.94	0.18	0.51	2,2,11,18	0
4	CYC	M	184	43/43	0.94	0.17	0.48	2,2,3,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CYC	L	184	43/43	0.93	0.17	0.46	2,5,15,23	0
4	CYC	B	184	43/43	0.91	0.18	0.45	2,3,10,13	0
4	CYC	G	184	43/43	0.96	0.17	0.43	2,2,2,2	0
4	CYC	L	255	43/43	0.94	0.19	0.32	2,2,2,11	0
4	CYC	J	255	43/43	0.93	0.20	0.30	2,2,2,7	0
4	CYC	X	255	43/43	0.94	0.20	0.19	2,2,7,10	0
4	CYC	T	255	43/43	0.95	0.17	0.10	2,2,5,8	0
4	CYC	K	184	43/43	0.95	0.16	0.04	2,2,3,6	0
5	BLA	B	255	43/43	0.93	0.18	0.04	2,4,9,15	0
4	CYC	N	184	43/43	0.92	0.18	0.03	2,5,12,14	0
4	CYC	H	255	43/43	0.95	0.17	0.02	2,2,7,10	0
4	CYC	D	255	43/43	0.94	0.18	-0.05	3,8,17,18	0
4	CYC	O	184	43/43	0.96	0.15	-0.16	2,2,2,2	0
4	CYC	U	184	43/43	0.96	0.15	-0.24	2,2,2,5	0
4	CYC	V	255	43/43	0.93	0.17	-0.25	2,2,10,15	0
4	CYC	W	184	43/43	0.97	0.14	-0.34	2,2,2,2	0
4	CYC	A	184	43/43	0.95	0.15	-0.39	2,2,2,3	0
4	CYC	R	255	43/43	0.95	0.16	-0.41	2,2,7,9	0
4	CYC	P	255	43/43	0.95	0.16	-0.46	2,3,10,11	0
4	CYC	E	184	43/43	0.96	0.14	-0.48	2,2,2,2	0
4	CYC	F	255	43/43	0.96	0.15	-0.48	2,2,2,2	0
4	CYC	Q	184	43/43	0.95	0.15	-0.52	2,2,5,7	0
4	CYC	S	184	43/43	0.95	0.15	-0.59	2,6,11,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.