wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2016 – 06:27 PM EDT

PDB ID	:	5AQD
Title	:	Crystal structure of Phormidium Phycoerythrin at pH 8.5
Authors	:	Kumar, V.; Sharma, M.; Sonani, R.R.; Gupta, G.D.; Madamwar, D.
Deposited on	:	2015-09-22
Resolution	:	2.12 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

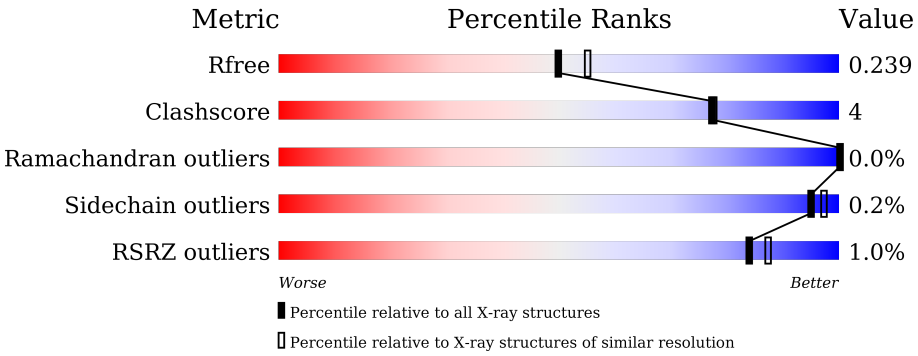
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.12 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}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (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 <=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	164	96% .
1	B	164	93% 7%
1	C	164	91% 9%
1	D	164	98% .
1	E	164	95% 5%
1	F	164	97% .

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Mol	Chain	Length	Quality of chain
1	G	164	96%
1	H	164	95% 5%
1	I	164	96%
1	J	164	95% 5%
1	K	164	93% 7%
1	L	164	93% 7%
2	M	184	2% 92% 8%
2	N	184	2% 96%
2	O	184	2% 95% 5%
2	P	184	% 90% 10%
2	Q	184	3% 91% 9%
2	R	184	2% 92% 8%
2	S	184	2% 96%
2	T	184	3% 93% 7%
2	U	184	% 90% 10%
2	V	184	3% 91% 9%
2	W	184	% 92% 8%
2	X	184	2% 93% 7%

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	PEB	C	167	-	-	-	X
3	PEB	D	167	-	-	-	X
4	GOL	A	1165	-	-	-	X
4	GOL	B	1165	-	-	-	X
4	GOL	C	1165	-	-	-	X
4	GOL	D	1165	-	-	-	X
4	GOL	E	1165	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	1165	-	-	-	X
4	GOL	I	1165	-	-	-	X
4	GOL	K	1165	-	-	-	X
5	SO4	E	1200	-	-	-	X
5	SO4	H	1200	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 37483 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 PHYCOERYTHRIN ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	B	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	C	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	D	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	E	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	F	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	G	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	H	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	I	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	J	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	K	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	L	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
A	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
A	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
A	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
B	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
C	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
C	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
D	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
D	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
E	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
E	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
F	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
F	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
G	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
G	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
H	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
H	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
I	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
I	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
J	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
J	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
K	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
K	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
L	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01

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Chain	Residue	Modelled	Actual	Comment	Reference
L	164	SER	-	SEE REMARK 999	UNP A0A0E3W01

- Molecule 2 is a protein called PHYCOERYTHRIN BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	N	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	O	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	P	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	Q	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	R	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	S	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	T	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	U	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	V	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	W	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	X	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
M	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
M	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
M	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
M	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
M	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
M	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
N	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
N	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

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Chain	Residue	Modelled	Actual	Comment	Reference
N	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
N	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
N	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
N	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
N	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
O	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
O	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
O	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
O	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
O	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
O	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
O	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
P	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
P	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
P	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
P	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
P	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
P	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
P	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
Q	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
Q	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
Q	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
Q	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
Q	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
Q	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
Q	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
R	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
R	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
R	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
R	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
R	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
R	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
R	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
S	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
S	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
S	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
S	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
S	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
S	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
S	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
T	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
T	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

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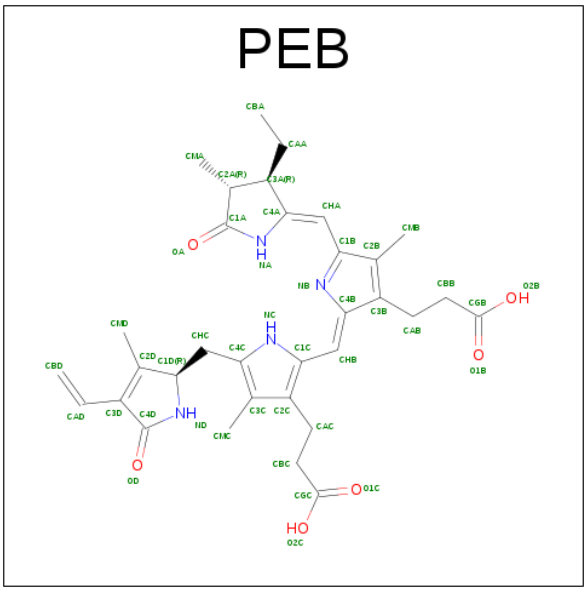
Chain	Residue	Modelled	Actual	Comment	Reference
T	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
T	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
T	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
T	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
T	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
U	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
U	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
U	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
U	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
U	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
U	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
U	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
V	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
V	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
V	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
V	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
V	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
V	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
V	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
W	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
W	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
W	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
W	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
W	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
W	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
W	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
X	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
X	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
X	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
X	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
X	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
X	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
X	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	J	1	Total	C	N	O	0	0
			43	33	4	6		
3	J	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	L	1	Total	C	N	O	0	0
			43	33	4	6		
3	L	1	Total	C	N	O	0	0
			43	33	4	6		
3	M	1	Total	C	N	O	0	0
			43	33	4	6		
3	M	1	Total	C	N	O	0	0
			43	33	4	6		
3	M	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		
3	N	1	Total	C	N	O	0	0
			43	33	4	6		
3	O	1	Total	C	N	O	0	0
			43	33	4	6		
3	O	1	Total	C	N	O	0	0
			43	33	4	6		
3	O	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		

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

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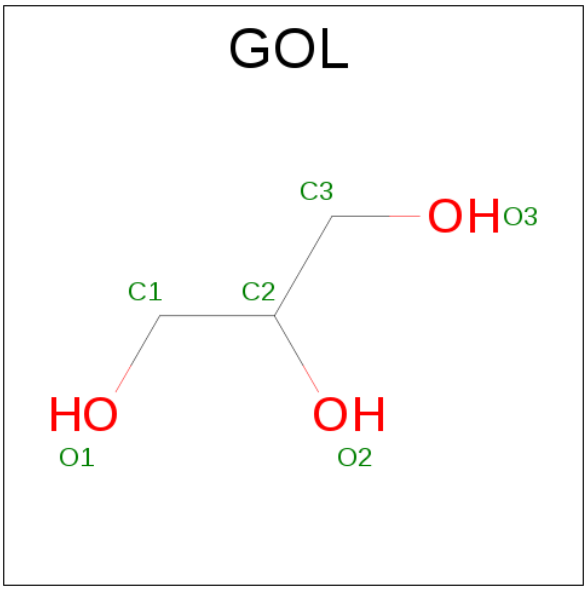
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	O		0	0
			6	3	3			
4	D	1	Total	C	O		0	0
			6	3	3			
4	E	1	Total	C	O		0	0
			6	3	3			
4	F	1	Total	C	O		0	0
			6	3	3			
4	G	1	Total	C	O		0	0
			6	3	3			

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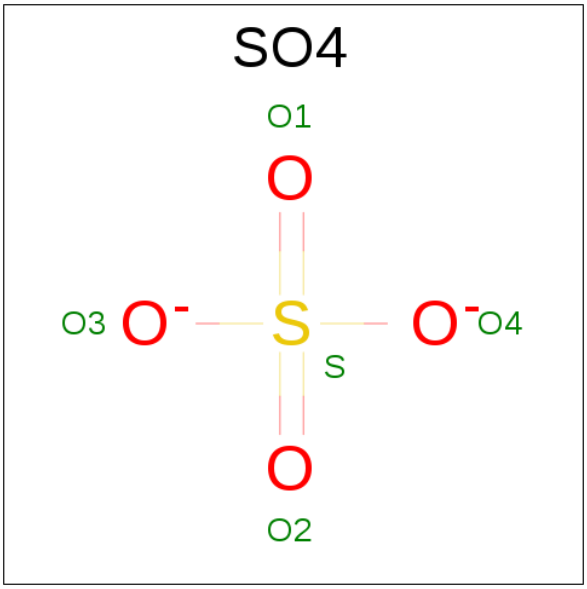
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	U	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	W	1	Total O S 5 4 1	0	0
5	X	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	0
6	B	194	Total O 194 194	0	0
6	C	178	Total O 178 178	0	0
6	D	168	Total O 168 168	0	0
6	E	167	Total O 167 167	0	0
6	F	161	Total O 161 161	0	0
6	G	206	Total O 206 206	0	0

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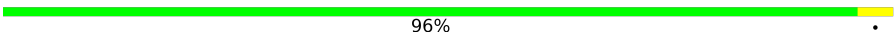
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	208	Total O 208 208	0	0
6	I	188	Total O 188 188	0	0
6	J	163	Total O 163 163	0	0
6	K	133	Total O 133 133	0	0
6	L	148	Total O 148 148	0	0
6	M	149	Total O 149 149	0	0
6	N	140	Total O 140 140	0	0
6	O	121	Total O 121 121	0	0
6	P	144	Total O 144 144	0	0
6	Q	134	Total O 134 134	0	0
6	R	118	Total O 118 118	0	0
6	S	134	Total O 134 134	0	0
6	T	107	Total O 107 107	0	0
6	U	123	Total O 123 123	0	0
6	V	153	Total O 153 153	0	0
6	W	134	Total O 134 134	0	0
6	X	126	Total O 126 126	0	0

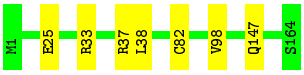
3 Residue-property plots (i)

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.

- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

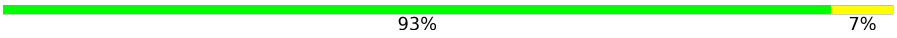
Chain A:

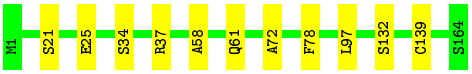




- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain B:



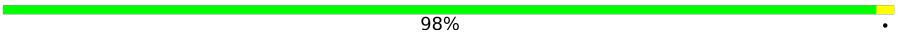


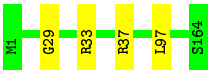
- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain C:

- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

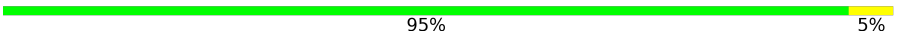
Chain D:

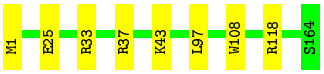




- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

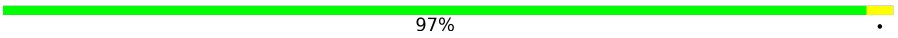
Chain E:

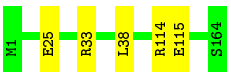




- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

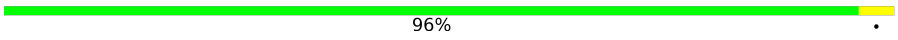
Chain F:





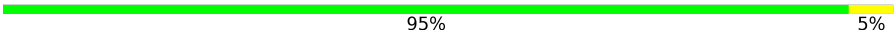
• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain G:



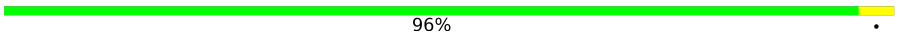
• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain H:



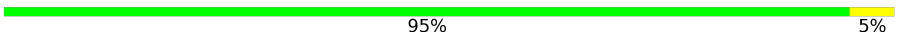
• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain I:



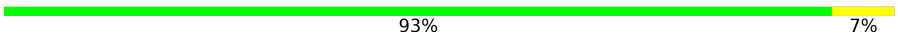
• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain J:



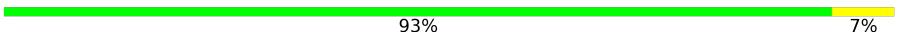
• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

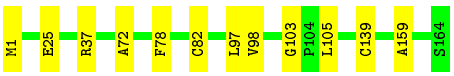
Chain K:



• Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

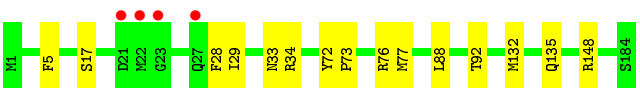
Chain L:





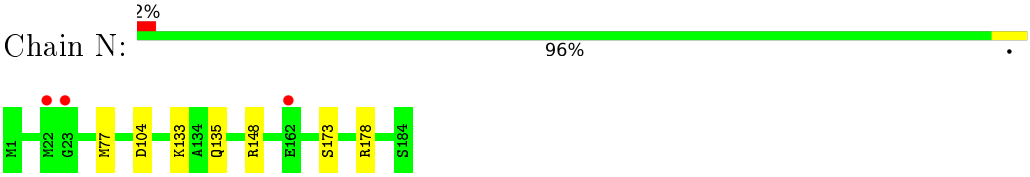
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain M:



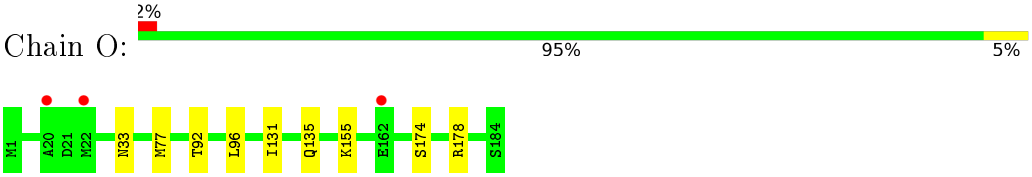
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain N:



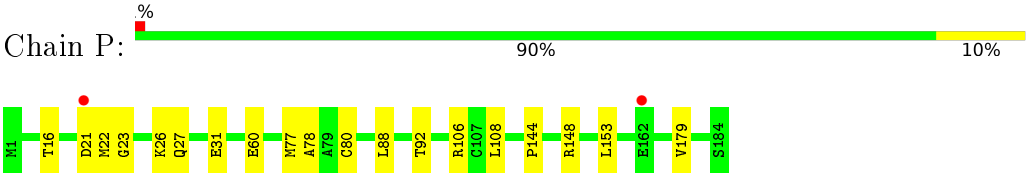
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain O:



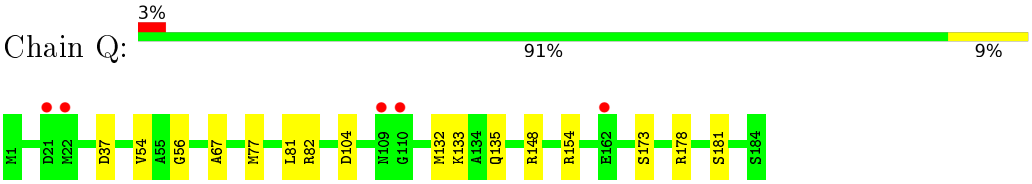
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain P:



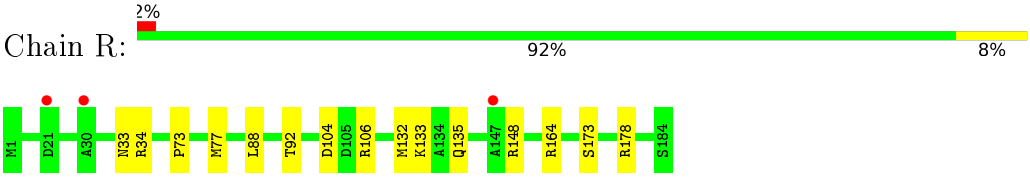
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain Q:



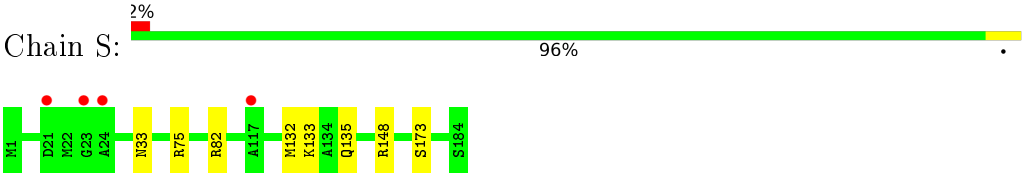
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain R:



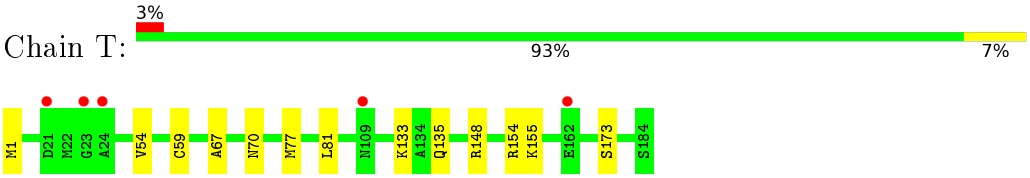
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain S:



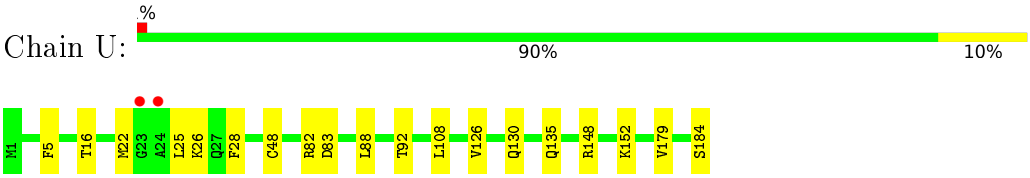
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain T:



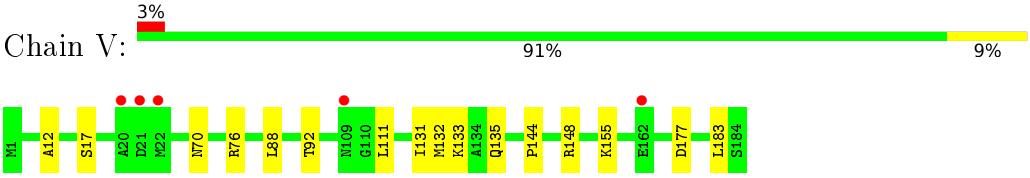
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain U:



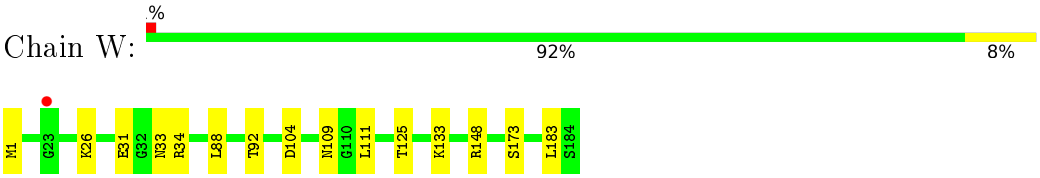
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain V:



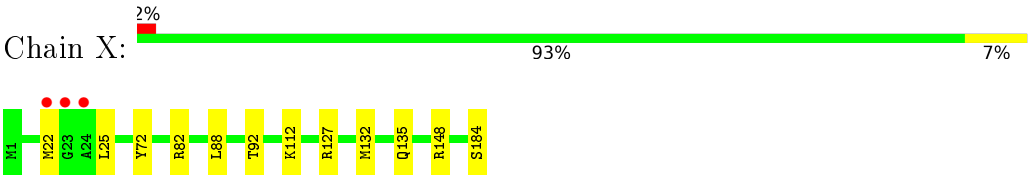
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain W:



• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	108.30Å 108.36Å 116.59Å 78.94° 82.50° 60.34°	Depositor
Resolution (Å)	29.29 – 2.12 29.29 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.29-2.12) 91.2 (29.29-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.239 0.176 , 0.239	Depositor DCC
R_{free} test set	12527 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for h-k,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	37483	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MEN, SO4, PEB

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	0.40	0/1259	0.54	0/1706
1	B	0.41	0/1259	0.54	0/1706
1	C	0.39	0/1259	0.52	0/1706
1	D	0.40	0/1259	0.52	0/1706
1	E	0.39	0/1259	0.51	0/1706
1	F	0.41	0/1259	0.51	0/1706
1	G	0.42	0/1259	0.53	0/1706
1	H	0.40	0/1259	0.52	0/1706
1	I	0.38	0/1259	0.52	0/1706
1	J	0.38	0/1259	0.51	0/1706
1	K	0.38	0/1259	0.52	0/1706
1	L	0.39	0/1259	0.53	0/1706
2	M	0.38	0/1349	0.50	0/1820
2	N	0.38	0/1349	0.50	0/1820
2	O	0.37	0/1349	0.50	0/1820
2	P	0.40	0/1349	0.52	0/1820
2	Q	0.36	0/1349	0.51	0/1820
2	R	0.35	0/1349	0.50	0/1820
2	S	0.36	0/1349	0.50	0/1820
2	T	0.33	0/1349	0.49	0/1820
2	U	0.39	0/1349	0.51	0/1820
2	V	0.38	0/1349	0.50	0/1820
2	W	0.36	0/1349	0.48	0/1820
2	X	0.37	0/1349	0.51	0/1820
All	All	0.38	0/31296	0.51	0/42312

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	1239	0	1221	7	0
1	B	1239	0	1221	10	0
1	C	1239	0	1221	10	0
1	D	1239	0	1221	3	0
1	E	1239	0	1221	10	0
1	F	1239	0	1221	5	0
1	G	1239	0	1221	6	0
1	H	1239	0	1221	6	0
1	I	1239	0	1221	5	0
1	J	1239	0	1221	7	0
1	K	1239	0	1221	10	0
1	L	1239	0	1221	8	0
2	M	1347	0	1359	10	0
2	N	1347	0	1359	6	0
2	O	1347	0	1359	7	0
2	P	1347	0	1359	15	0
2	Q	1347	0	1359	12	0
2	R	1347	0	1359	11	0
2	S	1347	0	1359	7	0
2	T	1347	0	1359	12	0
2	U	1347	0	1359	14	0
2	V	1347	0	1359	10	0
2	W	1347	0	1359	9	0
2	X	1347	0	1359	8	0
3	A	86	0	74	2	0
3	B	86	0	74	2	0
3	C	86	0	74	4	0
3	D	86	0	73	2	0
3	E	86	0	74	7	0
3	F	86	0	74	1	0
3	G	86	0	74	3	0
3	H	86	0	74	3	0
3	I	86	0	74	3	0
3	J	86	0	74	4	0
3	K	86	0	74	3	0
3	L	86	0	74	2	0
3	M	129	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	110	6	0
3	O	129	0	110	6	0
3	P	129	0	110	8	0
3	Q	129	0	110	12	0
3	R	129	0	110	6	0
3	S	129	0	110	7	0
3	T	129	0	110	8	0
3	U	129	0	110	9	0
3	V	129	0	109	6	0
3	W	129	0	110	6	0
3	X	129	0	110	4	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	1	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	0	0
4	L	6	0	8	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	0	0
5	I	5	0	0	1	0
5	L	5	0	0	0	0
5	M	5	0	0	0	0
5	N	5	0	0	0	0
5	O	5	0	0	0	0
5	P	5	0	0	1	0
5	Q	5	0	0	0	0
5	R	5	0	0	1	0
5	S	5	0	0	0	0
5	T	5	0	0	0	0
5	U	5	0	0	0	0
5	V	5	0	0	0	0
5	W	5	0	0	0	0
5	X	5	0	0	0	0
6	A	212	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	194	0	0	1	0
6	C	178	0	0	0	0
6	D	168	0	0	0	0
6	E	167	0	0	1	0
6	F	161	0	0	0	0
6	G	206	0	0	0	0
6	H	208	0	0	1	0
6	I	188	0	0	0	0
6	J	163	0	0	0	0
6	K	133	0	0	2	0
6	L	148	0	0	0	0
6	M	149	0	0	1	0
6	N	140	0	0	0	0
6	O	121	0	0	0	0
6	P	144	0	0	0	0
6	Q	134	0	0	0	0
6	R	118	0	0	1	0
6	S	134	0	0	1	0
6	T	107	0	0	0	0
6	U	123	0	0	0	0
6	V	153	0	0	0	0
6	W	134	0	0	0	0
6	X	126	0	0	0	0
All	All	37483	0	33262	247	0

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 4.

The worst 5 of 247 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:P:16:THR:HG23	2:Q:67:ALA:HB2	1.66	0.77
2:T:54:VAL:HG21	2:T:81:LEU:HD23	1.72	0.72
2:X:22:MET:HG2	2:X:25:LEU:HD12	1.72	0.71
2:M:88:LEU:O	2:M:92:THR:HG23	1.98	0.64
3:Q:186:PEB:HNA	3:Q:186:PEB:HMB2	1.63	0.63

There are no symmetry-related clashes.

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	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	B	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	C	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	D	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	E	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	F	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	G	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	H	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	I	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	J	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	K	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	L	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	M	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	30	24
2	N	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
2	O	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	P	181/184 (98%)	175 (97%)	5 (3%)	1 (1%)	30	24
2	Q	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
2	R	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
2	S	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
2	T	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
2	U	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	V	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	W	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	X	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
All	All	4116/4176 (99%)	4018 (98%)	96 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	23	GLY
2	M	73	PRO

5.3.2 Protein sidechains (i)

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	127/127 (100%)	127 (100%)	0	100	100
1	B	127/127 (100%)	127 (100%)	0	100	100
1	C	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	D	127/127 (100%)	127 (100%)	0	100	100
1	E	127/127 (100%)	127 (100%)	0	100	100
1	F	127/127 (100%)	127 (100%)	0	100	100
1	G	127/127 (100%)	127 (100%)	0	100	100
1	H	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	I	127/127 (100%)	127 (100%)	0	100	100
1	J	127/127 (100%)	127 (100%)	0	100	100
1	K	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	L	127/127 (100%)	127 (100%)	0	100	100
2	M	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	N	138/138 (100%)	138 (100%)	0	100	100
2	O	138/138 (100%)	138 (100%)	0	100	100
2	P	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	Q	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	R	138/138 (100%)	138 (100%)	0	100	100
2	S	138/138 (100%)	138 (100%)	0	100	100
2	T	138/138 (100%)	138 (100%)	0	100	100
2	U	138/138 (100%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	V	138/138 (100%)	138 (100%)	0	100 100
2	W	138/138 (100%)	137 (99%)	1 (1%)	88 92
2	X	138/138 (100%)	138 (100%)	0	100 100
All	All	3180/3180 (100%)	3173 (100%)	7 (0%)	95 97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	17	SER
2	W	26	LYS
2	P	21	ASP
1	H	30	SER
2	Q	181	SER

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

12 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	M	70	2	6,8,9	0.51	0	6,9,11	1.25	1 (16%)
2	MEN	N	70	2	6,8,9	0.44	0	6,9,11	1.25	1 (16%)
2	MEN	O	70	2	6,8,9	0.55	0	6,9,11	1.13	1 (16%)
2	MEN	P	70	2	6,8,9	0.46	0	6,9,11	1.07	1 (16%)
2	MEN	Q	70	2	6,8,9	0.53	0	6,9,11	1.27	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MEN	R	70	2	6,8,9	0.46	0	6,9,11	1.16	1 (16%)
2	MEN	S	70	2	6,8,9	0.57	0	6,9,11	1.06	1 (16%)
2	MEN	T	70	2	6,8,9	0.48	0	6,9,11	1.17	1 (16%)
2	MEN	U	70	2	6,8,9	0.53	0	6,9,11	1.08	1 (16%)
2	MEN	V	70	2	6,8,9	0.63	0	6,9,11	1.17	1 (16%)
2	MEN	W	70	2	6,8,9	0.43	0	6,9,11	1.12	1 (16%)
2	MEN	X	70	2	6,8,9	0.44	0	6,9,11	1.16	1 (16%)

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	M	70	2	-	0/6/8/10	0/0/0/0
2	MEN	N	70	2	-	0/6/8/10	0/0/0/0
2	MEN	O	70	2	-	0/6/8/10	0/0/0/0
2	MEN	P	70	2	-	0/6/8/10	0/0/0/0
2	MEN	Q	70	2	-	0/6/8/10	0/0/0/0
2	MEN	R	70	2	-	0/6/8/10	0/0/0/0
2	MEN	S	70	2	-	0/6/8/10	0/0/0/0
2	MEN	T	70	2	-	0/6/8/10	0/0/0/0
2	MEN	U	70	2	-	0/6/8/10	0/0/0/0
2	MEN	V	70	2	-	0/6/8/10	0/0/0/0
2	MEN	W	70	2	-	0/6/8/10	0/0/0/0
2	MEN	X	70	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	70	MEN	O-C-CA	-3.03	117.61	125.72
2	N	70	MEN	O-C-CA	-3.00	117.68	125.72
2	M	70	MEN	O-C-CA	-2.98	117.72	125.72
2	R	70	MEN	O-C-CA	-2.83	118.14	125.72
2	T	70	MEN	O-C-CA	-2.77	118.29	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	70	MEN	1	0
2	V	70	MEN	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

90 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	GOL	A	1165	-	5,5,5	0.23	0	5,5,5	0.53	0
5	SO4	A	1200	-	4,4,4	0.16	0	6,6,6	0.14	0
3	PEB	A	166	1	37,46,46	3.47	10 (27%)	36,67,67	2.76	19 (52%)
3	PEB	A	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	15 (41%)
4	GOL	B	1165	-	5,5,5	0.31	0	5,5,5	0.50	0
3	PEB	B	166	1	37,46,46	3.44	10 (27%)	36,67,67	2.66	17 (47%)
3	PEB	B	167	1	37,46,46	3.38	11 (29%)	36,67,67	2.32	16 (44%)
4	GOL	C	1165	-	5,5,5	0.32	0	5,5,5	0.27	0
3	PEB	C	166	1	37,46,46	3.39	9 (24%)	36,67,67	2.68	19 (52%)
3	PEB	C	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	14 (38%)
4	GOL	D	1165	-	5,5,5	0.28	0	5,5,5	0.42	0
5	SO4	D	1200	-	4,4,4	0.29	0	6,6,6	0.11	0
3	PEB	D	166	1	37,46,46	3.47	10 (27%)	36,67,67	2.60	18 (50%)
3	PEB	D	167	1	37,46,46	3.39	11 (29%)	36,67,67	2.67	17 (47%)
4	GOL	E	1165	-	5,5,5	0.25	0	5,5,5	0.43	0
5	SO4	E	1200	-	4,4,4	0.24	0	6,6,6	0.16	0
3	PEB	E	166	1	37,46,46	3.44	10 (27%)	36,67,67	2.58	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEB	E	167	1	37,46,46	3.45	11 (29%)	36,67,67	2.33	16 (44%)
4	GOL	F	1165	-	5,5,5	0.30	0	5,5,5	0.36	0
3	PEB	F	166	1	37,46,46	3.24	9 (24%)	36,67,67	2.74	16 (44%)
3	PEB	F	167	1	37,46,46	3.56	9 (24%)	36,67,67	2.18	13 (36%)
4	GOL	G	1165	-	5,5,5	0.26	0	5,5,5	0.35	0
3	PEB	G	166	1	37,46,46	3.26	9 (24%)	36,67,67	2.73	15 (41%)
3	PEB	G	167	1	37,46,46	3.49	11 (29%)	36,67,67	2.23	14 (38%)
4	GOL	H	1165	-	5,5,5	0.37	0	5,5,5	0.50	0
5	SO4	H	1200	-	4,4,4	0.25	0	6,6,6	0.14	0
3	PEB	H	166	1	37,46,46	3.44	11 (29%)	36,67,67	2.62	17 (47%)
3	PEB	H	167	1	37,46,46	3.38	11 (29%)	36,67,67	2.29	16 (44%)
4	GOL	I	1165	-	5,5,5	0.31	0	5,5,5	0.31	0
5	SO4	I	1200	-	4,4,4	0.19	0	6,6,6	0.25	0
3	PEB	I	166	1	37,46,46	3.48	11 (29%)	36,67,67	2.65	16 (44%)
3	PEB	I	167	1	37,46,46	3.35	11 (29%)	36,67,67	2.65	17 (47%)
4	GOL	J	1165	-	5,5,5	0.33	0	5,5,5	0.40	0
3	PEB	J	166	1	37,46,46	3.54	10 (27%)	36,67,67	2.65	15 (41%)
3	PEB	J	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	14 (38%)
4	GOL	K	1165	-	5,5,5	0.33	0	5,5,5	0.34	0
3	PEB	K	166	1	37,46,46	3.35	11 (29%)	36,67,67	2.81	17 (47%)
3	PEB	K	167	1	37,46,46	3.37	12 (32%)	36,67,67	2.33	16 (44%)
4	GOL	L	1165	-	5,5,5	0.33	0	5,5,5	0.31	0
5	SO4	L	1200	-	4,4,4	0.21	0	6,6,6	0.25	0
3	PEB	L	166	1	37,46,46	3.37	9 (24%)	36,67,67	2.74	16 (44%)
3	PEB	L	167	1	37,46,46	3.24	9 (24%)	36,67,67	2.35	15 (41%)
3	PEB	M	186	2	37,46,46	3.48	9 (24%)	36,67,67	2.46	16 (44%)
3	PEB	M	187	2	37,46,46	3.31	9 (24%)	36,67,67	2.41	13 (36%)
3	PEB	M	188	2	37,46,46	3.54	11 (29%)	36,67,67	2.32	16 (44%)
5	SO4	M	189	-	4,4,4	0.17	0	6,6,6	0.18	0
3	PEB	N	186	2	37,46,46	3.48	11 (29%)	36,67,67	2.43	13 (36%)
3	PEB	N	187	2	37,46,46	3.46	10 (27%)	36,67,67	2.25	14 (38%)
3	PEB	N	188	2	37,46,46	3.41	8 (21%)	36,67,67	2.33	14 (38%)
5	SO4	N	189	-	4,4,4	0.11	0	6,6,6	0.14	0
3	PEB	O	186	2	37,46,46	3.44	11 (29%)	36,67,67	2.56	16 (44%)
3	PEB	O	187	2	37,46,46	3.37	10 (27%)	36,67,67	2.15	14 (38%)
3	PEB	O	188	2	37,46,46	3.44	10 (27%)	36,67,67	2.35	16 (44%)
5	SO4	O	189	-	4,4,4	0.11	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEB	P	186	2	37,46,46	3.50	9 (24%)	36,67,67	2.37	17 (47%)
3	PEB	P	187	2	37,46,46	3.46	9 (24%)	36,67,67	2.23	16 (44%)
3	PEB	P	188	2	37,46,46	3.47	10 (27%)	36,67,67	2.26	16 (44%)
5	SO4	P	189	-	4,4,4	0.11	0	6,6,6	0.15	0
3	PEB	Q	186	2	37,46,46	3.44	10 (27%)	36,67,67	2.46	15 (41%)
3	PEB	Q	187	2	37,46,46	3.61	11 (29%)	36,67,67	2.34	15 (41%)
3	PEB	Q	188	2	37,46,46	3.52	10 (27%)	36,67,67	2.24	13 (36%)
5	SO4	Q	189	-	4,4,4	0.11	0	6,6,6	0.22	0
3	PEB	R	186	2	37,46,46	3.55	10 (27%)	36,67,67	2.31	15 (41%)
3	PEB	R	187	2	37,46,46	3.35	10 (27%)	36,67,67	2.34	14 (38%)
3	PEB	R	188	2	37,46,46	3.49	10 (27%)	36,67,67	2.33	16 (44%)
5	SO4	R	189	-	4,4,4	0.12	0	6,6,6	0.17	0
3	PEB	S	186	2	37,46,46	3.57	9 (24%)	36,67,67	2.40	14 (38%)
3	PEB	S	187	2	37,46,46	3.43	10 (27%)	36,67,67	2.28	16 (44%)
3	PEB	S	188	2	37,46,46	3.54	11 (29%)	36,67,67	2.25	16 (44%)
5	SO4	S	189	-	4,4,4	0.10	0	6,6,6	0.13	0
3	PEB	T	186	2	37,46,46	3.39	10 (27%)	36,67,67	2.66	16 (44%)
3	PEB	T	187	2	37,46,46	3.41	10 (27%)	36,67,67	2.32	16 (44%)
3	PEB	T	188	2	37,46,46	3.57	10 (27%)	36,67,67	2.27	15 (41%)
5	SO4	T	189	-	4,4,4	0.19	0	6,6,6	0.08	0
3	PEB	U	186	2	37,46,46	3.61	10 (27%)	36,67,67	2.53	13 (36%)
3	PEB	U	187	2	37,46,46	3.47	9 (24%)	36,67,67	2.42	16 (44%)
3	PEB	U	188	2	37,46,46	3.47	10 (27%)	36,67,67	2.28	16 (44%)
5	SO4	U	189	-	4,4,4	0.09	0	6,6,6	0.19	0
3	PEB	V	186	2	37,46,46	3.40	11 (29%)	36,67,67	2.64	17 (47%)
3	PEB	V	187	2	37,46,46	3.42	11 (29%)	36,67,67	2.39	16 (44%)
3	PEB	V	188	2	37,46,46	3.50	12 (32%)	36,67,67	2.20	16 (44%)
5	SO4	V	189	-	4,4,4	0.11	0	6,6,6	0.25	0
3	PEB	W	186	2	37,46,46	3.49	9 (24%)	36,67,67	2.35	15 (41%)
3	PEB	W	187	2	37,46,46	3.31	10 (27%)	36,67,67	2.36	15 (41%)
3	PEB	W	188	2	37,46,46	3.49	8 (21%)	36,67,67	2.10	15 (41%)
5	SO4	W	189	-	4,4,4	0.06	0	6,6,6	0.18	0
3	PEB	X	186	2	37,46,46	3.44	9 (24%)	36,67,67	2.47	15 (41%)
3	PEB	X	187	2	37,46,46	3.35	11 (29%)	36,67,67	2.35	15 (41%)
3	PEB	X	188	2	37,46,46	3.56	10 (27%)	36,67,67	2.30	17 (47%)
5	SO4	X	189	-	4,4,4	0.17	0	6,6,6	0.14	0

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	GOL	A	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	A	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	A	166	1	-	2/19/74/74	0/4/4/4
3	PEB	A	167	1	-	2/19/74/74	0/4/4/4
4	GOL	B	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	B	166	1	-	2/19/74/74	0/4/4/4
3	PEB	B	167	1	-	2/19/74/74	0/4/4/4
4	GOL	C	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	C	166	1	-	2/19/74/74	0/4/4/4
3	PEB	C	167	1	-	2/19/74/74	0/4/4/4
4	GOL	D	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	D	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	D	166	1	-	2/19/74/74	0/4/4/4
3	PEB	D	167	1	-	2/19/74/74	0/4/4/4
4	GOL	E	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	E	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	E	166	1	-	2/19/74/74	0/4/4/4
3	PEB	E	167	1	-	2/19/74/74	0/4/4/4
4	GOL	F	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	F	166	1	-	2/19/74/74	0/4/4/4
3	PEB	F	167	1	-	2/19/74/74	0/4/4/4
4	GOL	G	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	G	166	1	-	2/19/74/74	0/4/4/4
3	PEB	G	167	1	-	2/19/74/74	0/4/4/4
4	GOL	H	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	H	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	H	166	1	-	2/19/74/74	0/4/4/4
3	PEB	H	167	1	-	2/19/74/74	0/4/4/4
4	GOL	I	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	I	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	I	166	1	-	2/19/74/74	0/4/4/4
3	PEB	I	167	1	-	2/19/74/74	0/4/4/4
4	GOL	J	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	J	166	1	-	2/19/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	J	167	1	-	2/19/74/74	0/4/4/4
4	GOL	K	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	K	166	1	-	2/19/74/74	0/4/4/4
3	PEB	K	167	1	-	2/19/74/74	0/4/4/4
4	GOL	L	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	L	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	L	166	1	-	2/19/74/74	0/4/4/4
3	PEB	L	167	1	-	2/19/74/74	0/4/4/4
3	PEB	M	186	2	-	2/19/74/74	0/4/4/4
3	PEB	M	187	2	-	2/19/74/74	0/4/4/4
3	PEB	M	188	2	-	2/19/74/74	0/4/4/4
5	SO4	M	189	-	-	0/0/0/0	0/0/0/0
3	PEB	N	186	2	-	2/19/74/74	0/4/4/4
3	PEB	N	187	2	-	2/19/74/74	0/4/4/4
3	PEB	N	188	2	-	2/19/74/74	0/4/4/4
5	SO4	N	189	-	-	0/0/0/0	0/0/0/0
3	PEB	O	186	2	-	2/19/74/74	0/4/4/4
3	PEB	O	187	2	-	2/19/74/74	0/4/4/4
3	PEB	O	188	2	-	2/19/74/74	0/4/4/4
5	SO4	O	189	-	-	0/0/0/0	0/0/0/0
3	PEB	P	186	2	-	2/19/74/74	0/4/4/4
3	PEB	P	187	2	-	2/19/74/74	0/4/4/4
3	PEB	P	188	2	-	2/19/74/74	0/4/4/4
5	SO4	P	189	-	-	0/0/0/0	0/0/0/0
3	PEB	Q	186	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	187	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	188	2	-	2/19/74/74	0/4/4/4
5	SO4	Q	189	-	-	0/0/0/0	0/0/0/0
3	PEB	R	186	2	-	2/19/74/74	0/4/4/4
3	PEB	R	187	2	-	2/19/74/74	0/4/4/4
3	PEB	R	188	2	-	2/19/74/74	0/4/4/4
5	SO4	R	189	-	-	0/0/0/0	0/0/0/0
3	PEB	S	186	2	-	2/19/74/74	0/4/4/4
3	PEB	S	187	2	-	2/19/74/74	0/4/4/4
3	PEB	S	188	2	-	2/19/74/74	0/4/4/4
5	SO4	S	189	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	T	186	2	-	2/19/74/74	0/4/4/4
3	PEB	T	187	2	-	2/19/74/74	0/4/4/4
3	PEB	T	188	2	-	2/19/74/74	0/4/4/4
5	SO4	T	189	-	-	0/0/0/0	0/0/0/0
3	PEB	U	186	2	-	2/19/74/74	0/4/4/4
3	PEB	U	187	2	-	2/19/74/74	0/4/4/4
3	PEB	U	188	2	-	2/19/74/74	0/4/4/4
5	SO4	U	189	-	-	0/0/0/0	0/0/0/0
3	PEB	V	186	2	-	2/19/74/74	0/4/4/4
3	PEB	V	187	2	-	2/19/74/74	0/4/4/4
3	PEB	V	188	2	-	2/19/74/74	0/4/4/4
5	SO4	V	189	-	-	0/0/0/0	0/0/0/0
3	PEB	W	186	2	-	2/19/74/74	0/4/4/4
3	PEB	W	187	2	-	2/19/74/74	0/4/4/4
3	PEB	W	188	2	-	2/19/74/74	0/4/4/4
5	SO4	W	189	-	-	0/0/0/0	0/0/0/0
3	PEB	X	186	2	-	2/19/74/74	0/4/4/4
3	PEB	X	187	2	-	2/19/74/74	0/4/4/4
3	PEB	X	188	2	-	2/19/74/74	0/4/4/4
5	SO4	X	189	-	-	0/0/0/0	0/0/0/0

The worst 5 of 603 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	166	PEB	C2A-C1A	-4.42	1.47	1.52
3	W	187	PEB	C1A-NA	-3.83	1.32	1.37
3	T	188	PEB	C1A-NA	-3.58	1.33	1.37
3	K	167	PEB	C1A-NA	-3.58	1.33	1.37
3	M	187	PEB	C1A-NA	-3.56	1.33	1.37

The worst 5 of 934 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	166	PEB	OA-C1A-C2A	-7.04	120.64	126.30
3	J	166	PEB	OA-C1A-C2A	-6.89	120.76	126.30
3	F	166	PEB	CHA-C1B-NB	-6.81	112.17	124.89
3	K	166	PEB	CHA-C1B-NB	-6.77	112.25	124.89
3	D	167	PEB	CHC-C4C-C3C	-6.66	121.99	130.95

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	167	PEB	C4A-CHA-C1B-C2B
3	L	167	PEB	C4A-CHA-C1B-C2B
3	K	167	PEB	C4A-CHA-C1B-C2B
3	A	167	PEB	C4A-CHA-C1B-C2B
3	J	167	PEB	C4A-CHA-C1B-C2B

There are no ring outliers.

62 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	166	PEB	2	0
3	B	166	PEB	1	0
3	B	167	PEB	1	0
3	C	166	PEB	3	0
3	C	167	PEB	1	0
3	D	166	PEB	2	0
4	E	1165	GOL	1	0
3	E	166	PEB	3	0
3	E	167	PEB	4	0
3	F	166	PEB	1	0
3	G	166	PEB	2	0
3	G	167	PEB	1	0
4	H	1165	GOL	1	0
3	H	166	PEB	2	0
3	H	167	PEB	1	0
5	I	1200	SO4	1	0
3	I	166	PEB	2	0
3	I	167	PEB	1	0
3	J	166	PEB	2	0
3	J	167	PEB	2	0
3	K	166	PEB	2	0
3	K	167	PEB	1	0
3	L	166	PEB	1	0
3	L	167	PEB	1	0
3	M	186	PEB	1	0
3	M	187	PEB	3	0
3	M	188	PEB	1	0
3	N	186	PEB	1	0
3	N	187	PEB	2	0
3	N	188	PEB	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	186	PEB	1	0
3	O	187	PEB	3	0
3	O	188	PEB	2	0
3	P	186	PEB	2	0
3	P	187	PEB	3	0
3	P	188	PEB	3	0
5	P	189	SO4	1	0
3	Q	186	PEB	3	0
3	Q	187	PEB	5	0
3	Q	188	PEB	4	0
3	R	186	PEB	1	0
3	R	187	PEB	2	0
3	R	188	PEB	3	0
5	R	189	SO4	1	0
3	S	186	PEB	2	0
3	S	187	PEB	2	0
3	S	188	PEB	3	0
3	T	186	PEB	2	0
3	T	187	PEB	1	0
3	T	188	PEB	5	0
3	U	186	PEB	4	0
3	U	187	PEB	2	0
3	U	188	PEB	3	0
3	V	186	PEB	2	0
3	V	187	PEB	1	0
3	V	188	PEB	3	0
3	W	186	PEB	1	0
3	W	187	PEB	3	0
3	W	188	PEB	2	0
3	X	186	PEB	2	0
3	X	187	PEB	1	0
3	X	188	PEB	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, 95^{th} 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	164/164 (100%)	-0.41	0	100	100	8, 13, 20, 27	0
1	B	164/164 (100%)	-0.45	0	100	100	8, 14, 22, 27	0
1	C	164/164 (100%)	-0.45	0	100	100	10, 16, 23, 31	0
1	D	164/164 (100%)	-0.39	0	100	100	8, 14, 24, 30	0
1	E	164/164 (100%)	-0.44	0	100	100	9, 14, 23, 29	0
1	F	164/164 (100%)	-0.40	0	100	100	10, 15, 22, 33	0
1	G	164/164 (100%)	-0.44	0	100	100	9, 14, 21, 29	0
1	H	164/164 (100%)	-0.49	0	100	100	9, 14, 21, 28	0
1	I	164/164 (100%)	-0.38	0	100	100	9, 15, 26, 33	0
1	J	164/164 (100%)	-0.47	0	100	100	11, 15, 23, 29	0
1	K	164/164 (100%)	-0.41	0	100	100	10, 16, 25, 30	0
1	L	164/164 (100%)	-0.37	0	100	100	9, 14, 23, 28	0
2	M	183/184 (99%)	-0.39	4 (2%)	65	71	8, 14, 29, 53	0
2	N	183/184 (99%)	-0.31	3 (1%)	74	79	9, 16, 29, 41	0
2	O	183/184 (99%)	-0.25	3 (1%)	74	79	10, 18, 30, 42	0
2	P	183/184 (99%)	-0.31	2 (1%)	82	86	6, 14, 29, 52	0
2	Q	183/184 (99%)	-0.22	5 (2%)	58	65	9, 17, 30, 47	0
2	R	183/184 (99%)	-0.24	3 (1%)	74	79	12, 19, 34, 54	0
2	S	183/184 (99%)	-0.24	4 (2%)	65	71	10, 16, 30, 55	0
2	T	183/184 (99%)	-0.10	5 (2%)	58	65	13, 21, 36, 49	0
2	U	183/184 (99%)	-0.33	2 (1%)	82	86	8, 14, 28, 42	0
2	V	183/184 (99%)	-0.34	5 (2%)	58	65	9, 15, 29, 48	0
2	W	183/184 (99%)	-0.29	1 (0%)	91	93	10, 17, 31, 50	0
2	X	183/184 (99%)	-0.34	3 (1%)	74	79	9, 15, 28, 47	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4164/4176 (99%)	-0.35	40 (0%)	84	87	6, 15, 27, 55	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	21	ASP	3.6
2	W	23	GLY	3.6
2	M	21	ASP	3.5
2	P	21	ASP	3.4
2	M	23	GLY	3.2

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, 95^{th} 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	R	70	9/10	0.97	0.06	-	16,17,19,23	0
2	MEN	T	70	9/10	0.98	0.07	-	18,21,23,24	0
2	MEN	W	70	9/10	0.96	0.09	-	8,11,14,16	0
2	MEN	V	70	9/10	0.98	0.07	-	13,14,17,18	0
2	MEN	Q	70	9/10	0.97	0.09	-	14,17,20,21	0
2	MEN	X	70	9/10	0.98	0.09	-	8,13,16,16	0
2	MEN	M	70	9/10	0.98	0.09	-	10,12,13,16	0
2	MEN	U	70	9/10	0.97	0.07	-	9,11,13,15	0
2	MEN	O	70	9/10	0.96	0.07	-	12,16,17,20	0
2	MEN	N	70	9/10	0.96	0.09	-	10,13,17,18	0
2	MEN	P	70	9/10	0.96	0.07	-	8,11,17,17	0
2	MEN	S	70	9/10	0.95	0.08	-	9,14,17,17	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, 95^{th} 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	GOL	K	1165	6/6	0.93	0.14	6.75	15,25,26,29	0
4	GOL	E	1165	6/6	0.87	0.22	4.88	25,30,33,37	0
4	GOL	I	1165	6/6	0.85	0.20	4.51	24,28,28,33	0
4	GOL	A	1165	6/6	0.95	0.16	4.22	21,23,25,30	0
3	PEB	C	167	43/43	0.92	0.13	4.00	11,19,26,27	0
5	SO4	H	1200	5/5	0.97	0.14	3.77	21,26,33,36	0
4	GOL	H	1165	6/6	0.86	0.18	3.69	25,28,33,36	0
4	GOL	D	1165	6/6	0.84	0.17	3.25	23,28,31,35	0
4	GOL	C	1165	6/6	0.87	0.15	2.68	25,27,32,34	0
5	SO4	E	1200	5/5	0.97	0.13	2.20	18,18,30,38	0
4	GOL	B	1165	6/6	0.89	0.13	2.02	16,23,31,33	0
3	PEB	D	167	43/43	0.90	0.13	2.00	12,18,26,35	0
4	GOL	F	1165	6/6	0.90	0.14	2.00	27,29,31,37	0
4	GOL	G	1165	6/6	0.82	0.13	1.95	27,30,31,37	0
3	PEB	B	167	43/43	0.94	0.13	1.84	10,18,28,31	0
3	PEB	J	167	43/43	0.91	0.13	1.62	10,21,29,32	0
3	PEB	X	186	43/43	0.92	0.13	1.58	8,14,24,41	0
4	GOL	L	1165	6/6	0.89	0.14	1.55	22,28,33,34	0
4	GOL	J	1165	6/6	0.92	0.10	1.45	18,24,27,27	0
3	PEB	I	167	43/43	0.89	0.14	1.36	12,18,23,26	0
3	PEB	K	167	43/43	0.90	0.15	1.32	15,24,29,32	0
3	PEB	N	186	43/43	0.93	0.13	1.15	7,15,23,35	0
3	PEB	M	186	43/43	0.92	0.11	1.06	8,14,23,45	0
5	SO4	I	1200	5/5	0.97	0.11	1.03	24,31,37,38	0
3	PEB	K	166	43/43	0.94	0.10	1.02	8,12,17,21	0
3	PEB	U	186	43/43	0.92	0.13	1.01	9,13,24,33	0
3	PEB	C	166	43/43	0.94	0.10	0.97	7,13,17,28	0
3	PEB	P	186	43/43	0.91	0.13	0.96	9,14,24,34	0
5	SO4	D	1200	5/5	0.98	0.11	0.91	20,26,34,34	0
3	PEB	R	186	43/43	0.92	0.11	0.90	9,17,25,32	0
3	PEB	V	186	43/43	0.89	0.12	0.88	8,17,28,36	0
3	PEB	A	167	43/43	0.93	0.11	0.84	8,15,21,28	0
5	SO4	L	1200	5/5	0.96	0.10	0.83	20,24,32,35	0
3	PEB	G	166	43/43	0.94	0.10	0.75	7,10,15,19	0
3	PEB	W	186	43/43	0.93	0.12	0.73	8,15,23,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PEB	Q	186	43/43	0.90	0.13	0.70	12,17,25,38	0
3	PEB	O	186	43/43	0.90	0.11	0.69	7,17,27,37	0
3	PEB	T	186	43/43	0.91	0.13	0.65	14,22,29,37	0
3	PEB	R	187	43/43	0.88	0.15	0.65	12,20,31,40	0
3	PEB	A	166	43/43	0.95	0.10	0.64	8,12,16,20	0
3	PEB	B	166	43/43	0.95	0.09	0.64	6,10,14,18	0
3	PEB	H	166	43/43	0.93	0.11	0.63	9,14,20,25	0
3	PEB	S	186	43/43	0.91	0.12	0.59	10,16,27,38	0
3	PEB	E	166	43/43	0.94	0.11	0.58	8,15,19,30	0
3	PEB	P	187	43/43	0.89	0.13	0.49	9,15,27,31	0
3	PEB	S	187	43/43	0.91	0.14	0.48	11,17,26,30	0
3	PEB	G	167	43/43	0.95	0.09	0.48	8,15,20,27	0
3	PEB	U	187	43/43	0.91	0.12	0.42	7,15,25,38	0
3	PEB	L	167	43/43	0.92	0.12	0.40	10,16,25,32	0
3	PEB	F	166	43/43	0.94	0.10	0.40	6,12,15,18	0
3	PEB	W	187	43/43	0.93	0.12	0.39	8,16,25,38	0
3	PEB	Q	187	43/43	0.91	0.13	0.38	7,16,34,39	0
3	PEB	N	188	43/43	0.94	0.10	0.34	9,15,22,25	0
3	PEB	X	187	43/43	0.91	0.12	0.32	8,16,23,34	0
3	PEB	S	188	43/43	0.95	0.10	0.24	9,14,20,25	0
3	PEB	T	187	43/43	0.90	0.13	0.19	11,20,31,35	0
3	PEB	X	188	43/43	0.95	0.10	0.18	10,13,22,24	0
3	PEB	L	166	43/43	0.95	0.09	0.12	7,12,17,18	0
3	PEB	O	188	43/43	0.94	0.11	0.08	10,16,24,31	0
3	PEB	U	188	43/43	0.94	0.10	0.08	8,11,16,28	0
3	PEB	W	188	43/43	0.94	0.10	0.07	9,16,23,24	0
3	PEB	Q	188	43/43	0.94	0.10	0.07	9,16,25,31	0
3	PEB	N	187	43/43	0.92	0.11	0.05	10,15,22,24	0
3	PEB	J	166	43/43	0.95	0.09	0.02	9,13,19,24	0
3	PEB	F	167	43/43	0.95	0.10	-0.04	10,15,19,25	0
3	PEB	I	166	43/43	0.94	0.10	-0.05	11,17,25,28	0
3	PEB	T	188	43/43	0.92	0.11	-0.08	13,22,30,40	0
3	PEB	M	187	43/43	0.92	0.10	-0.09	9,14,20,36	0
3	PEB	E	167	43/43	0.95	0.09	-0.13	11,15,20,24	0
3	PEB	O	187	43/43	0.90	0.12	-0.15	12,20,26,31	0
3	PEB	D	166	43/43	0.94	0.09	-0.16	9,15,22,31	0
3	PEB	V	187	43/43	0.92	0.11	-0.19	13,17,23,25	0
3	PEB	P	188	43/43	0.93	0.10	-0.20	6,12,16,19	0
3	PEB	R	188	43/43	0.93	0.10	-0.28	11,17,21,35	0
3	PEB	V	188	43/43	0.94	0.09	-0.46	8,14,19,23	0
3	PEB	M	188	43/43	0.96	0.08	-0.52	10,13,19,20	0
3	PEB	H	167	43/43	0.96	0.08	-0.56	8,14,17,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	A	1200	5/5	0.97	0.08	-0.96	23,24,34,40	0
5	SO4	S	189	5/5	0.92	0.28	-	32,38,53,56	0
5	SO4	Q	189	5/5	0.87	0.23	-	32,46,54,57	0
5	SO4	W	189	5/5	0.88	0.22	-	25,37,52,54	0
5	SO4	V	189	5/5	0.91	0.27	-	27,31,51,54	0
5	SO4	U	189	5/5	0.81	0.21	-	40,41,51,63	0
5	SO4	N	189	5/5	0.92	0.21	-	28,34,47,52	0
5	SO4	R	189	5/5	0.89	0.23	-	35,51,58,64	0
5	SO4	X	189	5/5	0.96	0.15	-	30,33,43,52	0
5	SO4	T	189	5/5	0.96	0.32	-	42,46,49,60	0
5	SO4	P	189	5/5	0.93	0.20	-	28,35,56,56	0
5	SO4	M	189	5/5	0.92	0.18	-	26,31,38,46	0
5	SO4	O	189	5/5	0.91	0.26	-	30,41,48,58	0

6.5 Other polymers

There are no such residues in this entry.