



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 28, 2018 – 03:38 PM EST

PDB ID : 5NB3  
Title : High resolution C-phycoerythrin from marine cyanobacterium Phormidium sp. A09DM at pH 7.5  
Authors : Sonani, R.R.; Roszak, A.W.; Ortmann de Percin Northumberland, C.; Madamwar, D.; Cogdell, R.J.  
Deposited on : 2017-03-01  
Resolution : 1.38 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

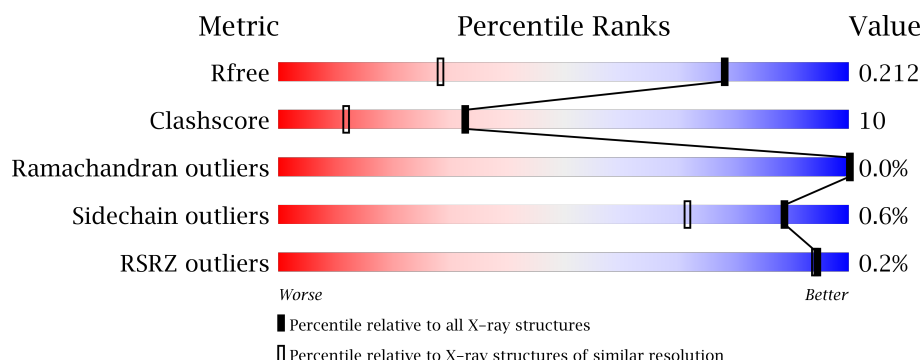
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.38 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.



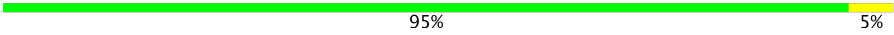
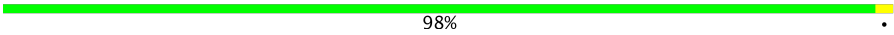
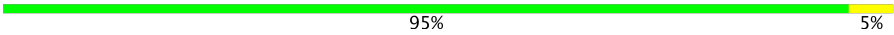
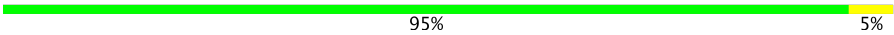
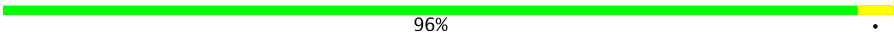
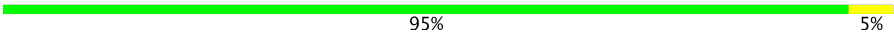
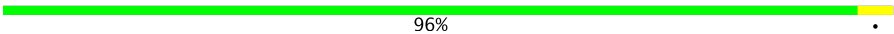
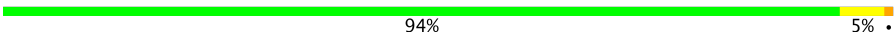




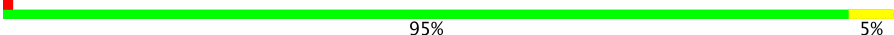



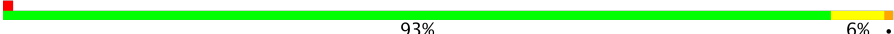

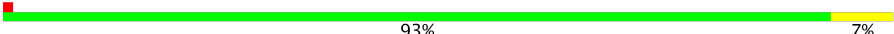
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2133 (1.40-1.36)
Clashscore	112137	2266 (1.40-1.36)
Ramachandran outliers	110173	2215 (1.40-1.36)
Sidechain outliers	110143	2214 (1.40-1.36)
RSRZ outliers	101464	2141 (1.40-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	164	<div> <div>95%</div> <div>5%</div> </div>
1	B	164	<div> <div>96%</div> <div>..</div> </div>
1	C	164	<div> <div>95%</div> <div>5%</div> </div>
1	D	164	<div> <div>94%</div> <div>5%</div> <div>.</div> </div>
1	E	164	<div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	164	 95% 5%
1	G	164	 98% .
1	H	164	 95% 5%
1	I	164	 95% 5%
1	J	164	 96% .
1	K	164	 95% 5%
1	L	164	 96% .
2	M	184	 94% 5% .
2	N	184	 92% 7% .
2	O	184	 .% 91% 9% .
2	P	184	 92% 8%
2	Q	184	 91% 9%
2	R	184	 .% 95% 5%
2	S	184	 .% 93% 7% .
2	T	184	 .% 91% 8% .
2	U	184	 .% 90% 9% .
2	V	184	 .% 93% 6% .
2	W	184	 92% 8%
2	X	184	 .% 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
4	FMT	A	203	-	-	-	X
4	FMT	A	204	-	-	X	X
4	FMT	H	203	-	-	X	-
4	FMT	J	203	-	-	X	X
4	FMT	K	203	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	N	206	-	-	-	X
4	FMT	O	205	-	-	X	X
4	FMT	P	205	-	-	-	X
4	FMT	Q	205	-	-	-	X
4	FMT	U	205	-	-	X	-
4	FMT	V	205	-	-	-	X
4	FMT	V	206	-	-	X	-
4	FMT	W	206	-	-	X	X
5	NA	Q	206	-	-	-	X
6	CL	A	206	-	-	X	X
6	CL	C	205	-	-	-	X
6	CL	I	204	-	-	X	X
6	CL	J	206	-	-	X	X
6	CL	L	204	-	-	X	X
7	MPD	M	204	-	-	X	X
7	MPD	N	204	-	-	X	X
7	MPD	N	205	-	-	X	X
7	MPD	O	204	-	-	-	X
7	MPD	P	204	-	-	-	X
7	MPD	Q	204	-	-	X	X
7	MPD	R	204	-	-	-	X
7	MPD	S	204	-	-	X	X
7	MPD	U	204	-	-	X	X
7	MPD	W	204	-	-	X	X
7	MPD	W	205	-	-	-	X
7	MPD	X	204	-	-	X	X
8	MRD	T	204	-	-	X	X
8	MRD	V	204	-	-	X	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 43181 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,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	10	0
			1298	810	227	254	7			
1	B	164	Total	C	N	O	S	0	10	0
			1304	813	229	255	7			
1	C	164	Total	C	N	O	S	0	8	0
			1287	803	224	253	7			
1	D	164	Total	C	N	O	S	0	9	0
			1293	809	224	253	7			
1	E	164	Total	C	N	O	S	0	9	0
			1303	813	231	252	7			
1	F	164	Total	C	N	O	S	0	11	0
			1310	817	229	257	7			
1	G	164	Total	C	N	O	S	0	10	0
			1301	812	228	254	7			
1	H	164	Total	C	N	O	S	0	10	0
			1304	813	229	255	7			
1	I	164	Total	C	N	O	S	0	10	0
			1304	815	228	254	7			
1	J	164	Total	C	N	O	S	0	10	0
			1304	813	228	256	7			
1	K	164	Total	C	N	O	S	0	10	0
			1304	813	228	256	7			
1	L	164	Total	C	N	O	S	0	9	0
			1295	808	227	253	7			

- Molecule 2 is a protein called Phycoerythrin Beta subunit,Phycoerythrin Beta subunit.

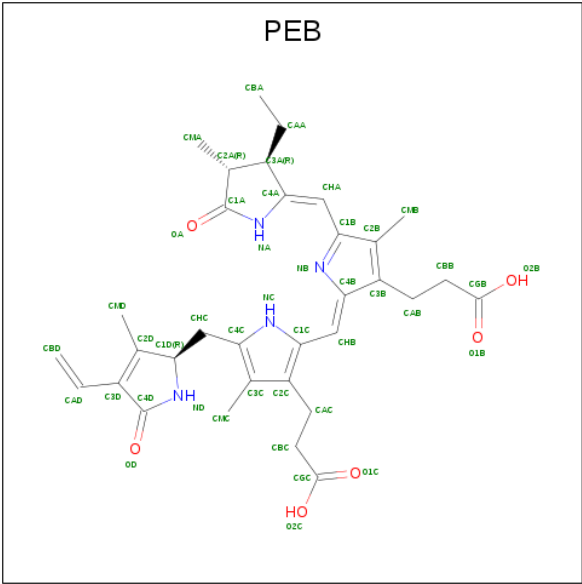
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	184	Total	C	N	O	S	0	12	0
			1417	880	250	273	14			
2	N	184	Total	C	N	O	S	0	16	0
			1432	884	257	277	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	184	Total	C	N	O	S	0	13	0
			1413	873	254	273	13			
2	P	184	Total	C	N	O	S	0	13	0
			1415	876	250	275	14			
2	Q	184	Total	C	N	O	S	0	15	0
			1422	882	251	276	13			
2	R	184	Total	C	N	O	S	0	10	0
			1395	860	250	272	13			
2	S	184	Total	C	N	O	S	0	16	0
			1434	887	254	279	14			
2	T	184	Total	C	N	O	S	0	14	0
			1421	880	251	277	13			
2	U	184	Total	C	N	O	S	0	12	0
			1408	865	255	275	13			
2	V	184	Total	C	N	O	S	0	16	0
			1436	889	253	280	14			
2	W	184	Total	C	N	O	S	0	17	0
			1436	890	254	278	14			
2	X	184	Total	C	N	O	S	0	8	0
			1384	854	248	269	13			

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0

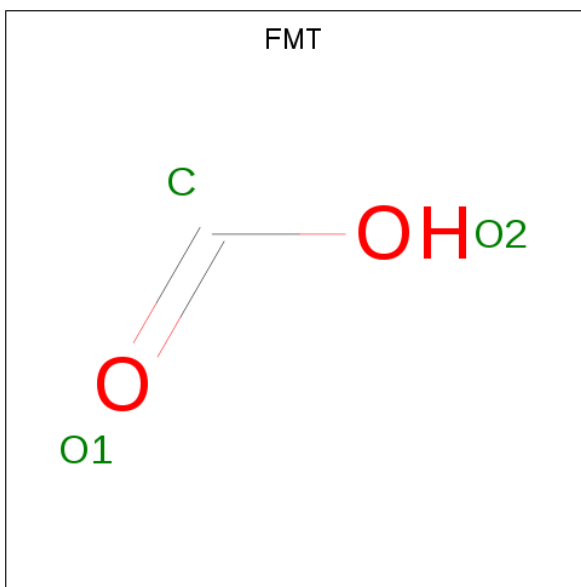
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		
4	J	1	Total	C	O	0	0
			3	1	2		
4	K	1	Total	C	O	0	0
			3	1	2		
4	N	1	Total	C	O	0	0
			3	1	2		
4	O	1	Total	C	O	0	0
			3	1	2		
4	P	1	Total	C	O	0	0
			3	1	2		
4	Q	1	Total	C	O	0	0
			3	1	2		
4	U	1	Total	C	O	0	0
			3	1	2		
4	U	1	Total	C	O	0	0
			3	1	2		
4	V	1	Total	C	O	0	0
			3	1	2		
4	V	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	W	1	Total	C	O	0	0
			3	1	2		

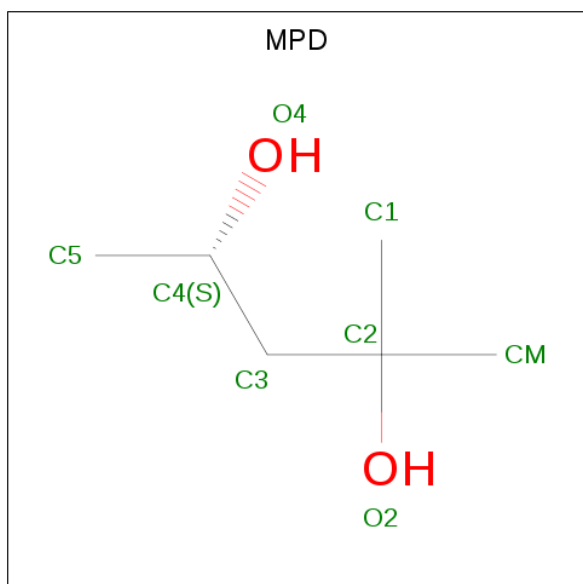
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		
5	J	2	Total	Na	0	0
			2	2		
5	Q	1	Total	Na	0	0
			1	1		
5	D	2	Total	Na	0	0
			2	2		
5	K	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	V	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	N	1	Total	Na	0	0
			1	1		
5	R	1	Total	Na	0	0
			1	1		
5	L	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	I	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0
6	L	1	Total Cl 1 1	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



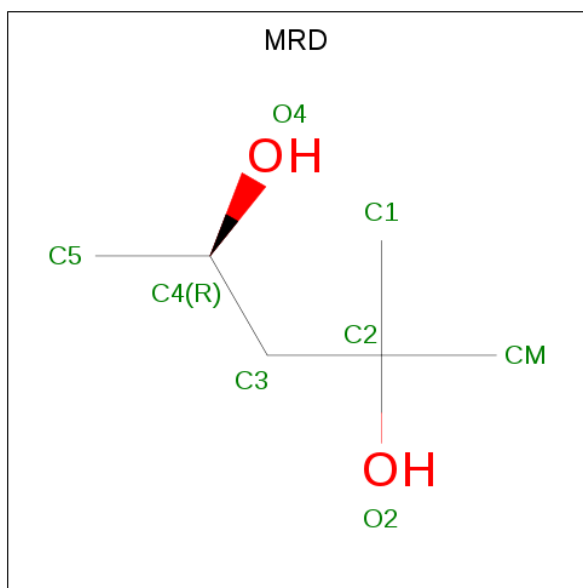
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C O 8 6 2	0	0
7	N	1	Total C O 8 6 2	0	0
7	N	1	Total C O 8 6 2	0	0
7	O	1	Total C O 8 6 2	0	0
7	P	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	Q	1	Total	C	O	0	0
			8	6	2		
7	R	1	Total	C	O	0	0
			8	6	2		
7	S	1	Total	C	O	0	0
			8	6	2		
7	U	1	Total	C	O	0	0
			8	6	2		
7	W	1	Total	C	O	0	0
			8	6	2		
7	W	1	Total	C	O	0	0
			8	6	2		
7	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	T	1	Total	C	O	0	0
			8	6	2		
8	V	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	342	Total 342	O 342	0	0
9	B	310	Total 310	O 310	0	0
9	C	327	Total 327	O 327	0	0
9	D	348	Total 348	O 348	0	0
9	E	311	Total 311	O 311	0	0
9	F	336	Total 336	O 336	0	0
9	G	338	Total 338	O 338	0	0
9	H	328	Total 328	O 328	0	0
9	I	323	Total 323	O 323	0	0
9	J	325	Total 325	O 325	0	0
9	K	303	Total 303	O 303	0	0
9	L	334	Total 334	O 334	0	0
9	M	346	Total 346	O 346	0	0
9	N	342	Total 342	O 342	0	0
9	O	351	Total 351	O 351	0	0
9	P	328	Total 328	O 328	0	0
9	Q	300	Total 300	O 300	0	0
9	R	279	Total 279	O 279	0	0
9	S	314	Total 314	O 314	0	0
9	T	277	Total 277	O 277	0	0
9	U	318	Total 318	O 318	0	0
9	V	360	Total 360	O 360	0	0

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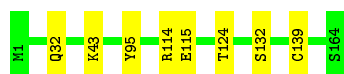
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	W	343	Total 343	O 343	0	0
9	X	316	Total 316	O 316	0	0

### 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: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain A: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain B: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain C: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain D: 



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain E: 





- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain F:  95% 5%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain G:  98% .



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain H:  95% 5%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain I:  95% 5%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain J:  96% .



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain K:  95% 5%



- Molecule 1: Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit,Phycoerythrin Alpha subunit

Chain L:  96% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain M: 94% 5% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain N: 92% 7% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain O: 91% 9% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain P: 92% 8% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain Q: 91% 9% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

Chain R: 95% 5% .

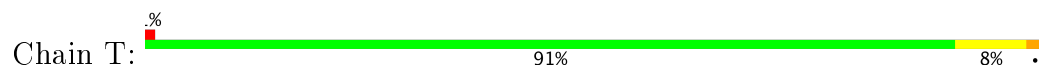


- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit

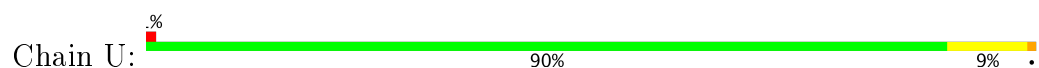
Chain S: 93% 7% .



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



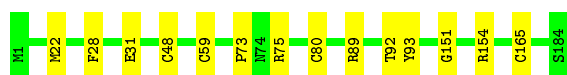
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



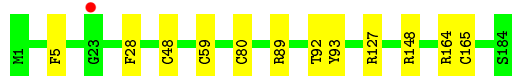
- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



- Molecule 2: Phycoerythrin Beta subunit,Phycoerythrin Beta subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.05Å 110.17Å 118.52Å 78.76° 82.28° 60.43°	Depositor
Resolution (Å)	95.42 – 1.38 93.40 – 1.38	Depositor EDS
% Data completeness (in resolution range)	94.7 (95.42-1.38) 89.5 (93.40-1.38)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.155 , 0.211 0.157 , 0.212	Depositor DCC
$R_{free}$ test set	46444 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.4	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h-k,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	43181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, CL, NA, FMT, MEN, MRD, 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	0.98	0/1339	0.90	3/1810 (0.2%)
1	B	0.95	0/1342	0.93	2/1814 (0.1%)
1	C	0.94	1/1322 (0.1%)	0.89	3/1788 (0.2%)
1	D	0.95	0/1337	0.90	2/1807 (0.1%)
1	E	0.92	0/1344	0.85	3/1816 (0.2%)
1	F	0.92	0/1351	0.87	0/1826
1	G	0.94	0/1342	0.92	1/1814 (0.1%)
1	H	0.91	0/1342	0.85	0/1814
1	I	0.90	0/1348	0.87	2/1821 (0.1%)
1	J	0.86	0/1342	0.80	0/1814
1	K	0.84	0/1342	0.85	0/1814
1	L	0.88	0/1333	0.93	1/1802 (0.1%)
2	M	0.90	0/1463	0.95	4/1971 (0.2%)
2	N	0.89	0/1468	0.93	3/1977 (0.2%)
2	O	0.86	0/1443	0.92	3/1943 (0.2%)
2	P	0.93	1/1443 (0.1%)	0.91	2/1944 (0.1%)
2	Q	0.85	0/1459	0.94	8/1967 (0.4%)
2	R	0.77	0/1416	0.85	3/1909 (0.2%)
2	S	0.86	0/1468	0.93	2/1978 (0.1%)
2	T	0.78	0/1455	0.84	4/1961 (0.2%)
2	U	0.89	0/1431	0.88	3/1929 (0.2%)
2	V	0.92	0/1473	0.86	1/1985 (0.1%)
2	W	0.85	0/1476	0.89	2/1989 (0.1%)
2	X	0.91	0/1411	0.91	3/1903 (0.2%)
All	All	0.89	2/33490 (0.0%)	0.89	55/45196 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	TYR	CB-CG	5.55	1.59	1.51
2	P	51	SER	CB-OG	-5.09	1.35	1.42

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	163	ASP	CB-CG-OD1	8.24	125.72	118.30
2	R	164	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	S	163	ASP	CB-CG-OD1	7.99	125.49	118.30
2	O	164	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	N	164	ARG	NE-CZ-NH1	7.64	124.12	120.30

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	1298	0	1305	14	0
1	B	1304	0	1308	18	0
1	C	1287	0	1289	13	0
1	D	1293	0	1306	17	0
1	E	1303	0	1317	19	0
1	F	1310	0	1314	12	0
1	G	1301	0	1309	11	0
1	H	1304	0	1309	21	0
1	I	1304	0	1319	21	0
1	J	1304	0	1306	13	0
1	K	1304	0	1307	26	0
1	L	1295	0	1301	15	0
2	M	1417	0	1466	40	0
2	N	1432	0	1474	42	0
2	O	1413	0	1454	32	0
2	P	1415	0	1443	24	0
2	Q	1422	0	1459	30	0
2	R	1395	0	1423	15	0
2	S	1434	0	1461	33	0
2	T	1421	0	1451	43	0
2	U	1408	0	1440	30	0
2	V	1436	0	1466	28	0
2	W	1436	0	1476	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1384	0	1417	27	0
3	A	86	0	75	5	0
3	B	86	0	75	8	0
3	C	86	0	76	9	0
3	D	86	0	75	9	0
3	E	86	0	76	12	0
3	F	86	0	75	6	0
3	G	86	0	76	12	0
3	H	86	0	76	11	0
3	I	86	0	76	11	0
3	J	86	0	75	8	0
3	K	86	0	76	10	0
3	L	86	0	76	10	0
3	M	129	0	112	16	0
3	N	129	0	113	18	0
3	O	129	0	113	21	0
3	P	129	0	112	21	0
3	Q	129	0	113	21	0
3	R	129	0	114	16	0
3	S	129	0	112	17	0
3	T	129	0	114	20	0
3	U	129	0	114	24	0
3	V	129	0	111	12	0
3	W	129	0	112	18	0
3	X	129	0	114	26	0
4	A	6	0	2	3	0
4	C	3	0	1	1	0
4	H	3	0	1	5	0
4	J	3	0	1	4	0
4	K	3	0	1	2	0
4	N	3	0	1	0	0
4	O	3	0	1	3	0
4	P	3	0	1	1	0
4	Q	3	0	1	1	0
4	U	6	0	2	2	0
4	V	6	0	2	4	0
4	W	3	0	1	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	V	1	0	0	0	0
6	A	1	0	0	2	0
6	B	1	0	0	1	0
6	C	1	0	0	0	0
6	I	1	0	0	2	0
6	J	1	0	0	2	0
6	L	1	0	0	2	0
7	M	8	0	14	17	0
7	N	16	0	28	32	0
7	O	8	0	12	2	0
7	P	8	0	14	0	0
7	Q	8	0	11	6	0
7	R	8	0	14	5	0
7	S	8	0	14	11	0
7	U	8	0	14	7	0
7	W	16	0	25	11	0
7	X	8	0	14	12	0
8	T	8	0	14	21	0
8	V	8	0	14	20	0
9	A	342	0	0	8	0
9	B	310	0	0	8	0
9	C	327	0	0	1	0
9	D	348	0	0	6	0
9	E	311	0	0	1	0
9	F	336	0	0	4	0
9	G	338	0	0	2	0
9	H	328	0	0	6	1
9	I	323	0	0	10	1
9	J	325	0	0	4	0
9	K	303	0	0	8	0
9	L	334	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	346	0	0	9	0
9	N	342	0	0	19	0
9	O	351	0	0	15	0
9	P	328	0	0	6	0
9	Q	300	0	0	5	0
9	R	279	0	0	5	0
9	S	314	0	0	7	0
9	T	277	0	0	7	0
9	U	318	0	0	14	0
9	V	360	0	0	23	0
9	W	343	0	0	17	0
9	X	316	0	0	7	0
All	All	43181	0	35584	700	1

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 10.

The worst 5 of 700 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:O:48:CYS:SG	3:O:188:PEB:HAA1	1.21	1.75
2:Q:80:CYS:SG	3:Q:186:PEB:HAA2	1.19	1.74
1:B:139:CYS:SG	3:B:167:PEB:HAA2	1.19	1.74
1:E:139:CYS:SG	3:E:167:PEB:HAA2	1.17	1.72
1:C:82:CYS:SG	3:C:166:PEB:HAA2	1.21	1.72

All (1) 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)
9:H:469:HOH:O	9:I:515:HOH:O[1_455]	2.19	0.01

## 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	171/164 (104%)	168 (98%)	3 (2%)	0	100	100
1	B	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	C	169/164 (103%)	167 (99%)	2 (1%)	0	100	100
1	D	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	E	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	F	172/164 (105%)	169 (98%)	3 (2%)	0	100	100
1	G	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	H	171/164 (104%)	169 (99%)	2 (1%)	0	100	100
1	I	172/164 (105%)	169 (98%)	3 (2%)	0	100	100
1	J	171/164 (104%)	168 (98%)	3 (2%)	0	100	100
1	K	171/164 (104%)	168 (98%)	3 (2%)	0	100	100
1	L	170/164 (104%)	168 (99%)	2 (1%)	0	100	100
2	M	194/184 (105%)	190 (98%)	3 (2%)	1 (0%)	32	9
2	N	197/184 (107%)	191 (97%)	6 (3%)	0	100	100
2	O	194/184 (105%)	190 (98%)	4 (2%)	0	100	100
2	P	194/184 (105%)	190 (98%)	4 (2%)	0	100	100
2	Q	196/184 (106%)	191 (97%)	5 (3%)	0	100	100
2	R	191/184 (104%)	184 (96%)	7 (4%)	0	100	100
2	S	197/184 (107%)	191 (97%)	6 (3%)	0	100	100
2	T	195/184 (106%)	191 (98%)	4 (2%)	0	100	100
2	U	193/184 (105%)	186 (96%)	7 (4%)	0	100	100
2	V	198/184 (108%)	195 (98%)	3 (2%)	0	100	100
2	W	198/184 (108%)	190 (96%)	8 (4%)	0	100	100
2	X	189/184 (103%)	184 (97%)	5 (3%)	0	100	100
All	All	4387/4176 (105%)	4295 (98%)	91 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	73	PRO

### 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	137/127 (108%)	137 (100%)	0	100	100
1	B	137/127 (108%)	137 (100%)	0	100	100
1	C	135/127 (106%)	135 (100%)	0	100	100
1	D	137/127 (108%)	135 (98%)	2 (2%)	70	38
1	E	137/127 (108%)	137 (100%)	0	100	100
1	F	138/127 (109%)	134 (97%)	4 (3%)	48	13
1	G	137/127 (108%)	137 (100%)	0	100	100
1	H	137/127 (108%)	135 (98%)	2 (2%)	70	38
1	I	138/127 (109%)	136 (99%)	2 (1%)	71	41
1	J	137/127 (108%)	137 (100%)	0	100	100
1	K	137/127 (108%)	137 (100%)	0	100	100
1	L	136/127 (107%)	135 (99%)	1 (1%)	87	67
2	M	152/138 (110%)	152 (100%)	0	100	100
2	N	151/138 (109%)	149 (99%)	2 (1%)	73	44
2	O	148/138 (107%)	146 (99%)	2 (1%)	71	41
2	P	148/138 (107%)	145 (98%)	3 (2%)	60	25
2	Q	150/138 (109%)	150 (100%)	0	100	100
2	R	145/138 (105%)	144 (99%)	1 (1%)	87	67
2	S	151/138 (109%)	151 (100%)	0	100	100
2	T	149/138 (108%)	146 (98%)	3 (2%)	60	25
2	U	147/138 (106%)	146 (99%)	1 (1%)	87	67
2	V	152/138 (110%)	150 (99%)	2 (1%)	73	44
2	W	152/138 (110%)	151 (99%)	1 (1%)	87	67
2	X	146/138 (106%)	146 (100%)	0	100	100
All	All	3434/3180 (108%)	3408 (99%)	26 (1%)	89	63

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	92[A]	THR
2	O	178	ARG
2	V	178	ARG
2	N	92[B]	THR
2	O	153	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	68	ASN
1	D	61	GLN
2	P	62	GLN
2	R	62	GLN

### 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	8,8,9	1.33	1 (12%)	8,9,11	1.24	1 (12%)
2	MEN	N	70	2	8,8,9	1.21	1 (12%)	8,9,11	1.20	1 (12%)
2	MEN	O	70	2	8,8,9	0.89	1 (12%)	8,9,11	1.19	1 (12%)
2	MEN	P	70	2	8,8,9	0.65	0	8,9,11	1.25	1 (12%)
2	MEN	Q	70	2	8,8,9	0.60	0	8,9,11	1.22	1 (12%)
2	MEN	R	70	2	8,8,9	0.64	0	8,9,11	1.25	1 (12%)
2	MEN	S	70	2	8,8,9	0.90	0	8,9,11	1.48	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MEN	T	70	2	8,8,9	1.22	1 (12%)	8,9,11	1.24	2 (25%)
2	MEN	U	70	2	8,8,9	0.50	0	8,9,11	1.48	2 (25%)
2	MEN	V	70	2	8,8,9	1.02	1 (12%)	8,9,11	1.57	2 (25%)
2	MEN	W	70	2	8,8,9	1.08	1 (12%)	8,9,11	1.02	1 (12%)
2	MEN	X	70	2	8,8,9	0.95	1 (12%)	8,9,11	1.47	2 (25%)

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	70	MEN	CA-C	2.04	1.52	1.50
2	V	70	MEN	CA-C	2.11	1.53	1.50
2	N	70	MEN	CA-C	2.22	1.53	1.50
2	W	70	MEN	CA-C	2.38	1.53	1.50
2	X	70	MEN	CA-C	2.44	1.53	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	70	MEN	O-C-CA	-3.25	116.06	125.02
2	Q	70	MEN	O-C-CA	-2.71	117.53	125.02
2	V	70	MEN	O-C-CA	-2.70	117.55	125.02
2	P	70	MEN	O-C-CA	-2.68	117.61	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	70	MEN	O-C-CA	-2.65	117.69	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 25 are monoatomic - leaving 89 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	A	166	1	37,46,46	3.16	9 (24%)	39,67,67	1.81	12 (30%)
3	PEB	A	167	-	37,46,46	3.00	11 (29%)	39,67,67	2.27	15 (38%)
4	FMT	A	203	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	204	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	B	166	-	37,46,46	3.35	8 (21%)	39,67,67	2.03	13 (33%)
3	PEB	B	167	-	37,46,46	3.26	9 (24%)	39,67,67	2.90	19 (48%)
3	PEB	C	166	-	37,46,46	3.30	9 (24%)	39,67,67	2.37	17 (43%)
3	PEB	C	167	-	37,46,46	3.16	9 (24%)	39,67,67	2.36	16 (41%)
4	FMT	C	203	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	D	166	-	37,46,46	3.02	9 (24%)	39,67,67	2.05	11 (28%)
3	PEB	D	167	-	37,46,46	3.17	10 (27%)	39,67,67	2.53	17 (43%)
3	PEB	E	166	-	37,46,46	3.62	10 (27%)	39,67,67	2.15	13 (33%)
3	PEB	E	167	-	37,46,46	3.45	10 (27%)	39,67,67	2.04	17 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	F	166	-	37,46,46	3.08	9 (24%)	39,67,67	2.10	18 (46%)
3	PEB	F	167	-	37,46,46	3.30	10 (27%)	39,67,67	1.92	14 (35%)
3	PEB	G	166	-	37,46,46	2.93	8 (21%)	39,67,67	2.01	11 (28%)
3	PEB	G	167	-	37,46,46	3.49	9 (24%)	39,67,67	1.89	11 (28%)
3	PEB	H	166	-	37,46,46	3.19	9 (24%)	39,67,67	2.24	16 (41%)
3	PEB	H	167	-	37,46,46	3.14	10 (27%)	39,67,67	2.08	12 (30%)
4	FMT	H	203	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	I	166	-	37,46,46	3.50	9 (24%)	39,67,67	2.35	15 (38%)
3	PEB	I	167	-	37,46,46	3.34	10 (27%)	39,67,67	1.98	12 (30%)
3	PEB	J	166	-	37,46,46	3.01	10 (27%)	39,67,67	2.28	15 (38%)
3	PEB	J	167	5	37,46,46	3.64	12 (32%)	39,67,67	2.31	15 (38%)
4	FMT	J	203	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	K	166	-	37,46,46	3.28	8 (21%)	39,67,67	1.95	12 (30%)
3	PEB	K	167	-	37,46,46	3.02	7 (18%)	39,67,67	2.28	16 (41%)
4	FMT	K	203	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	L	166	-	37,46,46	3.55	11 (29%)	39,67,67	2.15	11 (28%)
3	PEB	L	167	-	37,46,46	3.35	11 (29%)	39,67,67	2.51	17 (43%)
3	PEB	M	186	-	37,46,46	3.52	9 (24%)	39,67,67	2.20	17 (43%)
3	PEB	M	187	-	37,46,46	3.04	9 (24%)	39,67,67	1.81	13 (33%)
3	PEB	M	188	-	37,46,46	3.02	9 (24%)	39,67,67	1.98	14 (35%)
7	MPD	M	204	-	7,7,7	0.25	0	9,10,10	0.80	0
3	PEB	N	186	-	37,46,46	3.35	9 (24%)	39,67,67	2.20	18 (46%)
3	PEB	N	187	-	37,46,46	3.26	10 (27%)	39,67,67	1.62	7 (17%)
3	PEB	N	188	2	37,46,46	3.37	13 (35%)	39,67,67	2.06	14 (35%)
7	MPD	N	204	-	7,7,7	0.24	0	9,10,10	0.64	0
7	MPD	N	205	-	7,7,7	0.31	0	9,10,10	0.57	0
4	FMT	N	206	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	O	186	-	37,46,46	3.56	9 (24%)	39,67,67	2.22	16 (41%)
3	PEB	O	187	-	37,46,46	3.40	8 (21%)	39,67,67	2.00	12 (30%)
3	PEB	O	188	-	37,46,46	3.01	10 (27%)	39,67,67	2.20	14 (35%)
7	MPD	O	204	-	7,7,7	0.27	0	9,10,10	0.46	0
4	FMT	O	205	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	P	186	-	37,46,46	3.44	8 (21%)	39,67,67	2.24	15 (38%)
3	PEB	P	187	-	37,46,46	2.61	8 (21%)	39,67,67	1.93	14 (35%)
3	PEB	P	188	-	37,46,46	2.72	9 (24%)	39,67,67	1.96	13 (33%)
7	MPD	P	204	-	7,7,7	0.23	0	9,10,10	1.01	0
4	FMT	P	205	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	Q	186	-	37,46,46	3.46	9 (24%)	39,67,67	1.99	12 (30%)
3	PEB	Q	187	-	37,46,46	3.22	7 (18%)	39,67,67	1.79	11 (28%)
3	PEB	Q	188	-	37,46,46	2.94	11 (29%)	39,67,67	2.17	14 (35%)
7	MPD	Q	204	2	7,7,7	0.43	0	9,10,10	0.80	0
4	FMT	Q	205	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	R	186	-	37,46,46	3.32	9 (24%)	39,67,67	2.14	14 (35%)
3	PEB	R	187	-	37,46,46	3.50	9 (24%)	39,67,67	1.86	13 (33%)
3	PEB	R	188	-	37,46,46	3.37	9 (24%)	39,67,67	1.95	14 (35%)
7	MPD	R	204	-	7,7,7	0.19	0	9,10,10	0.80	0
3	PEB	S	186	-	37,46,46	3.41	9 (24%)	39,67,67	1.81	13 (33%)
3	PEB	S	187	-	37,46,46	3.15	11 (29%)	39,67,67	1.80	13 (33%)
3	PEB	S	188	-	37,46,46	3.38	10 (27%)	39,67,67	2.01	15 (38%)
7	MPD	S	204	-	7,7,7	0.18	0	9,10,10	0.60	0
3	PEB	T	186	-	37,46,46	3.39	10 (27%)	39,67,67	2.16	15 (38%)
3	PEB	T	187	-	37,46,46	3.39	11 (29%)	39,67,67	2.03	13 (33%)
3	PEB	T	188	-	37,46,46	3.19	12 (32%)	39,67,67	2.03	17 (43%)
8	MRD	T	204	-	7,7,7	0.43	0	9,10,10	0.48	0
3	PEB	U	186	-	37,46,46	3.19	9 (24%)	39,67,67	2.00	11 (28%)
3	PEB	U	187	-	37,46,46	2.98	8 (21%)	39,67,67	1.76	12 (30%)
3	PEB	U	188	-	37,46,46	3.57	9 (24%)	39,67,67	1.86	15 (38%)
7	MPD	U	204	-	7,7,7	0.19	0	9,10,10	0.57	0
4	FMT	U	205	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	U	206	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	V	186	-	37,46,46	3.40	10 (27%)	39,67,67	1.98	9 (23%)
3	PEB	V	187	2	37,46,46	3.31	8 (21%)	39,67,67	1.73	9 (23%)
3	PEB	V	188	2	37,46,46	2.84	13 (35%)	39,67,67	1.90	12 (30%)
8	MRD	V	204	-	7,7,7	0.41	0	9,10,10	0.54	0
4	FMT	V	205	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	V	206	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	W	186	-	37,46,46	2.96	9 (24%)	39,67,67	2.13	19 (48%)
3	PEB	W	187	-	37,46,46	3.27	9 (24%)	39,67,67	1.93	11 (28%)
3	PEB	W	188	-	37,46,46	3.14	8 (21%)	39,67,67	1.94	14 (35%)
7	MPD	W	204	2	7,7,7	0.33	0	9,10,10	0.73	0
7	MPD	W	205	-	7,7,7	0.28	0	9,10,10	0.50	0
4	FMT	W	206	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PEB	X	186	-	37,46,46	3.36	9 (24%)	39,67,67	2.21	10 (25%)
3	PEB	X	187	-	37,46,46	3.32	11 (29%)	39,67,67	1.70	10 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	X	188	-	37,46,46	3.06	12 (32%)	39,67,67	2.07	15 (38%)
7	MPD	X	204	-	7,7,7	0.28	0	9,10,10	1.11	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	A	166	1	-	2/19/74/74	0/4/4/4
3	PEB	A	167	-	-	2/19/74/74	0/4/4/4
4	FMT	A	203	-	-	0/0/0/0	0/0/0/0
4	FMT	A	204	-	-	0/0/0/0	0/0/0/0
3	PEB	B	166	-	-	2/19/74/74	0/4/4/4
3	PEB	B	167	-	-	2/19/74/74	0/4/4/4
3	PEB	C	166	-	-	2/19/74/74	0/4/4/4
3	PEB	C	167	-	-	2/19/74/74	0/4/4/4
4	FMT	C	203	-	-	0/0/0/0	0/0/0/0
3	PEB	D	166	-	-	2/19/74/74	0/4/4/4
3	PEB	D	167	-	-	2/19/74/74	0/4/4/4
3	PEB	E	166	-	-	2/19/74/74	0/4/4/4
3	PEB	E	167	-	-	2/19/74/74	0/4/4/4
3	PEB	F	166	-	-	2/19/74/74	0/4/4/4
3	PEB	F	167	-	-	2/19/74/74	0/4/4/4
3	PEB	G	166	-	-	2/19/74/74	0/4/4/4
3	PEB	G	167	-	-	2/19/74/74	0/4/4/4
3	PEB	H	166	-	-	2/19/74/74	0/4/4/4
3	PEB	H	167	-	-	2/19/74/74	0/4/4/4
4	FMT	H	203	-	-	0/0/0/0	0/0/0/0
3	PEB	I	166	-	-	2/19/74/74	0/4/4/4
3	PEB	I	167	-	-	2/19/74/74	0/4/4/4
3	PEB	J	166	-	-	2/19/74/74	0/4/4/4
3	PEB	J	167	5	-	2/19/74/74	0/4/4/4
4	FMT	J	203	-	-	0/0/0/0	0/0/0/0
3	PEB	K	166	-	-	2/19/74/74	0/4/4/4
3	PEB	K	167	-	-	2/19/74/74	0/4/4/4
4	FMT	K	203	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	L	166	-	-	2/19/74/74	0/4/4/4
3	PEB	L	167	-	-	2/19/74/74	0/4/4/4
3	PEB	M	186	-	-	2/19/74/74	0/4/4/4
3	PEB	M	187	-	-	2/19/74/74	0/4/4/4
3	PEB	M	188	-	-	2/19/74/74	0/4/4/4
7	MPD	M	204	-	-	0/5/5/5	0/0/0/0
3	PEB	N	186	-	-	2/19/74/74	0/4/4/4
3	PEB	N	187	-	-	2/19/74/74	0/4/4/4
3	PEB	N	188	2	-	2/19/74/74	0/4/4/4
7	MPD	N	204	-	-	0/5/5/5	0/0/0/0
7	MPD	N	205	-	-	0/5/5/5	0/0/0/0
4	FMT	N	206	-	-	0/0/0/0	0/0/0/0
3	PEB	O	186	-	-	2/19/74/74	0/4/4/4
3	PEB	O	187	-	-	2/19/74/74	0/4/4/4
3	PEB	O	188	-	-	2/19/74/74	0/4/4/4
7	MPD	O	204	-	-	0/5/5/5	0/0/0/0
4	FMT	O	205	-	-	0/0/0/0	0/0/0/0
3	PEB	P	186	-	-	2/19/74/74	0/4/4/4
3	PEB	P	187	-	-	2/19/74/74	0/4/4/4
3	PEB	P	188	-	-	2/19/74/74	0/4/4/4
7	MPD	P	204	-	-	0/5/5/5	0/0/0/0
4	FMT	P	205	-	-	0/0/0/0	0/0/0/0
3	PEB	Q	186	-	-	2/19/74/74	0/4/4/4
3	PEB	Q	187	-	-	2/19/74/74	0/4/4/4
3	PEB	Q	188	-	-	2/19/74/74	0/4/4/4
7	MPD	Q	204	2	-	0/5/5/5	0/0/0/0
4	FMT	Q	205	-	-	0/0/0/0	0/0/0/0
3	PEB	R	186	-	-	2/19/74/74	0/4/4/4
3	PEB	R	187	-	-	2/19/74/74	0/4/4/4
3	PEB	R	188	-	-	2/19/74/74	0/4/4/4
7	MPD	R	204	-	-	0/5/5/5	0/0/0/0
3	PEB	S	186	-	-	2/19/74/74	0/4/4/4
3	PEB	S	187	-	-	2/19/74/74	0/4/4/4
3	PEB	S	188	-	-	2/19/74/74	0/4/4/4
7	MPD	S	204	-	-	0/5/5/5	0/0/0/0
3	PEB	T	186	-	-	2/19/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	T	187	-	-	2/19/74/74	0/4/4/4
3	PEB	T	188	-	-	2/19/74/74	0/4/4/4
8	MRD	T	204	-	-	0/5/5/5	0/0/0/0
3	PEB	U	186	-	-	2/19/74/74	0/4/4/4
3	PEB	U	187	-	-	2/19/74/74	0/4/4/4
3	PEB	U	188	-	-	2/19/74/74	0/4/4/4
7	MPD	U	204	-	-	0/5/5/5	0/0/0/0
4	FMT	U	205	-	-	0/0/0/0	0/0/0/0
4	FMT	U	206	-	-	0/0/0/0	0/0/0/0
3	PEB	V	186	-	-	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
8	MRD	V	204	-	-	0/5/5/5	0/0/0/0
4	FMT	V	205	-	-	0/0/0/0	0/0/0/0
4	FMT	V	206	-	-	0/0/0/0	0/0/0/0
3	PEB	W	186	-	-	2/19/74/74	0/4/4/4
3	PEB	W	187	-	-	2/19/74/74	0/4/4/4
3	PEB	W	188	-	-	2/19/74/74	0/4/4/4
7	MPD	W	204	2	-	0/5/5/5	0/0/0/0
7	MPD	W	205	-	-	0/5/5/5	0/0/0/0
4	FMT	W	206	-	-	0/0/0/0	0/0/0/0
3	PEB	X	186	-	-	2/19/74/74	0/4/4/4
3	PEB	X	187	-	-	2/19/74/74	0/4/4/4
3	PEB	X	188	-	-	2/19/74/74	0/4/4/4
7	MPD	X	204	-	-	0/5/5/5	0/0/0/0

The worst 5 of 570 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	167	PEB	C2A-C1A	-5.18	1.47	1.52
3	W	187	PEB	C1A-NA	-5.09	1.31	1.37
3	D	167	PEB	C2A-C1A	-5.01	1.47	1.52
3	K	166	PEB	C2A-C1A	-5.01	1.47	1.52
3	E	166	PEB	C2A-C1A	-4.98	1.47	1.52

The worst 5 of 824 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	186	PEB	OA-C1A-C2A	-8.23	119.60	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	167	PEB	OA-C1A-C2A	-7.06	120.55	126.25
3	D	167	PEB	OA-C1A-C2A	-7.03	120.57	126.25
3	I	166	PEB	CHA-C1B-NB	-6.91	111.69	124.97
3	F	166	PEB	CHA-C1B-NB	-6.34	112.80	124.97

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	188	PEB	C4A-CHA-C1B-C2B
3	T	188	PEB	C4A-CHA-C1B-C2B
3	R	188	PEB	C4A-CHA-C1B-C2B
3	O	188	PEB	C4A-CHA-C1B-C2B
3	V	188	PEB	C4A-CHA-C1B-C2B

There are no ring outliers.

83 monomers are involved in 516 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	166	PEB	1	0
3	A	167	PEB	4	0
4	A	204	FMT	3	0
3	B	166	PEB	3	0
3	B	167	PEB	5	0
3	C	166	PEB	5	0
3	C	167	PEB	4	0
4	C	203	FMT	1	0
3	D	166	PEB	3	0
3	D	167	PEB	6	0
3	E	166	PEB	6	0
3	E	167	PEB	6	0
3	F	167	PEB	6	0
3	G	166	PEB	5	0
3	G	167	PEB	7	0
3	H	166	PEB	5	0
3	H	167	PEB	6	0
4	H	203	FMT	5	0
3	I	166	PEB	5	0
3	I	167	PEB	6	0
3	J	166	PEB	3	0
3	J	167	PEB	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	203	FMT	4	0
3	K	166	PEB	5	0
3	K	167	PEB	5	0
4	K	203	FMT	2	0
3	L	166	PEB	5	0
3	L	167	PEB	5	0
3	M	186	PEB	4	0
3	M	187	PEB	6	0
3	M	188	PEB	6	0
7	M	204	MPD	17	0
3	N	186	PEB	6	0
3	N	187	PEB	7	0
3	N	188	PEB	5	0
7	N	204	MPD	21	0
7	N	205	MPD	11	0
3	O	186	PEB	4	0
3	O	187	PEB	5	0
3	O	188	PEB	12	0
7	O	204	MPD	2	0
4	O	205	FMT	3	0
3	P	186	PEB	6	0
3	P	187	PEB	5	0
3	P	188	PEB	10	0
4	P	205	FMT	1	0
3	Q	186	PEB	7	0
3	Q	187	PEB	6	0
3	Q	188	PEB	8	0
7	Q	204	MPD	6	0
4	Q	205	FMT	1	0
3	R	186	PEB	4	0
3	R	187	PEB	4	0
3	R	188	PEB	8	0
7	R	204	MPD	5	0
3	S	186	PEB	4	0
3	S	187	PEB	7	0
3	S	188	PEB	6	0
7	S	204	MPD	11	0
3	T	186	PEB	6	0
3	T	187	PEB	5	0
3	T	188	PEB	9	0
8	T	204	MRD	21	0
3	U	186	PEB	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	187	PEB	6	0
3	U	188	PEB	12	0
7	U	204	MPD	7	0
4	U	205	FMT	2	0
3	V	186	PEB	4	0
3	V	187	PEB	2	0
3	V	188	PEB	6	0
8	V	204	MRD	20	0
4	V	205	FMT	1	0
4	V	206	FMT	3	0
3	W	186	PEB	3	0
3	W	187	PEB	7	0
3	W	188	PEB	8	0
7	W	204	MPD	11	0
4	W	206	FMT	5	0
3	X	186	PEB	7	0
3	X	187	PEB	7	0
3	X	188	PEB	12	0
7	X	204	MPD	12	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	-0.47	0	100   100	6, 9, 16, 27	0
1	B	164/164 (100%)	-0.50	0	100   100	6, 10, 18, 26	0
1	C	164/164 (100%)	-0.41	0	100   100	9, 14, 21, 28	0
1	D	164/164 (100%)	-0.51	0	100   100	6, 10, 18, 27	0
1	E	164/164 (100%)	-0.47	0	100   100	6, 12, 21, 32	0
1	F	164/164 (100%)	-0.48	0	100   100	8, 12, 18, 25	0
1	G	164/164 (100%)	-0.52	0	100   100	7, 10, 17, 25	0
1	H	164/164 (100%)	-0.46	0	100   100	7, 11, 19, 27	0
1	I	164/164 (100%)	-0.47	0	100   100	8, 12, 23, 36	0
1	J	164/164 (100%)	-0.47	0	100   100	7, 12, 24, 39	0
1	K	164/164 (100%)	-0.46	0	100   100	8, 13, 22, 29	0
1	L	164/164 (100%)	-0.44	0	100   100	8, 11, 20, 26	0
2	M	183/184 (99%)	-0.37	0	100   100	6, 10, 22, 37	0
2	N	183/184 (99%)	-0.40	0	100   100	8, 12, 21, 36	0
2	O	183/184 (99%)	-0.30	2 (1%)	80   82	7, 13, 29, 49	0
2	P	183/184 (99%)	-0.38	0	100   100	6, 11, 26, 35	0
2	Q	183/184 (99%)	-0.40	0	100   100	7, 12, 25, 38	0
2	R	183/184 (99%)	-0.25	1 (0%)	90   91	11, 18, 32, 53	0
2	S	183/184 (99%)	-0.36	1 (0%)	90   91	8, 12, 28, 38	0
2	T	183/184 (99%)	-0.21	2 (1%)	80   82	11, 18, 32, 50	0
2	U	183/184 (99%)	-0.39	1 (0%)	90   91	8, 12, 25, 42	0
2	V	183/184 (99%)	-0.35	1 (0%)	90   91	7, 11, 25, 48	0
2	W	183/184 (99%)	-0.39	0	100   100	7, 12, 25, 41	0
2	X	183/184 (99%)	-0.37	1 (0%)	90   91	7, 12, 25, 38	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4164/4176 (99%)	-0.41	9 (0%) 94 94	6, 12, 25, 53	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	184	SER	3.2
2	S	22[A]	MET	2.7
2	O	150[A]	GLY	2.6
2	O	184	SER	2.5
2	R	184	SER	2.3

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MEN	S	70	9/10	0.98	0.05	-	11,12,16,18	0
2	MEN	U	70	9/10	0.98	0.05	-	10,11,14,16	0
2	MEN	V	70	9/10	0.99	0.04	-	9,11,16,18	0
2	MEN	W	70	9/10	0.98	0.05	-	9,11,13,13	0
2	MEN	P	70	9/10	0.98	0.05	-	9,11,15,16	0
2	MEN	X	70	9/10	0.97	0.06	-	11,12,15,17	0
2	MEN	T	70	9/10	0.97	0.06	-	14,16,19,20	0
2	MEN	M	70	9/10	0.98	0.05	-	9,10,11,14	0
2	MEN	N	70	9/10	0.97	0.06	-	11,12,14,14	0
2	MEN	O	70	9/10	0.98	0.05	-	10,11,14,16	0
2	MEN	Q	70	9/10	0.98	0.05	-	11,12,13,13	0
2	MEN	R	70	9/10	0.98	0.06	-	14,15,19,19	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MPD	W	205	8/8	0.74	0.25	25.62	20,21,23,25	8
7	MPD	X	204	8/8	0.69	0.25	20.53	12,19,23,26	8
7	MPD	N	205	8/8	0.87	0.22	20.28	19,21,23,24	8
5	NA	Q	206	1/1	0.96	0.12	15.05	30,30,30,30	1
7	MPD	U	204	8/8	0.61	0.30	14.04	23,28,35,36	8
4	FMT	A	203	3/3	0.91	0.18	11.85	10,10,12,17	3
7	MPD	R	204	8/8	0.73	0.25	11.46	24,26,31,36	8
4	FMT	V	205	3/3	0.94	0.13	10.88	22,22,27,29	3
4	FMT	Q	205	3/3	0.92	0.18	10.10	21,21,21,22	3
6	CL	I	204	1/1	0.99	0.10	9.89	36,36,36,36	0
7	MPD	M	204	8/8	0.76	0.31	8.68	16,18,19,19	8
4	FMT	O	205	3/3	0.91	0.12	7.11	25,25,27,27	3
7	MPD	O	204	8/8	0.64	0.28	7.02	30,35,36,36	8
7	MPD	N	204	8/8	0.82	0.19	6.92	19,21,29,40	8
7	MPD	W	204	8/8	0.79	0.20	6.78	18,19,25,26	8
7	MPD	S	204	8/8	0.78	0.21	5.97	21,24,27,28	8
8	MRD	V	204	8/8	0.63	0.24	5.68	25,26,30,30	8
4	FMT	P	205	3/3	0.90	0.13	5.04	24,24,24,27	3
8	MRD	T	204	8/8	0.81	0.20	4.85	19,20,24,28	8
7	MPD	Q	204	8/8	0.73	0.19	4.25	16,18,19,21	8
6	CL	C	205	1/1	0.99	0.09	4.19	32,32,32,32	0
4	FMT	W	206	3/3	0.89	0.12	4.02	23,23,25,26	3
4	FMT	N	206	3/3	0.94	0.10	3.90	22,22,23,25	3
6	CL	L	204	1/1	0.99	0.09	3.71	27,27,27,27	0
4	FMT	A	204	3/3	0.83	0.17	3.48	24,24,26,31	3
4	FMT	J	203	3/3	0.91	0.18	3.31	10,10,13,17	3
7	MPD	P	204	8/8	0.79	0.17	3.27	21,25,26,27	8
4	FMT	K	203	3/3	0.87	0.16	3.02	21,21,23,25	3
6	CL	J	206	1/1	0.99	0.10	2.69	33,33,33,33	0
6	CL	A	206	1/1	0.99	0.09	2.66	30,30,30,30	0
4	FMT	H	203	3/3	0.89	0.12	1.80	21,21,21,23	3
5	NA	D	203	1/1	0.95	0.14	1.55	36,36,36,36	0
5	NA	N	207	1/1	0.99	0.11	1.36	32,32,32,32	0
6	CL	B	204	1/1	0.99	0.08	1.27	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEB	Q	187	43/43	0.96	0.08	1.25	7,10,20,38	0
3	PEB	Q	186	43/43	0.96	0.07	1.14	9,12,24,37	0
3	PEB	I	166	43/43	0.96	0.06	1.03	11,14,19,28	0
3	PEB	R	186	43/43	0.94	0.07	0.97	13,18,27,41	0
3	PEB	J	167	43/43	0.94	0.09	0.92	14,24,33,39	0
3	PEB	S	186	43/43	0.95	0.07	0.87	9,12,24,40	0
3	PEB	C	166	43/43	0.97	0.06	0.74	10,11,14,17	0
3	PEB	U	187	43/43	0.96	0.07	0.68	10,12,20,36	0
3	PEB	B	166	43/43	0.97	0.06	0.65	7,9,14,21	0
5	NA	C	204	1/1	0.99	0.11	0.62	27,27,27,27	0
5	NA	L	203	1/1	0.99	0.10	0.60	26,26,26,26	0
3	PEB	I	167	43/43	0.95	0.08	0.56	11,15,25,28	0
3	PEB	S	187	43/43	0.95	0.07	0.55	10,13,22,37	0
5	NA	F	203	1/1	0.99	0.09	0.51	21,21,21,21	0
3	PEB	P	187	43/43	0.96	0.07	0.50	7,10,19,45	0
3	PEB	T	188	43/43	0.94	0.09	0.50	11,18,28,35	0
3	PEB	E	166	43/43	0.97	0.06	0.45	10,13,18,23	0
3	PEB	M	188	43/43	0.97	0.07	0.42	6,8,17,27	0
5	NA	A	205	1/1	0.99	0.09	0.41	26,26,26,26	0
3	PEB	L	166	43/43	0.97	0.06	0.41	8,9,12,14	0
3	PEB	X	186	43/43	0.96	0.07	0.39	9,13,24,36	0
3	PEB	D	166	43/43	0.97	0.06	0.38	8,10,14,21	0
3	PEB	T	187	43/43	0.95	0.09	0.36	10,15,25,49	0
3	PEB	R	188	43/43	0.94	0.08	0.35	12,17,27,34	0
3	PEB	O	187	43/43	0.96	0.07	0.35	9,13,23,31	0
3	PEB	K	166	43/43	0.97	0.06	0.34	9,12,15,21	0
3	PEB	X	187	43/43	0.96	0.07	0.33	8,11,17,30	0
3	PEB	T	186	43/43	0.95	0.07	0.32	13,17,28,48	0
3	PEB	F	166	43/43	0.97	0.06	0.30	7,9,12,16	0
3	PEB	G	166	43/43	0.97	0.06	0.28	7,9,13,17	0
3	PEB	O	186	43/43	0.96	0.07	0.26	8,13,25,38	0
3	PEB	R	187	43/43	0.95	0.08	0.25	12,17,29,32	0
3	PEB	V	186	43/43	0.96	0.07	0.24	8,11,21,35	0
3	PEB	U	188	43/43	0.96	0.07	0.23	7,10,18,29	0
3	PEB	J	166	43/43	0.97	0.06	0.18	9,12,17,25	0
3	PEB	N	187	43/43	0.96	0.07	0.17	7,10,19,30	0
3	PEB	S	188	43/43	0.96	0.07	0.15	9,11,15,20	0
3	PEB	Q	188	43/43	0.96	0.07	0.14	6,10,16,22	0
3	PEB	X	188	43/43	0.96	0.07	0.13	7,10,17,22	0
3	PEB	V	187	43/43	0.97	0.07	0.13	8,10,16,28	0
3	PEB	C	167	43/43	0.95	0.08	0.09	12,18,27,32	0
3	PEB	N	188	43/43	0.97	0.07	0.09	7,11,17,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEB	A	166	43/43	0.98	0.06	0.07	6,9,12,17	0
3	PEB	P	188	43/43	0.97	0.06	0.03	6,9,16,24	0
3	PEB	D	167	43/43	0.95	0.07	-0.00	9,15,23,25	0
3	PEB	P	186	43/43	0.97	0.06	-0.00	7,12,27,39	0
3	PEB	K	167	43/43	0.96	0.07	-0.00	13,17,25,31	0
3	PEB	L	167	43/43	0.95	0.08	-0.01	12,18,28,33	0
3	PEB	M	186	43/43	0.97	0.07	-0.02	6,11,21,35	0
3	PEB	W	188	43/43	0.97	0.06	-0.10	8,11,17,30	0
3	PEB	U	186	43/43	0.97	0.06	-0.10	7,13,25,41	0
3	PEB	N	186	43/43	0.97	0.06	-0.11	8,11,21,35	0
3	PEB	H	167	43/43	0.96	0.07	-0.12	11,13,24,35	0
3	PEB	W	187	43/43	0.97	0.06	-0.13	8,11,19,31	0
3	PEB	M	187	43/43	0.97	0.06	-0.14	7,10,16,27	0
3	PEB	O	188	43/43	0.97	0.06	-0.23	7,10,17,18	0
3	PEB	W	186	43/43	0.97	0.06	-0.23	8,12,21,33	0
3	PEB	A	167	43/43	0.97	0.06	-0.24	8,12,18,28	0
3	PEB	H	166	43/43	0.97	0.06	-0.24	8,10,15,23	0
3	PEB	E	167	43/43	0.96	0.06	-0.26	10,14,24,37	0
3	PEB	B	167	43/43	0.97	0.06	-0.26	8,12,19,31	0
3	PEB	G	167	43/43	0.97	0.06	-0.27	9,12,18,23	0
3	PEB	V	188	43/43	0.97	0.06	-0.36	7,9,13,18	0
3	PEB	F	167	43/43	0.97	0.06	-0.53	9,13,20,27	0
5	NA	G	203	1/1	0.99	0.05	-1.30	25,25,25,25	0
4	FMT	C	203	3/3	0.92	0.19	-	18,18,21,26	3
5	NA	R	205	1/1	0.99	0.18	-	26,26,26,26	0
5	NA	I	203	1/1	0.99	0.11	-	26,26,26,26	0
5	NA	D	204	1/1	0.99	0.09	-	24,24,24,24	0
5	NA	P	206	1/1	0.99	0.10	-	24,24,24,24	0
5	NA	H	204	1/1	0.93	0.14	-	34,34,34,34	0
5	NA	J	205	1/1	0.90	0.28	-	34,34,34,34	1
5	NA	V	207	1/1	0.99	0.06	-	22,22,22,22	0
5	NA	B	203	1/1	0.99	0.12	-	26,26,26,26	0
4	FMT	U	205	3/3	0.81	0.16	-	19,19,21,21	3
5	NA	J	204	1/1	0.99	0.09	-	25,25,25,25	0
5	NA	K	204	1/1	0.99	0.16	-	34,34,34,34	0
4	FMT	V	206	3/3	0.94	0.16	-	14,14,15,16	3
5	NA	E	203	1/1	0.97	0.09	-	34,34,34,34	0
4	FMT	U	206	3/3	0.87	0.16	-	23,23,23,25	3

## 6.5 Other polymers ⓘ

There are no such residues in this entry.