



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2017 – 02:05 PM EDT

PDB ID : 5TJF  
Title : The crystal structure of Allophycocyanin from the red algae *Gracilaria chilensis*  
Authors : Figueroa, M.; Dagnino, J.; Kerff, F.; Chartier, P.; Bunster, M.; Martinez-Oyanedel, J.  
Deposited on : 2016-10-04  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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-20029077  
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-20029077

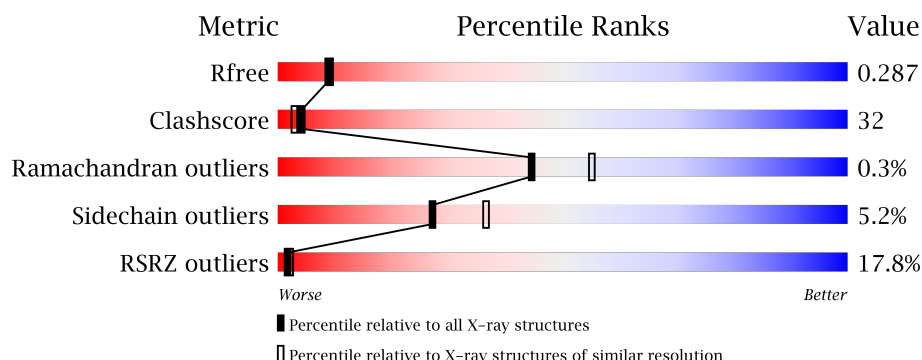
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	160	<div> <div>19%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
2	B	161	<div> <div>17%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYC	B	201	-	-	-	X
4	PEG	A	202	-	-	-	X
6	CL	A	209	-	-	-	X
6	CL	B	216	-	-	X	-
6	CL	B	218	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5535 atoms, of which 2500 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.

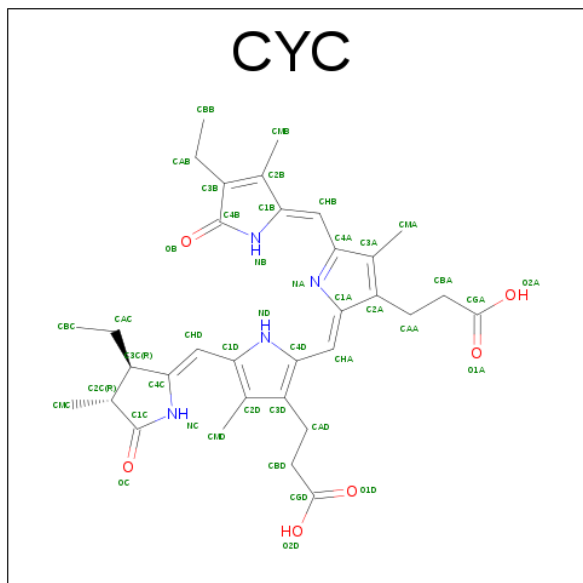
- Molecule 1 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	H	N	O	S	0	0	0
			2386	754	1185	205	236	6			

- Molecule 2 is a protein called Allophycocyanin beta subunit.

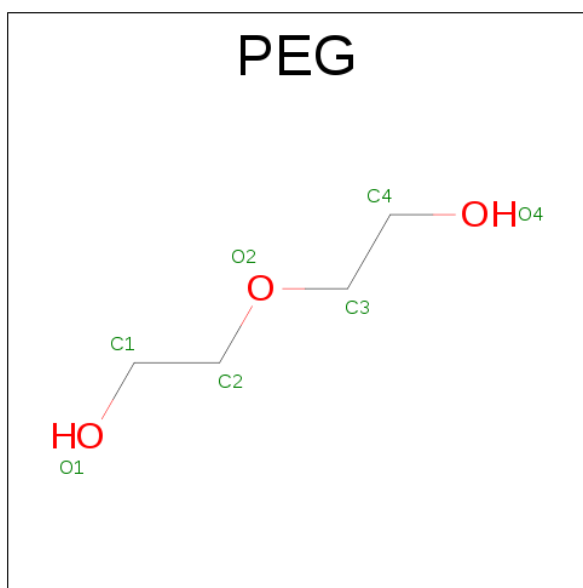
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	161	Total	C	H	N	O	S	0	0	0
			2425	764	1204	207	243	7			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		0	0
			79	33	36	4	6			
3	B	1	Total	C	H	N	O		0	0
			80	33	37	4	6			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	12	Total	Na	0	0
			12	12		
5	A	5	Total	Na	0	0
			5	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Cl	0	0
			4	4		
6	A	1	Total	Cl	0	0
			1	1		

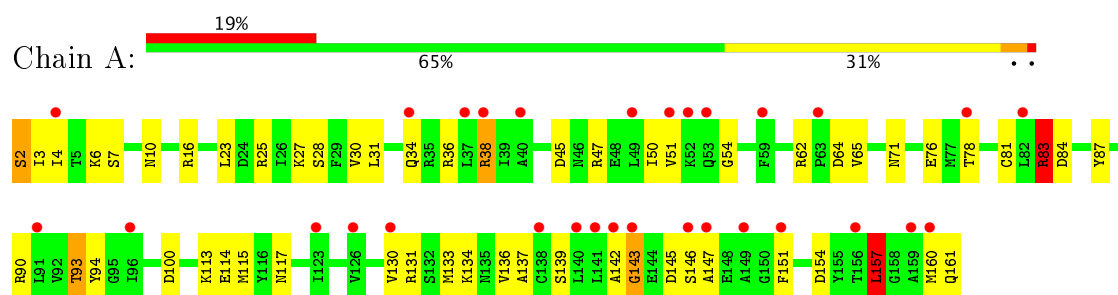
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	222	Total 222	O 222	0	0
7	B	256	Total 256	O 256	0	0

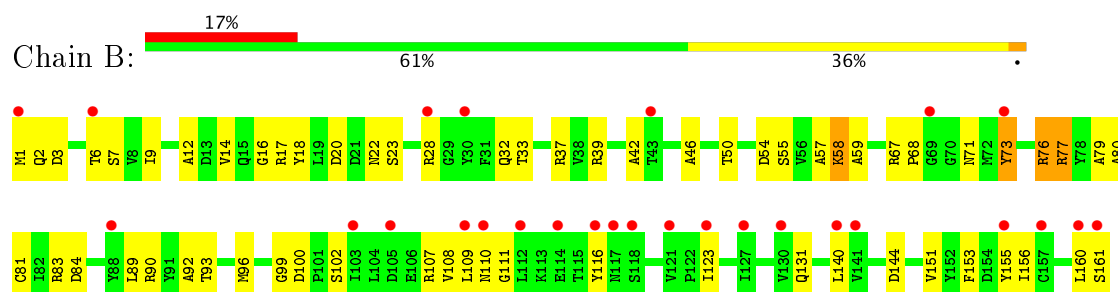
### 3 Residue-property plots [i](#)

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



#### • Molecule 2: Allophycocyanin beta subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.41 Å 97.41 Å 63.83 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.18 – 2.30 42.18 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.18-2.30) 97.2 (42.18-2.02)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.01 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.257 , 0.284 0.264 , 0.287	Depositor DCC
$R_{free}$ test set	783 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, NA, MEN, PEG, CL

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	0.45	2/1215 (0.2%)	0.56	3/1637 (0.2%)
2	B	0.63	4/1227 (0.3%)	0.57	1/1659 (0.1%)
All	All	0.55	6/2442 (0.2%)	0.56	4/3296 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	ARG	CZ-NH1	6.83	1.42	1.33
2	B	76	ARG	CZ-NH2	6.46	1.41	1.33
2	B	77	ARG	CZ-NH1	6.31	1.41	1.33
1	A	83	ARG	CZ-NH1	6.08	1.41	1.33
2	B	77	ARG	CZ-NH2	5.64	1.40	1.33
1	A	83	ARG	CZ-NH2	5.12	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	83	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	A	157	LEU	CA-CB-CG	5.44	127.81	115.30
2	B	77	ARG	NE-CZ-NH1	-5.40	117.60	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	1201	1185	1186	69	0
2	B	1221	1204	1208	81	1
3	A	43	36	37	12	1
3	B	43	37	38	10	0
4	A	13	18	17	2	0
4	B	14	20	19	0	0
5	A	5	0	0	0	0
5	B	12	0	0	0	0
6	A	1	0	0	0	0
6	B	4	0	0	7	0
7	A	222	0	0	58	6
7	B	256	0	0	67	9
All	All	3035	2500	2505	164	11

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 32.

All (164) 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:B:76:ARG:HD2	7:B:315:HOH:O	1.42	1.19
2:B:76:ARG:CD	7:B:315:HOH:O	1.96	1.14
1:A:28:SER:O	7:A:302:HOH:O	1.72	1.06
2:B:99:GLY:O	7:B:301:HOH:O	1.71	1.05
6:B:218:CL:CL	7:B:436:HOH:O	2.11	1.04
2:B:50:THR:OG1	7:B:302:HOH:O	1.75	1.03
2:B:54:ASP:O	7:B:303:HOH:O	1.75	1.02
1:A:38:ARG:NH2	7:A:308:HOH:O	1.92	1.02
1:A:3:ILE:O	7:A:303:HOH:O	1.79	1.00
1:A:23:LEU:O	7:A:304:HOH:O	1.80	0.98
2:B:55:SER:O	7:B:305:HOH:O	1.80	0.97
2:B:68:PRO:O	7:B:304:HOH:O	1.80	0.97
1:A:136:VAL:N	7:A:312:HOH:O	1.97	0.95
1:A:30:VAL:O	7:A:305:HOH:O	1.86	0.94
1:A:147:ALA:O	7:A:307:HOH:O	1.88	0.91
1:A:45:ASP:O	7:A:306:HOH:O	1.87	0.91
6:B:218:CL:CL	7:B:366:HOH:O	2.26	0.90
7:A:371:HOH:O	6:B:216:CL:CL	2.27	0.89
1:A:25:ARG:NH1	7:A:319:HOH:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ARG:NE	7:B:317:HOH:O	2.05	0.87
2:B:161:SER:OXT	7:B:306:HOH:O	1.92	0.86
2:B:156:ILE:N	7:B:319:HOH:O	2.06	0.86
1:A:50:ILE:O	7:A:309:HOH:O	1.92	0.86
1:A:134:LYS:NZ	7:A:321:HOH:O	2.10	0.85
1:A:146:SER:N	7:A:316:HOH:O	2.01	0.85
1:A:161:GLN:O	7:A:310:HOH:O	1.94	0.84
2:B:58:LYS:N	7:B:303:HOH:O	2.03	0.83
2:B:76:ARG:NE	7:B:315:HOH:O	2.04	0.83
2:B:77:ARG:NH2	7:B:323:HOH:O	2.12	0.83
2:B:22:ASN:O	7:B:308:HOH:O	1.97	0.82
1:A:133:MET:O	7:A:312:HOH:O	1.96	0.82
3:B:201:CYC:HBB3	3:B:201:CYC:HMB1	1.61	0.81
1:A:34:GLN:OE1	7:A:313:HOH:O	1.98	0.81
2:B:46:ALA:O	7:B:307:HOH:O	1.97	0.81
2:B:28:ARG:NH1	7:B:318:HOH:O	2.06	0.81
1:A:34:GLN:NE2	7:A:324:HOH:O	2.14	0.81
1:A:47:ARG:O	7:A:314:HOH:O	1.98	0.80
6:B:217:CL:CL	7:B:457:HOH:O	2.37	0.79
1:A:54:GLY:N	7:A:309:HOH:O	2.16	0.79
2:B:109:LEU:O	7:B:309:HOH:O	2.02	0.78
1:A:114:GLU:OE2	7:A:315:HOH:O	2.00	0.78
2:B:76:ARG:NH1	7:B:320:HOH:O	2.10	0.78
2:B:110:ASN:O	7:B:311:HOH:O	2.03	0.77
1:A:36:ARG:NH1	7:A:328:HOH:O	2.18	0.76
2:B:16:GLY:O	7:B:310:HOH:O	2.02	0.76
6:B:218:CL:CL	7:B:435:HOH:O	2.40	0.76
1:A:62:ARG:NH1	7:A:326:HOH:O	2.18	0.76
2:B:18:TYR:O	7:B:316:HOH:O	2.05	0.75
2:B:37:ARG:NH1	7:B:324:HOH:O	2.18	0.75
2:B:77:ARG:NH1	7:B:332:HOH:O	2.19	0.75
2:B:100:ASP:O	7:B:312:HOH:O	2.03	0.75
2:B:144:ASP:OD2	7:B:313:HOH:O	2.03	0.74
1:A:4:ILE:O	7:A:303:HOH:O	2.06	0.73
2:B:2:GLN:O	7:B:314:HOH:O	2.04	0.73
1:A:25:ARG:NH2	7:A:331:HOH:O	2.21	0.73
2:B:76:ARG:NH2	3:B:201:CYC:O1D	2.17	0.73
1:A:54:GLY:N	7:A:329:HOH:O	2.20	0.72
4:A:203:PEG:O4	7:A:317:HOH:O	2.04	0.72
1:A:7:SER:N	7:A:303:HOH:O	2.14	0.72
2:B:81:CYS:SG	3:B:201:CYC:H2C	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:216:CL:CL	7:B:345:HOH:O	2.45	0.71
1:A:137:ALA:N	7:A:312:HOH:O	2.16	0.70
2:B:83:ARG:NH1	2:B:84:ASP:OD1	2.23	0.70
1:A:2:SER:N	1:A:100:ASP:OD1	2.25	0.69
2:B:84:ASP:OD2	2:B:116:TYR:OH	2.08	0.69
2:B:151:VAL:O	7:B:321:HOH:O	2.10	0.68
2:B:39:ARG:NH2	7:B:334:HOH:O	2.22	0.68
1:A:83:ARG:HH12	3:A:201:CYC:CGA	2.07	0.68
1:A:31:LEU:O	7:A:322:HOH:O	2.11	0.68
1:A:64:ASP:OD1	7:A:323:HOH:O	2.11	0.68
2:B:107:ARG:NH1	6:B:216:CL:CL	2.63	0.68
2:B:100:ASP:OD2	7:B:325:HOH:O	2.12	0.67
2:B:42:ALA:O	7:B:326:HOH:O	2.12	0.67
2:B:96:MET:O	7:B:324:HOH:O	2.12	0.67
2:B:155:TYR:C	7:B:319:HOH:O	2.31	0.66
1:A:117:ASN:ND2	7:A:336:HOH:O	2.28	0.66
2:B:155:TYR:HD1	7:B:319:HOH:O	1.79	0.66
2:B:14:VAL:O	7:B:328:HOH:O	2.13	0.65
2:B:81:CYS:SG	3:B:201:CYC:HAC2	2.37	0.65
2:B:1:MET:HB2	7:B:365:HOH:O	1.97	0.64
2:B:22:ASN:ND2	7:B:342:HOH:O	2.30	0.64
2:B:102:SER:OG	7:B:322:HOH:O	2.11	0.63
2:B:59:ALA:N	7:B:305:HOH:O	2.31	0.63
2:B:54:ASP:OD2	7:B:330:HOH:O	2.15	0.62
2:B:131:GLN:NE2	7:B:331:HOH:O	2.18	0.61
2:B:92:ALA:HB1	7:B:347:HOH:O	2.00	0.61
1:A:147:ALA:N	7:A:341:HOH:O	2.34	0.61
2:B:54:ASP:C	7:B:303:HOH:O	2.29	0.60
2:B:57:ALA:N	7:B:303:HOH:O	2.33	0.60
3:A:201:CYC:HMA1	3:A:201:CYC:HB	1.66	0.60
1:A:71:ASN:OD1	3:A:201:CYC:HMD2	2.01	0.60
1:A:27:LYS:N	7:A:304:HOH:O	2.35	0.59
2:B:107:ARG:NH2	7:B:345:HOH:O	2.36	0.58
2:B:153:PHE:N	7:B:347:HOH:O	2.36	0.58
7:A:311:HOH:O	2:B:90:ARG:N	2.37	0.58
2:B:17:ARG:CZ	7:B:317:HOH:O	2.49	0.57
1:A:113:LYS:NZ	7:A:327:HOH:O	2.18	0.57
2:B:108:VAL:HA	3:B:201:CYC:HAB1	1.87	0.56
1:A:133:MET:C	7:A:312:HOH:O	2.40	0.56
2:B:76:ARG:HH22	3:B:201:CYC:CGD	2.16	0.56
2:B:17:ARG:NH1	7:B:317:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:311:HOH:O	2:B:89:LEU:HG	2.06	0.56
1:A:151:PHE:HB2	7:A:307:HOH:O	2.06	0.54
1:A:115:MET:HE1	3:A:201:CYC:CMA	2.38	0.54
1:A:7:SER:CB	7:A:303:HOH:O	2.55	0.54
1:A:65:VAL:HB	3:A:201:CYC:OC	2.07	0.53
3:A:201:CYC:HMD1	3:A:201:CYC:HBD2	1.89	0.53
2:B:23:SER:HB2	7:B:358:HOH:O	2.10	0.52
1:A:16:ARG:NH2	7:A:347:HOH:O	2.42	0.52
2:B:155:TYR:HB3	7:B:319:HOH:O	2.09	0.52
1:A:81:CYS:HB3	7:A:330:HOH:O	2.09	0.51
1:A:131:ARG:NE	7:A:342:HOH:O	2.34	0.51
2:B:93:THR:HG22	7:B:368:HOH:O	2.10	0.51
1:A:83:ARG:HD3	1:A:87:TYR:CZ	2.45	0.51
3:B:201:CYC:HMA1	3:B:201:CYC:HB	1.76	0.50
2:B:67:ARG:O	2:B:73:TYR:HB2	2.11	0.50
4:A:203:PEG:O4	7:A:318:HOH:O	2.05	0.50
1:A:4:ILE:C	7:A:303:HOH:O	2.49	0.49
2:B:108:VAL:HG12	3:B:201:CYC:HBB1	1.95	0.49
2:B:33:THR:HA	7:B:352:HOH:O	2.13	0.48
1:A:136:VAL:CA	7:A:312:HOH:O	2.56	0.47
1:A:10:ASN:HB3	7:A:347:HOH:O	2.13	0.47
2:B:79:ALA:HB1	7:B:349:HOH:O	2.15	0.47
7:A:311:HOH:O	2:B:89:LEU:C	2.54	0.47
2:B:20:ASP:HB2	7:B:455:HOH:O	2.14	0.46
1:A:3:ILE:CG1	7:A:353:HOH:O	2.63	0.46
1:A:6:LYS:HD2	7:A:391:HOH:O	2.15	0.46
2:B:111:GLY:O	7:B:333:HOH:O	2.21	0.46
1:A:143:GLY:O	1:A:145:ASP:N	2.46	0.46
2:B:107:ARG:NH1	7:B:345:HOH:O	2.48	0.46
1:A:36:ARG:N	7:A:352:HOH:O	2.50	0.45
1:A:6:LYS:CD	7:A:391:HOH:O	2.65	0.45
1:A:51:VAL:CG1	7:A:314:HOH:O	2.64	0.45
1:A:130:VAL:HG23	1:A:157:LEU:HB3	1.99	0.44
1:A:94:TYR:OH	2:B:12:ALA:O	2.34	0.44
2:B:32:GLN:HB3	7:B:336:HOH:O	2.17	0.44
1:A:78:THR:O	7:A:330:HOH:O	2.21	0.44
1:A:154:ASP:O	1:A:157:LEU:HD22	2.17	0.44
3:A:201:CYC:C2A	3:A:201:CYC:O1A	2.66	0.44
1:A:16:ARG:NH2	7:A:354:HOH:O	2.51	0.43
1:A:83:ARG:NH1	3:A:201:CYC:O2A	2.50	0.43
3:B:201:CYC:HMA3	3:B:201:CYC:HBA1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASP:O	2:B:58:LYS:CB	2.67	0.43
2:B:80:ALA:HA	7:B:395:HOH:O	2.19	0.43
1:A:145:ASP:HB2	7:A:316:HOH:O	2.17	0.43
1:A:31:LEU:HD11	7:B:379:HOH:O	2.18	0.43
1:A:142:ALA:C	7:A:316:HOH:O	2.57	0.43
2:B:81:CYS:SG	3:B:201:CYC:CAC	3.07	0.43
1:A:83:ARG:NH1	3:A:201:CYC:O1A	2.47	0.43
1:A:115:MET:HE1	3:A:201:CYC:HMA1	2.00	0.42
2:B:59:ALA:CB	7:B:305:HOH:O	2.66	0.42
1:A:90:ARG:O	1:A:93:THR:HG22	2.19	0.42
1:A:142:ALA:O	7:A:316:HOH:O	2.22	0.41
2:B:3:ASP:N	2:B:6:THR:OG1	2.48	0.41
1:A:114:GLU:OE1	1:A:114:GLU:N	2.47	0.41
1:A:115:MET:HE1	3:A:201:CYC:C3A	2.51	0.41
2:B:32:GLN:C	7:B:336:HOH:O	2.58	0.41
3:A:201:CYC:HAD2	3:A:201:CYC:HHA	1.91	0.41
2:B:155:TYR:CB	7:B:319:HOH:O	2.69	0.41
2:B:71:MEN:O	2:B:77:ARG:HD3	2.21	0.41
2:B:9:ILE:O	2:B:12:ALA:N	2.49	0.41
1:A:51:VAL:HG12	7:A:314:HOH:O	2.21	0.40
2:B:156:ILE:CA	7:B:319:HOH:O	2.65	0.40
2:B:3:ASP:O	2:B:7:SER:N	2.44	0.40

All (11) 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)
7:A:422:HOH:O	7:A:441:HOH:O[5_799]	1.57	0.63
7:B:432:HOH:O	7:B:476:HOH:O[3_695]	1.76	0.44
7:A:403:HOH:O	7:B:459:HOH:O[2_985]	1.78	0.42
7:A:457:HOH:O	7:B:459:HOH:O[2_985]	1.85	0.35
7:A:459:HOH:O	7:B:446:HOH:O[2_985]	1.99	0.21
7:A:418:HOH:O	7:B:355:HOH:O[3_585]	2.03	0.17
7:A:346:HOH:O	7:B:402:HOH:O[3_585]	2.05	0.15
7:B:502:HOH:O	7:B:502:HOH:O[5_7910]	2.07	0.13
7:B:413:HOH:O	7:B:461:HOH:O[5_7910]	2.07	0.13
7:B:304:HOH:O	7:B:407:HOH:O[3_695]	2.16	0.04
2:B:73:TYR:O	3:A:201:CYC:OB[3_695]	2.18	0.02

## 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	156/160 (98%)	146 (94%)	9 (6%)	1 (1%)	28	34
2	B	157/161 (98%)	147 (94%)	10 (6%)	0	100	100
All	All	313/321 (98%)	293 (94%)	19 (6%)	1 (0%)	44	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY

### 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	124/130 (95%)	116 (94%)	8 (6%)	20	26
2	B	126/127 (99%)	121 (96%)	5 (4%)	36	50
All	All	250/257 (97%)	237 (95%)	13 (5%)	27	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	38	ARG
1	A	76	GLU
1	A	83	ARG
1	A	93	THR

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Mol	Chain	Res	Type
1	A	139	SER
1	A	157	LEU
1	A	160	MET
2	B	58	LYS
2	B	73	TYR
2	B	123	ILE
2	B	140	LEU
2	B	160	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MEN	B	71	2	8,8,9	1.07	1 (12%)	8,9,11	1.25	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	B	71	2	-	0/6/8/10	0/0/0/0

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	71	MEN	CA-C	2.02	1.52	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	MEN	CB-CA-C	-2.53	106.54	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	71	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 22 are monoatomic - leaving 6 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	CYC	A	201	1	38,46,46	3.38	14 (36%)	46,67,67	3.97	24 (52%)
4	PEG	A	202	-	5,5,6	0.50	0	4,4,5	0.25	0
4	PEG	A	203	-	6,6,6	0.45	0	5,5,5	0.17	0
3	CYC	B	201	-	38,46,46	3.44	16 (42%)	46,67,67	3.85	23 (50%)
4	PEG	B	202	-	6,6,6	0.43	0	5,5,5	0.31	0
4	PEG	B	203	5	6,6,6	0.41	0	5,5,5	0.30	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
3	CYC	A	201	1	-	3/21/74/74	0/4/4/4
4	PEG	A	202	-	-	0/3/3/4	0/0/0/0
4	PEG	A	203	-	-	0/4/4/4	0/0/0/0
3	CYC	B	201	-	-	3/21/74/74	0/4/4/4
4	PEG	B	202	-	-	0/4/4/4	0/0/0/0
4	PEG	B	203	5	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	CYC	C2C-C1C	-5.13	1.47	1.52
3	B	201	CYC	C1C-NC	-4.48	1.31	1.37
3	A	201	CYC	C1A-NA	-3.84	1.30	1.38
3	A	201	CYC	C2C-C1C	-3.74	1.48	1.52
3	B	201	CYC	C1B-NB	-3.41	1.31	1.37
3	B	201	CYC	C4B-NB	-3.19	1.31	1.37
3	B	201	CYC	C4D-ND	-2.99	1.31	1.36
3	B	201	CYC	C4C-NC	-2.83	1.31	1.37
3	A	201	CYC	C4D-ND	-2.27	1.32	1.36
3	A	201	CYC	C1C-NC	-2.02	1.35	1.37
3	B	201	CYC	C1B-C2B	2.30	1.49	1.45
3	B	201	CYC	C1D-CHD	2.62	1.53	1.45
3	A	201	CYC	C1B-C2B	2.86	1.50	1.45
3	B	201	CYC	C3D-C2D	2.90	1.46	1.37
3	A	201	CYC	C1D-CHD	2.95	1.54	1.45
3	A	201	CYC	C4A-C3A	3.04	1.52	1.45
3	B	201	CYC	C2A-C3A	3.04	1.43	1.36
3	A	201	CYC	C3D-C2D	3.06	1.46	1.37
3	A	201	CYC	OB-C4B	3.20	1.29	1.23
3	B	201	CYC	OB-C4B	3.22	1.29	1.23
3	B	201	CYC	C4A-C3A	3.48	1.53	1.45
3	B	201	CYC	C3B-C2B	4.25	1.45	1.36
3	A	201	CYC	CHB-C1B	4.81	1.49	1.37
3	A	201	CYC	CHB-C4A	5.23	1.53	1.40
3	A	201	CYC	C3B-C2B	5.46	1.48	1.36
3	B	201	CYC	CHB-C4A	5.50	1.53	1.40
3	A	201	CYC	C2A-C3A	5.70	1.49	1.36
3	B	201	CYC	CHB-C1B	5.86	1.51	1.37
3	B	201	CYC	CHA-C1A	14.64	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	CYC	CHA-C1A	14.85	1.48	1.35

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CYC	C4B-C3B-C2B	-11.98	101.13	108.01
3	B	201	CYC	C4B-C3B-C2B	-8.75	102.98	108.01
3	B	201	CYC	OC-C1C-C2C	-8.71	119.22	126.25
3	A	201	CYC	OB-C4B-C3B	-6.80	120.52	128.11
3	A	201	CYC	OC-C1C-C2C	-6.29	121.17	126.25
3	A	201	CYC	C1D-C2D-C3D	-6.13	102.86	107.04
3	B	201	CYC	OB-C4B-C3B	-5.88	121.55	128.11
3	A	201	CYC	CHB-C4A-NA	-5.70	114.03	124.97
3	B	201	CYC	CMA-C3A-C2A	-4.94	112.41	126.09
3	B	201	CYC	C1D-C2D-C3D	-4.84	103.75	107.04
3	B	201	CYC	CHB-C4A-NA	-4.76	115.82	124.97
3	B	201	CYC	C1B-C2B-C3B	-3.44	104.06	107.83
3	B	201	CYC	CAD-CBD-CGD	-3.26	107.09	112.66
3	A	201	CYC	CMD-C2D-C3D	-3.14	119.03	124.94
3	A	201	CYC	CHA-C1A-NA	-3.13	124.05	128.79
3	B	201	CYC	CMD-C2D-C3D	-3.01	119.27	124.94
3	A	201	CYC	C1A-C2A-C3A	-2.94	103.51	106.81
3	B	201	CYC	C1A-C2A-C3A	-2.88	103.57	106.81
3	B	201	CYC	CHA-C1A-C2A	-2.88	118.57	125.39
3	A	201	CYC	C1B-NB-C4B	-2.84	106.92	110.70
3	A	201	CYC	C4A-C3A-C2A	-2.76	103.31	106.51
3	B	201	CYC	CHB-C1B-NB	-2.76	120.28	126.18
3	A	201	CYC	C3C-C4C-NC	-2.16	105.93	107.97
3	A	201	CYC	CAC-C3C-C4C	-2.05	107.42	112.67
3	A	201	CYC	C2A-C1A-NA	2.05	113.06	109.93
3	B	201	CYC	C2B-C1B-NB	2.06	110.10	107.04
3	A	201	CYC	C1A-NA-C4A	2.09	110.65	106.52
3	B	201	CYC	CBD-CAD-C3D	2.13	116.55	112.48
3	A	201	CYC	CAA-C2A-C3A	2.15	131.87	127.88
3	A	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
3	A	201	CYC	CMC-C2C-C1C	2.37	117.42	112.43
3	A	201	CYC	C2B-C1B-NB	2.65	110.99	107.04
3	B	201	CYC	C2A-C1A-NA	3.03	114.56	109.93
3	B	201	CYC	CAA-C2A-C1A	3.67	131.55	125.00
3	B	201	CYC	CHB-C4A-C3A	3.71	133.75	124.81
3	A	201	CYC	OC-C1C-NC	4.85	130.66	124.87
3	A	201	CYC	CHB-C4A-C3A	4.86	136.51	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	CYC	OC-C1C-NC	5.01	130.85	124.87
3	B	201	CYC	CMB-C2B-C1B	5.07	130.78	124.17
3	B	201	CYC	CMD-C2D-C1D	5.56	136.98	128.49
3	B	201	CYC	CAB-C3B-C4B	5.64	126.28	121.53
3	A	201	CYC	CMD-C2D-C1D	6.30	138.10	128.49
3	A	201	CYC	CMA-C3A-C4A	6.41	135.02	125.04
3	B	201	CYC	C3B-C4B-NB	7.88	113.42	106.75
3	A	201	CYC	CAB-C3B-C4B	9.42	129.47	121.53
3	A	201	CYC	C3B-C4B-NB	9.99	115.20	106.75
3	B	201	CYC	CMA-C3A-C4A	11.17	142.44	125.04

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	CYC	12	1
4	A	203	PEG	2	0
3	B	201	CYC	10	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	160/160 (100%)	1.25	30 (18%) <b>1</b> <b>2</b>	16, 31, 46, 60	0
2	B	160/161 (99%)	1.13	27 (16%) <b>2</b> <b>2</b>	15, 31, 45, 58	0
All	All	320/321 (99%)	1.19	57 (17%) <b>2</b> <b>2</b>	15, 31, 45, 60	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ILE	4.8
2	B	109	LEU	4.2
1	A	147	ALA	4.0
1	A	143	GLY	3.7
2	B	1	MET	3.6
1	A	40	ALA	3.6
1	A	96	ILE	3.6
1	A	82	LEU	3.6
2	B	28	ARG	3.6
2	B	160	LEU	3.5
1	A	38	ARG	3.4
1	A	151	PHE	3.2
2	B	140	LEU	3.1
2	B	6	THR	2.9
1	A	149	ALA	2.8
1	A	34	GLN	2.8
2	B	130	VAL	2.8
2	B	127	ILE	2.7
2	B	157	CYS	2.7
1	A	78	THR	2.7
1	A	140	LEU	2.6
2	B	69	GLY	2.5
2	B	155	TYR	2.5
1	A	130	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	2.5
1	A	59	PHE	2.5
1	A	142	ALA	2.4
1	A	63	PRO	2.4
1	A	4	ILE	2.4
1	A	52	LYS	2.4
2	B	73	TYR	2.4
1	A	53	GLN	2.4
2	B	105	ASP	2.4
2	B	43	THR	2.3
1	A	146	SER	2.3
2	B	123	ILE	2.3
1	A	160	MET	2.3
1	A	126	VAL	2.3
1	A	138	CYS	2.3
1	A	141	LEU	2.3
1	A	156	THR	2.3
2	B	118	SER	2.3
2	B	117	ASN	2.3
2	B	116	TYR	2.2
2	B	112	LEU	2.2
2	B	88	TYR	2.2
2	B	114	GLU	2.2
1	A	159	ALA	2.1
2	B	30	TYR	2.1
2	B	141	VAL	2.1
2	B	103	ILE	2.1
1	A	91	LEU	2.1
2	B	121	VAL	2.1
1	A	37	LEU	2.0
1	A	49	LEU	2.0
2	B	110	ASN	2.0
2	B	161	SER	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	MEN	B	71	9/10	0.69	0.30	-	30,32,32,32	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<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( $\text{\AA}^2$ )	Q<0.9
6	CL	A	209	1/1	0.77	0.48	10.50	30,30,30,30	0
4	PEG	A	202	6/7	0.74	0.28	2.80	26,26,32,32	0
3	CYC	B	201	43/43	0.66	0.32	2.25	27,29,34,36	80
3	CYC	A	201	43/43	0.71	0.28	1.35	19,23,28,29	79
5	NA	B	215	1/1	0.55	0.25	1.06	32,32,32,32	1
4	PEG	B	202	7/7	0.83	0.21	-0.30	29,31,38,39	0
4	PEG	B	203	7/7	0.84	0.20	-0.37	30,32,49,49	0
5	NA	B	209	1/1	0.93	0.18	-0.47	30,30,30,30	0
5	NA	A	208	1/1	0.94	0.17	-1.20	30,30,30,30	0
6	CL	B	219	1/1	0.94	0.12	-2.03	30,30,30,30	0
5	NA	B	208	1/1	0.90	0.13	-2.37	29,29,29,29	0
5	NA	A	204	1/1	0.91	0.09	-3.81	30,30,30,30	0
5	NA	B	214	1/1	0.87	0.15	-	29,29,29,29	0
5	NA	B	204	1/1	0.97	0.06	-	28,28,28,28	0
6	CL	B	217	1/1	0.81	0.14	-	30,30,30,30	0
5	NA	B	213	1/1	0.92	0.25	-	24,24,24,24	0
5	NA	B	210	1/1	0.78	0.27	-	30,30,30,30	0
5	NA	A	207	1/1	0.70	0.38	-	30,30,30,30	0
5	NA	B	205	1/1	0.90	0.11	-	35,35,35,35	0
5	NA	A	206	1/1	0.93	0.13	-	28,28,28,28	0
4	PEG	A	203	7/7	0.61	0.38	-	34,42,66,66	0
6	CL	B	216	1/1	0.97	0.12	-	30,30,30,30	0
5	NA	B	211	1/1	0.92	0.16	-	30,30,30,30	0
5	NA	B	212	1/1	0.93	0.12	-	35,35,35,35	0
5	NA	A	205	1/1	0.71	0.22	-	35,35,35,35	0
5	NA	B	207	1/1	0.91	0.10	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	B	218	1/1	0.94	0.22	-	30,30,30,30	0
5	NA	B	206	1/1	0.89	0.09	-	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.