



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:35 AM GMT

PDB ID : 1B8D
Title : CRYSTAL STRUCTURE OF A PHYCOUROBILIN-CONTAININGPHY-COERYTHRIN
Authors : Ritter, S.; Hiller, R.G.; Wrench, P.M.; Welte, W.; Diederichs, K.
Deposited on : 1999-01-29
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

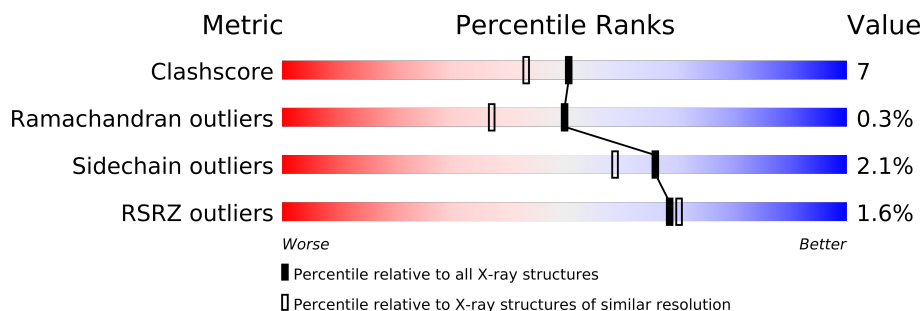
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	164	
1	K	164	
2	B	177	
2	L	177	
3	G	6	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7734 atoms, of which 1879 are hydrogens and 0 are deuterium.

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 PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	H	N	O	S	290	0	0
			1530	771	290	217	245	7			
1	K	164	Total	C	H	N	O	S	290	0	0
			1530	771	290	217	245	7			

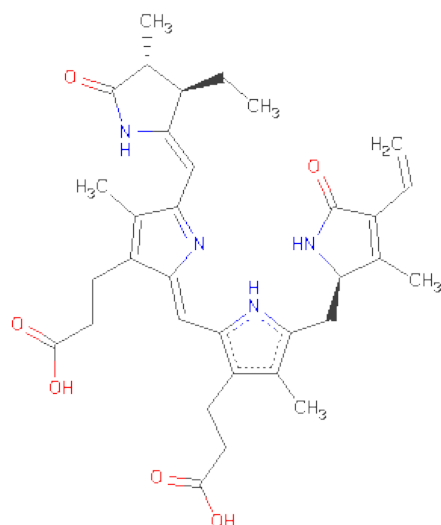
- Molecule 2 is a protein called PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	177	Total	C	H	N	O	S	299	0	0
			1590	797	299	223	261	10			
2	L	177	Total	C	H	N	O	S	299	0	0
			1590	797	299	223	261	10			

- Molecule 3 is a protein called PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (GAMMA CHAIN)).

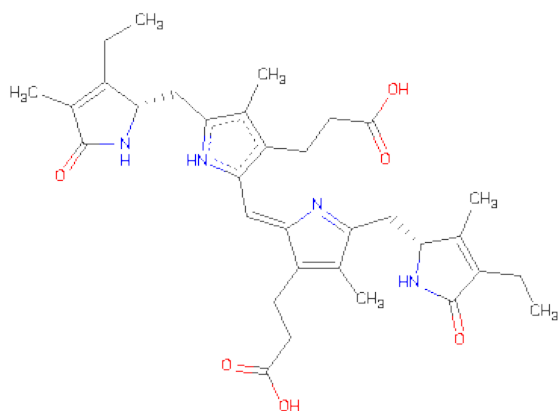
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	5	Total	C	H	N	O	5	0	2
			35	20	5	5	5			

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	A	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	B	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	B	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	K	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	K	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	L	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
4	L	1	Total	C	H	N	O	3	0
			46	33	3	4	6		

- Molecule 5 is PHYCOUROBILIN (three-letter code: PUB) (formula: C₃₃H₄₂N₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	3	0
			46	33	3	4	6		
5	L	1	Total	C	H	N	O	3	0
			46	33	3	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	80	Total	H	O	160	0
			240	160	80		
6	B	74	Total	H	O	148	0
			222	148	74		
6	K	80	Total	H	O	160	0
			240	160	80		
6	L	99	Total	H	O	198	0
			297	198	99		

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 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.

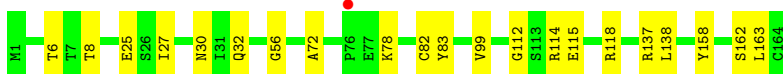
- Molecule 1: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN))

Chain A: 



- Molecule 1: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN))

Chain K: 



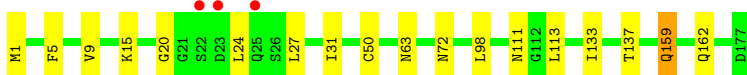
- Molecule 2: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN))

Chain B: 



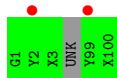
- Molecule 2: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN))

Chain L: 



- Molecule 3: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (GAMMA CHAIN))

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	187.35Å 187.35Å 59.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 1.90 31.53 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.0 (100.00-1.90) 73.9 (31.53-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.175 , 0.227 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.0	EDS
Estimated twinning fraction	0.004 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 67710 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7734	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 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, PEB, PUB

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	0.46	0/1261	0.63	0/1704
1	K	0.46	0/1261	0.61	0/1704
2	B	0.46	0/1294	0.63	0/1748
2	L	0.46	0/1294	0.63	0/1748
3	G	0.89	0/28	0.86	0/35
All	All	0.46	0/5138	0.62	0/6939

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1240	290	921	23	0
1	K	1240	290	921	19	0
2	B	1291	299	988	15	0
2	L	1291	299	988	16	0
3	G	30	5	18	0	0
4	A	86	6	70	7	0
4	B	86	6	70	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	86	6	70	3	0
4	L	86	6	70	5	0
5	B	43	3	35	4	0
5	L	43	3	35	2	0
6	A	80	160	0	3	0
6	B	74	148	0	1	0
6	K	80	160	0	2	0
6	L	99	198	0	3	0
All	All	5855	1879	4186	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:GLN:HG3	1:K:32:GLN:HG3	1.48	0.93
2:B:137:THR:HG21	6:B:364:HOH:O	1.82	0.79
2:L:137:THR:HG21	6:L:401:HOH:O	1.88	0.73
1:A:140:VAL:HG11	1:A:146:SER:HA	1.72	0.72
1:A:32:GLN:CG	1:K:32:GLN:HG3	2.21	0.71
2:L:137:THR:HG22	5:L:210:PUB:C4B	2.21	0.70
2:B:137:THR:HG22	5:B:205:PUB:C4B	2.22	0.69
4:L:209:PEB:HBC2	6:L:525:HOH:O	1.95	0.67
1:A:32:GLN:HG3	1:K:32:GLN:CG	2.23	0.64
2:L:133:ILE:O	2:L:137:THR:HG23	1.98	0.64
1:A:38:LEU:HD22	2:B:24:LEU:HD22	1.84	0.60
2:L:1:MET:SD	6:L:597:HOH:O	2.56	0.60
2:B:133:ILE:O	2:B:137:THR:HG23	2.02	0.58
4:A:202:PEB:NA	4:A:202:PEB:HMB2	2.20	0.57
1:A:27:ILE:O	1:A:30:ASN:HB2	2.05	0.56
1:A:82:CYS:HA	4:A:201:PEB:HHA1	1.88	0.56
2:B:157:ASP:OD1	2:B:159:GLN:HG2	2.06	0.55
2:B:137:THR:HG22	5:B:205:PUB:NB	2.22	0.54
1:K:27:ILE:HD12	2:L:98:LEU:HD11	1.89	0.54
1:A:54:GLU:OE1	1:A:137:ARG:HD3	2.08	0.53
2:L:137:THR:HG22	5:L:210:PUB:NB	2.23	0.53
4:B:204:PEB:NA	4:B:204:PEB:HMB2	2.24	0.52
1:A:62:LYS:HD3	1:A:63:TYR:CE2	2.45	0.52
2:B:72:MEN:HB2	4:B:203:PEB:OA	2.09	0.51
1:A:56:GLY:HA3	1:A:83:TYR:CE2	2.46	0.50
1:A:139:CYS:HB2	4:A:202:PEB:HHA1	1.92	0.50
1:A:25:GLU:OE2	1:K:30:ASN:HA	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:ILE:HD13	2:B:98:LEU:HD11	1.95	0.48
1:K:137:ARG:HG3	4:K:207:PEB:HHC1	1.94	0.48
1:K:82:CYS:HA	4:K:206:PEB:HHA1	1.94	0.48
1:K:56:GLY:HA3	1:K:83:TYR:CE2	2.48	0.48
1:A:45:SER:O	1:A:48:HIS:HD2	1.97	0.48
1:K:114:ARG:HB3	1:K:114:ARG:NH1	2.28	0.48
2:B:51:ILE:HG23	2:B:137:THR:OG1	2.12	0.47
1:K:138:LEU:HA	4:K:207:PEB:HMD2	1.97	0.47
1:A:30:ASN:HA	1:K:25:GLU:OE2	2.15	0.47
4:B:204:PEB:HBD1	4:B:204:PEB:OD	2.14	0.46
2:B:15:LYS:HB2	2:B:15:LYS:HE3	1.58	0.46
1:A:88:HIS:HE1	6:A:406:HOH:O	1.98	0.46
1:K:6:THR:HG22	2:L:1:MET:HG3	1.98	0.46
1:A:140:VAL:HG13	1:A:144:MET:O	2.16	0.46
1:A:88:HIS:O	1:A:92:LEU:HG	2.16	0.46
1:K:158:TYR:HA	6:K:574:HOH:O	2.15	0.45
1:K:118:ARG:NH1	6:K:535:HOH:O	2.48	0.45
1:K:99:VAL:HG23	2:L:9:VAL:HG21	1.99	0.44
2:L:113:LEU:CD1	4:L:208:PEB:HMD3	2.47	0.44
2:B:137:THR:HG22	5:B:205:PUB:C1B	2.48	0.44
4:B:203:PEB:HBD1	4:B:203:PEB:OD	2.18	0.44
2:L:5:PHE:CZ	2:L:31:ILE:HD11	2.53	0.44
2:L:15:LYS:HB2	2:L:15:LYS:HE3	1.81	0.44
4:A:202:PEB:HHC2	6:A:546:HOH:O	2.17	0.44
1:A:78:LYS:HE3	4:A:201:PEB:O1B	2.18	0.44
2:B:24:LEU:O	2:B:28:LYS:HG3	2.18	0.43
2:L:27:LEU:O	2:L:31:ILE:HG12	2.19	0.43
1:A:35:ALA:HB3	6:A:367:HOH:O	2.19	0.43
1:A:99:VAL:HG23	2:B:9:VAL:HG21	1.99	0.43
1:K:27:ILE:O	1:K:30:ASN:HB2	2.18	0.43
1:K:162:SER:OG	1:K:163:LEU:HD22	2.18	0.42
4:B:203:PEB:HMB2	4:B:203:PEB:NA	2.34	0.42
2:L:72:MEN:HB2	4:L:208:PEB:OA	2.19	0.42
2:L:20:GLY:HA2	2:L:24:LEU:HG	2.01	0.42
1:K:112:GLY:HA2	1:K:115:GLU:OE1	2.20	0.42
4:L:209:PEB:HBC1	4:L:209:PEB:HBB1	2.01	0.42
1:A:88:HIS:CD2	1:A:91:ARG:NH2	2.88	0.41
2:B:137:THR:HG22	5:B:205:PUB:C3B	2.51	0.41
2:L:159:GLN:HA	2:L:159:GLN:NE2	2.34	0.41
2:L:72:MEN:HE22	4:L:208:PEB:HBB2	2.03	0.41
1:K:72:ALA:O	1:K:78:LYS:HB3	2.20	0.41
4:A:202:PEB:HMA1	4:A:202:PEB:HBA2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:204:PEB:HHA1	4:B:204:PEB:HBA3	2.02	0.41
1:A:137:ARG:HG2	4:A:202:PEB:HHC1	2.03	0.40
2:B:6:SER:HA	2:B:9:VAL:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	K	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	B	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	33	19
2	L	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	33	19
3	G	1/6 (17%)	1 (100%)	0	0	100	100
All	All	673/688 (98%)	655 (97%)	16 (2%)	2 (0%)	50	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	111	ASN
2	B	75	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/129 (100%)	126 (98%)	3 (2%)	63	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	129/129 (100%)	128 (99%)	1 (1%)	89	89
2	B	137/137 (100%)	134 (98%)	3 (2%)	64	57
2	L	137/137 (100%)	133 (97%)	4 (3%)	55	44
3	G	2/2 (100%)	2 (100%)	0	100	100
All	All	534/534 (100%)	523 (98%)	11 (2%)	66	59

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	137	ARG
1	A	138	LEU
2	B	50	CYS
2	B	63	ASN
2	B	152	GLU
1	K	8	THR
2	L	50	CYS
2	L	63	ASN
2	L	159	GLN
2	L	162	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	47	ASN
1	A	48	HIS
1	A	88	HIS
1	K	32	GLN
1	K	48	HIS
1	K	88	HIS
2	L	35	ASN
2	L	47	ASN
2	L	144	ASN
2	L	162	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	B	72	2	8,8,9	6.45	2 (25%)	7,9,11	0.92	1 (14%)
2	MEN	L	72	2	8,8,9	6.28	2 (25%)	7,9,11	0.65	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
2	MEN	B	72	2	-	0/6/8/10	0/0/0/0
2	MEN	L	72	2	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	O-C	17.99	1.23	1.11
2	L	72	MEN	O-C	17.52	1.23	1.11
2	L	72	MEN	CA-C	2.75	1.53	1.48
2	B	72	MEN	CA-C	2.73	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	MEN	C-CA-N	2.36	116.19	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	PEB	A	201	1	46,46,46	1.52	7 (15%)	66,67,67	1.61	13 (19%)
4	PEB	A	202	1	46,46,46	1.42	7 (15%)	66,67,67	1.43	8 (12%)
4	PEB	B	203	2	46,46,46	1.40	9 (19%)	66,67,67	1.58	13 (19%)
4	PEB	B	204	2	46,46,46	1.64	10 (21%)	66,67,67	1.46	9 (13%)
5	PUB	B	205	2	46,46,46	2.21	12 (26%)	66,67,67	1.96	16 (24%)
4	PEB	K	206	1	46,46,46	1.63	9 (19%)	66,67,67	1.60	14 (21%)
4	PEB	K	207	1	46,46,46	1.71	12 (26%)	66,67,67	1.61	13 (19%)
4	PEB	L	208	2	46,46,46	1.39	7 (15%)	66,67,67	1.64	15 (22%)
4	PEB	L	209	2	46,46,46	1.90	10 (21%)	66,67,67	1.45	10 (15%)
5	PUB	L	210	2	46,46,46	2.06	12 (26%)	66,67,67	1.87	12 (18%)

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	PEB	A	201	1	-	2/26/74/74	0/4/4/4
4	PEB	A	202	1	-	2/26/74/74	0/4/4/4
4	PEB	B	203	2	-	2/26/74/74	0/4/4/4
4	PEB	B	204	2	-	2/26/74/74	0/4/4/4
5	PUB	B	205	2	-	0/26/74/74	0/4/4/4
4	PEB	K	206	1	-	2/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEB	K	207	1	-	2/26/74/74	0/4/4/4
4	PEB	L	208	2	-	2/26/74/74	0/4/4/4
4	PEB	L	209	2	-	2/26/74/74	0/4/4/4
5	PUB	L	210	2	-	0/26/74/74	0/4/4/4

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	205	PUB	C3A-C2A	9.42	1.46	1.34
5	L	210	PUB	C3A-C2A	8.96	1.45	1.34
4	L	209	PEB	C4C-C3C	6.22	1.47	1.37
4	L	209	PEB	C4D-ND	5.65	1.42	1.34
4	B	204	PEB	C4C-C3C	5.53	1.46	1.37
4	K	206	PEB	C4C-C3C	5.37	1.46	1.37
4	A	202	PEB	C4C-C3C	5.08	1.45	1.37
5	B	205	PUB	C4D-ND	5.07	1.41	1.34
4	L	208	PEB	C4C-C3C	4.96	1.45	1.37
4	K	206	PEB	C2A-C1A	-4.93	1.47	1.52
4	A	201	PEB	C2A-C1A	-4.47	1.47	1.52
4	A	201	PEB	C4C-C3C	4.41	1.44	1.37
5	L	210	PUB	C4D-ND	4.37	1.40	1.34
5	B	205	PUB	C2D-C3D	4.29	1.47	1.36
4	K	207	PEB	C4D-ND	4.14	1.40	1.34
4	K	207	PEB	C2A-C1A	-4.07	1.48	1.52
4	L	209	PEB	C3B-C2B	3.85	1.44	1.36
5	B	205	PUB	C1C-C2C	-3.84	1.38	1.45
4	A	201	PEB	C4D-ND	3.68	1.39	1.34
5	L	210	PUB	C1B-C2B	3.64	1.43	1.37
4	B	203	PEB	C4D-ND	3.56	1.39	1.34
4	K	207	PEB	C3A-C4A	3.50	1.54	1.51
4	B	204	PEB	C2A-C1A	-3.44	1.48	1.52
5	L	210	PUB	C2D-C3D	3.38	1.44	1.36
4	K	207	PEB	C4C-C3C	3.30	1.43	1.37
4	B	203	PEB	C4C-C3C	3.26	1.43	1.37
4	B	204	PEB	C2D-C3D	3.24	1.46	1.35
4	B	203	PEB	C3A-C4A	3.23	1.54	1.51
4	K	207	PEB	CMD-C2D	3.23	1.55	1.50
4	L	209	PEB	C2A-C1A	-3.12	1.49	1.52
4	B	204	PEB	C4D-ND	3.07	1.38	1.34
5	L	210	PUB	C1A-NA	3.05	1.38	1.34
4	L	209	PEB	CAD-C3D	-3.04	1.37	1.48
5	L	210	PUB	C1C-C2C	-3.03	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	205	PUB	C1A-NA	2.95	1.38	1.34
4	B	203	PEB	CAD-C3D	-2.85	1.38	1.48
5	B	205	PUB	CHC-C1D	2.84	1.59	1.53
4	B	204	PEB	CAD-C3D	-2.76	1.38	1.48
4	K	207	PEB	C2D-C3D	2.76	1.44	1.35
4	L	209	PEB	C1C-C2C	-2.73	1.35	1.42
4	L	208	PEB	C4D-ND	2.72	1.38	1.34
5	L	210	PUB	C4D-C3D	-2.72	1.42	1.48
4	A	201	PEB	CAD-C3D	-2.65	1.38	1.48
4	A	202	PEB	C3A-C4A	-2.63	1.48	1.51
4	B	203	PEB	C3B-C2B	2.63	1.42	1.36
4	A	202	PEB	CAD-C3D	-2.60	1.39	1.48
4	K	207	PEB	CAD-C3D	-2.59	1.39	1.48
4	A	202	PEB	C2D-C3D	2.56	1.44	1.35
4	K	206	PEB	C2D-C3D	2.54	1.44	1.35
4	L	208	PEB	CAD-C3D	-2.52	1.39	1.48
4	L	209	PEB	C2D-C3D	2.52	1.44	1.35
5	B	205	PUB	C3C-C4C	2.51	1.48	1.42
4	K	206	PEB	CAD-C3D	-2.50	1.39	1.48
4	A	202	PEB	C1C-CHB	-2.49	1.36	1.46
4	K	207	PEB	CHB-C4B	2.49	1.36	1.35
5	L	210	PUB	C4B-CHB	-2.46	1.36	1.46
5	B	205	PUB	C4B-CHB	-2.46	1.36	1.46
4	L	209	PEB	CHC-C1D	2.45	1.60	1.54
4	L	209	PEB	C1C-CHB	-2.44	1.36	1.46
4	K	206	PEB	OD-C4D	-2.41	1.18	1.23
4	L	208	PEB	C1C-CHB	-2.41	1.36	1.46
4	K	207	PEB	C1C-CHB	-2.36	1.36	1.46
5	B	205	PUB	CHB-C1C	2.35	1.36	1.35
5	B	205	PUB	C2C-C3C	2.35	1.41	1.36
4	B	204	PEB	C1C-CHB	-2.34	1.37	1.46
4	B	203	PEB	C1C-CHB	-2.33	1.37	1.46
4	B	204	PEB	C3B-C2B	2.32	1.41	1.36
4	B	204	PEB	C3A-C4A	2.32	1.53	1.51
5	B	205	PUB	C4D-C3D	-2.31	1.43	1.48
4	K	207	PEB	CAC-C2C	-2.31	1.48	1.52
4	K	206	PEB	CHB-C4B	2.30	1.36	1.35
4	A	202	PEB	C2A-C1A	-2.29	1.49	1.52
4	B	204	PEB	CHB-C4B	2.28	1.36	1.35
4	B	203	PEB	CHB-C4B	2.28	1.36	1.35
4	A	201	PEB	C1C-CHB	-2.28	1.37	1.46
4	K	206	PEB	C1C-CHB	-2.26	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	PEB	C2D-C3D	2.26	1.43	1.35
4	A	202	PEB	C1C-C2C	-2.25	1.36	1.42
4	A	201	PEB	CHB-C4B	2.24	1.36	1.35
5	L	210	PUB	CHB-C1C	2.23	1.36	1.35
4	L	208	PEB	C2A-C1A	-2.20	1.49	1.52
5	L	210	PUB	C3C-C4C	2.20	1.47	1.42
4	B	203	PEB	OA-C1A	2.16	1.27	1.23
4	K	207	PEB	OA-C1A	2.15	1.27	1.23
4	K	207	PEB	C1C-C2C	-2.13	1.37	1.42
4	L	208	PEB	C2C-C3C	2.10	1.43	1.37
4	B	203	PEB	C2D-C3D	2.08	1.42	1.35
4	K	206	PEB	C3B-C2B	2.07	1.41	1.36
5	L	210	PUB	C4B-C3B	2.06	1.47	1.42
4	B	204	PEB	C2C-C3C	2.05	1.43	1.37
4	L	208	PEB	OD-C4D	-2.04	1.19	1.23
4	L	209	PEB	C1B-C2B	2.04	1.50	1.45
5	L	210	PUB	C4B-NB	2.04	1.38	1.36
5	B	205	PUB	C3B-C2B	2.04	1.43	1.37
4	K	206	PEB	C2C-C3C	2.02	1.43	1.37

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	205	PUB	CHB-C1C-NC	-8.83	112.28	128.59
5	L	210	PUB	CHB-C1C-NC	-8.77	112.39	128.59
4	L	209	PEB	C2C-C1C-NC	5.25	115.45	106.79
4	A	202	PEB	C2C-C1C-NC	4.90	114.88	106.79
4	B	204	PEB	C2C-C1C-NC	4.82	114.74	106.79
4	L	208	PEB	C2C-C1C-NC	4.52	114.26	106.79
4	K	207	PEB	C2C-C1C-NC	4.15	113.65	106.79
4	B	203	PEB	C2C-C1C-NC	3.99	113.37	106.79
4	A	201	PEB	C2C-C1C-NC	3.96	113.33	106.79
4	A	201	PEB	C3A-C4A-NA	-3.95	104.02	107.83
4	L	208	PEB	C1D-ND-C4D	-3.91	107.68	113.89
5	L	210	PUB	CHC-C1D-ND	-3.85	109.95	114.18
5	B	205	PUB	C4A-NA-C1A	-3.76	107.93	113.89
4	K	206	PEB	C2C-C1C-NC	3.71	112.91	106.79
4	B	203	PEB	CHC-C4C-C3C	-3.68	126.00	130.95
4	A	201	PEB	CHC-C4C-C3C	-3.65	126.04	130.95
5	B	205	PUB	CHA-C1B-C2B	-3.63	126.06	130.95
5	B	205	PUB	CHC-C1D-ND	-3.62	110.21	114.18
4	K	207	PEB	C1C-CHB-C4B	3.47	136.69	129.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	203	PEB	C1D-ND-C4D	-3.47	108.39	113.89
4	K	206	PEB	CHC-C4C-C3C	-3.44	126.32	130.95
5	L	210	PUB	C4A-NA-C1A	-3.44	108.44	113.89
5	B	205	PUB	CAD-C3D-C4D	3.43	124.35	121.49
5	L	210	PUB	CHB-C1C-C2C	3.37	134.09	125.48
4	K	207	PEB	C1D-ND-C4D	-3.32	108.62	113.89
5	B	205	PUB	C3C-C4C-NC	-3.26	108.95	112.14
4	L	208	PEB	CHC-C4C-C3C	-3.24	126.59	130.95
4	K	206	PEB	C1D-ND-C4D	-3.21	108.79	113.89
4	K	207	PEB	CHC-C4C-C3C	-3.20	126.64	130.95
5	B	205	PUB	OD-C4D-C3D	-3.19	124.60	128.20
4	A	201	PEB	OA-C1A-C2A	-3.13	123.67	126.25
4	A	201	PEB	C1D-ND-C4D	-3.12	108.94	113.89
5	L	210	PUB	CAD-C3D-C4D	3.11	124.08	121.49
4	K	206	PEB	C2C-C1C-CHB	3.08	134.47	125.72
5	L	210	PUB	C1D-ND-C4D	-3.08	108.99	113.89
5	B	205	PUB	CHB-C1C-C2C	3.05	133.29	125.48
5	L	210	PUB	OD-C4D-C3D	-3.05	124.76	128.20
4	K	207	PEB	C1C-NC-C4C	-3.05	103.63	109.01
4	L	209	PEB	C1C-NC-C4C	-3.00	103.71	109.01
4	B	203	PEB	C2A-C3A-C4A	2.97	105.27	101.08
4	B	203	PEB	C2C-C1C-CHB	2.94	134.07	125.72
4	A	201	PEB	C2C-C1C-CHB	2.92	134.02	125.72
5	L	210	PUB	C2A-C1A-NA	2.90	109.16	107.05
5	L	210	PUB	C3C-C4C-NC	-2.90	109.30	112.14
4	B	203	PEB	C4B-NB-C1B	2.89	112.16	106.55
4	B	204	PEB	CHC-C4C-C3C	-2.88	127.07	130.95
4	A	202	PEB	C1C-NC-C4C	-2.87	103.93	109.01
4	K	207	PEB	CBC-CAC-C2C	-2.88	107.63	112.69
4	L	208	PEB	C1C-CHB-C4B	2.86	135.51	129.92
5	B	205	PUB	C2C-C1C-NC	2.86	114.31	109.79
4	L	208	PEB	C2A-C3A-C4A	2.85	105.11	101.08
4	B	204	PEB	C1C-CHB-C4B	2.84	135.47	129.92
5	B	205	PUB	CHA-C4A-NA	-2.82	110.96	114.29
4	A	202	PEB	C1D-ND-C4D	-2.80	109.44	113.89
4	B	203	PEB	C1C-CHB-C4B	2.77	135.34	129.92
4	A	202	PEB	CHC-C4C-C3C	-2.74	127.26	130.95
4	K	207	PEB	C2C-C1C-CHB	2.72	133.45	125.72
4	K	206	PEB	C4B-NB-C1B	2.70	111.79	106.55
4	L	209	PEB	C1D-ND-C4D	-2.69	109.61	113.89
4	K	207	PEB	OA-C1A-C2A	-2.67	124.04	126.25
4	B	203	PEB	C1C-NC-C4C	-2.63	104.36	109.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	210	PUB	CHA-C1B-C2B	-2.60	127.45	130.95
4	L	209	PEB	C4B-NB-C1B	2.59	111.59	106.55
4	L	208	PEB	C2C-C1C-CHB	2.58	133.03	125.72
4	L	209	PEB	C2A-C3A-C4A	2.57	104.72	101.08
4	L	208	PEB	CMB-C2B-C1B	2.57	129.26	125.02
4	B	204	PEB	C4B-NB-C1B	2.56	111.53	106.55
4	L	208	PEB	C1C-NC-C4C	-2.53	104.55	109.01
4	L	209	PEB	C1C-CHB-C4B	2.53	134.85	129.92
4	A	202	PEB	C2C-C1C-CHB	2.53	132.89	125.72
4	B	203	PEB	CMB-C2B-C1B	2.53	129.19	125.02
4	B	204	PEB	CHC-C1D-ND	-2.52	111.31	114.29
4	A	201	PEB	C2A-C3A-C4A	2.49	104.60	101.08
4	K	207	PEB	C2A-C3A-C4A	2.49	104.60	101.08
4	B	204	PEB	C1C-NC-C4C	-2.48	104.63	109.01
4	K	206	PEB	C3A-C4A-NA	-2.47	105.45	107.83
4	K	206	PEB	C1C-CHB-C4B	2.46	134.73	129.92
4	L	209	PEB	CBC-CAC-C2C	-2.44	108.39	112.69
4	A	202	PEB	CHC-C1D-ND	-2.44	111.40	114.29
4	A	201	PEB	C1C-NC-C4C	-2.43	104.73	109.01
5	B	205	PUB	C3D-C4D-ND	2.42	110.16	107.19
4	B	204	PEB	C1D-ND-C4D	-2.42	110.05	113.89
4	L	208	PEB	C4B-NB-C1B	2.41	111.24	106.55
5	B	205	PUB	CAA-C3A-C4A	2.41	126.62	121.94
5	B	205	PUB	C1D-ND-C4D	-2.40	110.08	113.89
4	B	204	PEB	C2C-C1C-CHB	2.39	132.51	125.72
4	K	206	PEB	C2A-C3A-C4A	2.38	104.44	101.08
4	L	208	PEB	CHA-C1B-C2B	2.37	131.00	125.10
4	B	204	PEB	CMD-C2D-C1D	2.35	127.15	120.35
4	A	202	PEB	C1B-CHA-C4A	-2.33	121.23	126.65
4	K	206	PEB	CMD-C2D-C1D	2.33	127.08	120.35
4	L	209	PEB	CMD-C2D-C1D	2.32	127.05	120.35
5	L	210	PUB	C2C-C1C-NC	2.32	113.46	109.79
4	A	201	PEB	CBB-CAB-C3B	-2.30	105.91	112.71
4	K	207	PEB	CMD-C2D-C1D	2.28	126.95	120.35
4	B	203	PEB	C3C-C4C-NC	2.27	110.57	106.83
4	K	206	PEB	OA-C1A-C2A	-2.26	124.38	126.25
4	L	208	PEB	C3C-C4C-NC	2.25	110.54	106.83
4	L	209	PEB	CHC-C4C-C3C	-2.25	127.92	130.95
4	A	201	PEB	C3B-C4B-NB	-2.24	106.23	109.79
4	A	201	PEB	C4B-NB-C1B	2.24	110.90	106.55
4	L	208	PEB	CAD-C3D-C2D	-2.23	122.92	128.74
5	B	205	PUB	CMD-C2D-C1D	2.23	126.80	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	205	PUB	C2A-C1A-NA	2.23	108.67	107.05
5	B	205	PUB	C4B-CHB-C1C	2.22	134.25	129.92
4	L	208	PEB	CMD-C2D-C1D	2.22	126.76	120.35
4	K	206	PEB	C3B-C4B-NB	-2.19	106.31	109.79
5	L	210	PUB	CAA-C3A-C4A	2.19	126.19	121.94
4	A	201	PEB	CMD-C2D-C1D	2.15	126.56	120.35
4	L	209	PEB	C2C-C1C-CHB	2.13	131.77	125.72
4	A	202	PEB	C3A-C4A-NA	-2.13	105.77	107.83
4	B	203	PEB	CMD-C2D-C1D	2.11	126.44	120.35
4	L	208	PEB	C1C-C2C-C3C	-2.10	104.74	106.92
4	K	207	PEB	C4B-NB-C1B	2.09	110.62	106.55
4	B	203	PEB	CHA-C1B-C2B	2.08	130.27	125.10
4	K	206	PEB	C3C-C4C-NC	2.08	110.25	106.83
4	K	207	PEB	C3A-C2A-C1A	2.07	105.21	103.43
4	K	206	PEB	C3D-C4D-ND	2.05	110.18	106.85
4	K	206	PEB	CMB-C2B-C1B	2.05	128.40	125.02
4	K	207	PEB	CMB-C2B-C1B	2.04	128.40	125.02
4	A	201	PEB	CMB-C2B-C1B	2.02	128.36	125.02
4	L	208	PEB	C3B-C4B-NB	-2.02	106.59	109.79
4	B	203	PEB	C1C-C2C-C3C	-2.02	104.83	106.92

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	208	PEB	C4A-CHA-C1B-NB
4	B	204	PEB	C4A-CHA-C1B-NB
4	L	208	PEB	C4A-CHA-C1B-C2B
4	B	203	PEB	C4A-CHA-C1B-NB
4	B	204	PEB	C4A-CHA-C1B-C2B
4	A	202	PEB	C4A-CHA-C1B-NB
4	B	203	PEB	C4A-CHA-C1B-C2B
4	L	209	PEB	C4A-CHA-C1B-NB
4	K	207	PEB	C4A-CHA-C1B-NB
4	K	206	PEB	C4A-CHA-C1B-NB
4	A	202	PEB	C4A-CHA-C1B-C2B
4	K	207	PEB	C4A-CHA-C1B-C2B
4	A	201	PEB	C4A-CHA-C1B-NB
4	A	201	PEB	C4A-CHA-C1B-C2B
4	L	209	PEB	C4A-CHA-C1B-C2B
4	K	206	PEB	C4A-CHA-C1B-C2B

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.23	2 (1%) 75 78	12, 20, 34, 45	0
1	K	164/164 (100%)	-0.22	1 (0%) 86 88	12, 19, 34, 45	0
2	B	177/177 (100%)	-0.24	2 (1%) 77 79	12, 20, 39, 57	0
2	L	177/177 (100%)	-0.29	3 (1%) 67 69	11, 20, 39, 57	0
3	G	3/6 (50%)	1.40	2 (66%) 0 0	36, 36, 40, 40	0
All	All	685/688 (99%)	-0.24	10 (1%) 68 72	11, 20, 38, 57	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	147	SER	3.5
2	L	25	GLN	3.3
2	L	22	SER	3.0
2	B	159	GLN	2.5
1	A	140	VAL	2.3
3	G	2	TYR	2.3
1	K	76	PRO	2.3
1	A	139	CYS	2.1
3	G	99	TYR	2.1
2	L	23	ASP	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MEN	B	72	9/10	0.08	0.18	0,19,23,24	1
2	MEN	L	72	9/10	0.07	-0.59	0,19,23,24	1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PEB	A	202	43/43	0.22	1.05	0,47,59,63	3
4	PEB	L	209	43/43	0.11	0.79	0,18,43,56	3
4	PEB	K	207	43/43	0.09	0.32	0,23,38,47	3
5	PUB	L	210	43/43	0.09	0.26	0,19,32,35	3
4	PEB	A	201	43/43	0.08	0.20	0,19,27,40	3
4	PEB	L	208	43/43	0.10	0.19	0,17,29,37	3
4	PEB	B	203	43/43	0.09	0.13	0,17,28,38	3
4	PEB	B	204	43/43	0.11	0.02	0,19,44,52	3
5	PUB	B	205	43/43	0.09	-0.14	0,26,38,49	3
4	PEB	K	206	43/43	0.08	-0.33	0,16,27,34	3

6.5 Other polymers

There are no such residues in this entry.