Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:33 PM GMT

PDB ID	:	1B33
Title	:	STRUCTURE OF LIGHT HARVESTING COMPLEX OF ALLOPHYCOCYANIN ALPHA AND BETA CHAINS/CORE-LINKER COMPLEX AP*LC7.8
Authors	:	Reuter, W.; Wiegand, G.; Huber, R.; Than, M.E.
Deposited on	:	1998-12-15
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

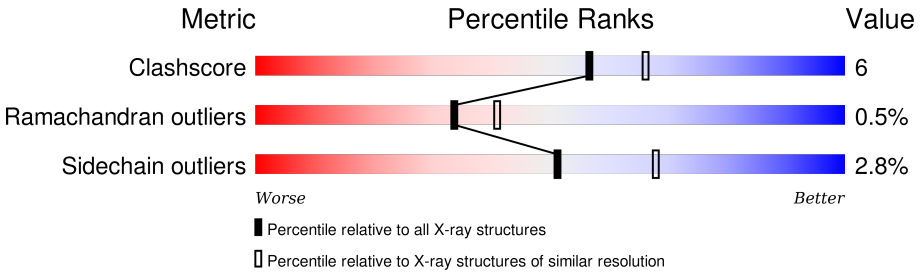
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	160	91% 9%
1	C	160	88% 12%
1	E	160	83% 16%
1	H	160	89% 11%
1	J	160	88% 12%
1	L	160	91% 9%
2	B	161	89% 10%

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Mol	Chain	Length	Quality of chain
2	D	161	89% 10%
2	F	161	91% 9%
2	I	161	92% 7%
2	K	161	83% 17%
2	M	161	90% 9%
3	N	67	73% 22%
3	O	67	66% 31%

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
5	CYC	C	203	X	-	-	-
5	CYC	D	204	X	-	-	-
5	CYC	E	205	X	-	-	-
5	CYC	F	206	X	-	-	-
5	CYC	H	207	X	-	-	-
5	CYC	I	208	X	-	-	-
5	CYC	J	209	X	-	-	-
5	CYC	K	210	X	-	-	-
5	CYC	L	211	X	-	-	-
5	CYC	M	212	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17502 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 ALLOPHYCOCYANIN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	22	0	0
			1203	754	206	239	4			
1	C	160	Total	C	N	O	S	19	0	0
			1203	754	206	239	4			
1	E	160	Total	C	N	O	S	12	0	0
			1203	754	206	239	4			
1	H	160	Total	C	N	O	S	13	0	0
			1203	754	206	239	4			
1	J	160	Total	C	N	O	S	18	0	0
			1203	754	206	239	4			
1	L	160	Total	C	N	O	S	11	0	0
			1203	754	206	239	4			

- Molecule 2 is a protein called ALLOPHYCOCYANIN, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	21	0	0
			1219	769	202	241	7			
2	D	161	Total	C	N	O	S	6	0	0
			1219	769	202	241	7			
2	F	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	I	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	K	161	Total	C	N	O	S	10	0	0
			1219	769	202	241	7			
2	M	161	Total	C	N	O	S	13	0	0
			1219	769	202	241	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	MEN	ASN	METHYLATED ASN	UNP P00318

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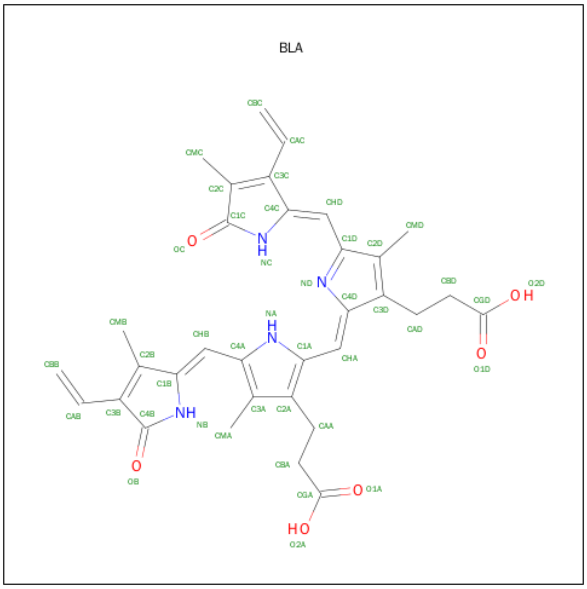
Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MEN	ASN	METHYLATED ASN	UNP P00318
F	71	MEN	ASN	METHYLATED ASN	UNP P00318
I	71	MEN	ASN	METHYLATED ASN	UNP P00318
K	71	MEN	ASN	METHYLATED ASN	UNP P00318
M	71	MEN	ASN	METHYLATED ASN	UNP P00318

- Molecule 3 is a protein called PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE.

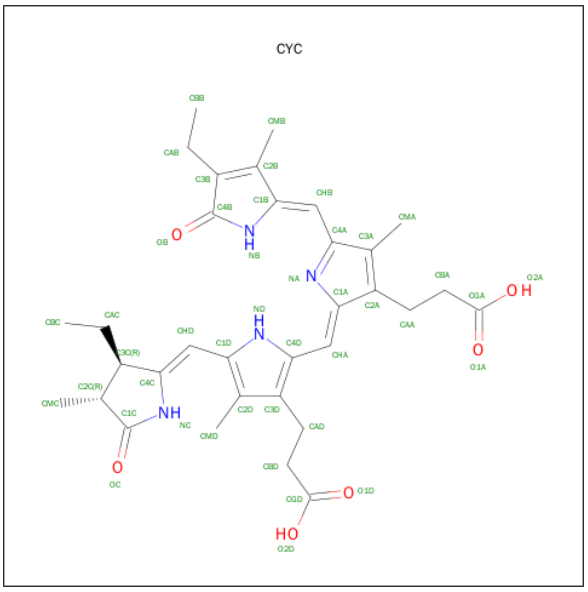
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	67	Total	C	N	O	S	13	0	0
			545	345	102	96	2			
3	O	67	Total	C	N	O	S	28	0	0
			545	345	102	96	2			

- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



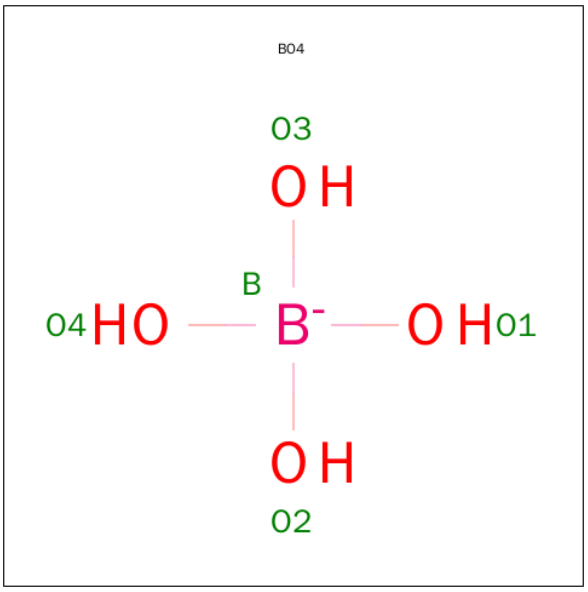
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	4	6		
4	B	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 6 is BORATE ION (three-letter code: BO4) (formula: BH_4O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total B O 5 1 4	0	0
6	J	1	Total B O 5 1 4	0	0
6	C	1	Total B O 5 1 4	0	0
6	E	1	Total B O 5 1 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	81	Total O 81 81	0	0
7	C	82	Total O 82 82	0	0
7	D	145	Total O 145 145	0	0
7	E	101	Total O 101 101	0	0
7	F	127	Total O 127 127	0	0
7	H	99	Total O 99 99	0	0
7	I	113	Total O 113 113	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	109	Total O 109 109	0	0
7	K	117	Total O 117 117	0	0
7	L	126	Total O 126 126	0	0
7	M	136	Total O 136 136	0	0
7	N	31	Total O 31 31	0	0
7	O	15	Total O 15 15	0	0

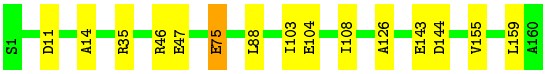
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

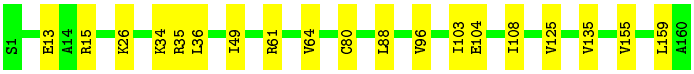
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain A:



- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain C:

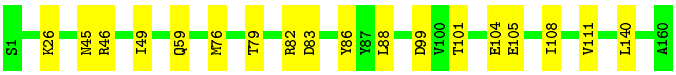


- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain E:

- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain H:

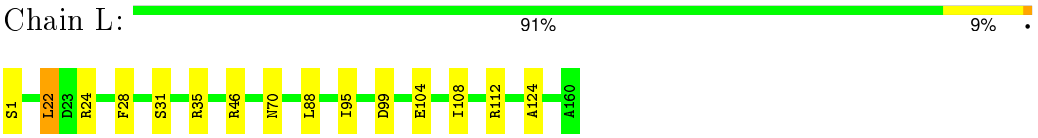


- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain J:

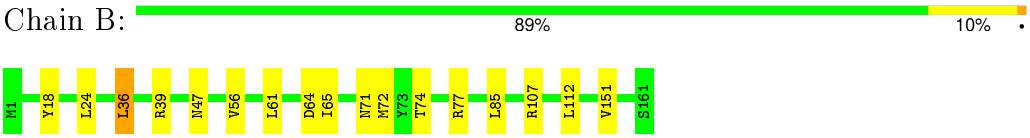
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain L:



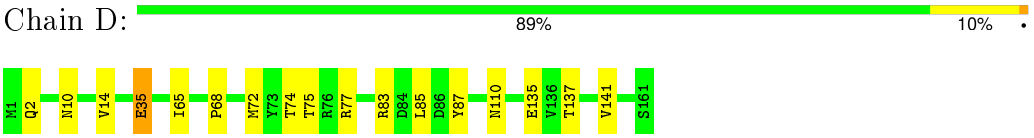
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain B:



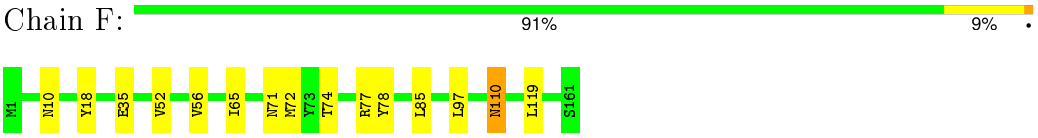
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain D:



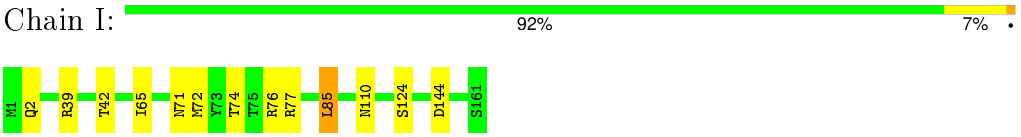
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain F:



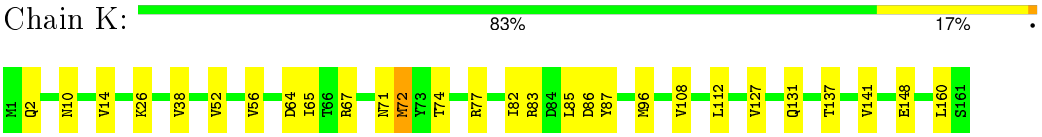
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain I:



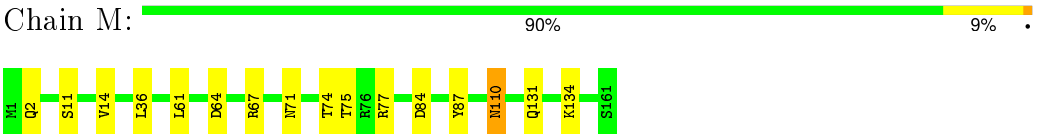
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain K:



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain M:



• Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain N:

• Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain O:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	176.12Å 151.90Å 137.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (25.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17502	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, BLA, MEN, BO4

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	0.37	0/1218	0.56	0/1647
1	C	0.39	0/1218	0.56	0/1647
1	E	0.38	0/1218	0.56	0/1647
1	H	0.41	0/1218	0.57	0/1647
1	J	0.40	0/1218	0.58	0/1647
1	L	0.40	0/1218	0.59	1/1647 (0.1%)
2	B	0.41	0/1226	0.61	0/1659
2	D	0.42	0/1226	0.64	0/1659
2	F	0.41	0/1226	0.65	0/1659
2	I	0.44	0/1226	0.65	0/1659
2	K	0.42	0/1226	0.62	0/1659
2	M	0.43	0/1226	0.66	0/1659
3	N	0.47	0/553	0.69	0/740
3	O	0.49	0/553	0.74	0/740
All	All	0.41	0/15770	0.61	1/21316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	22	LEU	CA-CB-CG	5.15	127.14	115.30

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	1203	0	1213	11	0
1	C	1203	0	1213	10	0
1	E	1203	0	1213	17	0
1	H	1203	0	1213	10	0
1	J	1203	0	1213	12	0
1	L	1203	0	1213	9	0
2	B	1219	0	1229	13	0
2	D	1219	0	1229	8	0
2	F	1219	0	1229	11	0
2	I	1219	0	1229	8	0
2	K	1219	0	1229	16	0
2	M	1219	0	1229	11	0
3	N	545	0	572	17	0
3	O	545	0	572	14	0
4	A	43	0	31	6	0
4	B	43	0	31	8	0
5	C	43	0	35	4	0
5	D	43	0	35	3	0
5	E	43	0	35	5	0
5	F	43	0	35	3	0
5	H	43	0	35	6	0
5	I	43	0	35	3	0
5	J	43	0	35	7	0
5	K	43	0	35	3	0
5	L	43	0	35	5	0
5	M	43	0	35	3	0
6	C	5	0	4	0	0
6	E	5	0	4	0	0
6	J	5	0	4	0	0
6	L	5	0	4	0	0
7	A	62	0	0	1	0
7	B	81	0	0	2	0
7	C	82	0	0	2	0
7	D	145	0	0	0	0
7	E	101	0	0	3	0
7	F	127	0	0	1	0
7	H	99	0	0	2	0
7	I	113	0	0	4	0
7	J	109	0	0	1	0
7	K	117	0	0	2	0
7	L	126	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	136	0	0	0	0
7	N	31	0	0	1	0
7	O	15	0	0	3	0
All	All	17502	0	16224	193	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (193) 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)
5:E:205:CYC:HMA1	5:E:205:CYC:HB	1.31	0.96
5:H:207:CYC:HMA1	5:H:207:CYC:HB	1.32	0.93
2:F:110:ASN:HD21	3:N:56:ALA:HB1	1.33	0.91
5:C:203:CYC:HMA1	5:C:203:CYC:HB	1.38	0.89
1:J:48:ARG:HH21	1:J:139:ILE:HD11	1.38	0.88
5:J:209:CYC:HMA1	5:J:209:CYC:HB	1.38	0.86
5:L:211:CYC:HB	5:L:211:CYC:HMA1	1.41	0.86
5:D:204:CYC:HB	5:D:204:CYC:HMA1	1.38	0.85
5:K:210:CYC:HMD2	5:K:210:CYC:HC	1.43	0.82
4:A:201:BLA:HB	4:A:201:BLA:HMA1	1.44	0.82
1:J:70:ASN:HD22	5:J:209:CYC:HC	1.28	0.81
1:E:140:LEU:HD22	1:E:144:ASP:HB3	1.65	0.78
5:E:205:CYC:HMD2	5:E:205:CYC:HC	1.49	0.77
4:A:201:BLA:HC	4:A:201:BLA:HMD2	1.48	0.76
2:F:119:LEU:HD11	5:F:206:CYC:HAA2	1.69	0.74
5:J:209:CYC:HC	5:J:209:CYC:HMD2	1.54	0.73
2:F:110:ASN:ND2	3:N:56:ALA:HB1	2.04	0.72
4:B:202:BLA:HMD2	4:B:202:BLA:HC	1.55	0.71
2:K:65:ILE:HG22	2:K:72:MET:HB2	1.74	0.70
5:H:207:CYC:HMD2	5:H:207:CYC:HC	1.58	0.68
5:L:211:CYC:HMD2	5:L:211:CYC:HC	1.57	0.68
5:F:206:CYC:HMD2	5:F:206:CYC:HC	1.57	0.67
2:B:65:ILE:HG22	2:B:72:MET:HB2	1.75	0.67
5:D:204:CYC:HMD2	5:D:204:CYC:HC	1.59	0.67
3:O:7:THR:HA	3:O:27:PHE:O	1.95	0.66
5:K:210:CYC:HMA1	5:K:210:CYC:HB	1.61	0.65
5:C:203:CYC:HMD2	5:C:203:CYC:HC	1.62	0.65
3:N:3:LEU:HD12	3:N:32:PRO:HA	1.79	0.64
7:C:2028:HOH:O	2:D:2:GLN:HA	1.98	0.64
1:A:14:ALA:HB2	3:N:19:GLN:HE21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:HA	1:C:108:ILE:HB	1.79	0.64
2:M:131:GLN:HE22	2:M:134:LYS:NZ	1.97	0.63
5:I:208:CYC:HMD2	5:I:208:CYC:HC	1.63	0.63
1:J:101:THR:O	1:J:105:GLU:HG2	1.99	0.62
2:D:65:ILE:HG22	2:D:72:MET:HB2	1.81	0.62
2:F:35:GLU:HG2	7:F:215:HOH:O	1.99	0.62
5:H:207:CYC:HMA1	5:H:207:CYC:NB	2.10	0.61
5:E:205:CYC:HMA1	5:E:205:CYC:NB	2.11	0.61
2:I:65:ILE:HG22	2:I:72:MET:HB2	1.83	0.61
2:F:65:ILE:HG22	2:F:72:MET:HB2	1.83	0.61
2:K:137:THR:O	2:K:141:VAL:HG22	2.02	0.60
3:N:34:GLU:CD	3:N:34:GLU:H	2.06	0.58
1:H:104:GLU:HA	1:H:108:ILE:HB	1.86	0.58
1:E:104:GLU:HA	1:E:108:ILE:HB	1.85	0.58
3:N:3:LEU:HB2	3:N:57:THR:HG23	1.87	0.57
2:F:119:LEU:CD1	5:F:206:CYC:HAA2	2.34	0.57
1:J:48:ARG:NH2	1:J:139:ILE:HD11	2.16	0.57
1:C:35:ARG:HD3	7:C:2065:HOH:O	2.05	0.57
2:I:76:ARG:HD2	7:I:308:HOH:O	2.05	0.57
2:K:71:MEN:O	2:K:77:ARG:HD2	2.05	0.56
1:E:112:ARG:HD2	7:E:2071:HOH:O	2.05	0.56
1:E:61:ARG:O	1:E:64:VAL:HG22	2.06	0.56
7:J:2013:HOH:O	2:K:2:GLN:HA	2.06	0.56
1:A:75:GLU:CD	1:A:75:GLU:H	2.09	0.56
3:O:40:GLN:O	3:O:44:GLN:HG3	2.07	0.55
3:N:52:LYS:HE3	3:N:54:GLU:HG2	1.89	0.55
5:M:212:CYC:HC	5:M:212:CYC:HMD2	1.72	0.54
1:E:45:ASN:OD1	1:E:139:ILE:HG12	2.07	0.54
2:D:10:ASN:O	2:D:14:VAL:HG23	2.07	0.54
3:O:34:GLU:CD	3:O:34:GLU:H	2.10	0.54
1:L:24:ARG:NH1	7:L:2106:HOH:O	2.41	0.53
2:B:112:LEU:HD13	4:B:202:BLA:HMB3	1.89	0.53
1:J:70:ASN:ND2	5:J:209:CYC:HC	2.00	0.53
5:D:204:CYC:NB	5:D:204:CYC:HMA1	2.17	0.53
2:B:47:ASN:ND2	2:I:42:THR:HG21	2.24	0.53
1:A:126:ALA:HB2	1:A:159:LEU:O	2.09	0.53
5:K:210:CYC:CMD	5:K:210:CYC:HC	2.17	0.52
3:O:6:ILE:HG21	3:O:36:TRP:CH2	2.43	0.52
2:B:39:ARG:NH2	7:B:245:HOH:O	2.42	0.52
1:H:45:ASN:O	1:H:49:ILE:HG13	2.09	0.52
2:I:39:ARG:HB2	7:I:293:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:ARG:HD2	1:L:95:ILE:O	2.07	0.52
5:J:209:CYC:HMA1	5:J:209:CYC:NB	2.17	0.52
2:F:10:ASN:OD1	3:N:63:ASN:HB2	2.09	0.52
4:B:202:BLA:C4B	3:N:22:LEU:HB2	2.39	0.51
2:M:2:GLN:HG2	3:O:65:GLY:HA3	1.93	0.51
4:A:201:BLA:HMC1	4:A:201:BLA:HBC1	1.92	0.51
1:E:76:MET:HG2	7:E:2026:HOH:O	2.10	0.51
5:H:207:CYC:HAA1	2:M:61:LEU:HD22	1.93	0.51
2:M:2:GLN:HG3	7:O:71:HOH:O	2.11	0.51
1:E:49:ILE:HA	1:E:135:VAL:HG11	1.93	0.51
2:K:83:ARG:O	2:K:87:TYR:HD1	1.93	0.50
1:J:48:ARG:NH1	1:J:52:GLN:OE1	2.44	0.50
2:B:71:MEN:O	2:B:77:ARG:HD3	2.11	0.50
1:C:26:LYS:HD2	2:D:35:GLU:HG2	1.94	0.49
1:L:112:ARG:HD2	7:L:2102:HOH:O	2.11	0.49
4:A:201:BLA:NB	4:A:201:BLA:HMA1	2.22	0.49
2:M:11:SER:O	2:M:14:VAL:HG12	2.12	0.49
1:A:46:ARG:HD3	2:B:18:TYR:CE1	2.46	0.49
5:C:203:CYC:HMA1	5:C:203:CYC:NB	2.18	0.48
1:L:70:ASN:HB3	5:L:211:CYC:OC	2.13	0.48
3:N:1:GLY:O	3:N:57:THR:HG21	2.13	0.48
1:C:61:ARG:O	1:C:64:VAL:HG22	2.13	0.48
1:L:104:GLU:HA	1:L:108:ILE:HB	1.94	0.48
1:A:104:GLU:HA	1:A:108:ILE:HB	1.94	0.48
2:K:127:VAL:O	2:K:131:GLN:HG2	2.13	0.48
2:I:71:MEN:O	2:I:77:ARG:HD3	2.13	0.48
3:O:6:ILE:O	3:O:28:THR:HA	2.14	0.48
3:N:23:GLN:HG3	3:N:23:GLN:H	1.44	0.48
2:K:96:MET:HG2	2:K:148:GLU:HG3	1.95	0.48
3:N:15:ARG:NH1	7:N:1340:HOH:O	2.46	0.48
2:B:112:LEU:CD1	4:B:202:BLA:HMB3	2.44	0.48
1:H:26:LYS:HE3	1:H:26:LYS:HB2	1.74	0.47
1:E:70:ASN:HD22	5:E:205:CYC:HC	1.61	0.47
2:B:107:ARG:HG3	2:B:107:ARG:HH11	1.77	0.47
2:D:83:ARG:O	2:D:87:TYR:HD1	1.96	0.47
3:O:45:LYS:NZ	7:O:82:HOH:O	2.43	0.47
1:H:46:ARG:HD2	7:H:289:HOH:O	2.14	0.47
2:I:124:SER:HB3	7:I:266:HOH:O	2.15	0.47
1:A:11:ASP:OD2	2:B:107:ARG:NH1	2.48	0.47
1:L:31:SER:OG	1:L:35:ARG:NH1	2.48	0.46
1:H:99:ASP:HB2	7:H:250:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:70:ASN:ND2	5:J:209:CYC:HMD2	2.31	0.46
2:M:64:ASP:OD1	2:M:67:ARG:NH1	2.48	0.46
4:B:202:BLA:HMA1	4:B:202:BLA:NB	2.30	0.46
2:B:77:ARG:NH1	7:B:215:HOH:O	2.45	0.46
1:C:13:GLU:HB2	1:C:15:ARG:HG2	1.97	0.46
1:C:36:LEU:HD23	1:C:96:VAL:HG22	1.98	0.46
2:K:67:ARG:NH2	7:K:302:HOH:O	2.48	0.46
1:C:125:VAL:HG12	1:C:159:LEU:HD13	1.97	0.46
2:B:107:ARG:HG3	2:B:107:ARG:NH1	2.32	0.45
2:I:2:GLN:HA	7:I:236:HOH:O	2.14	0.45
2:B:56:VAL:HG12	2:B:61:LEU:HG	1.98	0.45
2:K:108:VAL:O	2:K:112:LEU:HB2	2.16	0.45
2:M:131:GLN:HE22	2:M:134:LYS:HZ1	1.63	0.45
1:E:131:ALA:O	1:E:135:VAL:HG23	2.17	0.45
1:A:46:ARG:CG	1:A:47:GLU:N	2.79	0.45
2:K:64:ASP:OD1	2:K:67:ARG:NH1	2.49	0.45
1:J:4:THR:O	1:J:8:VAL:HG13	2.17	0.45
1:E:110:GLY:HA2	1:E:113:GLU:OE1	2.17	0.45
1:E:75:GLU:H	1:E:75:GLU:CD	2.20	0.45
5:H:207:CYC:HBC2	5:H:207:CYC:HMC1	1.98	0.45
2:D:75:THR:HG21	1:E:111:VAL:HG23	1.99	0.45
3:O:4:PHE:HE2	3:O:33:TYR:CD2	2.35	0.44
2:K:52:VAL:O	2:K:56:VAL:HG23	2.17	0.44
3:N:52:LYS:HE3	3:N:54:GLU:CG	2.46	0.44
1:J:103:ILE:HG21	1:J:155:VAL:HG22	1.99	0.44
3:O:2:ARG:HD3	7:O:72:HOH:O	2.17	0.44
2:K:83:ARG:O	2:K:86:ASP:HB2	2.17	0.44
4:B:202:BLA:HAD1	4:B:202:BLA:HMD1	1.85	0.44
3:N:49:LYS:HB3	3:N:49:LYS:HE3	1.77	0.44
2:D:77:ARG:HH22	3:N:63:ASN:HD21	1.65	0.44
1:C:49:ILE:HA	1:C:135:VAL:HG11	1.99	0.44
1:H:79:THR:O	1:H:82:ARG:HB3	2.18	0.44
5:I:208:CYC:C4B	3:O:22:LEU:HB2	2.48	0.44
1:A:35:ARG:NH1	7:A:255:HOH:O	2.42	0.44
4:B:202:BLA:HBC1	4:B:202:BLA:HMC1	1.99	0.43
3:N:46:MET:HB2	3:N:46:MET:HE3	1.87	0.43
2:M:84:ASP:O	2:M:87:TYR:HB2	2.18	0.43
5:H:207:CYC:HMD2	5:H:207:CYC:NC	2.31	0.43
2:M:71:MEN:HB2	5:M:212:CYC:OC	2.19	0.43
4:A:201:BLA:NC	4:A:201:BLA:HMD2	2.27	0.43
5:I:208:CYC:HAB1	5:I:208:CYC:HMB1	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:85:LEU:HA	2:I:85:LEU:HD12	1.87	0.43
1:H:101:THR:O	1:H:105:GLU:HG3	2.19	0.42
5:L:211:CYC:HMA1	5:L:211:CYC:NB	2.21	0.42
4:A:201:BLA:HMA2	2:F:78:TYR:CE2	2.54	0.42
3:O:13:GLN:CG	3:O:14:THR:H	2.32	0.42
2:B:36:LEU:HA	2:B:36:LEU:HD12	1.83	0.42
1:J:61:ARG:O	1:J:64:VAL:HG22	2.19	0.42
1:C:80:CYS:HA	5:C:203:CYC:CHD	2.49	0.42
2:D:137:THR:O	2:D:141:VAL:HG22	2.20	0.42
1:A:103:ILE:HG21	1:A:155:VAL:HG22	2.02	0.42
2:F:71:MEN:O	2:F:77:ARG:HD3	2.20	0.42
4:B:202:BLA:HC	4:B:202:BLA:CMD	2.30	0.42
1:H:111:VAL:HG23	2:M:75:THR:HG21	2.01	0.42
2:K:26:LYS:HD2	7:K:282:HOH:O	2.19	0.42
1:C:103:ILE:HG21	1:C:155:VAL:HG22	2.01	0.42
1:J:34:LYS:O	1:J:38:ILE:HG13	2.20	0.41
1:E:23:ASP:OD1	1:E:26:LYS:NZ	2.53	0.41
1:E:51:LYS:NZ	1:E:55:ASP:OD2	2.53	0.41
3:O:10:VAL:HG22	3:O:48:GLY:HA3	2.01	0.41
5:E:205:CYC:HC	5:E:205:CYC:CMD	2.25	0.41
3:O:37:PHE:O	3:O:41:GLN:HG3	2.20	0.41
2:M:71:MEN:O	2:M:77:ARG:HD3	2.20	0.41
1:E:46:ARG:HD3	2:F:18:TYR:CE1	2.56	0.41
3:N:20:ARG:HH12	3:N:22:LEU:HD23	1.85	0.41
3:O:40:GLN:HG3	3:O:50:ILE:CD1	2.50	0.41
1:A:46:ARG:HG2	1:A:47:GLU:N	2.36	0.41
5:J:209:CYC:CMD	5:J:209:CYC:HC	2.29	0.41
1:L:28:PHE:CE1	1:L:35:ARG:NH2	2.89	0.41
1:H:76:MET:HA	1:H:76:MET:CE	2.50	0.41
1:A:143:GLU:HG3	1:A:144:ASP:N	2.36	0.41
2:K:10:ASN:O	2:K:14:VAL:HG13	2.21	0.41
1:J:22:LEU:HD22	2:K:38:VAL:HG13	2.03	0.41
1:L:1:SER:HA	1:L:99:ASP:OD2	2.20	0.41
1:L:124:ALA:HB3	5:L:211:CYC:HMC3	2.03	0.41
2:F:52:VAL:O	2:F:56:VAL:HG23	2.21	0.41
5:M:212:CYC:HMC1	5:M:212:CYC:HBC2	2.04	0.40
1:E:41:ILE:HG13	1:E:42:LEU:N	2.36	0.40
1:E:2:ILE:N	7:E:2080:HOH:O	2.49	0.40
2:K:56:VAL:HG21	2:K:82:ILE:HG22	2.04	0.40
1:H:83:ASP:O	1:H:86:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
1	C	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
1	E	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
1	H	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
1	J	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
1	L	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
2	B	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	30	36
2	D	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	15	15
2	F	158/161 (98%)	152 (96%)	4 (2%)	2 (1%)	15	15
2	I	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	15	15
2	K	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	30	36
2	M	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	15	15
3	N	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
3	O	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
All	All	2026/2060 (98%)	1975 (98%)	41 (2%)	10 (0%)	34	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	110	ASN
2	D	110	ASN
2	F	110	ASN
2	I	110	ASN
2	F	74	THR
2	K	74	THR
2	B	74	THR
2	I	74	THR
2	M	74	THR

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Mol	Chain	Res	Type
2	D	74	THR

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	125/125 (100%)	123 (98%)	2 (2%)	70	84
1	C	125/125 (100%)	123 (98%)	2 (2%)	70	84
1	E	125/125 (100%)	121 (97%)	4 (3%)	46	62
1	H	125/125 (100%)	122 (98%)	3 (2%)	57	74
1	J	125/125 (100%)	121 (97%)	4 (3%)	46	62
1	L	125/125 (100%)	122 (98%)	3 (2%)	57	74
2	B	126/126 (100%)	121 (96%)	5 (4%)	38	52
2	D	126/126 (100%)	122 (97%)	4 (3%)	46	62
2	F	126/126 (100%)	124 (98%)	2 (2%)	70	84
2	I	126/126 (100%)	124 (98%)	2 (2%)	70	84
2	K	126/126 (100%)	123 (98%)	3 (2%)	57	74
2	M	126/126 (100%)	124 (98%)	2 (2%)	70	84
3	N	58/58 (100%)	53 (91%)	5 (9%)	13	15
3	O	58/58 (100%)	54 (93%)	4 (7%)	19	24
All	All	1622/1622 (100%)	1577 (97%)	45 (3%)	51	68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	88	LEU
2	B	24	LEU
2	B	36	LEU
2	B	64	ASP
2	B	85	LEU

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Mol	Chain	Res	Type
2	B	151	VAL
1	C	34	LYS
1	C	88	LEU
2	D	35	GLU
2	D	68	PRO
2	D	85	LEU
2	D	135	GLU
1	E	41	ILE
1	E	51	LYS
1	E	86	TYR
1	E	88	LEU
2	F	85	LEU
2	F	97	LEU
3	N	3	LEU
3	N	19	GLN
3	N	23	GLN
3	N	42	ARG
3	N	60	GLN
1	H	59	GLN
1	H	88	LEU
1	H	140	LEU
2	I	85	LEU
2	I	144	ASP
1	J	33	GLU
1	J	76	MET
1	J	88	LEU
1	J	90	LEU
2	K	72	MET
2	K	85	LEU
2	K	160	LEU
1	L	22	LEU
1	L	46	ARG
1	L	88	LEU
2	M	36	LEU
2	M	110	ASN
3	O	2	ARG
3	O	34	GLU
3	O	38	ARG
3	O	59	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
2	B	10	ASN
2	B	47	ASN
2	B	117	ASN
1	C	40	GLN
2	D	10	ASN
2	D	47	ASN
2	D	117	ASN
2	D	131	GLN
1	E	70	ASN
2	F	47	ASN
2	F	110	ASN
2	F	117	ASN
2	F	131	GLN
3	N	19	GLN
3	N	24	ASN
3	N	35	ASN
3	N	44	GLN
3	N	63	ASN
1	H	9	ASN
1	H	56	GLN
1	H	59	GLN
1	H	134	ASN
2	I	2	GLN
2	I	10	ASN
2	I	47	ASN
2	I	117	ASN
2	I	128	GLN
1	J	9	ASN
1	J	56	GLN
1	J	70	ASN
1	J	134	ASN
2	K	2	GLN
2	K	10	ASN
2	K	47	ASN
2	K	117	ASN
2	K	128	GLN
1	L	40	GLN
1	L	56	GLN
2	M	47	ASN
2	M	117	ASN
2	M	131	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 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	71	2	7,8,9	0.47	0	5,9,11	0.79	0
2	MEN	D	71	2	7,8,9	0.55	0	5,9,11	0.87	0
2	MEN	F	71	2	7,8,9	0.60	0	5,9,11	1.02	1 (20%)
2	MEN	I	71	2	7,8,9	0.59	0	5,9,11	0.90	0
2	MEN	K	71	2	7,8,9	0.48	0	5,9,11	0.88	0
2	MEN	M	71	2	7,8,9	0.39	0	5,9,11	0.87	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	71	2	-	0/6/8/10	0/0/0/0
2	MEN	D	71	2	-	0/6/8/10	0/0/0/0
2	MEN	F	71	2	-	0/6/8/10	0/0/0/0
2	MEN	I	71	2	-	0/6/8/10	0/0/0/0
2	MEN	K	71	2	-	0/6/8/10	0/0/0/0
2	MEN	M	71	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	71	MEN	O-C-CA	-2.07	120.10	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	71	MEN	1	0
2	F	71	MEN	1	0
2	I	71	MEN	1	0
2	K	71	MEN	1	0
2	M	71	MEN	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

16 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	BLA	A	201	1	35,46,46	1.89	7 (20%)	43,67,67	1.74	10 (23%)
4	BLA	B	202	2	35,46,46	1.97	7 (20%)	43,67,67	1.68	10 (23%)
6	BO4	C	2003	-	0,4,4	0.00	-	0,6,6	0.00	-
5	CYC	C	203	1	35,46,46	2.64	6 (17%)	47,67,67	2.41	17 (36%)
5	CYC	D	204	2	35,46,46	2.29	7 (20%)	47,67,67	2.45	18 (38%)
6	BO4	E	2004	-	0,4,4	0.00	-	0,6,6	0.00	-
5	CYC	E	205	1	35,46,46	2.20	7 (20%)	47,67,67	2.76	16 (34%)
5	CYC	F	206	2	35,46,46	2.30	7 (20%)	47,67,67	3.00	19 (40%)
5	CYC	H	207	1	35,46,46	2.34	8 (22%)	47,67,67	2.35	16 (34%)
5	CYC	I	208	2	35,46,46	2.76	7 (20%)	47,67,67	2.97	19 (40%)
6	BO4	J	2002	-	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CYC	J	209	1	35,46,46	2.55	7 (20%)	47,67,67	2.46	16 (34%)
5	CYC	K	210	2	35,46,46	2.87	6 (17%)	47,67,67	2.83	21 (44%)
6	BO4	L	2001	-	0,4,4	0.00	-	0,6,6	0.00	-
5	CYC	L	211	1	35,46,46	2.69	6 (17%)	47,67,67	2.69	19 (40%)
5	CYC	M	212	2	35,46,46	2.68	7 (20%)	47,67,67	3.12	19 (40%)

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	BLA	A	201	1	-	2/22/74/74	0/4/4/4
4	BLA	B	202	2	-	2/22/74/74	0/4/4/4
6	BO4	C	2003	-	-	0/0/0/0	0/0/0/0
5	CYC	C	203	1	2/2/14/19	2/21/74/74	0/4/4/4
5	CYC	D	204	2	1/1/14/19	2/21/74/74	0/4/4/4
6	BO4	E	2004	-	-	0/0/0/0	0/0/0/0
5	CYC	E	205	1	2/2/14/19	2/21/74/74	0/4/4/4
5	CYC	F	206	2	2/2/14/19	2/21/74/74	0/4/4/4
5	CYC	H	207	1	2/2/14/19	2/21/74/74	0/4/4/4
5	CYC	I	208	2	1/1/14/19	2/21/74/74	0/4/4/4
6	BO4	J	2002	-	-	0/0/0/0	0/0/0/0
5	CYC	J	209	1	1/1/14/19	2/21/74/74	0/4/4/4
5	CYC	K	210	2	1/1/14/19	2/21/74/74	0/4/4/4
6	BO4	L	2001	-	-	0/0/0/0	0/0/0/0
5	CYC	L	211	1	2/2/14/19	2/21/74/74	0/4/4/4
5	CYC	M	212	2	2/2/14/19	2/21/74/74	0/4/4/4

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	210	CYC	C2C-C1C	-11.60	1.41	1.52
5	I	208	CYC	C2C-C1C	-11.45	1.41	1.52
5	M	212	CYC	C2C-C1C	-11.31	1.41	1.52
5	C	203	CYC	C2C-C1C	-10.40	1.42	1.52
5	L	211	CYC	C2C-C1C	-8.96	1.43	1.52
5	F	206	CYC	C2C-C1C	-8.69	1.43	1.52
5	J	209	CYC	C2C-C1C	-8.44	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	204	CYC	C2C-C1C	-7.94	1.44	1.52
5	H	207	CYC	C2C-C1C	-7.12	1.45	1.52
5	E	205	CYC	C2C-C1C	-6.69	1.45	1.52
5	M	212	CYC	C2C-C3C	-6.11	1.36	1.54
5	D	204	CYC	C2C-C3C	-5.92	1.36	1.54
5	K	210	CYC	C2C-C3C	-5.78	1.37	1.54
5	J	209	CYC	C2C-C3C	-5.63	1.37	1.54
5	L	211	CYC	C2C-C3C	-5.25	1.38	1.54
5	I	208	CYC	C2C-C3C	-5.24	1.38	1.54
5	F	206	CYC	C2C-C3C	-5.23	1.38	1.54
5	E	205	CYC	C2C-C3C	-5.05	1.39	1.54
5	C	203	CYC	C2C-C3C	-4.88	1.39	1.54
5	H	207	CYC	C2C-C3C	-4.86	1.40	1.54
5	D	204	CYC	CAB-C3B	-4.51	1.38	1.51
5	J	209	CYC	CAB-C3B	-4.30	1.39	1.51
5	C	203	CYC	CAB-C3B	-4.21	1.39	1.51
5	M	212	CYC	CAB-C3B	-4.08	1.39	1.51
5	H	207	CYC	CAB-C3B	-3.99	1.40	1.51
5	F	206	CYC	CAB-C3B	-3.78	1.40	1.51
5	I	208	CYC	CAB-C3B	-3.78	1.40	1.51
5	K	210	CYC	CAB-C3B	-3.48	1.41	1.51
5	E	205	CYC	CAB-C3B	-3.18	1.42	1.51
5	L	211	CYC	CAB-C3B	-3.05	1.42	1.51
4	A	201	BLA	CAB-C3B	-2.63	1.39	1.47
5	H	207	CYC	C4B-C3B	-2.47	1.43	1.48
5	M	212	CYC	CBB-CAB	-2.46	1.39	1.51
5	I	208	CYC	CBB-CAB	-2.37	1.39	1.51
5	F	206	CYC	CBB-CAB	-2.34	1.40	1.51
5	J	209	CYC	C4B-C3B	-2.27	1.43	1.48
5	D	204	CYC	CBB-CAB	-2.27	1.40	1.51
5	H	207	CYC	CBB-CAB	-2.10	1.41	1.51
4	B	202	BLA	CAB-C3B	-2.08	1.41	1.47
5	E	205	CYC	C3B-C2B	2.42	1.41	1.36
5	D	204	CYC	CHA-C1A	2.50	1.37	1.35
4	B	202	BLA	CHB-C1B	2.51	1.39	1.34
4	B	202	BLA	CBB-CAB	2.51	1.42	1.30
4	A	201	BLA	CBB-CAB	2.56	1.42	1.30
5	M	212	CYC	OC-C1C	2.63	1.28	1.23
4	A	201	BLA	CHB-C1B	2.99	1.41	1.34
5	I	208	CYC	OC-C1C	3.24	1.29	1.23
5	H	207	CYC	CHA-C1A	3.31	1.38	1.35
5	D	204	CYC	OC-C1C	3.47	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	209	CYC	OC-C1C	3.77	1.30	1.23
5	L	211	CYC	OC-C1C	3.82	1.30	1.23
5	F	206	CYC	OC-C1C	3.87	1.31	1.23
5	C	203	CYC	OC-C1C	3.89	1.31	1.23
5	F	206	CYC	CHA-C1A	4.08	1.38	1.35
5	M	212	CYC	CHA-C1A	4.09	1.38	1.35
4	B	202	BLA	CBC-CAC	4.12	1.50	1.30
4	A	201	BLA	OC-C1C	4.20	1.31	1.23
5	F	206	CYC	OB-C4B	4.25	1.31	1.23
4	B	202	BLA	OC-C1C	4.36	1.32	1.23
5	L	211	CYC	OB-C4B	4.45	1.32	1.23
4	A	201	BLA	CBC-CAC	4.47	1.52	1.30
5	E	205	CYC	OB-C4B	4.47	1.32	1.23
4	A	201	BLA	OB-C4B	4.67	1.32	1.23
5	E	205	CYC	OC-C1C	4.72	1.32	1.23
4	B	202	BLA	OB-C4B	4.73	1.32	1.23
5	E	205	CYC	CHA-C1A	4.86	1.39	1.35
5	J	209	CYC	OB-C4B	4.90	1.33	1.23
5	K	210	CYC	OC-C1C	4.94	1.33	1.23
4	A	201	BLA	CHA-C4D	5.15	1.39	1.35
5	C	203	CYC	CHA-C1A	5.25	1.39	1.35
5	M	212	CYC	OB-C4B	5.31	1.33	1.23
5	D	204	CYC	OB-C4B	5.37	1.33	1.23
5	K	210	CYC	OB-C4B	5.37	1.33	1.23
5	I	208	CYC	OB-C4B	5.40	1.33	1.23
5	H	207	CYC	OB-C4B	5.46	1.34	1.23
5	K	210	CYC	CHA-C1A	5.53	1.40	1.35
5	C	203	CYC	OB-C4B	5.57	1.34	1.23
5	H	207	CYC	OC-C1C	5.61	1.34	1.23
5	I	208	CYC	CHA-C1A	6.49	1.40	1.35
5	J	209	CYC	CHA-C1A	6.67	1.41	1.35
4	B	202	BLA	CHA-C4D	6.77	1.41	1.35
5	L	211	CYC	CHA-C1A	9.12	1.43	1.35

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	208	CYC	OC-C1C-C2C	-6.84	120.72	126.25
5	M	212	CYC	C4B-C3B-C2B	-6.64	104.26	108.05
5	F	206	CYC	OC-C1C-C2C	-6.38	121.10	126.25
5	E	205	CYC	C4B-C3B-C2B	-6.15	104.54	108.05
5	K	210	CYC	C4B-C3B-C2B	-6.02	104.61	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	210	CYC	OC-C1C-C2C	-5.83	121.54	126.25
5	I	208	CYC	C4B-C3B-C2B	-4.95	105.22	108.05
5	D	204	CYC	CHB-C4A-NA	-4.89	115.60	124.91
5	F	206	CYC	C4B-C3B-C2B	-4.82	105.29	108.05
5	L	211	CYC	C4B-C3B-C2B	-4.78	105.32	108.05
5	L	211	CYC	CHB-C4A-NA	-4.68	116.00	124.91
5	F	206	CYC	C1B-NB-C4B	-4.66	103.91	110.73
5	E	205	CYC	CHB-C4A-NA	-4.58	116.19	124.91
5	J	209	CYC	C4B-C3B-C2B	-4.43	105.52	108.05
5	C	203	CYC	CHB-C4A-NA	-4.28	116.76	124.91
5	H	207	CYC	CHB-C4A-NA	-4.16	116.98	124.91
4	B	202	BLA	C1B-NB-C4B	-4.15	104.66	110.73
5	M	212	CYC	C1B-NB-C4B	-4.15	104.66	110.73
4	A	201	BLA	C4C-NC-C1C	-4.06	104.79	110.73
5	M	212	CYC	OC-C1C-C2C	-4.00	123.02	126.25
4	B	202	BLA	C4C-NC-C1C	-3.86	105.08	110.73
5	K	210	CYC	CHB-C4A-NA	-3.80	117.68	124.91
4	A	201	BLA	C1B-NB-C4B	-3.71	105.30	110.73
5	L	211	CYC	C1B-NB-C4B	-3.49	105.62	110.73
5	C	203	CYC	C1B-NB-C4B	-3.34	105.85	110.73
5	D	204	CYC	C1B-NB-C4B	-3.32	105.87	110.73
5	J	209	CYC	CHB-C4A-NA	-3.17	118.87	124.91
5	K	210	CYC	CAD-C3D-C4D	-3.17	123.57	127.01
4	A	201	BLA	CAA-C2A-C1A	-3.02	123.72	127.01
5	I	208	CYC	C1B-NB-C4B	-2.98	106.37	110.73
5	I	208	CYC	OB-C4B-NB	-2.98	117.24	125.14
5	D	204	CYC	OB-C4B-C3B	-2.92	124.59	128.09
5	E	205	CYC	C1B-NB-C4B	-2.90	106.48	110.73
5	H	207	CYC	OB-C4B-C3B	-2.88	124.64	128.09
5	H	207	CYC	C4B-C3B-C2B	-2.83	106.43	108.05
4	A	201	BLA	CBC-CAC-C3C	-2.82	112.71	127.01
4	B	202	BLA	CAD-C3D-C2D	-2.75	123.21	128.01
5	K	210	CYC	OB-C4B-C3B	-2.74	124.81	128.09
5	K	210	CYC	C1B-NB-C4B	-2.70	106.78	110.73
5	J	209	CYC	C1B-NB-C4B	-2.68	106.81	110.73
4	A	201	BLA	CAC-C3C-C4C	-2.66	117.57	124.80
5	C	203	CYC	C1B-C2B-C3B	-2.65	104.99	107.81
5	K	210	CYC	CHA-C1A-NA	-2.64	123.95	128.67
5	M	212	CYC	CHA-C1A-NA	-2.60	124.02	128.67
4	B	202	BLA	CBC-CAC-C3C	-2.55	114.06	127.01
5	H	207	CYC	C1B-NB-C4B	-2.49	107.09	110.73
5	F	206	CYC	CHB-C4A-NA	-2.48	120.19	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	212	CYC	OB-C4B-NB	-2.41	118.74	125.14
5	D	204	CYC	CHA-C1A-NA	-2.39	124.41	128.67
4	B	202	BLA	CAC-C3C-C4C	-2.38	118.34	124.80
5	E	205	CYC	CAA-C2A-C1A	-2.38	120.81	125.06
5	L	211	CYC	CAD-C3D-C4D	-2.27	124.54	127.01
5	I	208	CYC	CMD-C2D-C3D	-2.27	120.50	125.24
5	M	212	CYC	CHB-C4A-NA	-2.27	120.60	124.91
5	J	209	CYC	OC-C1C-NC	-2.24	122.12	124.83
5	C	203	CYC	CHB-C1B-C2B	-2.22	122.28	126.89
5	L	211	CYC	CBD-CAD-C3D	-2.22	108.55	112.53
5	F	206	CYC	CAA-C2A-C3A	-2.20	124.18	128.01
5	I	208	CYC	CHB-C4A-NA	-2.11	120.89	124.91
5	L	211	CYC	OB-C4B-C3B	-2.09	125.59	128.09
4	A	201	BLA	CHD-C1D-ND	-2.08	120.94	124.91
5	E	205	CYC	CBD-CAD-C3D	-2.06	108.83	112.53
5	J	209	CYC	CBD-CAD-C3D	-2.04	108.87	112.53
5	I	208	CYC	CHB-C1B-NB	-2.03	121.76	126.16
5	F	206	CYC	CHA-C1A-NA	-2.01	125.07	128.67
5	D	204	CYC	CBB-CAB-C3B	2.00	118.50	112.39
5	K	210	CYC	C2C-C1C-NC	2.01	110.22	108.30
5	H	207	CYC	CMA-C3A-C4A	2.01	128.33	125.06
5	I	208	CYC	CHB-C4A-C3A	2.01	129.79	124.88
4	B	202	BLA	CHD-C1D-C2D	2.03	129.84	124.88
4	A	201	BLA	C2B-C1B-NB	2.04	109.95	107.00
4	B	202	BLA	CMB-C2B-C1B	2.05	126.94	124.20
5	M	212	CYC	C1D-CHD-C4C	2.06	134.72	127.23
4	B	202	BLA	C4C-CHD-C1D	2.06	133.39	128.06
5	F	206	CYC	C2C-C3C-C4C	2.08	105.03	101.50
5	F	206	CYC	CHB-C4A-C3A	2.13	130.07	124.88
5	E	205	CYC	C2B-C1B-NB	2.17	110.14	107.00
5	F	206	CYC	CAA-C2A-C1A	2.19	128.97	125.06
5	H	207	CYC	C2C-C3C-C4C	2.19	105.21	101.50
5	L	211	CYC	CMB-C2B-C1B	2.19	127.12	124.20
5	E	205	CYC	CAC-C3C-C4C	2.19	118.31	112.67
5	F	206	CYC	CMB-C2B-C1B	2.24	127.18	124.20
5	M	212	CYC	CMB-C2B-C1B	2.29	127.24	124.20
5	I	208	CYC	C2B-C1B-NB	2.30	110.33	107.00
5	K	210	CYC	CMB-C2B-C1B	2.32	127.28	124.20
5	J	209	CYC	C2C-C1C-NC	2.33	110.53	108.30
5	L	211	CYC	C2B-C1B-NB	2.36	110.42	107.00
4	B	202	BLA	C2B-C1B-NB	2.38	110.45	107.00
4	A	201	BLA	CAC-C3C-C2C	2.41	136.50	128.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	208	CYC	CMA-C3A-C4A	2.44	129.04	125.06
5	H	207	CYC	CAC-C3C-C4C	2.46	118.98	112.67
5	K	210	CYC	CAC-C3C-C4C	2.50	119.09	112.67
5	D	204	CYC	C2B-C1B-NB	2.53	110.67	107.00
5	H	207	CYC	C1B-CHB-C4A	2.57	134.71	128.06
5	M	212	CYC	C2B-C1B-NB	2.58	110.74	107.00
5	I	208	CYC	CAC-C3C-C4C	2.60	119.36	112.67
5	C	203	CYC	C2C-C1C-NC	2.60	110.79	108.30
5	M	212	CYC	C2C-C3C-C4C	2.63	105.95	101.50
5	J	209	CYC	CMA-C3A-C4A	2.64	129.36	125.06
5	C	203	CYC	CBB-CAB-C3B	2.67	120.56	112.39
5	M	212	CYC	CAC-C3C-C4C	2.70	119.61	112.67
5	D	204	CYC	C3C-C2C-C1C	2.73	105.70	103.41
5	D	204	CYC	CAC-C3C-C4C	2.74	119.71	112.67
5	H	207	CYC	CBB-CAB-C3B	2.78	120.88	112.39
5	K	210	CYC	CMC-C2C-C1C	2.78	118.27	112.43
5	C	203	CYC	CAC-C3C-C4C	2.81	119.90	112.67
5	L	211	CYC	C1B-CHB-C4A	2.81	135.34	128.06
5	K	210	CYC	OC-C1C-NC	2.82	128.24	124.83
5	D	204	CYC	CMA-C3A-C4A	2.82	129.65	125.06
5	L	211	CYC	CAC-C3C-C4C	2.84	119.97	112.67
5	J	209	CYC	C3C-C2C-C1C	2.99	105.92	103.41
5	F	206	CYC	CAC-C3C-C4C	3.03	120.45	112.67
5	C	203	CYC	C3C-C2C-C1C	3.03	105.95	103.41
5	J	209	CYC	CAC-C3C-C4C	3.07	120.55	112.67
5	E	205	CYC	C1B-CHB-C4A	3.08	136.02	128.06
5	M	212	CYC	CMA-C3A-C4A	3.10	130.10	125.06
5	H	207	CYC	CAB-C3B-C4B	3.10	124.22	121.51
5	F	206	CYC	C2B-C1B-NB	3.12	111.52	107.00
5	C	203	CYC	C1B-CHB-C4A	3.15	136.22	128.06
5	J	209	CYC	CHB-C4A-C3A	3.19	132.66	124.88
4	B	202	BLA	CMD-C2D-C1D	3.19	130.25	125.06
5	K	210	CYC	CMA-C3A-C4A	3.20	130.26	125.06
5	K	210	CYC	CBB-CAB-C3B	3.24	122.30	112.39
5	D	204	CYC	C1B-CHB-C4A	3.31	136.61	128.06
5	E	205	CYC	C3C-C2C-C1C	3.32	106.19	103.41
5	C	203	CYC	CMA-C3A-C4A	3.34	130.50	125.06
4	A	201	BLA	CMD-C2D-C1D	3.37	130.55	125.06
5	K	210	CYC	C1B-CHB-C4A	3.38	136.81	128.06
5	J	209	CYC	CMC-C2C-C3C	3.39	129.34	114.35
5	D	204	CYC	CMB-C2B-C1B	3.40	128.72	124.20
5	C	203	CYC	C2B-C1B-NB	3.41	111.94	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	204	CYC	C2C-C1C-NC	3.41	111.56	108.30
5	J	209	CYC	C1B-CHB-C4A	3.41	136.89	128.06
5	E	205	CYC	CMC-C2C-C3C	3.42	129.49	114.35
5	D	204	CYC	C3B-C4B-NB	3.48	109.90	106.74
5	K	210	CYC	CHB-C4A-C3A	3.54	133.52	124.88
5	C	203	CYC	C3B-C4B-NB	3.54	109.96	106.74
5	H	207	CYC	CMC-C2C-C3C	3.57	130.14	114.35
5	D	204	CYC	CMC-C2C-C3C	3.58	130.19	114.35
5	L	211	CYC	CMA-C3A-C4A	3.60	130.91	125.06
5	L	211	CYC	C2C-C1C-NC	3.61	111.75	108.30
5	C	203	CYC	CMC-C2C-C3C	3.65	130.49	114.35
5	I	208	CYC	OB-C4B-C3B	3.70	132.54	128.09
5	H	207	CYC	CHB-C4A-C3A	3.71	133.94	124.88
5	C	203	CYC	CHB-C4A-C3A	3.71	133.94	124.88
5	F	206	CYC	CMC-C2C-C3C	3.75	130.94	114.35
5	I	208	CYC	C3B-C4B-NB	3.83	110.22	106.74
5	C	203	CYC	CAB-C3B-C4B	3.84	124.86	121.51
5	D	204	CYC	CHB-C4A-C3A	3.84	134.26	124.88
5	H	207	CYC	C3B-C4B-NB	3.85	110.24	106.74
5	M	212	CYC	CMC-C2C-C3C	3.85	131.40	114.35
5	L	211	CYC	CBB-CAB-C3B	3.90	124.30	112.39
4	A	201	BLA	CMB-C2B-C1B	3.92	129.42	124.20
5	L	211	CYC	CMC-C2C-C3C	3.95	131.84	114.35
5	I	208	CYC	CMC-C2C-C3C	4.13	132.62	114.35
5	L	211	CYC	CAB-C3B-C4B	4.14	125.13	121.51
5	E	205	CYC	CHB-C4A-C3A	4.16	135.04	124.88
5	E	205	CYC	CBB-CAB-C3B	4.19	125.19	112.39
5	D	204	CYC	CAB-C3B-C4B	4.21	125.19	121.51
5	L	211	CYC	CHB-C4A-C3A	4.29	135.36	124.88
5	I	208	CYC	CBB-CAB-C3B	4.32	125.57	112.39
5	K	210	CYC	CMC-C2C-C3C	4.35	133.60	114.35
5	F	206	CYC	CBB-CAB-C3B	4.45	125.97	112.39
5	M	212	CYC	CBB-CAB-C3B	4.45	125.99	112.39
5	M	212	CYC	C2C-C1C-NC	4.51	112.61	108.30
5	F	206	CYC	C2C-C1C-NC	4.58	112.68	108.30
5	I	208	CYC	C2C-C1C-NC	4.63	112.72	108.30
5	J	209	CYC	CAB-C3B-C4B	4.63	125.55	121.51
5	H	207	CYC	C3C-C2C-C1C	4.65	107.31	103.41
5	H	207	CYC	CMC-C2C-C1C	4.82	122.55	112.43
5	I	208	CYC	CMC-C2C-C1C	4.82	122.55	112.43
5	C	203	CYC	CMC-C2C-C1C	4.87	122.66	112.43
5	K	210	CYC	C3B-C4B-NB	4.99	111.27	106.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	209	CYC	C3B-C4B-NB	5.07	111.35	106.74
5	L	211	CYC	CMC-C2C-C1C	5.25	123.46	112.43
5	E	205	CYC	C3B-C4B-NB	5.32	111.58	106.74
5	D	204	CYC	CMC-C2C-C1C	5.49	123.96	112.43
5	M	212	CYC	CMC-C2C-C1C	5.52	124.02	112.43
5	K	210	CYC	C3C-C2C-C1C	5.55	108.06	103.41
5	E	205	CYC	CMC-C2C-C1C	5.65	124.29	112.43
5	F	206	CYC	CMC-C2C-C1C	5.71	124.42	112.43
5	E	205	CYC	CAB-C3B-C4B	5.77	126.55	121.51
5	J	209	CYC	CMC-C2C-C1C	5.79	124.60	112.43
5	L	211	CYC	C3B-C4B-NB	5.82	112.03	106.74
5	M	212	CYC	C3B-C4B-NB	6.07	112.26	106.74
5	K	210	CYC	CAB-C3B-C4B	6.44	127.14	121.51
5	F	206	CYC	C3B-C4B-NB	6.57	112.71	106.74
5	K	210	CYC	CAC-C3C-C2C	7.12	132.03	114.13
5	I	208	CYC	CAC-C3C-C2C	7.18	132.18	114.13
5	M	212	CYC	CAC-C3C-C2C	7.24	132.32	114.13
5	D	204	CYC	CAC-C3C-C2C	7.29	132.47	114.13
5	F	206	CYC	CAC-C3C-C2C	7.47	132.91	114.13
5	L	211	CYC	CAC-C3C-C2C	7.64	133.34	114.13
5	J	209	CYC	CAC-C3C-C2C	7.71	133.51	114.13
5	H	207	CYC	CAC-C3C-C2C	8.04	134.35	114.13
5	C	203	CYC	CAC-C3C-C2C	8.39	135.21	114.13
5	F	206	CYC	CAB-C3B-C4B	8.39	128.84	121.51
5	E	205	CYC	CAC-C3C-C2C	8.78	136.21	114.13
5	I	208	CYC	CAB-C3B-C4B	10.04	130.28	121.51
5	M	212	CYC	CAB-C3B-C4B	11.04	131.15	121.51

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	206	CYC	C3C
5	F	206	CYC	C2C
5	I	208	CYC	C2C
5	M	212	CYC	C3C
5	M	212	CYC	C2C
5	J	209	CYC	C2C
5	C	203	CYC	C3C
5	C	203	CYC	C2C
5	D	204	CYC	C2C
5	H	207	CYC	C3C
5	H	207	CYC	C2C

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Mol	Chain	Res	Type	Atom
5	L	211	CYC	C3C
5	L	211	CYC	C2C
5	E	205	CYC	C3C
5	E	205	CYC	C2C
5	K	210	CYC	C2C

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	208	CYC	C1B-CHB-C4A-C3A
5	F	206	CYC	C1B-CHB-C4A-C3A
5	M	212	CYC	C1B-CHB-C4A-C3A
5	I	208	CYC	C1B-CHB-C4A-NA
5	F	206	CYC	C1B-CHB-C4A-NA
5	M	212	CYC	C1B-CHB-C4A-NA
4	A	201	BLA	C4C-CHD-C1D-C2D
4	B	202	BLA	C4C-CHD-C1D-C2D
5	K	210	CYC	C1B-CHB-C4A-C3A
4	A	201	BLA	C4C-CHD-C1D-ND
4	B	202	BLA	C4C-CHD-C1D-ND
5	K	210	CYC	C1B-CHB-C4A-NA
5	L	211	CYC	C1B-CHB-C4A-C3A
5	H	207	CYC	C1B-CHB-C4A-C3A
5	D	204	CYC	C1B-CHB-C4A-C3A
5	E	205	CYC	C1B-CHB-C4A-C3A
5	J	209	CYC	C1B-CHB-C4A-C3A
5	L	211	CYC	C1B-CHB-C4A-NA
5	C	203	CYC	C1B-CHB-C4A-C3A
5	H	207	CYC	C1B-CHB-C4A-NA
5	D	204	CYC	C1B-CHB-C4A-NA
5	E	205	CYC	C1B-CHB-C4A-NA
5	C	203	CYC	C1B-CHB-C4A-NA
5	J	209	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

12 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	BLA	6	0
4	B	202	BLA	8	0
5	C	203	CYC	4	0
5	D	204	CYC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	205	CYC	5	0
5	F	206	CYC	3	0
5	H	207	CYC	6	0
5	I	208	CYC	3	0
5	J	209	CYC	7	0
5	K	210	CYC	3	0
5	L	211	CYC	5	0
5	M	212	CYC	3	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.