



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:18 PM GMT

PDB ID : 1EYX
Title : CRYSTAL STRUCTURE OF R-PHYCOERYTHRIN AT 2.2 ANGSTROMS
Authors : Contreras-Martel, C.; Legrand, P.; Piras, C.; Vernede, X.; Martinez-Oyanedel, J.; Bunster, M.; Fontecilla-Camps, J.C.
Deposited on : 2000-05-09
Resolution : 2.25 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

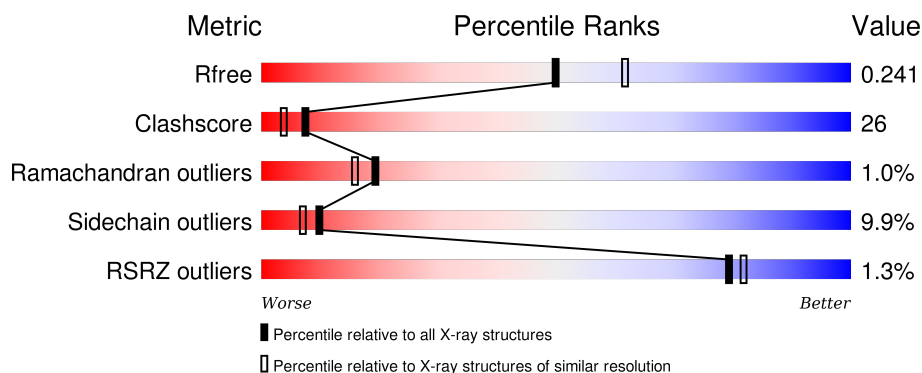
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	<div> <div>55%</div> <div>41%</div> <div>.</div> </div>
1	K	164	<div> <div>57%</div> <div>38%</div> <div>5%</div> </div>
2	B	177	<div> <div>%</div> <div>51%</div> <div>42%</div> <div>6%</div> </div>
2	L	177	<div> <div>%</div> <div>59%</div> <div>35%</div> <div>6%</div> </div>
3	G	6	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	6	

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
6	CYC	A	168	X	-	-	-
6	CYC	K	168	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5719 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 R-PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1247	775	218	248	6			
1	K	164	Total	C	N	O	S	0	0	0
			1247	775	218	248	6			

- Molecule 2 is a protein called R-PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1298	800	227	260	11			
2	L	177	Total	C	N	O	S	0	0	0
			1298	800	227	260	11			

- Molecule 3 is a protein called R-PHYCOERYTHRIN.

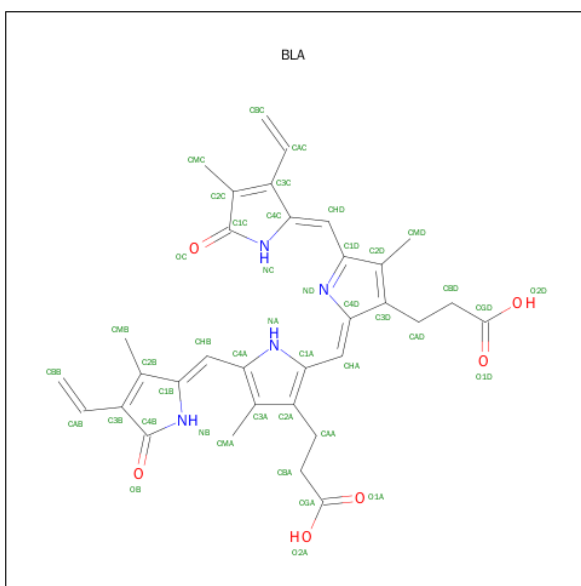
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	6	Total	C	N	O	0	0	0
			42	27	9	6			
3	H	5	Total	C	N	O	0	0	0
			37	24	8	5			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



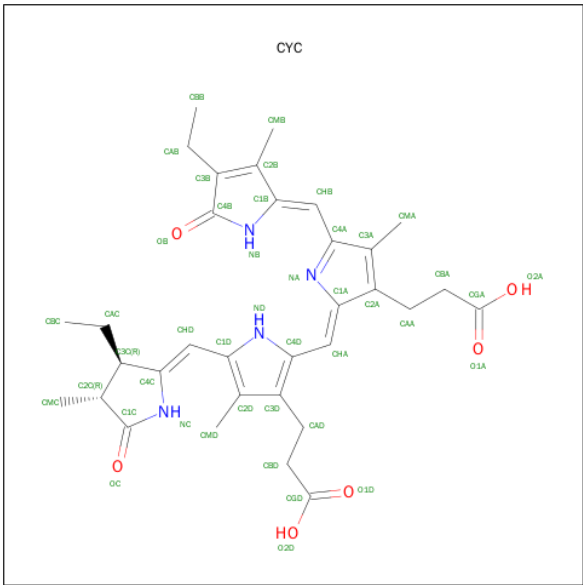
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



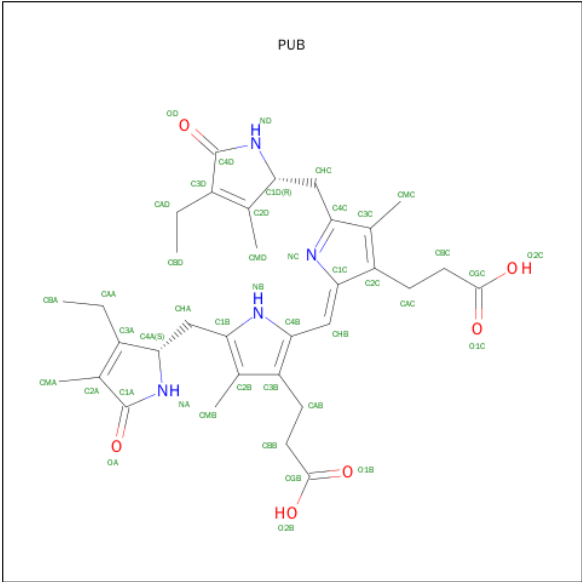
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	O	
			43	33	4	6	

- Molecule 6 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 7 is PHYCOUROBILIN (three-letter code: PUB) (formula: C₃₃H₄₂N₄O₆).



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

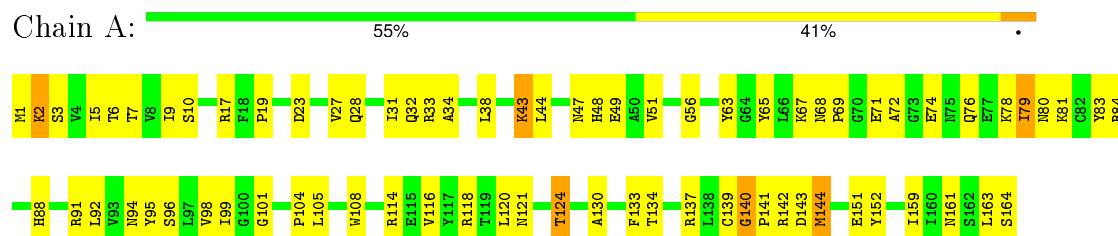
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	22	Total	O	0	0
			22	22		
8	H	1	Total	O	0	0
			1	1		
8	K	31	Total	O	0	0
			31	31		
8	L	29	Total	O	0	0
			29	29		

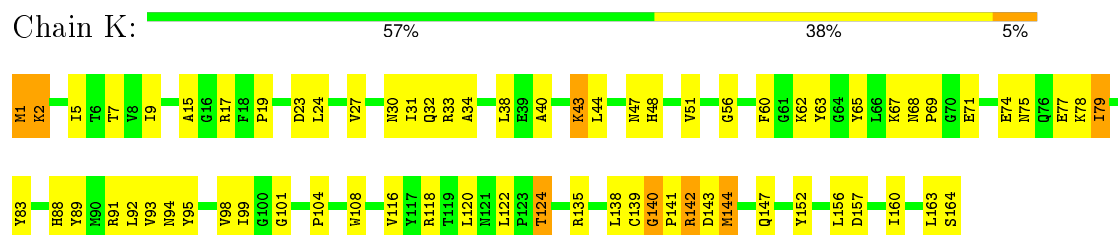
3 Residue-property plots

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.

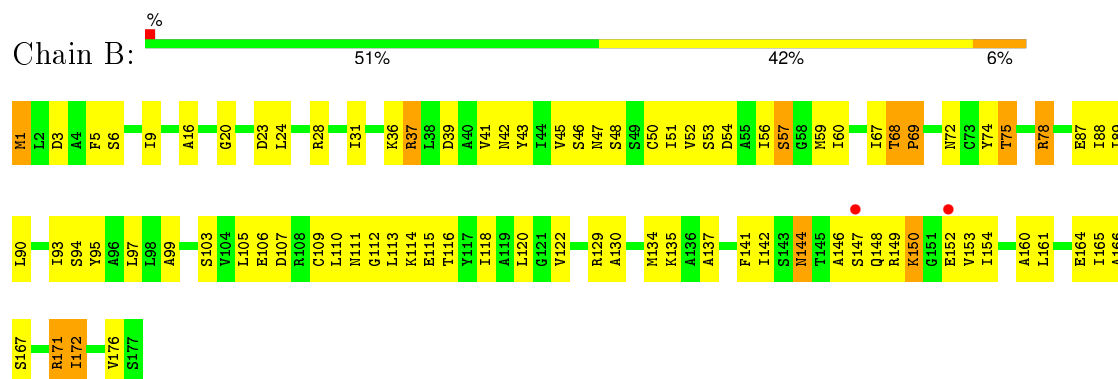
• Molecule 1: R-PHYCOERYTHRIN



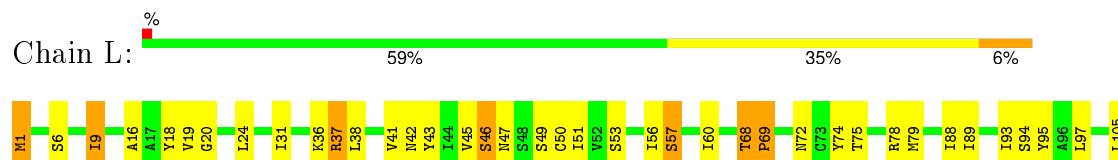
• Molecule 1: R-PHYCOERYTHRIN

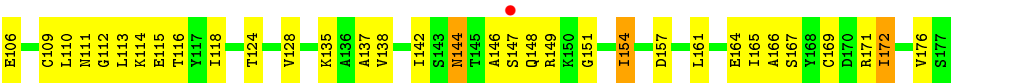


• Molecule 2: R-PHYCOERYTHRIN

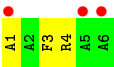


• Molecule 2: R-PHYCOERYTHRIN





● Molecule 3: R-PHYCOERYTHRIN



● Molecule 3: R-PHYCOERYTHRIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	187.27Å 187.27Å 59.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	999.00 – 2.25 19.80 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (999.00-2.25) 97.8 (19.80-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.26Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.180 , 0.279 0.153 , 0.241	Depositor DCC
R_{free} test set	1824 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.2	EDS
Estimated twinning fraction	0.460 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 36655 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC, MEN, BLA, SO4, 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	0.30	0/1268	0.55	0/1713
1	K	0.31	0/1268	0.57	0/1713
2	B	0.34	0/1300	0.56	0/1755
2	L	0.33	0/1300	0.55	0/1755
3	G	0.28	0/42	0.46	0/55
3	H	0.27	0/37	0.37	0/48
All	All	0.32	0/5215	0.56	0/7039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1247	0	1215	61	0
1	K	1247	0	1215	65	0
2	B	1298	0	1300	87	0
2	L	1298	0	1300	77	0
3	G	42	0	44	7	0
3	H	37	0	39	9	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	43	0	32	3	0
6	A	43	0	37	7	0
6	B	86	0	74	15	0
6	K	86	0	74	6	0
6	L	86	0	74	18	0
7	B	43	0	33	3	0
7	L	43	0	33	2	0
8	A	27	0	0	0	0
8	B	22	0	0	0	0
8	H	1	0	0	0	0
8	K	31	0	0	1	0
8	L	29	0	0	0	0
All	All	5719	0	5470	283	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 26.

All (283) 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:106:GLU:HG2	2:B:110:LEU:HD12	1.50	0.93
2:B:36:LYS:HD3	6:B:183:CYC:HMD3	1.52	0.91
2:L:114:LYS:HB2	2:L:176:VAL:HA	1.54	0.89
1:K:44:LEU:HD12	6:K:168:CYC:HBB1	1.53	0.89
1:A:32:GLN:HG3	1:K:32:GLN:HG3	1.55	0.87
1:A:44:LEU:HD12	6:A:168:CYC:HBB1	1.60	0.83
2:B:89:ILE:HG23	2:B:172:ILE:HD12	1.64	0.80
2:L:88:ILE:HG21	6:L:181:CYC:HAB1	1.64	0.80
2:L:53:SER:O	2:L:57:SER:HB2	1.82	0.79
2:B:47:ASN:O	2:B:51:ILE:HG13	1.84	0.76
2:B:20:GLY:O	2:B:24:LEU:HB2	1.86	0.76
1:K:75:ASN:OD1	1:K:78:LYS:HG3	1.86	0.75
2:L:20:GLY:O	2:L:24:LEU:HB2	1.85	0.75
1:K:94:ASN:O	1:K:98:VAL:HG23	1.86	0.75
1:K:68:ASN:O	1:K:71:GLU:HB2	1.87	0.74
1:K:27:VAL:O	1:K:30:ASN:HB2	1.88	0.74
1:A:68:ASN:O	1:A:71:GLU:HB2	1.88	0.74
2:B:154:ILE:HD11	6:B:183:CYC:HAD2	1.71	0.73
1:K:5:ILE:O	1:K:9:ILE:HG13	1.89	0.73
1:A:76:GLN:HG3	1:A:80:ASN:ND2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:89:ILE:HG23	2:L:172:ILE:HD12	1.71	0.72
3:G:1:ALA:HA	3:G:4:ARG:HD3	1.69	0.72
2:B:148:GLN:HB2	7:B:179:PUB:OA	1.89	0.72
3:G:3:PHE:HB3	3:G:4:ARG:NH1	2.05	0.72
3:G:4:ARG:N	3:G:4:ARG:HD2	2.05	0.71
2:B:43:TYR:HD2	2:B:142:ILE:HA	1.53	0.71
2:B:37:ARG:O	2:B:41:VAL:HG23	1.91	0.71
2:B:88:ILE:HG21	6:B:181:CYC:HAB1	1.71	0.70
1:A:33:ARG:NE	6:L:183:CYC:HAB1	2.05	0.70
2:L:146:ALA:HB3	2:L:149:ARG:O	1.92	0.70
1:A:99:ILE:HD12	1:A:104:PRO:HD3	1.74	0.70
2:B:75:THR:HG1	2:B:78:ARG:HG3	1.55	0.70
1:K:108:TRP:O	6:K:166:CYC:HAB2	1.91	0.70
1:K:99:ILE:HD13	2:L:6:SER:HB3	1.74	0.69
2:L:36:LYS:HD3	6:L:183:CYC:HMD3	1.75	0.69
1:K:89:TYR:O	1:K:93:VAL:HG23	1.94	0.68
3:G:3:PHE:HB3	3:G:4:ARG:HH11	1.59	0.68
2:B:146:ALA:HB3	2:B:149:ARG:O	1.94	0.68
2:L:148:GLN:HB2	7:L:179:PUB:OA	1.93	0.67
6:B:183:CYC:HAB1	1:K:33:ARG:NE	2.09	0.67
2:L:19:VAL:HG12	2:L:24:LEU:HD13	1.75	0.67
2:B:75:THR:OG1	2:B:78:ARG:HG3	1.95	0.67
1:A:47:ASN:O	1:A:51:VAL:HG23	1.94	0.66
1:K:104:PRO:O	1:K:108:TRP:HB2	1.94	0.66
3:G:4:ARG:HD2	3:G:4:ARG:H	1.58	0.66
1:K:88:HIS:O	1:K:92:LEU:HG	1.95	0.66
2:L:41:VAL:HG22	2:L:97:LEU:HD23	1.77	0.65
1:K:47:ASN:O	1:K:51:VAL:HG23	1.96	0.65
2:L:113:LEU:HD11	6:L:181:CYC:HMB3	1.79	0.64
2:B:113:LEU:HA	3:G:3:PHE:HE1	1.61	0.64
2:B:43:TYR:OH	2:B:153:VAL:HG11	1.96	0.64
1:K:44:LEU:HD11	1:K:152:TYR:HE1	1.62	0.63
1:A:76:GLN:HG3	1:A:80:ASN:HD21	1.62	0.63
2:B:144:ASN:HB2	6:B:183:CYC:HMC3	1.81	0.63
6:K:166:CYC:HMD1	6:K:166:CYC:HBD2	1.81	0.62
1:A:99:ILE:HD13	2:B:6:SER:HB3	1.80	0.62
2:L:47:ASN:O	2:L:51:ILE:HG13	1.99	0.62
2:B:142:ILE:O	6:B:183:CYC:HMC1	1.99	0.61
3:H:1:ALA:O	3:H:5:ALA:HB3	2.01	0.61
1:A:81:LYS:HE2	1:A:84:ARG:NH1	2.16	0.61
2:B:53:SER:O	2:B:57:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:VAL:HG21	6:A:168:CYC:HBB3	1.82	0.61
1:A:34:ALA:O	1:A:38:LEU:HG	2.00	0.60
2:B:167:SER:O	2:B:171:ARG:HG2	2.01	0.60
2:B:105:LEU:HD11	2:B:172:ILE:HD11	1.84	0.60
2:L:106:GLU:HG2	2:L:110:LEU:HD12	1.84	0.60
1:K:23:ASP:O	1:K:27:VAL:HG23	2.00	0.60
2:L:97:LEU:HD13	2:L:165:ILE:HD13	1.83	0.59
1:A:124:THR:HG21	1:A:163:LEU:O	2.01	0.59
1:A:44:LEU:O	1:A:48:HIS:HB3	2.03	0.59
2:B:110:LEU:HD21	2:B:172:ILE:HD13	1.85	0.59
2:L:113:LEU:HA	3:H:2:PHE:HE1	1.67	0.59
1:A:9:ILE:HD12	2:B:1:MET:HE3	1.84	0.59
1:K:68:ASN:O	1:K:74:GLU:HB3	2.04	0.58
1:K:44:LEU:HD11	1:K:152:TYR:CE1	2.39	0.58
2:B:105:LEU:O	2:B:109:CYS:HB3	2.04	0.57
2:B:148:GLN:HB2	7:B:179:PUB:C1A	2.33	0.57
2:L:43:TYR:HD2	2:L:142:ILE:HA	1.69	0.57
2:L:142:ILE:O	6:L:183:CYC:HMC1	2.04	0.57
1:K:19:PRO:HD3	2:L:95:TYR:CE1	2.40	0.56
2:B:154:ILE:HD11	6:B:183:CYC:CAD	2.35	0.56
1:A:44:LEU:HD11	1:A:152:TYR:HE2	1.70	0.56
1:K:124:THR:HG21	1:K:163:LEU:O	2.04	0.56
2:L:105:LEU:O	2:L:109:CYS:HB3	2.06	0.56
2:L:112:GLY:HA2	2:L:115:GLU:OE1	2.05	0.56
1:A:44:LEU:HD11	1:A:152:TYR:CE2	2.41	0.56
1:A:94:ASN:O	1:A:98:VAL:HG23	2.05	0.56
1:A:78:LYS:O	5:A:166:BLA:HMD3	2.05	0.56
1:A:43:LYS:HG2	1:A:144:MET:HG2	1.88	0.55
2:B:142:ILE:CD1	2:B:165:ILE:HG21	2.37	0.55
1:A:161:ASN:OD1	2:L:49:SER:HB2	2.06	0.55
6:L:183:CYC:HMD1	6:L:183:CYC:HBD2	1.87	0.55
1:K:67:LYS:HE3	1:K:79:ILE:HD11	1.89	0.55
1:K:95:TYR:O	1:K:99:ILE:HG13	2.07	0.55
1:A:81:LYS:HE2	1:A:84:ARG:HH12	1.72	0.55
1:A:51:VAL:HG21	6:A:168:CYC:CBB	2.37	0.54
2:B:74:TYR:O	2:B:78:ARG:HG3	2.07	0.54
2:L:56:ILE:O	2:L:60:ILE:HG13	2.06	0.54
2:L:154:ILE:HD11	6:L:183:CYC:HAD2	1.90	0.54
2:L:36:LYS:HD3	6:L:183:CYC:CMD	2.37	0.54
2:L:51:ILE:HG23	2:L:137:ALA:HB3	1.88	0.54
1:K:34:ALA:O	1:K:38:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:O	1:A:92:LEU:HG	2.08	0.54
2:L:105:LEU:HD11	2:L:172:ILE:CD1	2.38	0.54
2:L:113:LEU:CD1	6:L:181:CYC:HMB3	2.38	0.54
2:L:72:MEN:HE22	6:L:181:CYC:HBD2	1.90	0.53
2:B:68:THR:HG23	2:B:69:PRO:HD2	1.88	0.53
2:B:130:ALA:O	2:B:134:MET:HG3	2.08	0.53
3:H:3:ARG:HD2	3:H:3:ARG:N	2.23	0.53
1:A:143:ASP:O	1:A:144:MET:HG3	2.09	0.53
2:L:37:ARG:HH11	2:L:37:ARG:HB2	1.74	0.53
2:B:105:LEU:HD11	2:B:172:ILE:CD1	2.39	0.53
2:B:41:VAL:O	2:B:45:VAL:HG13	2.09	0.53
1:K:40:ALA:O	1:K:44:LEU:HD13	2.08	0.53
2:B:60:ILE:HG21	2:B:67:ILE:HD13	1.91	0.53
2:L:113:LEU:O	2:L:116:THR:HB	2.08	0.53
6:B:183:CYC:HBD2	6:B:183:CYC:HMD1	1.90	0.53
1:A:28:GLN:O	1:A:32:GLN:HG2	2.09	0.53
2:L:93:ILE:HG22	2:L:165:ILE:HD11	1.90	0.53
2:L:68:THR:HG23	2:L:69:PRO:HD2	1.92	0.52
2:L:41:VAL:O	2:L:45:VAL:HG13	2.09	0.52
1:A:44:LEU:CD1	6:A:168:CYC:HBB1	2.37	0.52
1:A:2:LYS:HE2	1:A:7:THR:OG1	2.09	0.52
1:A:31:ILE:HA	2:B:31:ILE:HG23	1.91	0.51
1:A:63:TYR:HB3	1:A:65:TYR:CE1	2.44	0.51
1:K:88:HIS:CD2	1:K:91:ARG:HH21	2.28	0.51
1:K:140:GLY:O	1:K:144:MET:O	2.29	0.51
1:K:9:ILE:HG21	2:L:1:MET:HE3	1.92	0.51
2:L:135:LYS:HE3	2:L:166:ALA:HB1	1.91	0.51
1:K:43:LYS:HG2	1:K:144:MET:HG2	1.93	0.51
2:B:93:ILE:HG22	2:B:165:ILE:HD11	1.92	0.51
1:K:56:GLY:HA3	1:K:83:TYR:CE2	2.46	0.50
1:A:95:TYR:O	1:A:99:ILE:HG13	2.12	0.50
2:B:106:GLU:O	2:B:111:ASN:HB2	2.11	0.50
2:B:3:ASP:HB3	2:B:99:ALA:HB1	1.93	0.50
2:L:144:ASN:HB2	6:L:183:CYC:HMC3	1.93	0.50
2:L:105:LEU:HD11	2:L:172:ILE:HD11	1.93	0.50
1:A:91:ARG:NH1	2:B:16:ALA:HA	2.27	0.50
1:A:9:ILE:HG23	2:B:95:TYR:CD1	2.47	0.49
1:A:140:GLY:O	1:A:144:MET:O	2.30	0.49
6:B:183:CYC:HMA2	1:K:147:GLN:HG3	1.94	0.49
1:K:60:PHE:HB3	1:K:67:LYS:NZ	2.28	0.49
1:K:116:VAL:O	1:K:120:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH22	6:A:168:CYC:CGD	2.26	0.49
2:B:56:ILE:O	2:B:60:ILE:HG13	2.13	0.49
1:K:62:LYS:HB2	8:K:383:HOH:O	2.13	0.48
6:L:181:CYC:HBB2	3:H:2:PHE:CE2	2.48	0.48
2:B:135:LYS:HE2	2:B:166:ALA:HB1	1.96	0.48
1:K:143:ASP:O	1:K:144:MET:HG3	2.13	0.48
1:K:44:LEU:O	1:K:48:HIS:HB3	2.14	0.48
1:A:96:SER:HB3	1:A:101:GLY:O	2.13	0.48
2:B:144:ASN:HB2	6:B:183:CYC:CMC	2.44	0.48
1:K:91:ARG:NH1	2:L:16:ALA:HA	2.29	0.48
1:K:15:ALA:CB	1:K:17:ARG:HD3	2.44	0.48
2:L:109:CYS:O	3:H:2:PHE:HZ	1.97	0.48
2:B:89:ILE:CG2	2:B:172:ILE:HD12	2.41	0.47
2:B:103:SER:O	2:B:107:ASP:HB2	2.15	0.47
1:K:91:ARG:HA	2:L:18:TYR:CE2	2.49	0.47
2:L:138:VAL:HG11	2:L:165:ILE:HG12	1.97	0.47
2:B:36:LYS:HD3	6:B:183:CYC:CMD	2.36	0.47
1:A:17:ARG:O	2:B:95:TYR:OH	2.30	0.47
2:L:89:ILE:CG2	2:L:172:ILE:HD12	2.42	0.47
2:L:89:ILE:HG23	2:L:172:ILE:CD1	2.43	0.47
1:K:9:ILE:HD12	2:L:1:MET:CE	2.45	0.47
2:L:154:ILE:HD11	6:L:183:CYC:CAD	2.45	0.47
1:K:19:PRO:HD3	2:L:95:TYR:HE1	1.80	0.47
2:B:176:VAL:HG23	2:B:176:VAL:O	2.15	0.47
1:A:133:PHE:O	1:A:137:ARG:N	2.48	0.46
2:L:106:GLU:O	2:L:111:ASN:HB2	2.14	0.46
2:L:37:ARG:NH2	2:L:164:GLU:OE1	2.48	0.46
2:B:39:ASP:OD2	2:B:153:VAL:HG21	2.16	0.46
1:K:122:LEU:CD2	6:K:166:CYC:HMD2	2.44	0.46
1:K:88:HIS:HD2	1:K:91:ARG:HH21	1.62	0.46
2:B:3:ASP:CB	2:B:99:ALA:HB1	2.46	0.46
1:A:130:ALA:O	1:A:134:THR:OG1	2.30	0.46
2:L:114:LYS:CB	2:L:176:VAL:HA	2.36	0.46
1:A:68:ASN:HB3	1:A:69:PRO:HD2	1.96	0.46
1:K:43:LYS:HA	1:K:43:LYS:HD2	1.75	0.46
1:K:135:ARG:NH1	1:K:160:ILE:HD13	2.30	0.46
1:K:19:PRO:HG2	2:L:45:VAL:HG11	1.97	0.46
1:K:24:LEU:N	1:K:24:LEU:HD23	2.31	0.46
2:L:9:ILE:CD1	2:L:19:VAL:HG21	2.46	0.46
2:L:36:LYS:NZ	2:L:157:ASP:O	2.47	0.46
1:A:116:VAL:HG13	1:A:120:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH1	1:A:95:TYR:OH	2.48	0.46
2:B:74:TYR:O	2:B:75:THR:OG1	2.28	0.46
2:L:38:LEU:HD12	6:L:183:CYC:C4B	2.45	0.46
2:B:3:ASP:HB2	2:B:99:ALA:O	2.16	0.46
2:B:161:LEU:HD12	2:B:161:LEU:N	2.31	0.46
1:A:5:ILE:O	1:A:9:ILE:HG13	2.16	0.45
2:B:60:ILE:CG2	2:B:67:ILE:HD13	2.46	0.45
2:B:161:LEU:HD12	2:B:161:LEU:H	1.81	0.45
1:K:2:LYS:O	1:K:101:GLY:HA3	2.15	0.45
2:B:160:ALA:O	2:B:164:GLU:HB2	2.16	0.45
2:L:88:ILE:CG2	6:L:181:CYC:HAB1	2.42	0.45
6:B:183:CYC:O1A	1:K:147:GLN:NE2	2.50	0.45
2:B:24:LEU:O	2:B:28:ARG:HG3	2.17	0.45
1:K:1:MET:HE3	1:K:104:PRO:HA	1.97	0.45
1:K:9:ILE:HB	2:L:1:MET:HE1	1.99	0.45
2:L:75:THR:HG1	2:L:78:ARG:HG3	1.82	0.45
2:L:147:SER:HB3	7:L:179:PUB:O1B	2.17	0.45
2:B:144:ASN:O	2:B:144:ASN:ND2	2.50	0.45
1:A:144:MET:HE2	1:A:144:MET:HB2	1.89	0.45
1:A:98:VAL:O	2:B:5:PHE:HD1	2.00	0.45
1:K:63:TYR:HB3	1:K:65:TYR:CE1	2.52	0.45
2:B:89:ILE:HG23	2:B:172:ILE:CD1	2.41	0.45
1:A:139:CYS:HA	6:A:168:CYC:HBC3	1.98	0.45
2:L:149:ARG:HG3	2:L:149:ARG:HH11	1.81	0.45
1:A:121:ASN:ND2	1:A:121:ASN:O	2.49	0.45
1:A:9:ILE:HB	2:B:1:MET:HE1	1.98	0.45
2:B:43:TYR:CD2	2:B:142:ILE:HA	2.44	0.44
1:A:72:ALA:O	1:A:78:LYS:HB3	2.16	0.44
2:B:147:SER:O	2:B:150:LYS:HE2	2.17	0.44
2:B:149:ARG:NH2	1:K:157:ASP:OD2	2.49	0.44
1:A:23:ASP:O	1:A:27:VAL:HG23	2.18	0.44
2:B:51:ILE:HG23	2:B:137:ALA:HB3	1.99	0.44
1:K:31:ILE:HA	2:L:31:ILE:HG23	1.99	0.44
2:B:90:LEU:HA	2:B:93:ILE:HD12	2.00	0.44
2:L:72:MEN:OD1	6:L:181:CYC:HMD2	2.17	0.44
2:L:161:LEU:HD12	2:L:161:LEU:N	2.33	0.44
2:B:37:ARG:HB2	2:B:37:ARG:HH11	1.82	0.44
3:H:3:ARG:H	3:H:3:ARG:HD2	1.83	0.44
1:A:9:ILE:HD12	2:B:1:MET:CE	2.46	0.43
1:K:135:ARG:HA	1:K:156:LEU:HD13	2.00	0.43
1:K:1:MET:HG3	1:K:99:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:ARG:CD	3:H:3:ARG:N	2.82	0.43
2:L:124:THR:O	2:L:128:VAL:HG23	2.19	0.43
2:B:42:ASN:O	2:B:46:SER:HB2	2.19	0.43
2:B:59:MET:HG2	2:B:59:MET:O	2.18	0.43
2:L:135:LYS:HD2	2:L:169:CYS:HB2	2.01	0.43
1:K:2:LYS:HE2	1:K:7:THR:OG1	2.19	0.43
1:K:1:MET:HE2	1:K:108:TRP:CZ2	2.54	0.43
2:L:144:ASN:HD21	2:L:151:GLY:H	1.67	0.43
2:L:41:VAL:HA	2:L:97:LEU:HD23	2.01	0.43
1:K:31:ILE:HG22	1:K:31:ILE:O	2.19	0.43
2:L:110:LEU:HD21	2:L:172:ILE:HG23	2.01	0.42
2:L:24:LEU:HA	2:L:24:LEU:HD12	1.86	0.42
1:A:68:ASN:O	1:A:74:GLU:HB3	2.18	0.42
2:L:60:ILE:HD13	2:L:79:MET:HE1	2.01	0.42
2:L:167:SER:O	2:L:171:ARG:HG3	2.19	0.42
2:L:106:GLU:HA	2:L:110:LEU:HB2	2.02	0.42
2:L:144:ASN:HB2	6:L:183:CYC:CMC	2.48	0.42
3:H:3:ARG:H	3:H:3:ARG:CD	2.32	0.42
1:K:1:MET:HG2	2:L:6:SER:HB2	2.00	0.42
1:K:139:CYS:SG	1:K:142:ARG:HB3	2.59	0.42
1:A:79:ILE:HG22	1:A:80:ASN:N	2.35	0.42
1:A:5:ILE:HG21	2:B:99:ALA:HA	2.01	0.42
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.20	0.42
1:A:3:SER:H	1:A:6:THR:HB	1.85	0.42
2:L:154:ILE:O	2:L:154:ILE:HG13	2.19	0.42
2:B:72:MEN:HE21	2:B:78:ARG:NH2	2.35	0.42
2:B:41:VAL:HA	2:B:97:LEU:HD23	2.02	0.42
3:G:4:ARG:N	3:G:4:ARG:CD	2.80	0.42
2:B:116:THR:HG22	2:B:120:LEU:CD1	2.49	0.42
2:B:97:LEU:HD13	2:B:165:ILE:HD13	2.02	0.41
1:K:68:ASN:HB3	1:K:69:PRO:HD2	2.02	0.41
1:A:56:GLY:HA3	1:A:83:TYR:CE2	2.55	0.41
2:B:122:VAL:HG13	6:B:181:CYC:NC	2.35	0.41
2:B:52:VAL:HG21	2:B:87:GLU:HA	2.02	0.41
2:B:120:LEU:CD2	6:B:181:CYC:HAA2	2.50	0.41
1:A:78:LYS:HB3	5:A:166:BLA:CMD	2.50	0.41
2:B:72:MEN:O	2:B:78:ARG:HD3	2.20	0.41
2:B:149:ARG:HH11	2:B:149:ARG:HG3	1.85	0.41
1:A:108:TRP:O	5:A:166:BLA:HAB	2.21	0.41
2:B:112:GLY:HA2	2:B:115:GLU:OE1	2.20	0.41
2:B:72:MEN:O	2:B:78:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:MET:HE2	1:K:144:MET:HB2	1.82	0.41
2:L:42:ASN:O	2:L:46:SER:HB2	2.19	0.41
2:B:43:TYR:HB3	2:B:141:PHE:O	2.21	0.41
6:A:168:CYC:HC	6:A:168:CYC:HMD2	1.86	0.41
1:K:78:LYS:HE2	6:K:166:CYC:CGD	2.51	0.41
2:L:74:TYR:O	2:L:78:ARG:HG3	2.20	0.41
1:A:63:TYR:CD1	1:A:65:TYR:HE1	2.38	0.41
1:A:105:LEU:HD21	1:A:159:ILE:HD11	2.02	0.41
2:L:105:LEU:HG	2:L:110:LEU:CD1	2.50	0.41
6:L:181:CYC:HMA1	3:H:2:PHE:HB2	2.03	0.41
2:B:88:ILE:HG21	6:B:181:CYC:CAB	2.44	0.41
1:K:138:LEU:HA	6:K:168:CYC:HMB2	2.03	0.41
2:B:97:LEU:HD22	2:B:165:ILE:HD13	2.02	0.40
2:B:114:LYS:HB2	2:B:176:VAL:HA	2.02	0.40
2:B:54:ASP:OD2	7:B:179:PUB:HHC1	2.21	0.40
2:B:154:ILE:O	2:B:154:ILE:HG13	2.22	0.40
1:K:15:ALA:HB3	1:K:17:ARG:HD3	2.03	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%)	153 (94%)	7 (4%)	2 (1%)	16	11
1	K	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	16	11
2	B	174/177 (98%)	167 (96%)	5 (3%)	2 (1%)	17	13
2	L	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	30	30
3	G	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	H	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	679/694 (98%)	646 (95%)	26 (4%)	7 (1%)	19	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	THR
1	K	140	GLY
2	L	69	PRO
1	A	140	GLY
2	B	69	PRO
1	A	141	PRO
1	K	141	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/129 (100%)	115 (89%)	14 (11%)	8	6
1	K	129/129 (100%)	119 (92%)	10 (8%)	16	14
2	B	138/138 (100%)	121 (88%)	17 (12%)	6	4
2	L	138/138 (100%)	126 (91%)	12 (9%)	13	11
3	G	2/2 (100%)	2 (100%)	0	100	100
3	H	2/2 (100%)	2 (100%)	0	100	100
All	All	538/538 (100%)	485 (90%)	53 (10%)	10	7

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	10	SER
1	A	19	PRO
1	A	43	LYS
1	A	49	GLU
1	A	67	LYS
1	A	79	ILE
1	A	114	ARG
1	A	118	ARG

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Mol	Chain	Res	Type
1	A	124	THR
1	A	142	ARG
1	A	144	MET
1	A	164	SER
2	B	1	MET
2	B	9	ILE
2	B	23	ASP
2	B	37	ARG
2	B	48	SER
2	B	50	CYS
2	B	57	SER
2	B	68	THR
2	B	78	ARG
2	B	94	SER
2	B	118	ILE
2	B	129	ARG
2	B	144	ASN
2	B	150	LYS
2	B	152	GLU
2	B	171	ARG
2	B	172	ILE
1	K	1	MET
1	K	2	LYS
1	K	43	LYS
1	K	77	GLU
1	K	79	ILE
1	K	118	ARG
1	K	124	THR
1	K	142	ARG
1	K	144	MET
1	K	164	SER
2	L	1	MET
2	L	9	ILE
2	L	37	ARG
2	L	46	SER
2	L	50	CYS
2	L	57	SER
2	L	68	THR
2	L	94	SER
2	L	118	ILE
2	L	144	ASN
2	L	154	ILE

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Mol	Chain	Res	Type
2	L	172	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	76	GLN
1	A	80	ASN
2	B	125	ASN
2	B	144	ASN
1	K	76	GLN
1	K	88	HIS
2	L	47	ASN
2	L	125	ASN
2	L	144	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	7,8,9	0.61	0	5,9,11	0.92	0
2	MEN	L	72	2	7,8,9	0.64	0	5,9,11	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	3	0
2	L	72	MEN	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	BLA	A	166	1	35,46,46	2.56	13 (37%)	43,67,67	2.17	12 (27%)
6	CYC	A	168	1	35,46,46	2.89	12 (34%)	47,67,67	2.28	17 (36%)
4	SO4	A	201	-	4,4,4	0.95	0	6,6,6	0.08	0
7	PUB	B	179	2	34,46,46	2.83	11 (32%)	30,67,67	3.38	7 (23%)
6	CYC	B	181	2	35,46,46	2.84	10 (28%)	47,67,67	2.31	18 (38%)
6	CYC	B	183	2	35,46,46	2.85	12 (34%)	47,67,67	2.24	18 (38%)
4	SO4	B	202	-	4,4,4	0.95	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	K	166	1	35,46,46	2.89	11 (31%)	47,67,67	2.24	19 (40%)
6	CYC	K	168	1	35,46,46	2.81	11 (31%)	47,67,67	2.21	14 (29%)
7	PUB	L	179	2	34,46,46	2.78	11 (32%)	30,67,67	3.31	9 (30%)
6	CYC	L	181	2	35,46,46	2.87	11 (31%)	47,67,67	2.41	20 (42%)
6	CYC	L	183	2	35,46,46	2.88	12 (34%)	47,67,67	2.34	16 (34%)

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
5	BLA	A	166	1	-	2/22/74/74	0/4/4/4
6	CYC	A	168	1	1/1/14/19	2/21/74/74	0/4/4/4
4	SO4	A	201	-	-	0/0/0/0	0/0/0/0
7	PUB	B	179	2	-	0/19/74/74	0/4/4/4
6	CYC	B	181	2	-	1/21/74/74	0/4/4/4
6	CYC	B	183	2	-	1/21/74/74	0/4/4/4
4	SO4	B	202	-	-	0/0/0/0	0/0/0/0
6	CYC	K	166	1	-	1/21/74/74	0/4/4/4
6	CYC	K	168	1	1/1/14/19	2/21/74/74	0/4/4/4
7	PUB	L	179	2	-	0/19/74/74	0/4/4/4
6	CYC	L	181	2	-	1/21/74/74	0/4/4/4
6	CYC	L	183	2	-	1/21/74/74	0/4/4/4

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	168	CYC	C2C-C1C	-13.02	1.39	1.52
6	L	183	CYC	C2C-C1C	-12.97	1.39	1.52
6	L	181	CYC	C2C-C1C	-12.89	1.40	1.52
6	K	166	CYC	C2C-C1C	-12.85	1.40	1.52
6	B	181	CYC	C2C-C1C	-12.80	1.40	1.52
6	B	183	CYC	C2C-C1C	-12.73	1.40	1.52
6	K	168	CYC	C2C-C1C	-12.47	1.40	1.52
7	B	179	PUB	CBA-CAA	-7.82	1.14	1.51
7	L	179	PUB	CBA-CAA	-7.67	1.14	1.51
7	B	179	PUB	CHC-C1D	-4.33	1.44	1.53
7	L	179	PUB	CHC-C1D	-4.11	1.45	1.53
7	L	179	PUB	C4D-C3D	-3.71	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	179	PUB	C4D-C3D	-3.62	1.40	1.48
7	B	179	PUB	CHA-C4A	-3.57	1.45	1.54
7	L	179	PUB	CHA-C4A	-3.37	1.45	1.54
6	K	168	CYC	C4B-C3B	-3.00	1.41	1.48
6	A	168	CYC	C4B-C3B	-2.97	1.41	1.48
6	L	181	CYC	C4B-C3B	-2.96	1.41	1.48
6	K	166	CYC	C4B-C3B	-2.90	1.42	1.48
6	B	181	CYC	C4B-C3B	-2.83	1.42	1.48
6	L	183	CYC	C4B-C3B	-2.81	1.42	1.48
6	B	183	CYC	C4B-C3B	-2.79	1.42	1.48
7	L	179	PUB	C4A-C3A	-2.49	1.42	1.50
5	A	166	BLA	C1C-C2C	-2.44	1.40	1.47
7	B	179	PUB	CHA-C1B	-2.43	1.44	1.50
6	K	168	CYC	C1C-NC	-2.39	1.34	1.37
5	A	166	BLA	C4D-C3D	-2.36	1.41	1.45
7	B	179	PUB	C4A-C3A	-2.34	1.42	1.50
6	K	166	CYC	C1C-NC	-2.34	1.34	1.37
6	L	183	CYC	C1C-NC	-2.33	1.34	1.37
6	A	168	CYC	C1C-NC	-2.33	1.34	1.37
6	B	181	CYC	C1C-NC	-2.30	1.34	1.37
7	L	179	PUB	CHA-C1B	-2.28	1.45	1.50
6	K	166	CYC	C4B-NB	-2.26	1.32	1.37
6	B	183	CYC	C1C-NC	-2.25	1.34	1.37
6	L	181	CYC	C1C-NC	-2.23	1.34	1.37
6	B	183	CYC	C4B-NB	-2.22	1.32	1.37
6	A	168	CYC	C4B-NB	-2.20	1.32	1.37
6	L	183	CYC	C4B-NB	-2.18	1.33	1.37
6	K	168	CYC	C4B-NB	-2.11	1.33	1.37
6	A	168	CYC	C4A-NA	2.02	1.41	1.37
6	L	183	CYC	C1B-NB	2.04	1.41	1.37
6	K	168	CYC	C4A-NA	2.09	1.41	1.37
6	B	183	CYC	C4A-NA	2.10	1.41	1.37
6	L	183	CYC	C4A-NA	2.16	1.41	1.37
6	L	181	CYC	C4A-NA	2.17	1.42	1.37
6	L	181	CYC	C1B-NB	2.18	1.41	1.37
6	K	166	CYC	C1B-NB	2.19	1.41	1.37
6	B	183	CYC	C1B-NB	2.24	1.41	1.37
6	B	181	CYC	C1B-NB	2.27	1.41	1.37
5	A	166	BLA	C1B-NB	2.31	1.41	1.37
7	L	179	PUB	C3B-C2B	2.33	1.44	1.37
6	A	168	CYC	C1B-NB	2.34	1.41	1.37
7	B	179	PUB	C3B-C2B	2.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	168	CYC	CHB-C1B	2.38	1.43	1.37
6	L	181	CYC	CAC-C3C	2.46	1.59	1.54
6	K	168	CYC	CAC-C3C	2.48	1.59	1.54
5	A	166	BLA	C2A-C3A	2.52	1.45	1.37
6	B	181	CYC	CAC-C3C	2.53	1.59	1.54
6	K	166	CYC	C4C-NC	2.69	1.43	1.37
6	K	168	CYC	C4C-NC	2.72	1.43	1.37
5	A	166	BLA	C3D-C2D	2.74	1.42	1.36
6	L	181	CYC	CHB-C1B	2.75	1.44	1.37
6	L	183	CYC	CHB-C1B	2.76	1.44	1.37
6	K	166	CYC	CHB-C1B	2.77	1.44	1.37
6	B	183	CYC	CHB-C1B	2.78	1.44	1.37
6	L	183	CYC	C4C-NC	2.80	1.43	1.37
6	B	183	CYC	C4C-NC	2.84	1.43	1.37
6	K	168	CYC	CHB-C1B	2.90	1.44	1.37
6	B	181	CYC	CHB-C1B	2.93	1.44	1.37
6	B	181	CYC	C4C-NC	2.96	1.44	1.37
6	L	181	CYC	C4C-NC	2.97	1.44	1.37
6	A	168	CYC	C3B-C2B	2.98	1.43	1.36
6	B	183	CYC	C3B-C2B	3.02	1.43	1.36
6	A	168	CYC	C4C-NC	3.06	1.44	1.37
6	L	183	CYC	C3B-C2B	3.07	1.43	1.36
6	L	183	CYC	CAC-C3C	3.08	1.60	1.54
6	B	183	CYC	CAC-C3C	3.08	1.60	1.54
6	A	168	CYC	CAC-C3C	3.14	1.60	1.54
6	K	168	CYC	C3B-C2B	3.19	1.43	1.36
5	A	166	BLA	C4C-NC	3.22	1.43	1.37
6	K	166	CYC	C3B-C2B	3.23	1.43	1.36
5	A	166	BLA	C3B-C2B	3.29	1.43	1.36
6	L	181	CYC	C3B-C2B	3.37	1.44	1.36
6	B	181	CYC	C3B-C2B	3.38	1.44	1.36
6	K	166	CYC	CAC-C3C	3.54	1.61	1.54
5	A	166	BLA	CAC-C3C	3.57	1.58	1.47
6	K	168	CYC	C2A-C3A	3.68	1.44	1.36
6	B	183	CYC	C2A-C3A	3.70	1.44	1.36
6	A	168	CYC	C2A-C3A	3.71	1.44	1.36
6	K	166	CYC	C2A-C3A	3.74	1.44	1.36
6	B	181	CYC	C2A-C3A	3.78	1.44	1.36
6	L	183	CYC	C2A-C3A	3.83	1.45	1.36
7	L	179	PUB	C2D-C3D	3.84	1.45	1.36
5	A	166	BLA	CBC-CAC	3.91	1.49	1.30
6	L	181	CYC	C2A-C3A	3.92	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	179	PUB	C2C-C3C	3.98	1.45	1.36
7	B	179	PUB	C2C-C3C	4.00	1.45	1.36
7	B	179	PUB	C2D-C3D	4.04	1.46	1.36
5	A	166	BLA	CHB-C1B	4.66	1.44	1.34
6	B	181	CYC	CHA-C1A	4.87	1.39	1.35
5	A	166	BLA	CBB-CAB	5.11	1.55	1.30
6	L	181	CYC	CHA-C1A	5.12	1.39	1.35
6	L	183	CYC	CHA-C1A	5.13	1.39	1.35
6	A	168	CYC	CHA-C1A	5.13	1.39	1.35
6	K	168	CYC	CHA-C1A	5.17	1.39	1.35
6	K	166	CYC	CHA-C1A	5.18	1.39	1.35
6	B	183	CYC	CHA-C1A	5.39	1.39	1.35
7	L	179	PUB	CHB-C1C	5.56	1.40	1.35
7	B	179	PUB	CHB-C1C	5.57	1.40	1.35
5	A	166	BLA	CHA-C4D	5.62	1.40	1.35
5	A	166	BLA	C3C-C2C	6.65	1.50	1.36
7	B	179	PUB	C3A-C2A	7.91	1.44	1.34
7	L	179	PUB	C3A-C2A	7.99	1.44	1.34

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	179	PUB	CAD-C3D-C4D	-13.69	109.55	121.51
7	L	179	PUB	CAD-C3D-C4D	-12.88	110.26	121.51
5	A	166	BLA	CAC-C3C-C2C	-6.19	107.67	128.41
6	L	181	CYC	C1B-C2B-C3B	-5.25	102.21	107.81
6	A	168	CYC	C1B-C2B-C3B	-5.09	102.38	107.81
6	K	168	CYC	C1B-C2B-C3B	-4.90	102.58	107.81
6	K	166	CYC	C1B-C2B-C3B	-4.79	102.70	107.81
6	B	183	CYC	C1B-C2B-C3B	-4.79	102.70	107.81
6	B	181	CYC	C1B-C2B-C3B	-4.76	102.73	107.81
6	L	183	CYC	C1B-C2B-C3B	-4.71	102.78	107.81
6	K	166	CYC	CAC-C3C-C2C	-4.21	103.54	114.13
6	A	168	CYC	CAC-C3C-C2C	-4.18	103.61	114.13
6	B	183	CYC	C3C-C4C-NC	-4.08	103.84	107.93
5	A	166	BLA	CBC-CAC-C3C	-4.06	106.41	127.01
6	B	183	CYC	CAC-C3C-C2C	-4.05	103.96	114.13
6	L	183	CYC	OC-C1C-C2C	-3.98	123.03	126.25
7	L	179	PUB	CBA-CAA-C3A	-3.91	107.48	113.15
6	L	183	CYC	C3C-C4C-NC	-3.81	104.11	107.93
6	L	181	CYC	C3C-C4C-NC	-3.77	104.15	107.93
7	B	179	PUB	CBA-CAA-C3A	-3.60	107.94	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	181	CYC	C3C-C4C-NC	-3.55	104.37	107.93
6	B	181	CYC	CAC-C3C-C2C	-3.50	105.33	114.13
6	K	166	CYC	OC-C1C-C2C	-3.44	123.47	126.25
6	L	183	CYC	CAC-C3C-C2C	-3.42	105.53	114.13
6	L	183	CYC	CBC-CAC-C3C	-3.42	105.22	113.57
6	L	181	CYC	C1B-NB-C4B	-3.40	105.76	110.73
6	A	168	CYC	C3C-C4C-NC	-3.39	104.53	107.93
6	B	181	CYC	C2D-C1D-ND	-3.35	104.80	110.29
6	L	181	CYC	CAC-C3C-C2C	-3.30	105.82	114.13
5	A	166	BLA	C1B-NB-C4B	-3.30	105.90	110.73
6	A	168	CYC	C1B-NB-C4B	-3.18	106.07	110.73
6	K	166	CYC	C1B-NB-C4B	-3.18	106.09	110.73
6	K	168	CYC	CAC-C3C-C2C	-3.11	106.32	114.13
6	K	166	CYC	CBC-CAC-C3C	-3.10	105.99	113.57
6	K	168	CYC	CBC-CAC-C3C	-3.09	106.02	113.57
6	B	183	CYC	CBC-CAC-C3C	-3.07	106.07	113.57
6	B	181	CYC	C1B-NB-C4B	-3.05	106.28	110.73
6	L	181	CYC	CBC-CAC-C3C	-2.95	106.35	113.57
6	K	168	CYC	C3C-C4C-NC	-2.94	104.98	107.93
6	K	166	CYC	C3C-C4C-NC	-2.94	104.98	107.93
6	B	181	CYC	CBC-CAC-C3C	-2.93	106.39	113.57
6	L	183	CYC	C1B-NB-C4B	-2.91	106.48	110.73
7	L	179	PUB	CHA-C1B-C2B	-2.89	125.53	130.41
6	A	168	CYC	CBC-CAC-C3C	-2.85	106.60	113.57
6	K	168	CYC	C1B-NB-C4B	-2.81	106.62	110.73
6	B	183	CYC	CHB-C4A-NA	-2.79	119.60	124.91
6	B	181	CYC	CHB-C4A-NA	-2.79	119.60	124.91
6	L	181	CYC	C2D-C1D-ND	-2.77	105.76	110.29
6	B	183	CYC	C1B-NB-C4B	-2.76	106.69	110.73
7	B	179	PUB	CHA-C1B-C2B	-2.72	125.82	130.41
5	A	166	BLA	C2D-C1D-ND	-2.69	104.41	110.55
6	L	181	CYC	C4B-C3B-C2B	-2.67	106.52	108.05
5	A	166	BLA	CAA-C2A-C1A	-2.63	124.15	127.01
6	A	168	CYC	C2D-C1D-ND	-2.57	106.07	110.29
5	A	166	BLA	CHB-C1B-NB	-2.54	121.46	130.87
5	A	166	BLA	CHD-C1D-ND	-2.50	120.15	124.91
6	L	181	CYC	CHB-C4A-NA	-2.48	120.19	124.91
6	B	183	CYC	C4B-C3B-C2B	-2.46	106.65	108.05
6	L	181	CYC	OC-C1C-C2C	-2.45	124.27	126.25
7	L	179	PUB	CHB-C1C-NC	-2.45	124.29	128.67
6	K	168	CYC	CHB-C4A-NA	-2.43	120.28	124.91
6	A	168	CYC	CHB-C4A-NA	-2.43	120.29	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	181	CYC	CHB-C1B-NB	-2.42	120.92	126.16
6	K	166	CYC	CHB-C4A-NA	-2.36	120.42	124.91
7	L	179	PUB	CMB-C2B-C1B	-2.34	124.78	127.14
6	B	183	CYC	C2D-C1D-ND	-2.29	106.53	110.29
6	K	166	CYC	CHB-C1B-NB	-2.25	121.30	126.16
6	L	183	CYC	CHB-C4A-NA	-2.24	120.64	124.91
6	B	181	CYC	OC-C1C-C2C	-2.24	124.44	126.25
7	B	179	PUB	CHB-C1C-NC	-2.23	124.68	128.67
6	B	183	CYC	CHB-C1B-NB	-2.22	121.35	126.16
6	K	166	CYC	C2D-C1D-ND	-2.21	106.66	110.29
5	A	166	BLA	C4C-C3C-C2C	-2.21	100.29	106.97
7	L	179	PUB	OD-C4D-ND	-2.14	122.42	126.00
6	K	166	CYC	CAD-CBD-CGD	-2.11	108.89	112.75
6	L	181	CYC	CHB-C1B-NB	-2.04	121.75	126.16
6	B	183	CYC	CMC-C2C-C3C	2.01	123.25	114.35
6	A	168	CYC	CBB-CAB-C3B	2.07	118.71	112.39
7	B	179	PUB	CMD-C2D-C3D	2.07	131.26	127.80
6	A	168	CYC	CHB-C4A-C3A	2.08	129.95	124.88
6	K	166	CYC	CMC-C2C-C3C	2.14	123.81	114.35
6	L	183	CYC	CMB-C2B-C1B	2.14	127.05	124.20
6	L	181	CYC	CHB-C4A-C3A	2.15	130.14	124.88
6	K	166	CYC	C3C-C2C-C1C	2.17	105.23	103.41
6	A	168	CYC	C3C-C2C-C1C	2.19	105.25	103.41
6	K	168	CYC	CBB-CAB-C3B	2.30	119.43	112.39
6	B	181	CYC	CBB-CAB-C3B	2.31	119.45	112.39
6	B	181	CYC	CMC-C2C-C3C	2.33	124.66	114.35
6	L	183	CYC	CMC-C2C-C3C	2.36	124.77	114.35
6	L	181	CYC	CBB-CAB-C3B	2.43	119.83	112.39
6	K	166	CYC	CBB-CAB-C3B	2.44	119.85	112.39
6	L	181	CYC	C3C-C2C-C1C	2.45	105.47	103.41
7	L	179	PUB	CMD-C2D-C3D	2.49	131.96	127.80
6	B	183	CYC	CMB-C2B-C1B	2.52	127.56	124.20
6	B	181	CYC	C3C-C2C-C1C	2.56	105.56	103.41
6	L	183	CYC	CBB-CAB-C3B	2.57	120.23	112.39
6	B	183	CYC	CBB-CAB-C3B	2.57	120.25	112.39
6	L	181	CYC	CMC-C2C-C3C	2.59	125.82	114.35
6	K	168	CYC	CMC-C2C-C3C	2.65	126.06	114.35
6	K	166	CYC	CAA-CBA-CGA	2.74	117.77	112.75
6	A	168	CYC	CMC-C2C-C3C	2.78	126.63	114.35
5	A	166	BLA	CMB-C2B-C1B	2.86	128.01	124.20
6	B	181	CYC	CMB-C2B-C1B	2.97	128.15	124.20
5	A	166	BLA	CAA-CBA-CGA	3.00	118.24	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	183	CYC	C1D-CHD-C4C	3.03	138.25	127.23
6	A	168	CYC	CMB-C2B-C1B	3.04	128.24	124.20
6	L	183	CYC	CAA-CBA-CGA	3.04	118.33	112.75
6	L	181	CYC	CMB-C2B-C1B	3.05	128.26	124.20
6	K	166	CYC	CMB-C2B-C1B	3.17	128.41	124.20
6	B	183	CYC	C1D-CHD-C4C	3.27	139.11	127.23
6	B	183	CYC	CAA-CBA-CGA	3.30	118.79	112.75
6	K	166	CYC	CAC-C3C-C4C	3.31	121.16	112.67
6	B	181	CYC	C3B-C4B-NB	3.35	109.79	106.74
6	K	168	CYC	C1D-CHD-C4C	3.37	139.48	127.23
6	B	181	CYC	CAA-CBA-CGA	3.47	119.11	112.75
6	K	168	CYC	C3B-C4B-NB	3.50	109.92	106.74
6	K	168	CYC	CMB-C2B-C1B	3.56	128.94	124.20
6	A	168	CYC	C1D-CHD-C4C	3.59	140.28	127.23
6	K	166	CYC	C3B-C4B-NB	3.63	110.04	106.74
6	A	168	CYC	CAC-C3C-C4C	3.70	122.18	112.67
6	B	181	CYC	C1D-CHD-C4C	3.87	141.30	127.23
6	L	181	CYC	C3B-C4B-NB	3.92	110.31	106.74
6	A	168	CYC	C3B-C4B-NB	3.93	110.31	106.74
6	L	181	CYC	C1D-CHD-C4C	3.94	141.56	127.23
5	A	166	BLA	CHD-C1D-C2D	4.00	134.63	124.88
6	A	168	CYC	CAA-CBA-CGA	4.01	120.09	112.75
6	L	183	CYC	C3B-C4B-NB	4.02	110.39	106.74
6	K	168	CYC	CAA-CBA-CGA	4.11	120.28	112.75
6	B	183	CYC	C3B-C4B-NB	4.15	110.51	106.74
6	B	183	CYC	C3C-C2C-C1C	4.16	106.90	103.41
6	B	183	CYC	CAC-C3C-C4C	4.21	123.47	112.67
6	L	181	CYC	CAA-CBA-CGA	4.43	120.86	112.75
6	L	183	CYC	CAC-C3C-C4C	4.61	124.50	112.67
6	K	166	CYC	C1D-CHD-C4C	4.79	144.66	127.23
6	L	183	CYC	C3C-C2C-C1C	4.92	107.53	103.41
6	B	183	CYC	CMC-C2C-C1C	4.93	122.79	112.43
6	B	181	CYC	CAC-C3C-C4C	5.22	126.08	112.67
6	L	183	CYC	CMC-C2C-C1C	5.27	123.50	112.43
6	L	181	CYC	CAC-C3C-C4C	5.32	126.33	112.67
6	K	168	CYC	CAC-C3C-C4C	5.38	126.48	112.67
6	K	166	CYC	CMC-C2C-C1C	5.58	124.14	112.43
6	L	181	CYC	CMC-C2C-C1C	5.68	124.35	112.43
6	B	181	CYC	CMC-C2C-C1C	5.71	124.42	112.43
6	K	168	CYC	CMC-C2C-C1C	5.81	124.62	112.43
7	L	179	PUB	C1D-CHC-C4C	5.87	126.38	113.72
6	A	168	CYC	CMC-C2C-C1C	6.16	125.36	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	166	BLA	C4C-CHD-C1D	6.56	145.04	128.06
7	B	179	PUB	C1D-CHC-C4C	6.58	127.91	113.72
7	B	179	PUB	CHC-C1D-ND	7.77	122.99	113.99
7	L	179	PUB	CHC-C1D-ND	7.90	123.13	113.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	K	168	CYC	C2C
6	A	168	CYC	C2C

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	181	CYC	C1B-CHB-C4A-NA
6	B	181	CYC	C1B-CHB-C4A-NA
6	A	168	CYC	C1B-CHB-C4A-C3A
6	K	166	CYC	C1B-CHB-C4A-NA
6	L	183	CYC	C1B-CHB-C4A-NA
6	A	168	CYC	C1B-CHB-C4A-NA
6	K	168	CYC	C1B-CHB-C4A-NA
6	B	183	CYC	C1B-CHB-C4A-NA
6	K	168	CYC	C1B-CHB-C4A-C3A
5	A	166	BLA	C4C-CHD-C1D-C2D
5	A	166	BLA	C4C-CHD-C1D-ND

There are no ring outliers.

10 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	166	BLA	3	0
6	A	168	CYC	7	0
7	B	179	PUB	3	0
6	B	181	CYC	4	0
6	B	183	CYC	11	0
6	K	166	CYC	4	0
6	K	168	CYC	2	0
7	L	179	PUB	2	0
6	L	181	CYC	8	0
6	L	183	CYC	10	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

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%)	-0.71	0 100 100	7, 20, 36, 53	0
1	K	164/164 (100%)	-0.68	0 100 100	7, 20, 36, 53	0
2	B	176/177 (99%)	-0.55	2 (1%) 82 84	11, 20, 43, 79	5 (2%)
2	L	176/177 (99%)	-0.60	1 (0%) 90 91	10, 20, 43, 79	4 (2%)
3	G	6/6 (100%)	4.03	3 (50%) 0 0	19, 22, 26, 28	6 (100%)
3	H	5/6 (83%)	3.89	3 (60%) 0 0	19, 21, 26, 28	4 (80%)
All	All	691/694 (99%)	-0.56	9 (1%) 79 82	7, 20, 42, 79	19 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	1	ALA	8.4
3	H	4	ALA	7.3
3	G	5	ALA	6.1
3	H	5	ALA	5.4
3	G	6	ALA	5.3
3	H	3	ARG	4.5
2	L	147	SER	3.7
2	B	152	GLU	2.3
2	B	147	SER	2.2

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MEN	L	72	9/10	0.99	0.08	-	0,9,27,27	0
2	MEN	B	72	9/10	0.97	0.11	-	0,9,27,29	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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CYC	A	168	43/43	0.92	0.16	0.60	15,31,57,62	0
5	BLA	A	166	43/43	0.96	0.11	0.53	3,19,30,57	0
6	CYC	B	181	43/43	0.97	0.12	0.49	7,14,32,37	0
6	CYC	K	166	43/43	0.97	0.11	0.32	3,18,30,57	0
6	CYC	L	183	43/43	0.95	0.11	0.15	3,20,36,57	0
6	CYC	L	181	43/43	0.97	0.11	0.08	6,14,32,37	0
6	CYC	K	168	43/43	0.94	0.11	0.04	15,32,57,62	0
7	PUB	L	179	43/43	0.94	0.11	-0.08	4,24,39,60	0
6	CYC	B	183	43/43	0.96	0.10	-0.29	4,20,37,57	0
7	PUB	B	179	43/43	0.95	0.11	-0.34	5,25,39,60	0
4	SO4	B	202	5/5	0.97	0.10	-	12,23,36,55	5
4	SO4	A	201	5/5	0.97	0.11	-	22,23,27,42	5

6.5 Other polymers [i](#)

There are no such residues in this entry.