



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 PM GMT

PDB ID : 4L1E
Title : Crystal structure of C-Phycocyanin from Leptolyngbya sp. N62DM
Authors : Singh, N.K.; Raj, I.; Gourinath, S.; Madamwar, D.
Deposited on : 2013-06-03
Resolution : 2.61 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

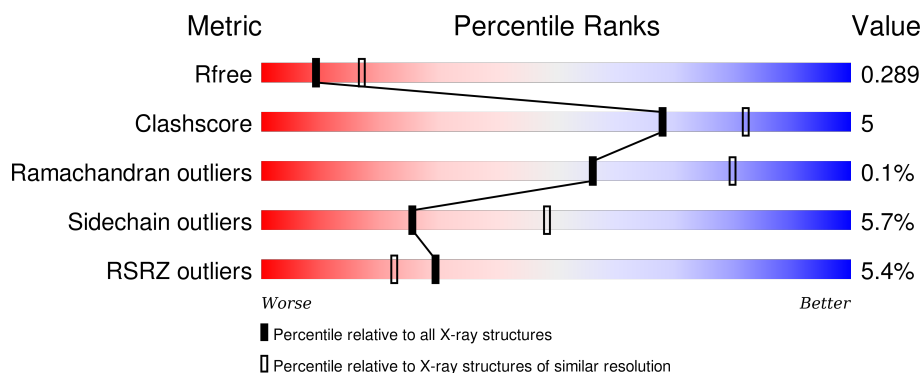
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	162	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	C	162	<div> <div>8%</div> <div>92%</div> <div>7%</div> </div>
1	E	162	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
1	G	162	<div> <div>4%</div> <div>94%</div> <div>6%</div> </div>
1	I	162	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	162	
2	B	172	
2	D	172	
2	F	172	
2	H	172	
2	J	172	
2	L	172	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYC	A	201	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31336 atoms, of which 15372 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.

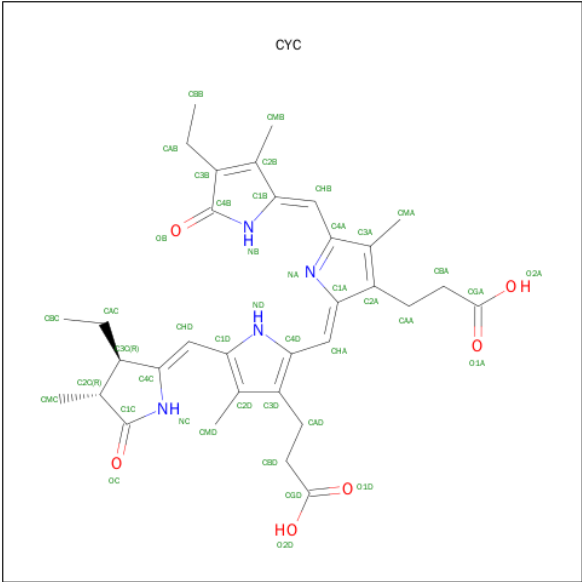
- Molecule 1 is a protein called Phycocyanin alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	H	N	O	S	0	0	0
			2440	778	1207	207	242	6			
1	C	162	Total	C	H	N	O	S	0	0	0
			2440	778	1207	207	242	6			
1	E	162	Total	C	H	N	O	S	0	0	0
			2440	778	1207	207	242	6			
1	G	162	Total	C	H	N	O	S	0	0	0
			2439	778	1206	207	242	6			
1	I	162	Total	C	H	N	O	S	0	0	0
			2440	778	1207	207	242	6			
1	K	162	Total	C	H	N	O	S	0	0	0
			2439	778	1206	207	242	6			

- Molecule 2 is a protein called Phycocyanin beta chain.

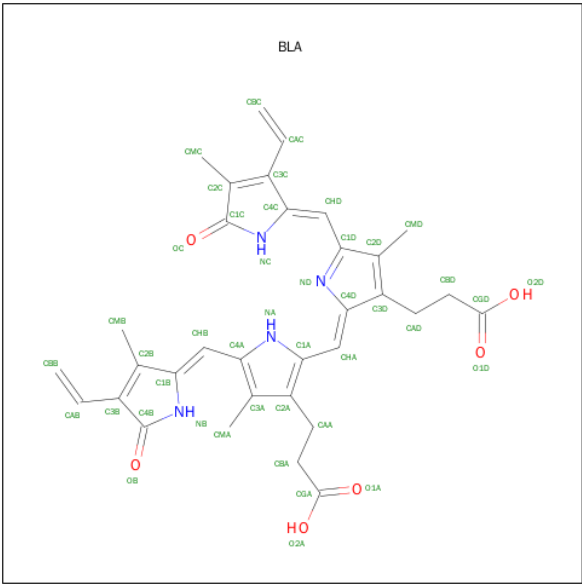
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	172	Total	C	H	N	O	S	0	0	0
			2512	779	1254	218	252	9			
2	D	172	Total	C	H	N	O	S	0	0	0
			2512	779	1254	218	252	9			
2	F	172	Total	C	H	N	O	S	0	0	0
			2512	779	1254	218	252	9			
2	H	172	Total	C	H	N	O	S	0	0	0
			2512	779	1254	218	252	9			
2	J	172	Total	C	H	N	O	S	0	0	0
			2513	779	1255	218	252	9			
2	L	172	Total	C	H	N	O	S	0	0	0
			2513	779	1255	218	252	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			81	33	38	4	6		
3	C	1	Total	C	H	N	O	0	0
			81	33	38	4	6		
3	E	1	Total	C	H	N	O	0	0
			81	33	38	4	6		
3	G	1	Total	C	H	N	O	0	0
			81	33	38	4	6		
3	K	1	Total	C	H	N	O	0	0
			81	33	38	4	6		

- Molecule 4 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	B	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	D	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	D	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	F	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	F	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	H	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	H	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	I	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	J	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	J	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	L	1	Total	C	H	N	O	0	0
			75	33	32	4	6		
4	L	1	Total	C	H	N	O	0	0
			75	33	32	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	18	Total	O	0	0
			18	18		
5	C	13	Total	O	0	0
			13	13		
5	D	23	Total	O	0	0
			23	23		
5	E	24	Total	O	0	0
			24	24		
5	F	17	Total	O	0	0
			17	17		
5	G	23	Total	O	0	0
			23	23		

Continued on next page...

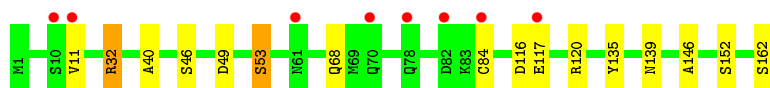
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	17	Total 17	O 17	0	0
5	I	16	Total 16	O 16	0	0
5	J	22	Total 22	O 22	0	0
5	K	26	Total 26	O 26	0	0
5	L	23	Total 23	O 23	0	0

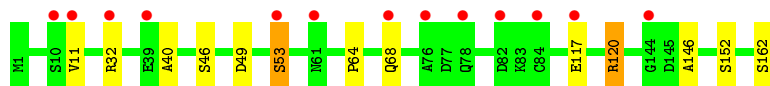
3 Residue-property plots [i](#)

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.

- Molecule 1: Phycocyanin alpha chain



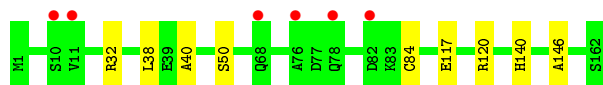
- Molecule 1: Phycocyanin alpha chain



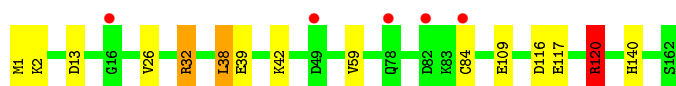
- Molecule 1: Phycocyanin alpha chain



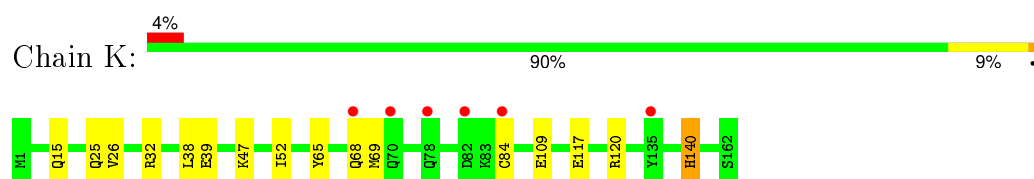
- Molecule 1: Phycocyanin alpha chain



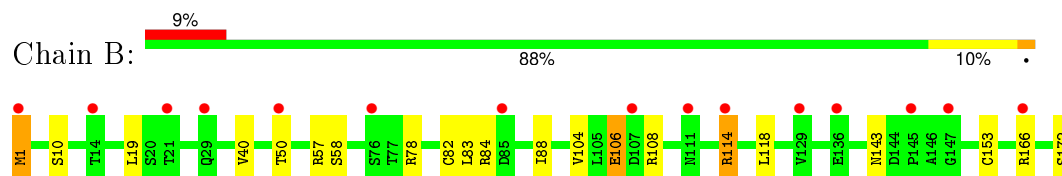
- Molecule 1: Phycocyanin alpha chain



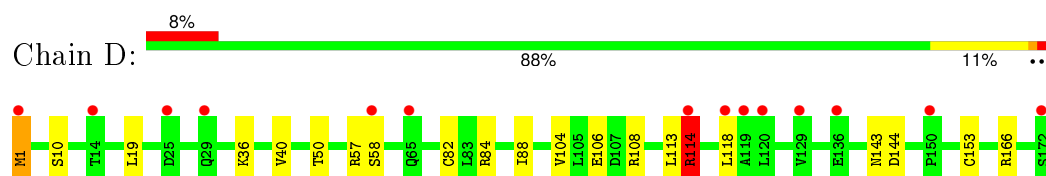
- Molecule 1: Phycocyanin alpha chain



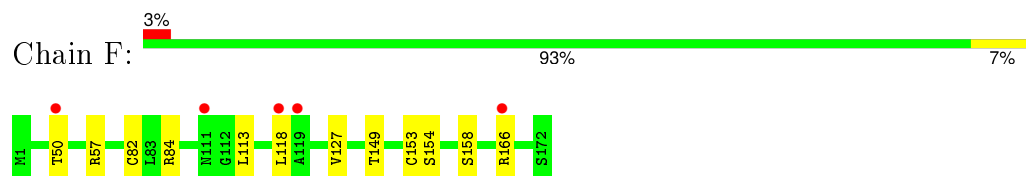
- Molecule 2: Phycocyanin beta chain



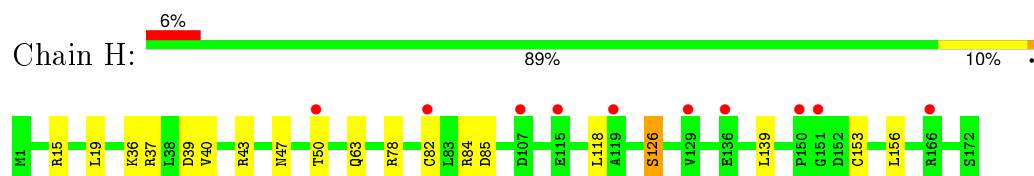
- Molecule 2: Phycocyanin beta chain



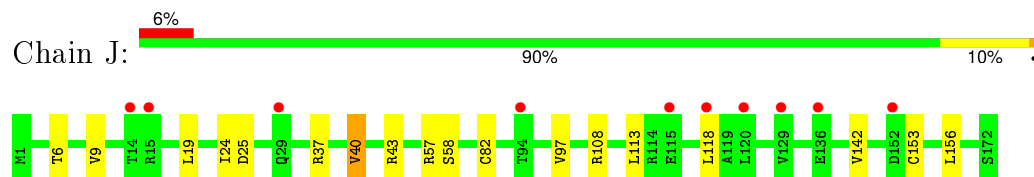
- Molecule 2: Phycocyanin beta chain



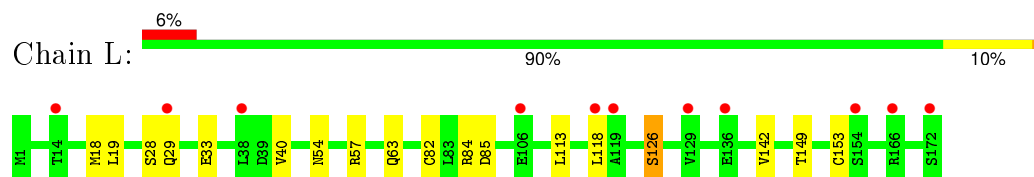
- Molecule 2: Phycocyanin beta chain



- Molecule 2: Phycocyanin beta chain



- Molecule 2: Phycocyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.47Å 107.11Å 111.09Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	24.98 – 2.61 24.98 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.5 (24.98-2.61) 95.6 (24.98-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.239 , 0.281 0.252 , 0.289	Depositor DCC
R_{free} test set	3141 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 28.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 61852 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31336	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, BLA

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	0.32	0/1256	0.42	0/1699
1	C	0.31	0/1256	0.42	0/1699
1	E	0.25	0/1256	0.40	0/1699
1	G	0.26	0/1256	0.41	0/1699
1	I	0.26	0/1256	0.48	1/1699 (0.1%)
1	K	0.25	0/1256	0.42	0/1699
2	B	0.28	0/1272	0.57	3/1724 (0.2%)
2	D	0.29	0/1272	0.67	4/1724 (0.2%)
2	F	0.27	0/1272	0.44	0/1724
2	H	0.26	0/1272	0.45	0/1724
2	J	0.26	0/1272	0.44	0/1724
2	L	0.26	0/1272	0.43	0/1724
All	All	0.27	0/15168	0.47	8/20538 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	114	ARG	NE-CZ-NH1	12.86	126.73	120.30
2	D	114	ARG	NE-CZ-NH2	-8.26	116.17	120.30
2	D	114	ARG	CG-CD-NE	7.92	128.43	111.80
1	I	120	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	114	ARG	NE-CZ-NH1	7.55	124.08	120.30
2	D	114	ARG	CD-NE-CZ	6.17	132.24	123.60
2	B	114	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	B	114	ARG	CG-CD-NE	5.07	122.45	111.80

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	1233	1207	1206	7	0
1	C	1233	1207	1206	4	0
1	E	1233	1207	1206	7	0
1	G	1233	1206	1206	4	0
1	I	1233	1207	1206	13	0
1	K	1233	1206	1206	6	0
2	B	1258	1254	1255	12	1
2	D	1258	1254	1255	15	0
2	F	1258	1254	1255	7	0
2	H	1258	1254	1255	8	1
2	J	1258	1255	1255	12	0
2	L	1258	1255	1255	9	0
3	A	43	38	38	5	0
3	C	43	38	38	3	0
3	E	43	38	38	7	0
3	G	43	38	38	4	0
3	K	43	38	38	3	0
4	B	86	64	64	13	0
4	D	86	64	64	12	0
4	F	86	64	64	12	0
4	H	86	64	64	10	0
4	I	43	32	32	5	0
4	J	86	64	64	10	0
4	L	86	64	64	11	0
5	A	22	0	0	1	0
5	B	18	0	0	0	0
5	C	13	0	0	0	0
5	D	23	0	0	1	0
5	E	24	0	0	0	0
5	F	17	0	0	0	0
5	G	23	0	0	0	0
5	H	17	0	0	0	0
5	I	16	0	0	2	0
5	J	22	0	0	0	0
5	K	26	0	0	0	0
5	L	23	0	0	0	0
All	All	15964	15372	15372	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (146) 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)
4:B:201:BLA:HMD2	4:B:201:BLA:HC	1.51	0.75
4:I:201:BLA:HC	4:I:201:BLA:HMD2	1.52	0.74
4:F:201:BLA:HC	4:F:201:BLA:HMD2	1.52	0.74
4:H:201:BLA:HMD2	4:H:201:BLA:HC	1.52	0.74
4:D:201:BLA:HC	4:D:201:BLA:HMD2	1.54	0.72
4:L:201:BLA:HC	4:L:201:BLA:HMD2	1.54	0.72
4:J:201:BLA:HMD2	4:J:201:BLA:HC	1.53	0.71
2:D:114:ARG:HH11	2:D:114:ARG:HB2	1.57	0.69
1:E:72:PRO:O	1:E:79:ARG:NH2	2.29	0.66
2:L:63:GLN:OE1	2:L:126:SER:OG	2.13	0.66
2:D:82:CYS:SG	4:D:201:BLA:HBC1	2.36	0.65
2:D:114:ARG:HH11	2:D:114:ARG:CB	2.11	0.64
2:D:36:LYS:NZ	5:D:306:HOH:O	2.30	0.64
2:B:57:ARG:NH1	4:I:201:BLA:O1D	2.30	0.64
2:F:57:ARG:NH1	3:K:201:CYC:O1D	2.31	0.64
4:D:202:BLA:HC	4:D:202:BLA:HMD2	1.62	0.63
3:E:201:CYC:HBC2	3:E:201:CYC:HMC1	1.80	0.63
1:I:84:CYS:SG	4:I:201:BLA:HAC	2.39	0.63
2:H:82:CYS:SG	4:H:201:BLA:HBC1	2.39	0.63
4:D:202:BLA:NC	4:D:202:BLA:HMD2	2.14	0.62
2:B:82:CYS:SG	4:B:201:BLA:HBC1	2.40	0.61
2:J:82:CYS:SG	4:J:201:BLA:HBC1	2.40	0.61
4:H:202:BLA:NC	4:H:202:BLA:HMD2	2.17	0.60
4:F:202:BLA:HC	4:F:202:BLA:HMD2	1.67	0.60
4:B:202:BLA:HMD2	4:B:202:BLA:NC	2.17	0.59
2:L:54:ASN:OD1	2:L:57:ARG:NH2	2.36	0.59
1:A:32:ARG:NH1	5:A:310:HOH:O	2.34	0.59
3:A:201:CYC:HBC2	3:A:201:CYC:HMC1	1.85	0.59
4:L:201:BLA:HMD2	4:L:201:BLA:NC	2.18	0.58
4:J:201:BLA:HMD2	4:J:201:BLA:NC	2.18	0.58
4:J:202:BLA:NC	4:J:202:BLA:HMD2	2.19	0.58
4:F:201:BLA:CB	4:F:201:BLA:HMC1	2.32	0.58
2:J:153:CYS:SG	4:J:202:BLA:HBC1	2.43	0.58
3:C:201:CYC:HMC1	3:C:201:CYC:HBC2	1.84	0.58
2:J:43:ARG:NH1	2:J:142:VAL:O	2.37	0.57
3:E:201:CYC:HC	3:E:201:CYC:HMD2	1.69	0.57
1:I:1:MET:N	5:I:306:HOH:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:202:BLA:HMD2	4:H:202:BLA:HC	1.70	0.57
2:H:63:GLN:OE1	2:H:126:SER:OG	2.23	0.56
3:C:201:CYC:HMD2	3:C:201:CYC:HC	1.70	0.56
4:J:202:BLA:HMD2	4:J:202:BLA:HC	1.70	0.56
4:H:201:BLA:HMD2	4:H:201:BLA:NC	2.21	0.56
2:L:113:LEU:HD13	4:L:201:BLA:HMB3	1.86	0.56
2:L:82:CYS:SG	4:L:201:BLA:HBC1	2.46	0.55
2:B:143:ASN:O	4:B:202:BLA:HMC3	2.05	0.55
3:G:201:CYC:O1D	2:J:57:ARG:NH1	2.39	0.55
4:F:202:BLA:HMD2	4:F:202:BLA:NC	2.21	0.55
1:A:135:TYR:CZ	1:A:139:ASN:OD1	2.59	0.55
2:L:153:CYS:SG	4:L:202:BLA:HBC1	2.47	0.55
2:L:84:ARG:NH2	2:L:85:ASP:OD1	2.39	0.55
4:L:202:BLA:NC	4:L:202:BLA:HMD2	2.22	0.55
4:D:201:BLA:NC	4:D:201:BLA:HMD2	2.22	0.55
2:D:153:CYS:SG	4:D:202:BLA:HBC1	2.47	0.55
2:L:149:THR:O	4:L:202:BLA:NC	2.41	0.54
3:K:201:CYC:HMC1	3:K:201:CYC:HBC2	1.90	0.54
2:F:153:CYS:SG	4:F:202:BLA:HBC1	2.48	0.54
4:L:201:BLA:CBC	4:L:201:BLA:HMC1	2.38	0.53
4:L:202:BLA:HMD2	4:L:202:BLA:HC	1.74	0.53
2:B:153:CYS:SG	4:B:202:BLA:HBC1	2.48	0.53
2:B:114:ARG:HH11	2:B:114:ARG:CB	2.22	0.53
1:G:117:GLU:OE1	1:G:117:GLU:N	2.38	0.53
3:A:201:CYC:HHA	3:A:201:CYC:HBD2	1.92	0.52
4:J:201:BLA:CBC	4:J:201:BLA:HMC1	2.40	0.51
4:H:201:BLA:HMC1	4:H:201:BLA:CBC	2.41	0.51
2:H:153:CYS:SG	4:H:202:BLA:HBC1	2.51	0.51
1:I:2:LYS:NZ	1:K:15:GLN:OE1	2.40	0.51
1:I:120:ARG:HH11	1:I:120:ARG:CB	2.24	0.50
4:B:201:BLA:CBC	4:B:201:BLA:HMC1	2.41	0.50
2:D:1:MET:SD	2:D:108:ARG:NH2	2.84	0.50
4:F:201:BLA:NC	4:F:201:BLA:HMD2	2.22	0.50
4:J:202:BLA:NB	4:J:202:BLA:HMA1	2.27	0.50
1:G:84:CYS:SG	3:G:201:CYC:HAC2	2.52	0.50
4:D:201:BLA:CBC	4:D:201:BLA:HMC1	2.41	0.49
4:F:201:BLA:HBC1	4:F:201:BLA:HMC1	1.93	0.49
1:K:47:LYS:NZ	1:K:140:HIS:O	2.31	0.49
2:B:1:MET:SD	2:B:108:ARG:NH2	2.85	0.49
4:H:202:BLA:NB	4:H:202:BLA:HMA1	2.28	0.49
1:I:42:LYS:NZ	2:J:25:ASP:OD1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:LEU:HG	2:J:24:ILE:HG23	1.94	0.49
4:B:201:BLA:HMD2	4:B:201:BLA:NC	2.23	0.49
2:D:143:ASN:O	4:D:202:BLA:HMC3	2.13	0.49
4:B:202:BLA:HMD2	4:B:202:BLA:HC	1.77	0.49
2:H:43:ARG:O	2:H:47:ASN:ND2	2.45	0.49
2:D:57:ARG:NH1	3:E:201:CYC:O1D	2.46	0.48
2:H:36:LYS:HE2	4:H:202:BLA:HMD3	1.96	0.48
1:A:84:CYS:SG	3:A:201:CYC:HAC2	2.54	0.48
4:I:201:BLA:NC	4:I:201:BLA:HMD2	2.24	0.48
1:E:128:TRP:CE3	3:E:201:CYC:H3C	2.48	0.47
2:H:84:ARG:NH2	2:H:85:ASP:OD1	2.46	0.47
2:F:127:VAL:HG22	4:F:201:BLA:CAC	2.44	0.47
1:K:84:CYS:SG	3:K:201:CYC:HAC2	2.54	0.47
1:E:84:CYS:SG	3:E:201:CYC:HAC2	2.54	0.47
2:B:106:GLU:HA	2:B:106:GLU:OE1	2.14	0.47
2:H:78:ARG:O	4:H:201:BLA:HMD3	2.15	0.47
2:D:88:ILE:HG21	4:D:201:BLA:HAB	1.96	0.47
1:I:117:GLU:OE1	1:I:117:GLU:N	2.46	0.47
1:I:13:ASP:OD2	2:J:108:ARG:NH1	2.47	0.46
2:F:113:LEU:HD13	4:F:201:BLA:HMB3	1.98	0.46
2:D:113:LEU:HD13	4:D:201:BLA:HMB3	1.98	0.46
2:J:113:LEU:HD13	4:J:201:BLA:HMB3	1.97	0.46
1:A:116:ASP:OD2	1:E:120:ARG:NH2	2.49	0.46
2:F:149:THR:O	4:F:202:BLA:NC	2.49	0.45
2:D:106:GLU:OE1	2:D:106:GLU:HA	2.16	0.45
3:E:201:CYC:HAB1	3:E:201:CYC:HMB1	1.82	0.45
2:L:82:CYS:SG	4:L:201:BLA:CBC	3.05	0.45
2:H:37:ARG:HA	2:H:156:LEU:HD21	1.99	0.45
1:E:112:ILE:HD13	1:E:112:ILE:N	2.32	0.45
4:B:202:BLA:HMC1	4:B:202:BLA:CBC	2.46	0.45
1:C:40:ALA:HB2	1:C:146:ALA:HB1	1.98	0.44
2:B:78:ARG:O	4:B:201:BLA:HMD3	2.18	0.44
2:F:127:VAL:HG22	4:F:201:BLA:HAC	1.98	0.44
2:D:36:LYS:CE	4:D:202:BLA:HMD3	2.46	0.44
2:D:36:LYS:HE3	4:D:202:BLA:HMD3	1.99	0.44
3:A:201:CYC:HMB1	3:A:201:CYC:HAB1	1.82	0.44
1:A:40:ALA:HB2	1:A:146:ALA:HB1	1.99	0.44
1:K:117:GLU:N	1:K:117:GLU:OE1	2.47	0.44
2:F:82:CYS:SG	4:F:201:BLA:CBC	3.06	0.44
1:G:40:ALA:HB2	1:G:146:ALA:HB1	1.99	0.44
1:C:49:ASP:O	1:C:53:SER:OG	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:ARG:HH11	1:I:120:ARG:CG	2.31	0.43
1:E:128:TRP:HE3	3:E:201:CYC:H3C	1.84	0.43
2:D:1:MET:CE	2:D:104:VAL:HB	2.49	0.43
1:A:49:ASP:O	1:A:53:SER:OG	2.37	0.43
2:B:88:ILE:HG21	4:B:201:BLA:HAB	1.99	0.43
2:L:40:VAL:HG12	2:L:142:VAL:HG13	2.00	0.43
2:J:82:CYS:SG	4:J:201:BLA:CB	3.06	0.42
1:E:40:ALA:HB2	1:E:146:ALA:HB1	2.01	0.42
3:A:201:CYC:CHA	3:A:201:CYC:HBD2	2.49	0.42
1:I:59:VAL:HG11	4:I:201:BLA:HMC1	2.00	0.42
4:B:202:BLA:NB	4:B:202:BLA:HMA1	2.35	0.42
2:B:1:MET:CE	2:B:104:VAL:HB	2.49	0.41
1:K:65:TYR:CD1	1:K:69:MET:HE3	2.55	0.41
1:G:84:CYS:HA	3:G:201:CYC:HHD	2.03	0.41
2:D:1:MET:SD	2:D:108:ARG:CZ	3.08	0.41
1:I:26:VAL:HG22	1:K:26:VAL:HG22	2.03	0.41
3:C:201:CYC:HAB1	3:C:201:CYC:HMB1	1.81	0.41
2:B:153:CYS:CB	4:B:202:BLA:HBC1	2.51	0.41
1:A:11:VAL:HG21	1:C:11:VAL:HG21	2.02	0.41
2:J:40:VAL:CG2	2:J:97:VAL:HG11	2.51	0.41
1:I:32:ARG:NH2	5:I:311:HOH:O	2.54	0.41
2:J:37:ARG:HA	2:J:156:LEU:HD21	2.03	0.41
3:G:201:CYC:HAB1	3:G:201:CYC:HMB1	1.82	0.41
2:B:1:MET:HE1	2:B:104:VAL:HG23	2.03	0.41
2:J:6:THR:HA	2:J:9:VAL:HB	2.02	0.40
4:L:202:BLA:NB	4:L:202:BLA:HMA1	2.36	0.40
1:C:120:ARG:NH1	1:I:116:ASP:OD2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:SER:O	2:H:15:ARG:NH1[4_444]	2.15	0.05

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	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	C	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	E	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
1	G	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	I	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
1	K	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
2	B	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
2	D	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	30	54
2	F	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	H	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	J	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
2	L	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
All	All	1980/2004 (99%)	1908 (96%)	71 (4%)	1 (0%)	56	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	144	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/125 (99%)	116 (94%)	8 (6%)	21	41
1	C	124/125 (99%)	115 (93%)	9 (7%)	17	34
1	E	124/125 (99%)	119 (96%)	5 (4%)	38	66
1	G	124/125 (99%)	119 (96%)	5 (4%)	38	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	124/125 (99%)	118 (95%)	6 (5%)	31	57
1	K	124/125 (99%)	115 (93%)	9 (7%)	17	34
2	B	131/133 (98%)	120 (92%)	11 (8%)	14	25
2	D	131/133 (98%)	121 (92%)	10 (8%)	16	31
2	F	131/133 (98%)	125 (95%)	6 (5%)	33	60
2	H	131/133 (98%)	124 (95%)	7 (5%)	28	52
2	J	131/133 (98%)	127 (97%)	4 (3%)	47	75
2	L	131/133 (98%)	124 (95%)	7 (5%)	28	52
All	All	1530/1548 (99%)	1443 (94%)	87 (6%)	25	48

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	46	SER
1	A	53	SER
1	A	68	GLN
1	A	117	GLU
1	A	120	ARG
1	A	152	SER
1	A	162	SER
2	B	1	MET
2	B	10	SER
2	B	19	LEU
2	B	40	VAL
2	B	50	THR
2	B	58	SER
2	B	83	LEU
2	B	84	ARG
2	B	106	GLU
2	B	118	LEU
2	B	166	ARG
1	C	32	ARG
1	C	46	SER
1	C	53	SER
1	C	64	PRO
1	C	68	GLN
1	C	117	GLU
1	C	120	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	152	SER
1	C	162	SER
2	D	1	MET
2	D	10	SER
2	D	19	LEU
2	D	40	VAL
2	D	50	THR
2	D	58	SER
2	D	84	ARG
2	D	114	ARG
2	D	118	LEU
2	D	166	ARG
1	E	10	SER
1	E	32	ARG
1	E	38	LEU
1	E	120	ARG
1	E	140	HIS
2	F	50	THR
2	F	84	ARG
2	F	118	LEU
2	F	154	SER
2	F	158	SER
2	F	166	ARG
1	G	32	ARG
1	G	38	LEU
1	G	50	SER
1	G	120	ARG
1	G	140	HIS
2	H	19	LEU
2	H	39	ASP
2	H	40	VAL
2	H	50	THR
2	H	118	LEU
2	H	126	SER
2	H	139	LEU
1	I	32	ARG
1	I	38	LEU
1	I	39	GLU
1	I	109	GLU
1	I	120	ARG
1	I	140	HIS
2	J	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	40	VAL
2	J	58	SER
2	J	118	LEU
1	K	25	GLN
1	K	32	ARG
1	K	38	LEU
1	K	39	GLU
1	K	52	ILE
1	K	68	GLN
1	K	109	GLU
1	K	120	ARG
1	K	140	HIS
2	L	18	MET
2	L	19	LEU
2	L	28	SER
2	L	29	GLN
2	L	33	GLU
2	L	118	LEU
2	L	126	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

18 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
3	CYC	A	201	-	37,46,46	4.03	14 (37%)	47,67,67	3.45	21 (44%)
4	BLA	B	201	-	37,46,46	4.13	12 (32%)	44,67,67	2.22	11 (25%)
4	BLA	B	202	-	37,46,46	4.12	13 (35%)	44,67,67	2.20	10 (22%)
3	CYC	C	201	-	37,46,46	3.92	14 (37%)	47,67,67	3.29	17 (36%)
4	BLA	D	201	-	37,46,46	4.11	13 (35%)	44,67,67	2.25	11 (25%)
4	BLA	D	202	-	37,46,46	4.13	13 (35%)	44,67,67	2.19	10 (22%)
3	CYC	E	201	-	37,46,46	3.93	14 (37%)	47,67,67	3.28	18 (38%)
4	BLA	F	201	-	37,46,46	4.11	13 (35%)	44,67,67	2.25	12 (27%)
4	BLA	F	202	-	37,46,46	4.15	13 (35%)	44,67,67	2.18	11 (25%)
3	CYC	G	201	-	37,46,46	3.96	15 (40%)	47,67,67	3.35	20 (42%)
4	BLA	H	201	-	37,46,46	4.09	13 (35%)	44,67,67	2.24	11 (25%)
4	BLA	H	202	-	37,46,46	4.13	13 (35%)	44,67,67	2.15	9 (20%)
4	BLA	I	201	-	37,46,46	4.11	12 (32%)	44,67,67	2.32	12 (27%)
4	BLA	J	201	-	37,46,46	4.12	13 (35%)	44,67,67	2.18	11 (25%)
4	BLA	J	202	-	37,46,46	4.16	13 (35%)	44,67,67	2.23	14 (31%)
3	CYC	K	201	-	37,46,46	3.94	15 (40%)	47,67,67	3.33	19 (40%)
4	BLA	L	201	-	37,46,46	4.12	13 (35%)	44,67,67	2.21	10 (22%)
4	BLA	L	202	-	37,46,46	4.12	13 (35%)	44,67,67	2.17	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	A	201	-	-	3/21/74/74	0/4/4/4
4	BLA	B	201	-	-	3/22/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BLA	B	202	-	-	3/22/74/74	0/4/4/4
3	CYC	C	201	-	-	3/21/74/74	0/4/4/4
4	BLA	D	201	-	-	3/22/74/74	0/4/4/4
4	BLA	D	202	-	-	3/22/74/74	0/4/4/4
3	CYC	E	201	-	-	3/21/74/74	0/4/4/4
4	BLA	F	201	-	-	3/22/74/74	0/4/4/4
4	BLA	F	202	-	-	3/22/74/74	0/4/4/4
3	CYC	G	201	-	-	3/21/74/74	0/4/4/4
4	BLA	H	201	-	-	3/22/74/74	0/4/4/4
4	BLA	H	202	-	-	3/22/74/74	0/4/4/4
4	BLA	I	201	-	-	3/22/74/74	0/4/4/4
4	BLA	J	201	-	-	3/22/74/74	0/4/4/4
4	BLA	J	202	-	-	3/22/74/74	0/4/4/4
3	CYC	K	201	-	-	3/21/74/74	0/4/4/4
4	BLA	L	201	-	-	3/22/74/74	0/4/4/4
4	BLA	L	202	-	-	3/22/74/74	0/4/4/4

All (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	BLA	C3C-C2C	-9.03	1.18	1.36
4	D	201	BLA	C3B-C2B	-8.97	1.18	1.36
4	F	202	BLA	C3B-C2B	-8.97	1.18	1.36
4	J	201	BLA	C3B-C2B	-8.97	1.18	1.36
4	I	201	BLA	C3B-C2B	-8.96	1.18	1.36
4	F	201	BLA	C3B-C2B	-8.96	1.18	1.36
4	B	201	BLA	C3B-C2B	-8.95	1.18	1.36
4	B	202	BLA	C3C-C2C	-8.94	1.18	1.36
4	H	202	BLA	C3B-C2B	-8.93	1.18	1.36
4	L	202	BLA	C3B-C2B	-8.90	1.18	1.36
4	L	201	BLA	C3B-C2B	-8.89	1.18	1.36
4	H	202	BLA	C3C-C2C	-8.88	1.18	1.36
4	F	202	BLA	C3C-C2C	-8.86	1.18	1.36
4	D	202	BLA	C3B-C2B	-8.85	1.18	1.36
4	L	202	BLA	C3C-C2C	-8.85	1.18	1.36
4	I	201	BLA	C3C-C2C	-8.84	1.18	1.36
4	D	201	BLA	C3C-C2C	-8.83	1.18	1.36
4	H	201	BLA	C3B-C2B	-8.80	1.18	1.36
4	J	202	BLA	C3B-C2B	-8.78	1.18	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	BLA	C3C-C2C	-8.77	1.18	1.36
4	B	202	BLA	C3B-C2B	-8.76	1.18	1.36
4	J	202	BLA	C3C-C2C	-8.73	1.18	1.36
4	H	201	BLA	C3C-C2C	-8.73	1.18	1.36
4	J	201	BLA	C3C-C2C	-8.68	1.18	1.36
4	L	201	BLA	C3C-C2C	-8.62	1.18	1.36
4	F	201	BLA	C3C-C2C	-8.34	1.19	1.36
3	C	201	CYC	C3B-C2B	-7.90	1.19	1.36
3	A	201	CYC	C3B-C2B	-7.89	1.19	1.36
3	G	201	CYC	C3B-C2B	-7.84	1.19	1.36
3	K	201	CYC	C3B-C2B	-7.79	1.19	1.36
3	E	201	CYC	C3B-C2B	-7.76	1.19	1.36
3	K	201	CYC	C4C-NC	-5.53	1.25	1.37
3	G	201	CYC	C4C-NC	-5.50	1.25	1.37
3	A	201	CYC	C4C-NC	-5.47	1.25	1.37
3	E	201	CYC	C4C-NC	-5.45	1.25	1.37
3	C	201	CYC	C4C-NC	-5.44	1.25	1.37
4	B	201	BLA	C3D-C2D	-3.94	1.28	1.36
4	D	202	BLA	C3D-C2D	-3.87	1.28	1.36
4	L	202	BLA	C3D-C2D	-3.86	1.28	1.36
4	H	202	BLA	C3D-C2D	-3.86	1.28	1.36
4	H	201	BLA	C3D-C2D	-3.83	1.28	1.36
4	F	201	BLA	C3D-C2D	-3.81	1.28	1.36
4	B	202	BLA	C3D-C2D	-3.81	1.28	1.36
4	L	201	BLA	C3D-C2D	-3.79	1.28	1.36
4	F	202	BLA	C3D-C2D	-3.77	1.28	1.36
4	I	201	BLA	C3D-C2D	-3.74	1.28	1.36
4	J	201	BLA	C3D-C2D	-3.67	1.28	1.36
4	D	201	BLA	C3D-C2D	-3.66	1.28	1.36
3	K	201	CYC	CMC-C2C	-3.57	1.44	1.53
4	J	202	BLA	C3D-C2D	-3.54	1.28	1.36
3	G	201	CYC	CMC-C2C	-3.51	1.45	1.53
3	C	201	CYC	CMC-C2C	-3.50	1.45	1.53
3	E	201	CYC	CMC-C2C	-3.46	1.45	1.53
3	A	201	CYC	CMC-C2C	-3.41	1.45	1.53
3	K	201	CYC	C2A-C3A	-3.35	1.29	1.36
3	E	201	CYC	C2A-C3A	-3.34	1.29	1.36
3	C	201	CYC	C2A-C3A	-3.28	1.29	1.36
3	G	201	CYC	C2A-C3A	-3.22	1.29	1.36
3	A	201	CYC	C2A-C3A	-3.21	1.29	1.36
4	J	202	BLA	C1D-ND	-2.52	1.31	1.37
4	B	202	BLA	C1D-ND	-2.50	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	BLA	C1D-ND	-2.47	1.31	1.37
3	A	201	CYC	C4B-C3B	-2.42	1.43	1.48
4	H	202	BLA	C1D-ND	-2.38	1.31	1.37
4	L	202	BLA	C1D-ND	-2.37	1.31	1.37
4	F	202	BLA	C1D-ND	-2.36	1.31	1.37
3	K	201	CYC	C4B-C3B	-2.30	1.43	1.48
3	C	201	CYC	C4B-C3B	-2.30	1.43	1.48
3	G	201	CYC	C4B-C3B	-2.29	1.43	1.48
4	J	201	BLA	C1D-ND	-2.17	1.31	1.37
4	H	201	BLA	C1D-ND	-2.16	1.32	1.37
4	D	201	BLA	C1D-ND	-2.16	1.32	1.37
3	E	201	CYC	C4B-C3B	-2.09	1.43	1.48
4	F	201	BLA	C1D-ND	-2.07	1.32	1.37
4	L	201	BLA	C1D-ND	-2.05	1.32	1.37
3	G	201	CYC	C1D-ND	2.01	1.39	1.36
4	I	201	BLA	C1A-CHA	2.01	1.51	1.45
3	K	201	CYC	C1D-ND	2.05	1.39	1.36
4	B	201	BLA	C1A-CHA	2.06	1.51	1.45
4	H	201	BLA	C1A-CHA	2.06	1.51	1.45
4	D	201	BLA	C4A-CHB	2.07	1.51	1.45
4	H	202	BLA	C1A-CHA	2.08	1.51	1.45
4	L	201	BLA	C1A-CHA	2.11	1.51	1.45
4	F	201	BLA	C1A-CHA	2.14	1.51	1.45
4	D	202	BLA	C1A-CHA	2.15	1.51	1.45
4	H	201	BLA	C4A-CHB	2.15	1.51	1.45
4	F	201	BLA	C4A-CHB	2.16	1.51	1.45
4	J	201	BLA	C1A-CHA	2.18	1.51	1.45
4	D	201	BLA	C1A-CHA	2.19	1.52	1.45
4	L	202	BLA	C1A-CHA	2.20	1.52	1.45
4	I	201	BLA	C4A-CHB	2.20	1.52	1.45
4	F	202	BLA	C1A-CHA	2.21	1.52	1.45
4	L	201	BLA	C4A-CHB	2.22	1.52	1.45
4	B	202	BLA	C1A-CHA	2.23	1.52	1.45
4	J	201	BLA	C4A-CHB	2.23	1.52	1.45
4	B	201	BLA	C4A-CHB	2.24	1.52	1.45
4	D	202	BLA	C4A-CHB	2.27	1.52	1.45
4	L	202	BLA	C4A-CHB	2.34	1.52	1.45
4	B	202	BLA	C4A-CHB	2.38	1.52	1.45
4	F	202	BLA	C4A-CHB	2.38	1.52	1.45
4	J	202	BLA	C1A-CHA	2.40	1.52	1.45
4	H	202	BLA	C4A-CHB	2.44	1.52	1.45
4	J	202	BLA	C4A-CHB	2.46	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	CYC	C4D-CHA	3.27	1.55	1.45
3	E	201	CYC	C4D-CHA	3.30	1.55	1.45
3	K	201	CYC	C4D-CHA	3.32	1.55	1.45
3	G	201	CYC	C4D-CHA	3.44	1.55	1.45
3	A	201	CYC	C1D-CHD	3.45	1.55	1.45
3	A	201	CYC	C4D-CHA	3.51	1.56	1.45
3	E	201	CYC	C1D-CHD	3.51	1.56	1.45
3	C	201	CYC	C1D-CHD	3.52	1.56	1.45
3	G	201	CYC	C1D-CHD	3.52	1.56	1.45
3	K	201	CYC	C1D-CHD	3.53	1.56	1.45
4	B	202	BLA	CHD-C1D	4.27	1.51	1.40
4	H	202	BLA	CHD-C1D	4.42	1.51	1.40
3	C	201	CYC	CHA-C1A	4.43	1.39	1.35
4	D	202	BLA	CHD-C1D	4.45	1.51	1.40
4	L	202	BLA	CHD-C1D	4.46	1.51	1.40
4	F	202	BLA	CHD-C1D	4.52	1.51	1.40
4	J	202	BLA	CHD-C1D	4.64	1.52	1.40
3	K	201	CYC	CHA-C1A	4.67	1.39	1.35
4	H	201	BLA	CHD-C1D	4.75	1.52	1.40
4	F	201	BLA	CHD-C1D	4.81	1.52	1.40
3	E	201	CYC	CHA-C1A	4.85	1.39	1.35
4	L	201	BLA	CHD-C1D	4.87	1.52	1.40
4	J	201	BLA	CHD-C1D	4.88	1.52	1.40
4	D	201	BLA	CHD-C1D	4.88	1.52	1.40
4	B	201	BLA	CHD-C1D	4.97	1.52	1.40
3	G	201	CYC	CHA-C1A	5.03	1.39	1.35
4	I	201	BLA	CHD-C1D	5.08	1.53	1.40
4	I	201	BLA	C4D-C3D	5.24	1.54	1.45
4	H	201	BLA	C4D-C3D	5.50	1.55	1.45
4	B	201	BLA	C4D-C3D	5.52	1.55	1.45
4	L	201	BLA	C4D-C3D	5.62	1.55	1.45
4	D	201	BLA	C4D-C3D	5.72	1.55	1.45
4	F	201	BLA	C4D-C3D	5.72	1.55	1.45
3	E	201	CYC	CHB-C4A	5.80	1.54	1.40
3	A	201	CYC	CHA-C1A	5.83	1.40	1.35
3	C	201	CYC	CHB-C4A	5.85	1.55	1.40
4	J	201	BLA	C4D-C3D	5.89	1.55	1.45
3	G	201	CYC	CHB-C4A	5.90	1.55	1.40
3	K	201	CYC	CHB-C4A	5.91	1.55	1.40
4	L	202	BLA	C4D-C3D	5.97	1.55	1.45
4	H	202	BLA	C4D-C3D	5.97	1.55	1.45
4	D	202	BLA	C4D-ND	5.98	1.51	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	BLA	C4D-C3D	5.99	1.55	1.45
4	B	202	BLA	C4D-ND	6.05	1.51	1.38
4	L	202	BLA	C4D-ND	6.05	1.51	1.38
3	A	201	CYC	CHB-C4A	6.05	1.55	1.40
4	H	202	BLA	C4D-ND	6.07	1.51	1.38
4	J	202	BLA	C4D-ND	6.07	1.51	1.38
4	J	201	BLA	C4D-ND	6.12	1.51	1.38
4	F	202	BLA	C4D-ND	6.15	1.51	1.38
4	H	201	BLA	C4D-ND	6.17	1.51	1.38
4	D	201	BLA	C4D-ND	6.17	1.51	1.38
4	B	202	BLA	C4D-C3D	6.20	1.56	1.45
4	F	202	BLA	C4D-C3D	6.21	1.56	1.45
4	F	201	BLA	C4D-ND	6.22	1.52	1.38
4	I	201	BLA	C4D-ND	6.24	1.52	1.38
4	B	201	BLA	C4D-ND	6.26	1.52	1.38
4	L	201	BLA	C4D-ND	6.29	1.52	1.38
4	J	202	BLA	C4D-C3D	6.53	1.56	1.45
3	K	201	CYC	C1A-NA	6.65	1.52	1.38
3	E	201	CYC	C1A-NA	6.68	1.53	1.38
3	C	201	CYC	C1A-NA	6.69	1.53	1.38
3	G	201	CYC	C1A-NA	6.72	1.53	1.38
3	A	201	CYC	C1A-NA	6.80	1.53	1.38
3	C	201	CYC	C1A-C2A	7.07	1.57	1.45
3	E	201	CYC	C1A-C2A	7.19	1.58	1.45
3	K	201	CYC	C1A-C2A	7.21	1.58	1.45
3	G	201	CYC	C1A-C2A	7.33	1.58	1.45
3	A	201	CYC	C1A-C2A	7.43	1.58	1.45
4	D	202	BLA	C1C-NC	7.71	1.55	1.37
4	L	202	BLA	C1C-NC	7.74	1.55	1.37
4	H	202	BLA	C1C-NC	7.74	1.55	1.37
4	B	202	BLA	C1C-NC	7.76	1.55	1.37
4	J	201	BLA	C1C-NC	7.77	1.55	1.37
4	D	201	BLA	C4B-NB	7.80	1.55	1.37
4	F	202	BLA	C1C-NC	7.81	1.55	1.37
4	J	202	BLA	C1C-NC	7.81	1.55	1.37
4	D	201	BLA	C1C-NC	7.81	1.55	1.37
4	B	201	BLA	C4B-NB	7.81	1.55	1.37
4	F	202	BLA	C4B-NB	7.82	1.55	1.37
4	L	202	BLA	C4B-NB	7.82	1.55	1.37
4	H	201	BLA	C1C-NC	7.83	1.55	1.37
4	F	201	BLA	C1C-NC	7.83	1.55	1.37
4	I	201	BLA	C1C-NC	7.83	1.55	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	201	BLA	C4B-NB	7.84	1.55	1.37
4	B	202	BLA	C4B-NB	7.84	1.55	1.37
4	L	201	BLA	C4B-NB	7.86	1.55	1.37
4	F	201	BLA	C4B-NB	7.87	1.55	1.37
4	H	201	BLA	C4B-NB	7.87	1.55	1.37
4	H	202	BLA	C4B-NB	7.88	1.55	1.37
4	B	201	BLA	C1C-NC	7.89	1.55	1.37
4	D	202	BLA	C4B-NB	7.90	1.55	1.37
4	J	202	BLA	C4B-NB	7.91	1.55	1.37
4	J	201	BLA	C4B-NB	7.92	1.55	1.37
4	L	201	BLA	C1C-NC	7.92	1.55	1.37
3	E	201	CYC	C4B-NB	7.96	1.55	1.37
3	K	201	CYC	C4B-NB	8.01	1.55	1.37
3	C	201	CYC	C4B-NB	8.04	1.56	1.37
3	A	201	CYC	C4B-NB	8.10	1.56	1.37
3	G	201	CYC	C4B-NB	8.15	1.56	1.37
3	G	201	CYC	C2C-C1C	8.95	1.60	1.52
3	K	201	CYC	C2C-C1C	9.09	1.60	1.52
3	C	201	CYC	C2C-C1C	9.09	1.60	1.52
3	A	201	CYC	C2C-C1C	9.37	1.60	1.52
3	E	201	CYC	C2C-C1C	9.38	1.60	1.52
4	B	202	BLA	C4C-NC	10.06	1.55	1.37
4	H	201	BLA	C1B-NB	10.19	1.55	1.37
4	H	201	BLA	C4C-NC	10.22	1.55	1.37
4	L	202	BLA	C1B-NB	10.23	1.55	1.37
4	D	201	BLA	C4C-NC	10.24	1.55	1.37
4	L	201	BLA	C1B-NB	10.24	1.55	1.37
4	I	201	BLA	C4C-NC	10.24	1.55	1.37
4	B	201	BLA	C1B-NB	10.24	1.55	1.37
4	F	202	BLA	C4C-NC	10.24	1.55	1.37
4	D	202	BLA	C4C-NC	10.25	1.55	1.37
4	J	201	BLA	C4C-NC	10.25	1.55	1.37
4	D	201	BLA	C1B-NB	10.26	1.55	1.37
4	H	202	BLA	C4C-NC	10.27	1.55	1.37
4	I	201	BLA	C1B-NB	10.28	1.55	1.37
4	F	201	BLA	C1B-NB	10.31	1.55	1.37
4	L	202	BLA	C4C-NC	10.32	1.55	1.37
4	D	202	BLA	C1B-NB	10.32	1.55	1.37
4	J	201	BLA	C1B-NB	10.34	1.55	1.37
4	F	202	BLA	C1B-NB	10.35	1.55	1.37
3	E	201	CYC	C1B-NB	10.35	1.55	1.37
4	B	202	BLA	C1B-NB	10.35	1.55	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	202	BLA	C1B-NB	10.35	1.55	1.37
4	J	202	BLA	C4C-NC	10.36	1.55	1.37
4	L	201	BLA	C4C-NC	10.38	1.55	1.37
4	H	202	BLA	C1B-NB	10.39	1.55	1.37
4	F	201	BLA	C4C-NC	10.41	1.55	1.37
4	B	201	BLA	C4C-NC	10.48	1.56	1.37
3	K	201	CYC	C1B-NB	10.51	1.56	1.37
3	C	201	CYC	C1B-NB	10.56	1.56	1.37
3	G	201	CYC	C1B-NB	10.57	1.56	1.37
3	A	201	CYC	C1B-NB	10.59	1.56	1.37

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CYC	C2A-C1A-NA	-7.99	97.45	109.86
4	I	201	BLA	C3D-C4D-ND	-7.89	97.61	109.86
4	F	201	BLA	C3D-C4D-ND	-7.75	97.82	109.86
4	D	201	BLA	C3D-C4D-ND	-7.66	97.96	109.86
3	G	201	CYC	C2A-C1A-NA	-7.61	98.04	109.86
4	J	202	BLA	C3D-C4D-ND	-7.58	98.09	109.86
4	H	201	BLA	C3D-C4D-ND	-7.55	98.14	109.86
4	J	201	BLA	C3D-C4D-ND	-7.54	98.15	109.86
4	L	201	BLA	C3D-C4D-ND	-7.54	98.15	109.86
4	L	202	BLA	C3D-C4D-ND	-7.54	98.16	109.86
4	B	201	BLA	C3D-C4D-ND	-7.53	98.17	109.86
4	F	202	BLA	C3D-C4D-ND	-7.51	98.20	109.86
3	K	201	CYC	C2A-C1A-NA	-7.51	98.20	109.86
3	E	201	CYC	C2A-C1A-NA	-7.46	98.27	109.86
4	B	202	BLA	C3D-C4D-ND	-7.41	98.36	109.86
3	C	201	CYC	C2A-C1A-NA	-7.37	98.42	109.86
4	H	202	BLA	C3D-C4D-ND	-7.35	98.44	109.86
4	D	202	BLA	C3D-C4D-ND	-7.31	98.52	109.86
3	G	201	CYC	C3C-C2C-C1C	-7.18	97.39	103.41
3	K	201	CYC	C3C-C2C-C1C	-7.15	97.42	103.41
3	E	201	CYC	C3C-C2C-C1C	-6.92	97.61	103.41
3	C	201	CYC	C3C-C2C-C1C	-6.24	98.18	103.41
3	A	201	CYC	C3C-C2C-C1C	-5.92	98.45	103.41
3	C	201	CYC	C1B-NB-C4B	-5.46	102.74	110.73
4	D	201	BLA	C1B-NB-C4B	-5.42	102.81	110.73
3	G	201	CYC	C1B-NB-C4B	-5.40	102.84	110.73
3	A	201	CYC	C1B-NB-C4B	-5.36	102.89	110.73
3	E	201	CYC	C1B-NB-C4B	-5.36	102.89	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	201	CYC	C1B-NB-C4B	-5.34	102.91	110.73
4	B	202	BLA	C4C-NC-C1C	-5.31	102.96	110.73
4	F	201	BLA	C1B-NB-C4B	-5.29	102.98	110.73
4	J	201	BLA	C1B-NB-C4B	-5.29	102.99	110.73
4	H	201	BLA	C1B-NB-C4B	-5.29	103.00	110.73
4	I	201	BLA	C1B-NB-C4B	-5.29	103.00	110.73
4	B	201	BLA	C1B-NB-C4B	-5.28	103.01	110.73
4	L	202	BLA	C4C-NC-C1C	-5.27	103.02	110.73
4	L	201	BLA	C1B-NB-C4B	-5.25	103.04	110.73
4	D	202	BLA	C1B-NB-C4B	-5.20	103.12	110.73
4	H	202	BLA	C4C-NC-C1C	-5.19	103.14	110.73
4	L	202	BLA	C1B-NB-C4B	-5.17	103.17	110.73
4	D	202	BLA	C4C-NC-C1C	-5.17	103.17	110.73
4	F	202	BLA	C4C-NC-C1C	-5.16	103.18	110.73
4	J	202	BLA	C4C-NC-C1C	-5.13	103.22	110.73
4	D	201	BLA	C4C-NC-C1C	-5.10	103.27	110.73
4	L	201	BLA	C4C-NC-C1C	-5.10	103.28	110.73
4	H	201	BLA	C4C-NC-C1C	-5.09	103.28	110.73
4	F	202	BLA	C1B-NB-C4B	-5.08	103.30	110.73
4	B	202	BLA	C1B-NB-C4B	-5.08	103.30	110.73
4	H	202	BLA	C1B-NB-C4B	-5.08	103.31	110.73
4	J	201	BLA	C4C-NC-C1C	-5.05	103.34	110.73
4	J	202	BLA	C1B-NB-C4B	-5.01	103.40	110.73
4	F	201	BLA	C4C-NC-C1C	-4.97	103.46	110.73
4	B	201	BLA	C4C-NC-C1C	-4.95	103.48	110.73
4	I	201	BLA	C4C-NC-C1C	-4.60	104.00	110.73
3	E	201	CYC	CMB-C2B-C1B	-3.83	119.12	124.20
3	K	201	CYC	CMB-C2B-C1B	-3.72	119.26	124.20
3	C	201	CYC	CMB-C2B-C1B	-3.64	119.37	124.20
3	G	201	CYC	CMB-C2B-C1B	-3.56	119.47	124.20
3	A	201	CYC	CAD-CBD-CGD	-3.47	106.39	112.75
3	A	201	CYC	C2B-C1B-NB	-3.38	102.10	107.00
3	A	201	CYC	CMB-C2B-C1B	-3.37	119.73	124.20
4	J	202	BLA	C2B-C1B-NB	-3.37	102.12	107.00
4	H	202	BLA	C2B-C1B-NB	-3.34	102.16	107.00
4	F	202	BLA	C2B-C1B-NB	-3.29	102.23	107.00
4	B	202	BLA	C2B-C1B-NB	-3.27	102.27	107.00
3	K	201	CYC	C2B-C1B-NB	-3.26	102.27	107.00
3	G	201	CYC	C2B-C1B-NB	-3.26	102.28	107.00
3	C	201	CYC	C2B-C1B-NB	-3.22	102.33	107.00
3	E	201	CYC	C2B-C1B-NB	-3.16	102.43	107.00
4	D	202	BLA	C2B-C1B-NB	-3.14	102.46	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	202	BLA	C2B-C1B-NB	-3.13	102.46	107.00
4	B	202	BLA	C4C-CHD-C1D	-3.03	120.21	128.06
3	G	201	CYC	C3B-C4B-NB	-3.03	103.98	106.74
3	A	201	CYC	CAD-C3D-C2D	-3.01	120.41	129.00
4	L	201	BLA	C2B-C1B-NB	-3.00	102.66	107.00
3	K	201	CYC	C3B-C4B-NB	-2.99	104.02	106.74
4	J	201	BLA	C2B-C1B-NB	-2.99	102.66	107.00
4	B	201	BLA	C2B-C1B-NB	-2.99	102.67	107.00
3	A	201	CYC	C3B-C4B-NB	-2.99	104.02	106.74
4	F	201	BLA	C2B-C1B-NB	-2.99	102.67	107.00
4	I	201	BLA	C2B-C1B-NB	-2.92	102.77	107.00
4	L	202	BLA	C4C-CHD-C1D	-2.92	120.52	128.06
3	C	201	CYC	C3B-C4B-NB	-2.91	104.09	106.74
3	K	201	CYC	C2C-C1C-NC	-2.91	105.52	108.30
4	H	201	BLA	C2B-C1B-NB	-2.90	102.80	107.00
3	E	201	CYC	C3B-C4B-NB	-2.87	104.13	106.74
3	K	201	CYC	CBD-CAD-C3D	-2.84	107.44	112.53
4	D	202	BLA	C4C-CHD-C1D	-2.80	120.81	128.06
3	G	201	CYC	CAD-C3D-C4D	-2.80	123.29	127.24
4	I	201	BLA	CAD-C3D-C4D	-2.78	120.10	125.06
4	J	202	BLA	C4C-CHD-C1D	-2.69	121.09	128.06
4	D	201	BLA	C2B-C1B-NB	-2.69	103.10	107.00
4	H	202	BLA	C4C-CHD-C1D	-2.68	121.14	128.06
3	C	201	CYC	CBD-CAD-C3D	-2.63	107.81	112.53
3	E	201	CYC	C2C-C1C-NC	-2.62	105.79	108.30
3	A	201	CYC	C2C-C1C-NC	-2.62	105.80	108.30
4	J	202	BLA	CAD-C3D-C2D	-2.61	123.45	128.01
3	K	201	CYC	CAD-C3D-C4D	-2.61	123.55	127.24
3	C	201	CYC	CAD-C3D-C4D	-2.55	123.64	127.24
4	H	202	BLA	CMB-C2B-C3B	-2.53	121.68	128.48
3	E	201	CYC	C1B-CHB-C4A	-2.52	121.55	128.06
4	F	202	BLA	CMB-C2B-C3B	-2.51	121.75	128.48
4	F	201	BLA	CAC-C3C-C4C	-2.50	118.02	124.80
3	G	201	CYC	C2C-C1C-NC	-2.49	105.92	108.30
4	J	202	BLA	CMB-C2B-C3B	-2.49	121.78	128.48
4	D	202	BLA	CMC-C2C-C3C	-2.48	121.82	128.48
4	F	202	BLA	C4C-CHD-C1D	-2.48	121.66	128.06
3	A	201	CYC	CAB-C3B-C4B	-2.45	119.37	121.51
4	L	202	BLA	CMB-C2B-C3B	-2.41	122.01	128.48
3	E	201	CYC	CBD-CAD-C3D	-2.40	108.22	112.53
4	B	202	BLA	CMB-C2B-C3B	-2.39	122.07	128.48
4	J	201	BLA	CMB-C2B-C3B	-2.36	122.14	128.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	CYC	C2C-C1C-NC	-2.34	106.06	108.30
4	D	202	BLA	CMB-C2B-C3B	-2.33	122.22	128.48
4	F	201	BLA	CMB-C2B-C3B	-2.31	122.27	128.48
4	J	202	BLA	CBA-CAA-C2A	-2.31	108.39	112.53
4	L	201	BLA	CMB-C2B-C3B	-2.30	122.32	128.48
3	G	201	CYC	C2C-C3C-C4C	-2.29	97.61	101.50
4	B	201	BLA	CMB-C2B-C3B	-2.27	122.38	128.48
3	G	201	CYC	CBD-CAD-C3D	-2.27	108.46	112.53
3	G	201	CYC	CAB-C3B-C4B	-2.26	119.54	121.51
4	H	201	BLA	CMB-C2B-C3B	-2.22	122.52	128.48
4	D	201	BLA	CMB-C2B-C3B	-2.21	122.56	128.48
3	G	201	CYC	C1B-CHB-C4A	-2.18	122.41	128.06
4	I	201	BLA	CMB-C2B-C3B	-2.14	122.74	128.48
4	F	202	BLA	CBA-CAA-C2A	-2.11	108.74	112.53
3	K	201	CYC	C2C-C3C-C4C	-2.11	97.92	101.50
3	A	201	CYC	CAA-C2A-C3A	-2.10	124.35	128.01
3	K	201	CYC	C1B-CHB-C4A	-2.09	122.64	128.06
3	E	201	CYC	CAD-C3D-C4D	-2.09	124.30	127.24
4	J	202	BLA	CAC-C3C-C2C	-2.07	121.46	128.41
4	F	202	BLA	CMC-C2C-C3C	-2.07	122.93	128.48
4	L	202	BLA	CMC-C2C-C3C	-2.01	123.08	128.48
4	L	201	BLA	C4D-ND-C1D	2.00	110.47	106.51
4	H	201	BLA	C4D-ND-C1D	2.05	110.58	106.51
4	B	201	BLA	C4D-ND-C1D	2.07	110.61	106.51
4	J	201	BLA	CHD-C4C-NC	2.08	130.66	126.16
3	C	201	CYC	CMA-C3A-C4A	2.08	128.44	125.06
4	F	201	BLA	C4D-ND-C1D	2.10	110.66	106.51
4	J	201	BLA	C4D-ND-C1D	2.11	110.69	106.51
3	E	201	CYC	CMA-C3A-C4A	2.15	128.55	125.06
4	H	201	BLA	CHD-C4C-NC	2.16	130.83	126.16
4	D	201	BLA	CHD-C4C-NC	2.16	130.84	126.16
3	A	201	CYC	OC-C1C-NC	2.16	127.44	124.83
4	D	201	BLA	C4D-ND-C1D	2.18	110.82	106.51
4	J	202	BLA	C4D-ND-C1D	2.18	110.83	106.51
4	B	202	BLA	CHA-C4D-C3D	2.19	130.69	125.55
4	I	201	BLA	CHD-C4C-NC	2.19	130.91	126.16
3	A	201	CYC	C1A-NA-C4A	2.22	110.90	106.51
3	E	201	CYC	C4A-C3A-C2A	2.22	109.16	106.50
3	K	201	CYC	CMA-C3A-C4A	2.23	128.68	125.06
3	A	201	CYC	C4A-C3A-C2A	2.23	109.17	106.50
3	C	201	CYC	C4A-C3A-C2A	2.28	109.23	106.50
4	J	201	BLA	CHA-C4D-ND	2.29	132.76	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	201	BLA	C4D-ND-C1D	2.32	111.11	106.51
3	C	201	CYC	OC-C1C-NC	2.33	127.65	124.83
3	G	201	CYC	C4A-C3A-C2A	2.36	109.33	106.50
3	K	201	CYC	OC-C1C-NC	2.37	127.70	124.83
3	E	201	CYC	OC-C1C-NC	2.38	127.70	124.83
3	K	201	CYC	C4A-C3A-C2A	2.40	109.39	106.50
4	B	202	BLA	C1D-C2D-C3D	2.44	109.43	106.50
4	D	202	BLA	C1D-C2D-C3D	2.48	109.47	106.50
4	D	201	BLA	CHA-C4D-ND	2.50	133.14	128.67
4	I	201	BLA	C1D-C2D-C3D	2.56	109.58	106.50
4	H	202	BLA	C1D-C2D-C3D	2.56	109.58	106.50
4	F	201	BLA	CHD-C4C-NC	2.58	131.76	126.16
4	B	201	BLA	CHD-C4C-NC	2.61	131.82	126.16
3	G	201	CYC	OC-C1C-NC	2.62	127.99	124.83
3	A	201	CYC	CAD-C3D-C4D	2.62	130.93	127.24
4	D	202	BLA	C4C-C3C-C2C	2.66	115.01	106.97
3	A	201	CYC	CHA-C1A-NA	2.66	133.43	128.67
4	L	202	BLA	C1D-C2D-C3D	2.69	109.72	106.50
4	F	201	BLA	C1D-C2D-C3D	2.73	109.77	106.50
3	G	201	CYC	CHA-C1A-NA	2.73	133.54	128.67
4	D	201	BLA	C1D-C2D-C3D	2.76	109.81	106.50
3	K	201	CYC	CHA-C1A-NA	2.78	133.64	128.67
4	H	202	BLA	C4C-C3C-C2C	2.80	115.43	106.97
4	H	201	BLA	C1D-C2D-C3D	2.80	109.86	106.50
4	L	202	BLA	C4C-C3C-C2C	2.80	115.45	106.97
4	B	202	BLA	C4C-C3C-C2C	2.80	115.45	106.97
3	G	201	CYC	CAC-C3C-C4C	2.81	119.88	112.67
4	J	202	BLA	C4C-C3C-C2C	2.82	115.49	106.97
4	J	202	BLA	CHA-C4D-C3D	2.82	132.16	125.55
4	F	202	BLA	C1D-C2D-C3D	2.83	109.89	106.50
4	F	201	BLA	C4C-C3C-C2C	2.83	115.53	106.97
4	J	201	BLA	C4C-C3C-C2C	2.84	115.56	106.97
4	F	202	BLA	C4C-C3C-C2C	2.87	115.67	106.97
4	H	201	BLA	C4C-C3C-C2C	2.89	115.71	106.97
4	J	201	BLA	C1D-C2D-C3D	2.90	109.98	106.50
4	D	201	BLA	C4C-C3C-C2C	2.91	115.78	106.97
4	L	201	BLA	C1D-C2D-C3D	2.92	110.00	106.50
4	L	201	BLA	C4C-C3C-C2C	2.92	115.81	106.97
4	F	201	BLA	CHA-C4D-ND	2.93	133.91	128.67
3	C	201	CYC	CHA-C1A-NA	2.94	133.92	128.67
3	E	201	CYC	CHA-C1A-NA	2.96	133.97	128.67
4	B	201	BLA	C4C-C3C-C2C	2.98	115.99	106.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	201	BLA	CHA-C4D-ND	3.00	134.03	128.67
4	L	201	BLA	CHA-C4D-ND	3.07	134.15	128.67
4	I	201	BLA	C4C-C3C-C2C	3.09	116.31	106.97
4	J	202	BLA	C4D-C3D-C2D	3.10	110.28	106.81
4	B	201	BLA	C1D-C2D-C3D	3.17	110.30	106.50
4	J	202	BLA	C1D-C2D-C3D	3.20	110.33	106.50
4	B	201	BLA	CHA-C4D-ND	3.34	134.63	128.67
3	A	201	CYC	CBD-CAD-C3D	3.58	118.95	112.53
4	F	202	BLA	C4D-C3D-C2D	3.61	110.85	106.81
4	B	202	BLA	C4D-C3D-C2D	3.68	110.93	106.81
4	D	202	BLA	C4D-C3D-C2D	3.72	110.97	106.81
4	H	202	BLA	C4D-C3D-C2D	3.73	110.98	106.81
4	J	201	BLA	C4D-C3D-C2D	3.78	111.03	106.81
4	L	202	BLA	C4D-C3D-C2D	3.82	111.08	106.81
4	B	201	BLA	C4D-C3D-C2D	3.98	111.27	106.81
4	L	201	BLA	C4D-C3D-C2D	4.01	111.29	106.81
4	D	201	BLA	C4D-C3D-C2D	4.07	111.36	106.81
4	I	201	BLA	CHA-C4D-ND	4.08	135.97	128.67
4	H	201	BLA	C4D-C3D-C2D	4.09	111.38	106.81
3	C	201	CYC	C1A-C2A-C3A	4.25	111.56	106.81
4	F	201	BLA	C4D-C3D-C2D	4.27	111.58	106.81
3	K	201	CYC	C1A-C2A-C3A	4.29	111.61	106.81
3	G	201	CYC	C1A-C2A-C3A	4.31	111.63	106.81
3	E	201	CYC	C1A-C2A-C3A	4.37	111.70	106.81
4	I	201	BLA	C4D-C3D-C2D	4.76	112.14	106.81
3	A	201	CYC	C1A-C2A-C3A	4.77	112.14	106.81
3	K	201	CYC	C3C-C4C-NC	5.22	113.16	107.93
3	G	201	CYC	C3C-C4C-NC	5.50	113.44	107.93
3	E	201	CYC	C3C-C4C-NC	5.99	113.93	107.93
3	C	201	CYC	C3C-C4C-NC	6.35	114.29	107.93
3	A	201	CYC	C3C-C4C-NC	6.43	114.37	107.93
3	K	201	CYC	C1B-C2B-C3B	7.17	115.46	107.81
3	G	201	CYC	C1B-C2B-C3B	7.19	115.48	107.81
3	C	201	CYC	C1B-C2B-C3B	7.23	115.52	107.81
3	E	201	CYC	C1B-C2B-C3B	7.24	115.54	107.81
3	A	201	CYC	C1B-C2B-C3B	7.25	115.55	107.81
3	E	201	CYC	C4B-C3B-C2B	12.17	114.99	108.05
3	C	201	CYC	C4B-C3B-C2B	12.71	115.30	108.05
3	K	201	CYC	C4B-C3B-C2B	12.76	115.33	108.05
3	G	201	CYC	C4B-C3B-C2B	12.89	115.40	108.05
3	A	201	CYC	C4B-C3B-C2B	12.94	115.43	108.05

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	202	BLA	C4C-CHD-C1D-C2D
4	F	202	BLA	C4C-CHD-C1D-C2D
4	J	202	BLA	C4C-CHD-C1D-C2D
4	H	202	BLA	C4C-CHD-C1D-C2D
4	B	202	BLA	C4C-CHD-C1D-C2D
3	K	201	CYC	C4C-CHD-C1D-ND
4	D	202	BLA	C4C-CHD-C1D-C2D
3	G	201	CYC	C4C-CHD-C1D-ND
4	L	202	BLA	C4C-CHD-C1D-ND
4	L	201	BLA	C4C-CHD-C1D-C2D
4	J	202	BLA	C4C-CHD-C1D-ND
4	F	202	BLA	C4C-CHD-C1D-ND
3	E	201	CYC	C1B-CHB-C4A-C3A
4	H	201	BLA	C4C-CHD-C1D-C2D
3	G	201	CYC	C1B-CHB-C4A-C3A
3	A	201	CYC	C4C-CHD-C1D-ND
3	E	201	CYC	C4C-CHD-C1D-ND
3	C	201	CYC	C1B-CHB-C4A-C3A
3	K	201	CYC	C1B-CHB-C4A-C3A
4	J	201	BLA	C4C-CHD-C1D-C2D
4	D	201	BLA	C4C-CHD-C1D-C2D
4	H	202	BLA	C4C-CHD-C1D-ND
4	B	202	BLA	C4C-CHD-C1D-ND
4	B	201	BLA	C4C-CHD-C1D-C2D
3	C	201	CYC	C4C-CHD-C1D-ND
4	I	201	BLA	C4C-CHD-C1D-C2D
4	F	201	BLA	C4C-CHD-C1D-C2D
4	D	202	BLA	C4C-CHD-C1D-ND
3	A	201	CYC	C1B-CHB-C4A-C3A
3	E	201	CYC	C1B-CHB-C4A-NA
4	D	201	BLA	C1B-CHB-C4A-NA
4	B	201	BLA	C1B-CHB-C4A-NA
4	L	201	BLA	C4C-CHD-C1D-ND
3	G	201	CYC	C1B-CHB-C4A-NA
3	C	201	CYC	C1B-CHB-C4A-NA
3	K	201	CYC	C1B-CHB-C4A-NA
4	H	201	BLA	C4C-CHD-C1D-ND
4	F	201	BLA	C1B-CHB-C4A-NA
4	F	202	BLA	C1B-CHB-C4A-NA
4	H	201	BLA	C1B-CHB-C4A-NA
4	L	201	BLA	C1B-CHB-C4A-NA
4	J	201	BLA	C1B-CHB-C4A-NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	201	BLA	C4C-CHD-C1D-ND
4	B	201	BLA	C4C-CHD-C1D-ND
4	D	201	BLA	C4C-CHD-C1D-ND
4	D	202	BLA	C1B-CHB-C4A-NA
4	I	201	BLA	C4C-CHD-C1D-ND
4	F	201	BLA	C4C-CHD-C1D-ND
4	I	201	BLA	C1B-CHB-C4A-NA
4	B	202	BLA	C1B-CHB-C4A-NA
4	L	202	BLA	C1B-CHB-C4A-NA
3	A	201	CYC	C1B-CHB-C4A-NA
4	H	202	BLA	C1B-CHB-C4A-NA
4	J	202	BLA	C1B-CHB-C4A-NA

There are no ring outliers.

18 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	CYC	5	0
4	B	201	BLA	6	0
4	B	202	BLA	7	0
3	C	201	CYC	3	0
4	D	201	BLA	6	0
4	D	202	BLA	6	0
3	E	201	CYC	7	0
4	F	201	BLA	8	0
4	F	202	BLA	4	0
3	G	201	CYC	4	0
4	H	201	BLA	5	0
4	H	202	BLA	5	0
4	I	201	BLA	5	0
4	J	201	BLA	6	0
4	J	202	BLA	4	0
3	K	201	CYC	3	0
4	L	201	BLA	6	0
4	L	202	BLA	5	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	162/162 (100%)	0.42	8 (4%)	33	26	20, 29, 46, 61	0
1	C	162/162 (100%)	0.50	13 (8%)	15	10	20, 29, 46, 61	0
1	E	162/162 (100%)	0.28	6 (3%)	45	37	19, 25, 41, 53	0
1	G	162/162 (100%)	0.30	6 (3%)	45	37	20, 28, 44, 65	0
1	I	162/162 (100%)	0.27	5 (3%)	52	45	21, 28, 42, 60	0
1	K	162/162 (100%)	0.28	6 (3%)	45	37	20, 25, 43, 68	0
2	B	172/172 (100%)	0.60	15 (8%)	13	9	21, 30, 47, 106	0
2	D	172/172 (100%)	0.65	14 (8%)	15	10	20, 29, 47, 106	0
2	F	172/172 (100%)	0.25	5 (2%)	55	48	19, 27, 44, 70	0
2	H	172/172 (100%)	0.35	10 (5%)	26	20	20, 28, 45, 63	0
2	J	172/172 (100%)	0.43	10 (5%)	26	20	21, 29, 49, 70	0
2	L	172/172 (100%)	0.35	11 (6%)	23	17	20, 27, 43, 60	0
All	All	2004/2004 (100%)	0.39	109 (5%)	29	22	19, 28, 46, 106	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	7.6
2	D	1	MET	6.2
2	L	129	VAL	4.3
2	L	14	THR	4.2
1	G	78	GLN	4.1
2	B	136	GLU	4.1
2	B	111	ASN	3.9
2	J	14	THR	3.8
1	C	78	GLN	3.6
2	J	136	GLU	3.6
1	C	144	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	14	THR	3.4
1	C	117	GLU	3.3
2	F	119	ALA	3.3
2	F	118	LEU	3.2
1	A	61	ASN	3.2
2	B	14	THR	3.1
1	K	68	GLN	3.1
1	A	82	ASP	3.1
1	G	76	ALA	3.1
1	E	78	GLN	3.0
2	D	29	GLN	3.0
2	B	129	VAL	3.0
1	C	82	ASP	2.9
1	I	49	ASP	2.9
1	A	117	GLU	2.9
2	D	172	SER	2.9
1	I	82	ASP	2.8
2	D	118	LEU	2.8
2	J	129	VAL	2.8
1	C	39	GLU	2.7
1	G	82	ASP	2.7
2	H	107	ASP	2.7
1	A	78	GLN	2.6
1	K	70	GLN	2.6
2	D	58	SER	2.6
2	H	136	GLU	2.6
1	E	10	SER	2.5
1	E	11	VAL	2.5
1	I	78	GLN	2.5
2	D	120	LEU	2.5
2	L	119	ALA	2.5
1	E	70	GLN	2.5
2	J	29	GLN	2.5
1	K	82	ASP	2.4
2	J	152	ASP	2.4
2	L	136	GLU	2.4
2	L	172	SER	2.4
1	A	84	CYS	2.4
2	J	120	LEU	2.4
2	F	111	ASN	2.4
2	H	166	ARG	2.4
1	C	76	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	84	CYS	2.4
2	H	150	PRO	2.4
1	C	84	CYS	2.3
1	C	10	SER	2.3
2	D	119	ALA	2.3
1	C	68	GLN	2.3
1	C	53	SER	2.3
1	E	76	ALA	2.3
1	G	11	VAL	2.3
2	J	115	GLU	2.3
2	F	50	THR	2.3
1	K	78	GLN	2.3
2	L	29	GLN	2.3
2	L	118	LEU	2.3
2	D	150	PRO	2.3
2	H	119	ALA	2.3
1	C	11	VAL	2.3
2	H	82	CYS	2.3
1	G	68	GLN	2.3
2	B	147	GLY	2.2
2	D	129	VAL	2.2
1	E	82	ASP	2.2
1	C	32	ARG	2.2
2	H	129	VAL	2.2
2	H	50	THR	2.2
1	A	70	GLN	2.2
2	J	94	THR	2.2
1	G	10	SER	2.2
2	B	29	GLN	2.2
2	B	166	ARG	2.2
2	B	107	ASP	2.2
2	H	151	GLY	2.1
2	D	114	ARG	2.1
1	A	11	VAL	2.1
2	B	21	THR	2.1
2	D	65	GLN	2.1
2	B	85	ASP	2.1
1	C	61	ASN	2.1
2	D	136	GLU	2.1
2	L	106	GLU	2.1
2	D	25	ASP	2.1
2	F	166	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	166	ARG	2.1
2	L	38	LEU	2.1
2	L	154	SER	2.1
2	H	115	GLU	2.1
2	B	76	SER	2.1
2	J	118	LEU	2.0
2	B	114	ARG	2.0
2	J	15	ARG	2.0
1	A	10	SER	2.0
1	K	84	CYS	2.0
2	B	50	THR	2.0
2	B	145	PRO	2.0
1	I	16	GLY	2.0
1	K	135	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CYC	A	201	43/43	0.87	0.29	2.32	22,32,40,42	0
4	BLA	L	201	43/43	0.76	0.26	1.76	31,40,48,50	0
4	BLA	F	201	43/43	0.81	0.26	1.76	29,38,47,53	0
4	BLA	H	201	43/43	0.79	0.28	1.73	31,40,46,51	0
3	CYC	E	201	43/43	0.85	0.28	1.63	18,28,36,38	0
4	BLA	J	201	43/43	0.78	0.27	1.55	31,38,46,57	0
4	BLA	L	202	43/43	0.85	0.26	1.18	21,29,42,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CYC	K	201	43/43	0.89	0.25	1.16	19,31,39,44	0
4	BLA	J	202	43/43	0.86	0.27	1.08	23,32,41,43	0
3	CYC	G	201	43/43	0.88	0.23	1.01	22,34,43,48	0
4	BLA	B	201	43/43	0.78	0.27	0.97	32,39,47,48	0
3	CYC	C	201	43/43	0.88	0.23	0.93	21,25,31,35	0
4	BLA	D	201	43/43	0.79	0.25	0.65	28,38,47,52	0
4	BLA	B	202	43/43	0.82	0.25	0.53	23,36,43,46	0
4	BLA	F	202	43/43	0.86	0.23	0.42	27,36,44,50	0
4	BLA	I	201	43/43	0.90	0.22	0.38	21,28,37,39	0
4	BLA	H	202	43/43	0.86	0.23	0.26	20,26,33,37	0
4	BLA	D	202	43/43	0.90	0.21	-0.17	20,24,30,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.