Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:02 AM GMT

PDB ID	:	2VML
Title	:	THE MONOCLINIC STRUCTURE OF PHYCOCYANIN FROM GLOEOBACTER VIOLACEUS
Authors	:	Murray, J.W.; Benson, S.; Barber, J.
Deposited on	:	2008-01-28
Resolution	:	2.40 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:

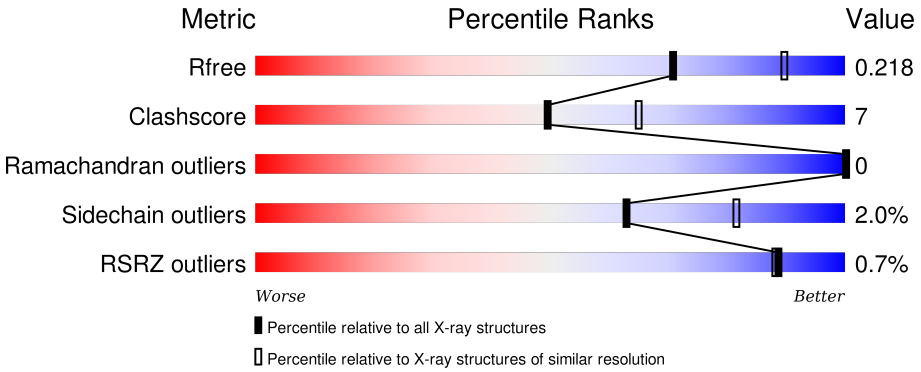
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	90% 9% •
1	C	162	90% 9% ••
1	E	162	93% 6% •
1	G	162	90% 9% •
1	I	162	88% 10% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	162	92% 8%
2	B	172	% 94% 5%
2	D	172	% 91% 8%
2	F	172	% 89% 10%
2	H	172	% 91% 8%
2	J	172	2% 92% 6%
2	L	172	3% 95% 5%

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	D	1082	-	-	-	X
3	CYC	J	1082	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16700 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.

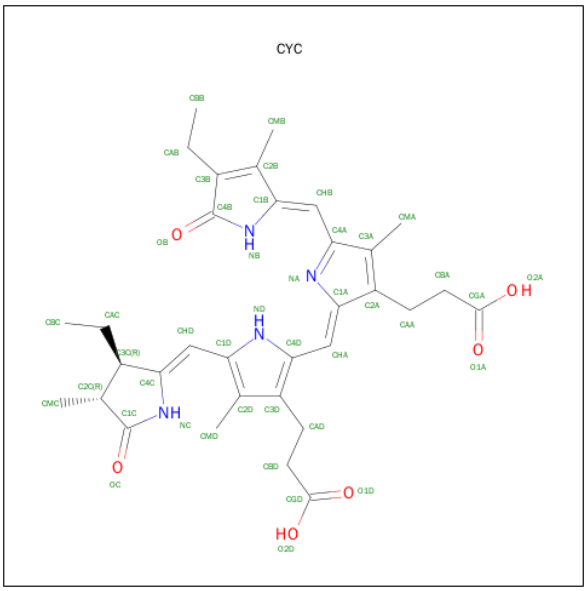
- Molecule 1 is a protein called PHYCOCYANIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			
1	C	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			
1	E	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			
1	G	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			
1	I	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			
1	K	162	Total	C	N	O	S	0	0	0
			1243	779	217	242	5			

- Molecule 2 is a protein called PHYCOCYANIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			
2	D	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			
2	F	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			
2	H	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			
2	J	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			
2	L	172	Total	C	N	O	S	0	0	0
			1293	802	229	255	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	J	1	Total	C	N	O	0	0
			43	33	4	6		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

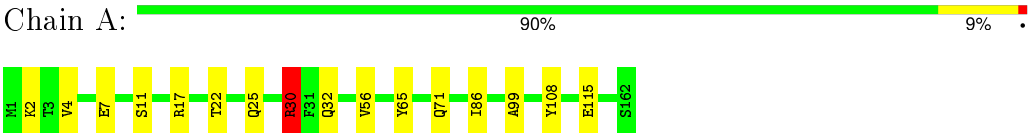
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total O 58 58	0	0
4	B	53	Total O 53 53	0	0
4	C	77	Total O 77 77	0	0
4	D	60	Total O 60 60	0	0
4	E	51	Total O 51 51	0	0
4	F	62	Total O 62 62	0	0
4	G	46	Total O 46 46	0	0
4	H	56	Total O 56 56	0	0
4	I	71	Total O 71 71	0	0
4	J	73	Total O 73 73	0	0
4	K	57	Total O 57 57	0	0
4	L	46	Total O 46 46	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.

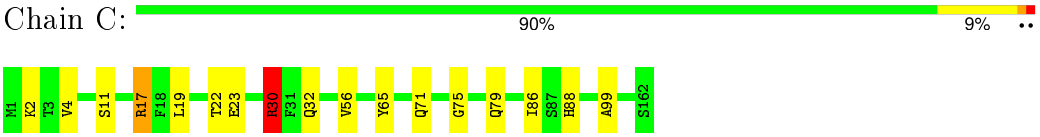
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

Chain A:



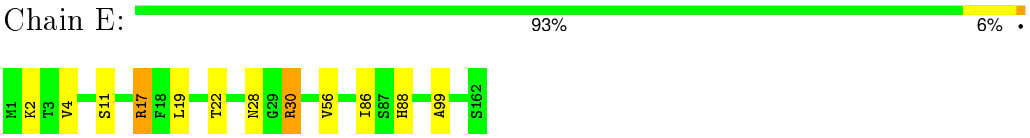
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

Chain C:



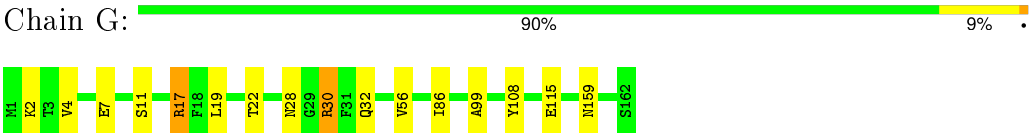
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

Chain E:



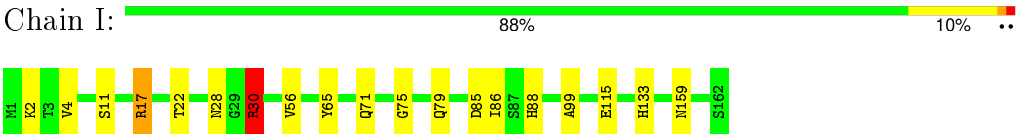
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

Chain G:



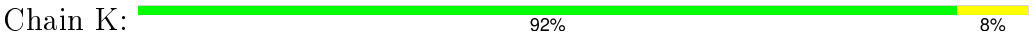
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

Chain I:



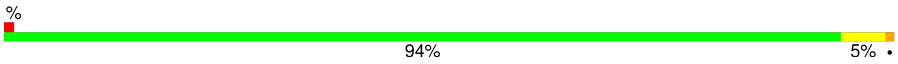
- Molecule 1: PHYCOCYANIN ALPHA CHAIN

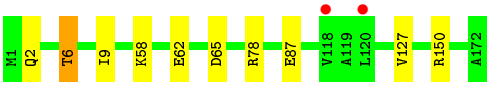
Chain K:



• Molecule 2: PHYCOCYANIN BETA CHAIN

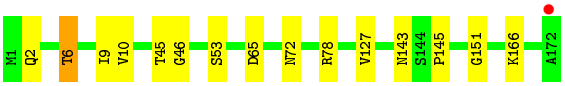
Chain B:





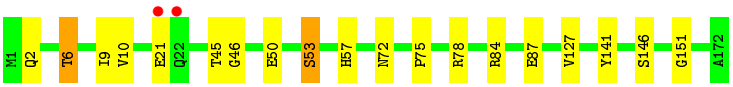
• Molecule 2: PHYCOCYANIN BETA CHAIN

Chain D:



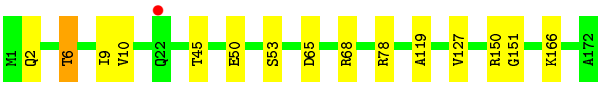
• Molecule 2: PHYCOCYANIN BETA CHAIN

Chain F:



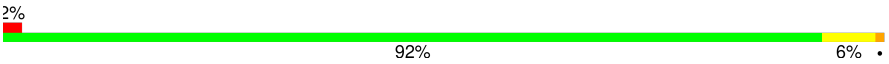
• Molecule 2: PHYCOCYANIN BETA CHAIN

Chain H:



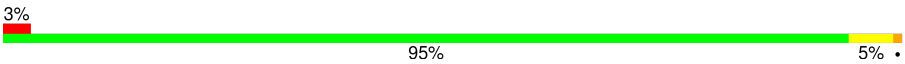
• Molecule 2: PHYCOCYANIN BETA CHAIN

Chain J:



• Molecule 2: PHYCOCYANIN BETA CHAIN

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.88Å 142.04Å 115.31Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	109.76 – 2.40 40.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (109.76-2.40) 98.9 (40.47-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.218 0.193 , 0.218	Depositor DCC
R_{free} test set	5148 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 102820 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16700	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	1/1265 (0.1%)	0.72	2/1713 (0.1%)
1	C	0.71	0/1265	0.74	2/1713 (0.1%)
1	E	0.67	0/1265	0.71	1/1713 (0.1%)
1	G	0.71	1/1265 (0.1%)	0.70	2/1713 (0.1%)
1	I	0.75	2/1265 (0.2%)	0.76	3/1713 (0.2%)
1	K	0.67	0/1265	0.68	0/1713
2	B	0.68	0/1307	0.70	3/1768 (0.2%)
2	D	0.72	0/1307	0.71	2/1768 (0.1%)
2	F	0.69	0/1307	0.70	1/1768 (0.1%)
2	H	0.76	1/1307 (0.1%)	0.71	2/1768 (0.1%)
2	J	0.80	1/1307 (0.1%)	0.72	2/1768 (0.1%)
2	L	0.71	2/1307 (0.2%)	0.69	2/1768 (0.1%)
All	All	0.72	8/15432 (0.1%)	0.71	22/20886 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	50	GLU	CG-CD	7.17	1.62	1.51
1	A	115	GLU	CD-OE1	6.32	1.32	1.25
2	J	47	ASN	CG-ND2	-5.66	1.18	1.32
2	L	47	ASN	CG-OD1	-5.66	1.11	1.24
1	G	115	GLU	CG-CD	5.51	1.60	1.51
1	I	115	GLU	CG-CD	5.48	1.60	1.51
1	I	115	GLU	CB-CG	5.31	1.62	1.52
2	L	47	ASN	CG-ND2	-5.16	1.20	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	78	ARG	NE-CZ-NH2	-6.62	116.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	78	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	L	78	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	I	30	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	L	78	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	C	17	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	78	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	30	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	F	78	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	H	78	ARG	NE-CZ-NH1	5.85	123.23	120.30
2	B	78	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	J	78	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	30	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	30	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	D	78	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	E	17	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	D	78	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	G	17	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	150	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	I	30	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	G	30	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	I	17	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	1243	0	1225	15	0
1	C	1243	0	1225	20	0
1	E	1243	0	1225	14	0
1	G	1243	0	1225	17	0
1	I	1243	0	1225	18	0
1	K	1243	0	1225	14	0
2	B	1293	0	1301	9	0
2	D	1293	0	1301	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1293	0	1301	17	0
2	H	1293	0	1301	11	0
2	J	1293	0	1301	14	0
2	L	1293	0	1301	10	0
3	A	43	0	36	6	0
3	B	86	0	74	12	0
3	C	43	0	37	6	0
3	D	86	0	74	14	0
3	E	43	0	36	7	0
3	F	86	0	74	14	0
3	G	43	0	36	6	0
3	H	86	0	74	10	0
3	I	43	0	36	5	0
3	J	86	0	74	13	0
3	K	43	0	36	6	0
3	L	86	0	74	12	0
4	A	58	0	0	1	0
4	B	53	0	0	1	0
4	C	77	0	0	2	0
4	D	60	0	0	0	0
4	E	51	0	0	2	0
4	F	62	0	0	2	0
4	G	46	0	0	1	0
4	H	56	0	0	2	0
4	I	71	0	0	4	0
4	J	73	0	0	1	0
4	K	57	0	0	0	0
4	L	46	0	0	2	0
All	All	16700	0	15817	226	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 7.

All (226) 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:J:2:GLN:OE1	2:J:6:THR:CG2	2.11	0.98
2:L:2:GLN:OE1	2:L:6:THR:CG2	2.12	0.96
2:B:2:GLN:OE1	2:B:6:THR:CG2	2.12	0.96
2:B:2:GLN:OE1	2:B:6:THR:HG23	1.65	0.96
2:H:2:GLN:OE1	2:H:6:THR:CG2	2.15	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:GLN:OE1	2:F:6:THR:CG2	2.14	0.94
2:J:2:GLN:OE1	2:J:6:THR:HG23	1.67	0.93
2:D:2:GLN:OE1	2:D:6:THR:CG2	2.17	0.93
3:F:1153:CYC:HC	3:F:1153:CYC:HMD2	1.36	0.89
4:H:2027:HOH:O	1:K:115:GLU:HG2	1.73	0.88
3:L:1153:CYC:HMD2	3:L:1153:CYC:HC	1.37	0.87
2:F:2:GLN:OE1	2:F:6:THR:HG23	1.77	0.84
2:L:2:GLN:OE1	2:L:6:THR:HG23	1.74	0.84
2:D:2:GLN:OE1	2:D:6:THR:HG23	1.74	0.83
3:D:1153:CYC:HMD2	3:D:1153:CYC:HC	1.43	0.83
3:A:1082:CYC:HC	3:A:1082:CYC:HMD3	1.44	0.82
3:K:1082:CYC:HC	3:K:1082:CYC:CMD	1.93	0.81
2:H:2:GLN:OE1	2:H:6:THR:HG23	1.78	0.80
3:B:1153:CYC:HC	3:B:1153:CYC:HMD2	1.46	0.80
3:E:1082:CYC:HC	3:E:1082:CYC:CMD	1.93	0.80
3:G:1082:CYC:HC	3:G:1082:CYC:CMD	1.94	0.80
3:A:1082:CYC:HC	3:A:1082:CYC:CMD	1.94	0.79
3:K:1082:CYC:HC	3:K:1082:CYC:HMD3	1.46	0.78
3:I:1082:CYC:HC	3:I:1082:CYC:CMD	1.98	0.77
2:L:26:GLN:NE2	4:L:2008:HOH:O	2.19	0.76
3:G:1082:CYC:HC	3:G:1082:CYC:HMD3	1.51	0.75
3:C:1082:CYC:CMD	3:C:1082:CYC:HC	1.99	0.75
3:E:1082:CYC:HC	3:E:1082:CYC:HMD3	1.53	0.73
3:I:1082:CYC:HMD3	3:I:1082:CYC:HC	1.54	0.72
3:H:1153:CYC:HC	3:H:1153:CYC:HMD2	1.54	0.71
1:E:30:ARG:NH2	4:E:2009:HOH:O	2.24	0.71
3:B:1153:CYC:HB	3:B:1153:CYC:HMA1	1.57	0.70
3:C:1082:CYC:HMD3	3:C:1082:CYC:HC	1.57	0.68
1:G:28:ASN:ND2	4:G:2009:HOH:O	2.14	0.68
1:E:28:ASN:ND2	4:E:2008:HOH:O	2.18	0.68
1:I:99:ALA:HB2	2:J:9:ILE:CD1	2.24	0.68
3:J:1153:CYC:HMA1	3:J:1153:CYC:HB	1.58	0.68
3:L:1082:CYC:HC	3:L:1082:CYC:HMD2	1.59	0.67
3:A:1082:CYC:HMA1	3:A:1082:CYC:NB	2.09	0.67
3:F:1153:CYC:HMA1	3:F:1153:CYC:HB	1.60	0.67
3:J:1082:CYC:NB	3:J:1082:CYC:HMA1	2.11	0.66
1:I:28:ASN:ND2	4:I:2010:HOH:O	2.18	0.65
3:J:1082:CYC:HB	3:J:1082:CYC:HMA1	1.63	0.64
3:E:1082:CYC:NB	3:E:1082:CYC:HMA1	2.11	0.64
3:C:1082:CYC:HMA1	3:C:1082:CYC:NB	2.13	0.64
1:C:2:LYS:NZ	1:G:17:ARG:CZ	2.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1082:CYC:HC	3:H:1082:CYC:HMD2	1.62	0.64
3:F:1082:CYC:HC	3:F:1082:CYC:HMD2	1.63	0.64
1:C:99:ALA:HB2	2:D:9:ILE:CD1	2.27	0.64
3:J:1153:CYC:HC	3:J:1153:CYC:HMD2	1.61	0.63
1:A:7:GLU:OE1	1:K:23:GLU:OE2	2.16	0.63
3:J:1082:CYC:HB	3:J:1082:CYC:CMA	2.11	0.63
1:C:30:ARG:NH2	4:C:2011:HOH:O	2.32	0.63
1:E:99:ALA:HB2	2:F:9:ILE:CD1	2.29	0.62
2:J:87:GLU:HG2	4:J:2030:HOH:O	2.00	0.62
1:I:56:VAL:HG22	1:I:86:ILE:HD12	1.81	0.62
1:C:56:VAL:HG22	1:C:86:ILE:HD12	1.82	0.62
3:L:1153:CYC:HB	3:L:1153:CYC:HMA1	1.65	0.62
3:A:1082:CYC:HB	3:A:1082:CYC:CMA	2.12	0.62
2:F:2:GLN:OE1	2:F:6:THR:HG22	1.96	0.61
3:D:1153:CYC:HMA1	3:D:1153:CYC:HB	1.65	0.61
3:C:1082:CYC:HMA1	3:C:1082:CYC:HB	1.66	0.61
3:E:1082:CYC:HB	3:E:1082:CYC:HMA1	1.66	0.60
2:H:2:GLN:OE1	2:H:6:THR:HG22	1.98	0.60
1:K:99:ALA:HB2	2:L:9:ILE:CD1	2.31	0.60
2:L:2:GLN:OE1	2:L:6:THR:HG22	1.99	0.60
3:I:1082:CYC:NB	3:I:1082:CYC:HMA1	2.17	0.60
3:A:1082:CYC:HMA1	3:A:1082:CYC:HB	1.66	0.60
3:K:1082:CYC:HMA1	3:K:1082:CYC:NB	2.17	0.60
3:E:1082:CYC:HB	3:E:1082:CYC:CMA	2.15	0.59
3:G:1082:CYC:NB	3:G:1082:CYC:HMA1	2.17	0.59
1:E:56:VAL:HG22	1:E:86:ILE:HD12	1.84	0.59
3:C:1082:CYC:CMA	3:C:1082:CYC:HB	2.15	0.59
3:D:1082:CYC:HMD2	3:D:1082:CYC:HC	1.66	0.59
2:F:50:GLU:HG2	2:F:141:TYR:OH	2.01	0.59
1:A:2:LYS:NZ	1:K:17:ARG:CZ	2.66	0.59
1:A:99:ALA:HB2	2:B:9:ILE:CD1	2.33	0.58
3:B:1082:CYC:HMA1	3:B:1082:CYC:NB	2.18	0.58
3:L:1153:CYC:HC	3:L:1153:CYC:CMD	2.12	0.58
3:B:1082:CYC:HB	3:B:1082:CYC:CMA	2.16	0.58
2:B:87:GLU:HG2	4:B:2030:HOH:O	2.02	0.58
3:H:1082:CYC:HMA1	3:H:1082:CYC:NB	2.19	0.58
3:D:1082:CYC:HMA1	3:D:1082:CYC:NB	2.19	0.57
3:K:1082:CYC:HB	3:K:1082:CYC:HMA1	1.70	0.57
1:K:56:VAL:HG22	1:K:86:ILE:HD12	1.85	0.57
1:I:30:ARG:NH2	4:I:2011:HOH:O	2.37	0.57
1:G:56:VAL:HG22	1:G:86:ILE:HD12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:ARG:HD2	4:F:2029:HOH:O	2.05	0.56
2:F:46:GLY:O	1:I:159:ASN:ND2	2.39	0.56
3:H:1082:CYC:HB	3:H:1082:CYC:CMA	2.19	0.56
3:B:1082:CYC:HB	3:B:1082:CYC:HMA1	1.70	0.56
1:A:30:ARG:NH2	4:A:2008:HOH:O	2.39	0.56
3:G:1082:CYC:HB	3:G:1082:CYC:HMA1	1.70	0.56
3:G:1082:CYC:HB	3:G:1082:CYC:CMA	2.19	0.56
3:I:1082:CYC:HB	3:I:1082:CYC:HMA1	1.71	0.55
1:C:17:ARG:CZ	1:G:2:LYS:NZ	2.69	0.55
1:C:2:LYS:HZ2	1:G:17:ARG:CZ	2.19	0.55
3:D:1082:CYC:CMA	3:D:1082:CYC:HB	2.20	0.55
2:D:151:GLY:HA3	3:D:1153:CYC:CMD	2.36	0.55
3:B:1153:CYC:HBC3	3:B:1153:CYC:HHD	1.88	0.55
2:L:127:VAL:HG22	3:L:1082:CYC:H3C	1.89	0.55
3:B:1082:CYC:HMD2	3:B:1082:CYC:HC	1.70	0.55
1:A:56:VAL:HG22	1:A:86:ILE:HD12	1.89	0.55
3:K:1082:CYC:HB	3:K:1082:CYC:CMA	2.20	0.55
3:I:1082:CYC:HB	3:I:1082:CYC:CMA	2.20	0.55
1:C:17:ARG:CZ	1:G:2:LYS:HZ1	2.20	0.54
1:C:32:GLN:HG2	4:C:2012:HOH:O	2.08	0.54
3:F:1153:CYC:NC	3:F:1153:CYC:HMD2	2.15	0.54
3:B:1153:CYC:NB	3:B:1153:CYC:HMA1	2.22	0.54
3:H:1082:CYC:HB	3:H:1082:CYC:HMA1	1.71	0.54
1:I:75:GLY:HA3	4:I:2027:HOH:O	2.07	0.54
3:J:1082:CYC:HC	3:J:1082:CYC:HMD2	1.74	0.53
1:A:17:ARG:CZ	1:K:2:LYS:NZ	2.71	0.53
2:J:21:GLU:HA	2:J:21:GLU:OE1	2.08	0.53
2:J:127:VAL:HG22	3:J:1082:CYC:H3C	1.91	0.53
1:C:23:GLU:OE2	1:G:7:GLU:OE1	2.27	0.53
3:D:1082:CYC:HMA1	3:D:1082:CYC:HB	1.74	0.53
2:H:119:ALA:HB3	4:H:2033:HOH:O	2.08	0.53
1:E:2:LYS:NZ	1:I:17:ARG:CZ	2.72	0.53
3:F:1082:CYC:HMA1	3:F:1082:CYC:NB	2.24	0.53
2:H:65:ASP:OD1	2:H:68:ARG:NH1	2.42	0.53
1:A:2:LYS:HZ1	1:K:17:ARG:CZ	2.22	0.52
1:G:99:ALA:HB2	2:H:9:ILE:CD1	2.39	0.52
2:D:2:GLN:OE1	2:D:6:THR:HG22	2.06	0.52
2:J:2:GLN:OE1	2:J:6:THR:HG22	2.05	0.52
3:L:1082:CYC:NB	3:L:1082:CYC:HMA1	2.25	0.52
2:H:127:VAL:HG22	3:H:1082:CYC:H3C	1.91	0.52
1:I:133:HIS:HD2	4:I:2022:HOH:O	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:GLY:O	1:I:79:GLN:HG3	2.11	0.51
3:J:1153:CYC:HMA1	3:J:1153:CYC:NB	2.26	0.51
2:D:2:GLN:HA	2:D:6:THR:HG21	1.93	0.51
3:L:1153:CYC:HBC3	3:L:1153:CYC:HHD	1.92	0.51
3:D:1153:CYC:HC	3:D:1153:CYC:CMD	2.21	0.51
3:F:1082:CYC:HB	3:F:1082:CYC:CMA	2.24	0.50
2:B:127:VAL:HG22	3:B:1082:CYC:H3C	1.94	0.50
1:E:17:ARG:CZ	1:I:2:LYS:NZ	2.74	0.50
3:H:1153:CYC:HB	3:H:1153:CYC:HMA1	1.77	0.50
3:F:1082:CYC:HC	3:F:1082:CYC:CMD	2.25	0.50
3:H:1082:CYC:HC	3:H:1082:CYC:CMD	2.24	0.49
2:B:2:GLN:HA	2:B:6:THR:HG21	1.94	0.49
3:L:1082:CYC:HB	3:L:1082:CYC:HMA1	1.78	0.49
2:F:127:VAL:HG22	3:F:1082:CYC:H3C	1.94	0.49
1:C:4:VAL:HG22	1:G:22:THR:O	2.13	0.49
3:L:1082:CYC:CMD	3:L:1082:CYC:HC	2.23	0.48
3:D:1082:CYC:CMD	3:D:1082:CYC:HC	2.26	0.48
3:L:1082:CYC:HB	3:L:1082:CYC:CMA	2.26	0.48
3:F:1082:CYC:HMA1	3:F:1082:CYC:HB	1.79	0.48
2:J:21:GLU:OE1	2:J:21:GLU:CA	2.61	0.48
1:C:56:VAL:CG2	1:C:86:ILE:HD12	2.43	0.48
1:E:56:VAL:CG2	1:E:86:ILE:HD12	2.44	0.48
2:L:151:GLY:HA3	3:L:1153:CYC:CMD	2.44	0.48
3:D:1153:CYC:NB	3:D:1153:CYC:HMA1	2.29	0.48
2:D:127:VAL:HG22	3:D:1082:CYC:H3C	1.94	0.48
1:C:88:HIS:HB3	3:C:1082:CYC:HBB3	1.96	0.47
1:G:19:LEU:O	2:H:45:THR:HG21	2.14	0.47
1:C:2:LYS:HZ1	1:G:17:ARG:CZ	2.25	0.47
1:K:56:VAL:CG2	1:K:86:ILE:HD12	2.44	0.47
1:A:108:TYR:O	2:F:75:PRO:HB2	2.15	0.47
3:D:1153:CYC:HHD	3:D:1153:CYC:HBC3	1.96	0.47
3:B:1153:CYC:HC	3:B:1153:CYC:CMD	2.19	0.47
1:E:88:HIS:CG	3:E:1082:CYC:HBB3	2.50	0.47
1:G:108:TYR:O	2:J:75:PRO:HB2	2.15	0.47
2:B:2:GLN:OE1	2:B:6:THR:HG22	2.09	0.46
2:B:2:GLN:HB3	2:B:6:THR:HG22	1.96	0.46
2:J:2:GLN:HA	2:J:6:THR:HG21	1.97	0.46
1:I:85:ASP:O	1:I:88:HIS:HB2	2.16	0.45
1:A:17:ARG:CZ	1:K:2:LYS:HZ1	2.29	0.45
1:I:56:VAL:CG2	1:I:86:ILE:HD12	2.44	0.45
3:J:1153:CYC:NC	3:J:1153:CYC:HMD2	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:O	1:G:4:VAL:HG22	2.16	0.45
3:F:1153:CYC:HMA1	3:F:1153:CYC:NB	2.29	0.45
3:H:1153:CYC:NC	3:H:1153:CYC:HMD2	2.27	0.45
2:J:2:GLN:HB3	2:J:6:THR:HG22	1.98	0.45
1:C:19:LEU:O	2:D:45:THR:HG21	2.17	0.45
1:A:4:VAL:HG22	1:K:22:THR:O	2.17	0.45
2:L:2:GLN:HA	2:L:6:THR:HG21	1.99	0.44
3:F:1153:CYC:HC	3:F:1153:CYC:CMD	2.19	0.44
2:H:151:GLY:HA3	3:H:1153:CYC:CMD	2.47	0.44
2:J:108:ARG:O	3:J:1082:CYC:HBB1	2.18	0.44
1:A:2:LYS:HZ2	1:K:17:ARG:CZ	2.31	0.44
1:E:2:LYS:HZ2	1:I:17:ARG:CZ	2.31	0.44
3:B:1082:CYC:HC	3:B:1082:CYC:CMD	2.31	0.44
2:F:53:SER:O	2:F:57:HIS:ND1	2.51	0.44
2:L:2:GLN:HB3	2:L:6:THR:HG22	2.00	0.44
2:D:151:GLY:HA3	3:D:1153:CYC:HMD1	1.99	0.44
3:E:1082:CYC:HC	3:E:1082:CYC:HMD2	1.80	0.43
2:D:2:GLN:HB3	2:D:6:THR:HG22	1.99	0.43
3:F:1153:CYC:HBC3	3:F:1153:CYC:HHD	1.99	0.43
2:F:87:GLU:HG2	4:F:2031:HOH:O	2.18	0.43
1:E:22:THR:O	1:I:4:VAL:HG22	2.18	0.43
2:L:125:ARG:HB2	4:L:2031:HOH:O	2.19	0.43
1:A:56:VAL:CG2	1:A:86:ILE:HD12	2.48	0.43
1:G:56:VAL:CG2	1:G:86:ILE:HD12	2.49	0.42
1:K:88:HIS:HB3	3:K:1082:CYC:HBB3	2.00	0.42
2:D:143:ASN:C	2:D:145:PRO:HD3	2.39	0.42
3:A:1082:CYC:NC	3:A:1082:CYC:CMD	2.74	0.42
3:B:1153:CYC:HB	3:B:1153:CYC:CMA	2.31	0.42
2:J:151:GLY:HA3	3:J:1153:CYC:CMD	2.50	0.42
1:C:99:ALA:HB2	2:D:9:ILE:HD11	2.02	0.42
2:D:46:GLY:O	1:G:159:ASN:ND2	2.52	0.42
1:I:65:TYR:O	1:I:71:GLN:HG3	2.20	0.42
1:A:25:GLN:HG2	1:K:33:ARG:HG2	2.02	0.42
3:G:1082:CYC:NC	3:G:1082:CYC:CMD	2.75	0.42
1:C:65:TYR:O	1:C:71:GLN:HG3	2.20	0.42
1:A:22:THR:O	1:K:4:VAL:HG22	2.19	0.42
3:L:1153:CYC:NB	3:L:1153:CYC:HMA1	2.33	0.41
2:F:72:ASN:O	3:F:1082:CYC:HMD2	2.20	0.41
1:E:4:VAL:HG22	1:I:22:THR:O	2.20	0.41
2:B:58:LYS:O	2:B:62:GLU:HG3	2.20	0.41
2:D:72:ASN:O	3:D:1082:CYC:HMD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:O	1:A:71:GLN:HG3	2.21	0.41
1:C:17:ARG:NH1	1:G:2:LYS:HZ1	2.19	0.41
2:F:2:GLN:HB3	2:F:6:THR:HG22	2.02	0.41
1:E:17:ARG:CZ	1:I:2:LYS:HZ2	2.34	0.41
1:E:19:LEU:O	2:F:45:THR:HG21	2.21	0.41
3:J:1082:CYC:HC	3:J:1082:CYC:CMD	2.33	0.41
2:J:72:ASN:O	3:J:1082:CYC:HMD2	2.20	0.41
1:C:75:GLY:O	1:C:79:GLN:HG3	2.20	0.41
2:D:6:THR:O	2:D:10:VAL:HG23	2.20	0.41
2:F:6:THR:O	2:F:10:VAL:HG23	2.20	0.41
2:F:2:GLN:HA	2:F:6:THR:HG21	2.02	0.41
2:F:151:GLY:HA3	3:F:1153:CYC:CMD	2.51	0.41
2:H:2:GLN:HB3	2:H:6:THR:HG22	2.03	0.40
1:E:2:LYS:HZ1	1:I:17:ARG:CZ	2.34	0.40
1:C:2:LYS:HZ1	1:G:17:ARG:NH1	2.19	0.40
2:H:6:THR:O	2:H:10:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/162 (99%)	160 (100%)	0	0	100	100
1	C	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	E	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	G	160/162 (99%)	160 (100%)	0	0	100	100
1	I	160/162 (99%)	160 (100%)	0	0	100	100
1	K	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	B	170/172 (99%)	166 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	F	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	H	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	J	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	L	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
All	All	1980/2004 (99%)	1954 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	130/130 (100%)	127 (98%)	3 (2%)	58	78
1	C	130/130 (100%)	128 (98%)	2 (2%)	72	87
1	E	130/130 (100%)	128 (98%)	2 (2%)	72	87
1	G	130/130 (100%)	127 (98%)	3 (2%)	58	78
1	I	130/130 (100%)	128 (98%)	2 (2%)	72	87
1	K	130/130 (100%)	128 (98%)	2 (2%)	72	87
2	B	134/134 (100%)	132 (98%)	2 (2%)	72	87
2	D	134/134 (100%)	130 (97%)	4 (3%)	48	70
2	F	134/134 (100%)	130 (97%)	4 (3%)	48	70
2	H	134/134 (100%)	130 (97%)	4 (3%)	48	70
2	J	134/134 (100%)	131 (98%)	3 (2%)	60	79
2	L	134/134 (100%)	133 (99%)	1 (1%)	88	95
All	All	1584/1584 (100%)	1552 (98%)	32 (2%)	63	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	30	ARG
1	A	32	GLN
2	B	6	THR
2	B	65	ASP
1	C	11	SER
1	C	30	ARG
2	D	6	THR
2	D	53	SER
2	D	65	ASP
2	D	166	LYS
1	E	11	SER
1	E	30	ARG
2	F	6	THR
2	F	21	GLU
2	F	53	SER
2	F	146	SER
1	G	11	SER
1	G	30	ARG
1	G	32	GLN
2	H	6	THR
2	H	53	SER
2	H	150	ARG
2	H	166	LYS
1	I	11	SER
1	I	30	ARG
2	J	6	THR
2	J	21	GLU
2	J	144	SER
1	K	11	SER
1	K	30	ARG
2	L	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	E	21	ASN
1	G	21	ASN
2	H	26	GLN
1	K	21	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	1082	1	35,46,46	3.38	12 (34%)	47,67,67	3.26	25 (53%)
3	CYC	B	1082	2	35,46,46	3.58	14 (40%)	47,67,67	3.17	20 (42%)
3	CYC	B	1153	2	35,46,46	3.32	12 (34%)	47,67,67	3.30	21 (44%)
3	CYC	C	1082	1	35,46,46	3.62	13 (37%)	47,67,67	3.29	21 (44%)
3	CYC	D	1082	2	35,46,46	3.52	14 (40%)	47,67,67	3.27	19 (40%)
3	CYC	D	1153	2	35,46,46	3.68	12 (34%)	47,67,67	3.21	18 (38%)
3	CYC	E	1082	1	35,46,46	3.60	12 (34%)	47,67,67	3.22	25 (53%)
3	CYC	F	1082	2	35,46,46	3.62	13 (37%)	47,67,67	2.99	19 (40%)
3	CYC	F	1153	2	35,46,46	3.31	12 (34%)	47,67,67	3.51	19 (40%)
3	CYC	G	1082	1	35,46,46	3.40	13 (37%)	47,67,67	3.15	21 (44%)
3	CYC	H	1082	2	35,46,46	3.56	12 (34%)	47,67,67	3.32	20 (42%)
3	CYC	H	1153	2	35,46,46	3.74	10 (28%)	47,67,67	3.36	16 (34%)
3	CYC	I	1082	1	35,46,46	3.53	12 (34%)	47,67,67	3.23	25 (53%)
3	CYC	J	1082	2	35,46,46	3.54	12 (34%)	47,67,67	3.46	22 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CYC	J	1153	2	35,46,46	3.73	12 (34%)	47,67,67	3.26	15 (31%)
3	CYC	K	1082	1	35,46,46	3.56	13 (37%)	47,67,67	3.09	23 (48%)
3	CYC	L	1082	2	35,46,46	3.59	13 (37%)	47,67,67	3.05	19 (40%)
3	CYC	L	1153	2	35,46,46	3.62	13 (37%)	47,67,67	3.32	15 (31%)

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	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	B	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	B	1153	2	-	2/21/74/74	0/4/4/4
3	CYC	C	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	D	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	D	1153	2	-	2/21/74/74	0/4/4/4
3	CYC	E	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	F	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	F	1153	2	-	2/21/74/74	0/4/4/4
3	CYC	G	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	H	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	H	1153	2	-	2/21/74/74	0/4/4/4
3	CYC	I	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	J	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	J	1153	2	-	2/21/74/74	0/4/4/4
3	CYC	K	1082	1	-	2/21/74/74	0/4/4/4
3	CYC	L	1082	2	-	2/21/74/74	0/4/4/4
3	CYC	L	1153	2	-	2/21/74/74	0/4/4/4

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1153	CYC	C1C-NC	-5.53	1.30	1.37
3	F	1082	CYC	C1C-NC	-4.66	1.31	1.37
3	A	1082	CYC	C1C-NC	-4.33	1.32	1.37
3	E	1082	CYC	C1C-NC	-4.30	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1082	CYC	C2C-C1C	-3.90	1.48	1.52
3	K	1082	CYC	C1C-NC	-3.84	1.32	1.37
3	C	1082	CYC	C1C-NC	-3.79	1.32	1.37
3	H	1153	CYC	C1C-NC	-3.65	1.33	1.37
3	K	1082	CYC	C2C-C1C	-3.59	1.48	1.52
3	J	1082	CYC	C2C-C1C	-3.52	1.48	1.52
3	L	1153	CYC	C1C-NC	-3.50	1.33	1.37
3	B	1153	CYC	C1C-NC	-3.36	1.33	1.37
3	J	1082	CYC	C1C-NC	-3.36	1.33	1.37
3	D	1082	CYC	C2C-C1C	-3.33	1.48	1.52
3	F	1153	CYC	C2C-C1C	-3.28	1.49	1.52
3	C	1082	CYC	C2C-C1C	-3.23	1.49	1.52
3	D	1153	CYC	C1C-NC	-3.22	1.33	1.37
3	G	1082	CYC	C1C-NC	-2.88	1.34	1.37
3	H	1082	CYC	C1C-NC	-2.85	1.34	1.37
3	I	1082	CYC	C2C-C1C	-2.67	1.49	1.52
3	D	1082	CYC	C1C-NC	-2.63	1.34	1.37
3	B	1082	CYC	C2C-C1C	-2.55	1.49	1.52
3	L	1082	CYC	C1C-NC	-2.55	1.34	1.37
3	F	1153	CYC	C1C-NC	-2.49	1.34	1.37
3	J	1153	CYC	C4C-NC	-2.43	1.32	1.37
3	C	1082	CYC	C1B-NB	-2.41	1.33	1.37
3	I	1082	CYC	C1C-NC	-2.29	1.34	1.37
3	B	1082	CYC	C1C-NC	-2.28	1.34	1.37
3	B	1153	CYC	C2C-C1C	-2.27	1.49	1.52
3	G	1082	CYC	C1B-NB	-2.26	1.33	1.37
3	H	1153	CYC	C4C-NC	-2.04	1.32	1.37
3	L	1153	CYC	C4B-NB	-2.03	1.33	1.37
3	B	1153	CYC	C4A-C3A	2.00	1.50	1.45
3	G	1082	CYC	C4D-CHA	2.05	1.48	1.40
3	K	1082	CYC	C4A-C3A	2.07	1.50	1.45
3	D	1153	CYC	C1A-C2A	2.08	1.49	1.45
3	A	1082	CYC	C4A-C3A	2.09	1.50	1.45
3	D	1082	CYC	C4A-C3A	2.10	1.50	1.45
3	K	1082	CYC	C1D-CHD	2.10	1.48	1.40
3	I	1082	CYC	C4A-C3A	2.11	1.50	1.45
3	A	1082	CYC	C1B-C2B	2.14	1.49	1.45
3	G	1082	CYC	C1A-C2A	2.16	1.49	1.45
3	J	1153	CYC	C1B-C2B	2.16	1.49	1.45
3	E	1082	CYC	C4A-C3A	2.16	1.50	1.45
3	F	1082	CYC	C4A-C3A	2.21	1.50	1.45
3	K	1082	CYC	C4D-CHA	2.21	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1153	CYC	C1B-C2B	2.22	1.49	1.45
3	C	1082	CYC	C4D-CHA	2.22	1.48	1.40
3	L	1153	CYC	C4A-C3A	2.23	1.50	1.45
3	I	1082	CYC	C1B-C2B	2.24	1.49	1.45
3	L	1082	CYC	C4D-CHA	2.25	1.48	1.40
3	F	1082	CYC	C1D-CHD	2.27	1.49	1.40
3	F	1082	CYC	C4D-CHA	2.30	1.49	1.40
3	F	1153	CYC	C1B-C2B	2.31	1.49	1.45
3	D	1082	CYC	C4D-CHA	2.34	1.49	1.40
3	C	1082	CYC	C1D-CHD	2.37	1.49	1.40
3	J	1153	CYC	C4D-CHA	2.37	1.49	1.40
3	F	1082	CYC	C1A-C2A	2.37	1.49	1.45
3	F	1153	CYC	C4A-C3A	2.42	1.51	1.45
3	D	1082	CYC	C1A-C2A	2.43	1.49	1.45
3	L	1153	CYC	C4D-CHA	2.44	1.49	1.40
3	G	1082	CYC	C1D-CHD	2.44	1.49	1.40
3	A	1082	CYC	C1A-C2A	2.45	1.49	1.45
3	A	1082	CYC	C1D-CHD	2.45	1.49	1.40
3	B	1082	CYC	C4D-CHA	2.46	1.49	1.40
3	K	1082	CYC	C1B-C2B	2.47	1.49	1.45
3	E	1082	CYC	C1D-CHD	2.48	1.49	1.40
3	D	1153	CYC	C4D-CHA	2.49	1.49	1.40
3	H	1082	CYC	C1D-CHD	2.49	1.49	1.40
3	L	1082	CYC	C1B-C2B	2.50	1.49	1.45
3	B	1153	CYC	C1B-C2B	2.51	1.49	1.45
3	B	1082	CYC	C4A-C3A	2.52	1.51	1.45
3	J	1082	CYC	C4D-CHA	2.52	1.49	1.40
3	F	1082	CYC	C1B-C2B	2.53	1.49	1.45
3	L	1153	CYC	OB-C4B	2.54	1.28	1.23
3	H	1082	CYC	C4D-CHA	2.54	1.50	1.40
3	H	1153	CYC	C1D-CHD	2.55	1.50	1.40
3	H	1082	CYC	C1B-C2B	2.56	1.49	1.45
3	L	1153	CYC	C1D-CHD	2.58	1.50	1.40
3	J	1082	CYC	C1D-CHD	2.60	1.50	1.40
3	I	1082	CYC	C1A-C2A	2.60	1.50	1.45
3	G	1082	CYC	C1B-C2B	2.63	1.50	1.45
3	L	1082	CYC	C1A-C2A	2.65	1.50	1.45
3	L	1082	CYC	C1D-CHD	2.65	1.50	1.40
3	D	1153	CYC	C1D-CHD	2.66	1.50	1.40
3	J	1082	CYC	OB-C4B	2.66	1.28	1.23
3	D	1153	CYC	C1B-C2B	2.67	1.50	1.45
3	H	1153	CYC	OB-C4B	2.68	1.28	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1153	CYC	C1D-CHD	2.72	1.50	1.40
3	B	1082	CYC	C1B-C2B	2.73	1.50	1.45
3	B	1153	CYC	OB-C4B	2.73	1.28	1.23
3	B	1082	CYC	C1D-CHD	2.78	1.50	1.40
3	L	1082	CYC	C4A-C3A	2.80	1.51	1.45
3	J	1082	CYC	C1B-C2B	2.81	1.50	1.45
3	E	1082	CYC	C1A-C2A	2.82	1.50	1.45
3	D	1082	CYC	C1B-C2B	2.86	1.50	1.45
3	J	1153	CYC	C1D-CHD	2.86	1.51	1.40
3	D	1082	CYC	C1D-CHD	2.89	1.51	1.40
3	A	1082	CYC	OB-C4B	2.93	1.29	1.23
3	B	1082	CYC	C1A-C2A	2.94	1.50	1.45
3	G	1082	CYC	OB-C4B	2.96	1.29	1.23
3	B	1153	CYC	C1D-CHD	3.02	1.51	1.40
3	L	1082	CYC	OB-C4B	3.05	1.29	1.23
3	F	1153	CYC	CHB-C4A	3.07	1.48	1.40
3	H	1082	CYC	OB-C4B	3.09	1.29	1.23
3	C	1082	CYC	C3D-C2D	3.10	1.46	1.37
3	C	1082	CYC	C1B-C2B	3.10	1.50	1.45
3	D	1082	CYC	C3D-C2D	3.12	1.46	1.37
3	D	1082	CYC	OB-C4B	3.14	1.29	1.23
3	J	1082	CYC	C3D-C2D	3.16	1.47	1.37
3	J	1153	CYC	OB-C4B	3.21	1.29	1.23
3	H	1082	CYC	C3D-C2D	3.23	1.47	1.37
3	B	1082	CYC	C3D-C2D	3.25	1.47	1.37
3	E	1082	CYC	C3D-C2D	3.27	1.47	1.37
3	F	1082	CYC	OB-C4B	3.30	1.29	1.23
3	E	1082	CYC	C1B-C2B	3.33	1.51	1.45
3	L	1082	CYC	C3D-C2D	3.37	1.47	1.37
3	H	1153	CYC	C3D-C2D	3.41	1.47	1.37
3	J	1153	CYC	CHB-C4A	3.41	1.48	1.40
3	F	1153	CYC	C3D-C2D	3.42	1.47	1.37
3	H	1153	CYC	CHB-C4A	3.42	1.48	1.40
3	C	1082	CYC	CHB-C4A	3.43	1.49	1.40
3	K	1082	CYC	C3D-C2D	3.45	1.47	1.37
3	B	1082	CYC	OB-C4B	3.46	1.30	1.23
3	I	1082	CYC	C3D-C2D	3.47	1.47	1.37
3	L	1153	CYC	CHB-C4A	3.48	1.49	1.40
3	F	1082	CYC	C3D-C2D	3.49	1.48	1.37
3	K	1082	CYC	OB-C4B	3.50	1.30	1.23
3	A	1082	CYC	C3D-C2D	3.52	1.48	1.37
3	B	1153	CYC	C3D-C2D	3.57	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1082	CYC	C3D-C2D	3.57	1.48	1.37
3	D	1153	CYC	OB-C4B	3.59	1.30	1.23
3	A	1082	CYC	CHB-C4A	3.61	1.49	1.40
3	I	1082	CYC	CHB-C4A	3.66	1.49	1.40
3	B	1153	CYC	CHB-C4A	3.67	1.49	1.40
3	F	1082	CYC	CHB-C4A	3.68	1.49	1.40
3	I	1082	CYC	OB-C4B	3.68	1.30	1.23
3	B	1082	CYC	CHB-C4A	3.69	1.49	1.40
3	J	1153	CYC	C3D-C2D	3.70	1.48	1.37
3	K	1082	CYC	CHB-C4A	3.76	1.49	1.40
3	L	1153	CYC	C3D-C2D	3.82	1.49	1.37
3	E	1082	CYC	OB-C4B	3.82	1.30	1.23
3	D	1153	CYC	C3D-C2D	3.87	1.49	1.37
3	J	1082	CYC	CHB-C4A	3.93	1.50	1.40
3	C	1082	CYC	OB-C4B	3.96	1.31	1.23
3	E	1082	CYC	CHB-C4A	3.97	1.50	1.40
3	D	1082	CYC	CHB-C4A	3.97	1.50	1.40
3	D	1153	CYC	CHB-C4A	3.99	1.50	1.40
3	G	1082	CYC	CHB-C4A	4.01	1.50	1.40
3	F	1153	CYC	CHB-C1B	4.01	1.47	1.37
3	H	1082	CYC	CHB-C4A	4.05	1.50	1.40
3	F	1153	CYC	OB-C4B	4.11	1.31	1.23
3	L	1082	CYC	CHB-C4A	4.21	1.50	1.40
3	J	1153	CYC	CHB-C1B	4.22	1.47	1.37
3	H	1153	CYC	CHB-C1B	4.41	1.48	1.37
3	D	1153	CYC	CHB-C1B	4.47	1.48	1.37
3	B	1153	CYC	CHB-C1B	4.58	1.48	1.37
3	J	1082	CYC	CHB-C1B	4.61	1.48	1.37
3	E	1082	CYC	CHB-C1B	4.75	1.49	1.37
3	D	1153	CYC	C2A-C3A	4.77	1.47	1.36
3	L	1153	CYC	CHB-C1B	4.83	1.49	1.37
3	F	1082	CYC	CHB-C1B	4.86	1.49	1.37
3	B	1153	CYC	C2A-C3A	4.90	1.47	1.36
3	H	1082	CYC	C2A-C3A	4.93	1.47	1.36
3	H	1153	CYC	C2A-C3A	4.94	1.47	1.36
3	A	1082	CYC	CHB-C1B	4.96	1.49	1.37
3	I	1082	CYC	CHB-C1B	5.00	1.49	1.37
3	F	1082	CYC	C2A-C3A	5.05	1.47	1.36
3	C	1082	CYC	CHB-C1B	5.07	1.49	1.37
3	K	1082	CYC	C2A-C3A	5.08	1.47	1.36
3	H	1082	CYC	CHB-C1B	5.10	1.49	1.37
3	L	1082	CYC	CHB-C1B	5.11	1.50	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1082	CYC	CHB-C1B	5.12	1.50	1.37
3	J	1082	CYC	C2A-C3A	5.16	1.47	1.36
3	K	1082	CYC	CHB-C1B	5.18	1.50	1.37
3	F	1153	CYC	C3B-C2B	5.20	1.48	1.36
3	D	1082	CYC	CHB-C1B	5.22	1.50	1.37
3	D	1153	CYC	C3B-C2B	5.30	1.48	1.36
3	L	1153	CYC	C2A-C3A	5.31	1.48	1.36
3	B	1082	CYC	CHB-C1B	5.38	1.50	1.37
3	D	1082	CYC	C2A-C3A	5.42	1.48	1.36
3	L	1082	CYC	C2A-C3A	5.42	1.48	1.36
3	H	1082	CYC	C3B-C2B	5.48	1.48	1.36
3	B	1082	CYC	C2A-C3A	5.50	1.48	1.36
3	A	1082	CYC	C2A-C3A	5.50	1.48	1.36
3	G	1082	CYC	C2A-C3A	5.52	1.48	1.36
3	I	1082	CYC	C2A-C3A	5.60	1.48	1.36
3	C	1082	CYC	C3B-C2B	5.69	1.49	1.36
3	J	1153	CYC	C3B-C2B	5.70	1.49	1.36
3	F	1153	CYC	C2A-C3A	5.70	1.49	1.36
3	E	1082	CYC	C2A-C3A	5.71	1.49	1.36
3	J	1153	CYC	C2A-C3A	5.76	1.49	1.36
3	H	1153	CYC	C3B-C2B	5.78	1.49	1.36
3	C	1082	CYC	C2A-C3A	5.86	1.49	1.36
3	D	1082	CYC	C3B-C2B	5.88	1.49	1.36
3	G	1082	CYC	C3B-C2B	5.90	1.49	1.36
3	L	1153	CYC	C3B-C2B	6.00	1.49	1.36
3	L	1082	CYC	C3B-C2B	6.06	1.49	1.36
3	B	1153	CYC	C3B-C2B	6.09	1.49	1.36
3	F	1082	CYC	C3B-C2B	6.28	1.50	1.36
3	K	1082	CYC	C3B-C2B	6.29	1.50	1.36
3	B	1082	CYC	C3B-C2B	6.30	1.50	1.36
3	I	1082	CYC	C3B-C2B	6.33	1.50	1.36
3	E	1082	CYC	C3B-C2B	6.41	1.50	1.36
3	J	1082	CYC	C3B-C2B	6.61	1.51	1.36
3	A	1082	CYC	C3B-C2B	6.86	1.51	1.36
3	A	1082	CYC	CHA-C1A	14.43	1.47	1.35
3	F	1153	CYC	CHA-C1A	14.71	1.48	1.35
3	B	1153	CYC	CHA-C1A	14.80	1.48	1.35
3	G	1082	CYC	CHA-C1A	15.07	1.48	1.35
3	D	1082	CYC	CHA-C1A	15.60	1.49	1.35
3	E	1082	CYC	CHA-C1A	15.69	1.49	1.35
3	J	1082	CYC	CHA-C1A	15.80	1.49	1.35
3	K	1082	CYC	CHA-C1A	15.82	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1082	CYC	CHA-C1A	15.84	1.49	1.35
3	B	1082	CYC	CHA-C1A	15.97	1.49	1.35
3	C	1082	CYC	CHA-C1A	16.16	1.49	1.35
3	H	1082	CYC	CHA-C1A	16.25	1.49	1.35
3	L	1082	CYC	CHA-C1A	16.34	1.49	1.35
3	F	1082	CYC	CHA-C1A	16.54	1.49	1.35
3	L	1153	CYC	CHA-C1A	16.80	1.50	1.35
3	J	1153	CYC	CHA-C1A	17.17	1.50	1.35
3	D	1153	CYC	CHA-C1A	17.55	1.50	1.35
3	H	1153	CYC	CHA-C1A	18.30	1.51	1.35

All (363) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1082	CYC	C4B-C3B-C2B	-12.34	101.01	108.05
3	L	1153	CYC	C4B-C3B-C2B	-11.90	101.26	108.05
3	C	1082	CYC	C4B-C3B-C2B	-11.88	101.27	108.05
3	J	1082	CYC	C4B-C3B-C2B	-11.85	101.28	108.05
3	G	1082	CYC	C4B-C3B-C2B	-11.63	101.41	108.05
3	D	1082	CYC	C4B-C3B-C2B	-11.59	101.43	108.05
3	B	1082	CYC	C4B-C3B-C2B	-11.43	101.53	108.05
3	L	1082	CYC	C4B-C3B-C2B	-11.19	101.66	108.05
3	E	1082	CYC	C4B-C3B-C2B	-11.17	101.67	108.05
3	K	1082	CYC	C4B-C3B-C2B	-10.94	101.81	108.05
3	H	1082	CYC	C4B-C3B-C2B	-10.89	101.83	108.05
3	J	1153	CYC	C4B-C3B-C2B	-10.71	101.93	108.05
3	I	1082	CYC	C4B-C3B-C2B	-10.68	101.95	108.05
3	F	1082	CYC	C4B-C3B-C2B	-10.54	102.03	108.05
3	B	1153	CYC	C4B-C3B-C2B	-10.44	102.09	108.05
3	H	1153	CYC	C4B-C3B-C2B	-10.37	102.13	108.05
3	F	1153	CYC	C4B-C3B-C2B	-9.60	102.57	108.05
3	H	1082	CYC	OC-C1C-C2C	-9.13	118.88	126.25
3	D	1153	CYC	C4B-C3B-C2B	-9.01	102.90	108.05
3	J	1082	CYC	OC-C1C-C2C	-8.64	119.27	126.25
3	F	1153	CYC	OB-C4B-C3B	-7.22	119.44	128.09
3	F	1153	CYC	OC-C1C-C2C	-6.73	120.81	126.25
3	B	1153	CYC	OB-C4B-C3B	-6.38	120.44	128.09
3	D	1082	CYC	OC-C1C-C2C	-6.24	121.21	126.25
3	B	1082	CYC	OC-C1C-C2C	-6.24	121.21	126.25
3	H	1153	CYC	OB-C4B-C3B	-6.21	120.64	128.09
3	F	1153	CYC	CHB-C4A-NA	-6.12	113.26	124.91
3	D	1153	CYC	OB-C4B-C3B	-5.86	121.07	128.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1082	CYC	OB-C4B-C3B	-5.66	121.31	128.09
3	L	1153	CYC	CHB-C4A-NA	-5.64	114.17	124.91
3	J	1153	CYC	CHB-C4A-NA	-5.58	114.28	124.91
3	H	1153	CYC	CHB-C4A-NA	-5.34	114.74	124.91
3	D	1082	CYC	OB-C4B-C3B	-5.26	121.78	128.09
3	B	1153	CYC	CHB-C4A-NA	-5.00	115.40	124.91
3	D	1153	CYC	CHB-C4A-NA	-4.94	115.49	124.91
3	F	1153	CYC	C4A-C3A-C2A	-4.56	101.04	106.50
3	E	1082	CYC	CBD-CAD-C3D	-4.55	104.38	112.53
3	J	1082	CYC	OB-C4B-C3B	-4.54	122.64	128.09
3	H	1153	CYC	C4A-C3A-C2A	-4.53	101.08	106.50
3	H	1153	CYC	C1B-C2B-C3B	-4.48	103.03	107.81
3	B	1153	CYC	C1B-C2B-C3B	-4.43	103.08	107.81
3	F	1082	CYC	OB-C4B-C3B	-4.40	122.82	128.09
3	J	1153	CYC	C4A-C3A-C2A	-4.32	101.34	106.50
3	L	1082	CYC	OB-C4B-C3B	-4.27	122.98	128.09
3	G	1082	CYC	CBD-CAD-C3D	-4.26	104.90	112.53
3	D	1153	CYC	C1B-C2B-C3B	-4.24	103.29	107.81
3	I	1082	CYC	CMC-C2C-C1C	-4.13	103.75	112.43
3	D	1153	CYC	OC-C1C-C2C	-4.11	122.93	126.25
3	J	1082	CYC	CBD-CAD-C3D	-4.11	105.17	112.53
3	D	1153	CYC	C4A-C3A-C2A	-4.09	101.61	106.50
3	A	1082	CYC	CBD-CAD-C3D	-4.07	105.24	112.53
3	L	1082	CYC	OC-C1C-C2C	-4.06	122.97	126.25
3	J	1153	CYC	C1B-C2B-C3B	-4.05	103.50	107.81
3	G	1082	CYC	OB-C4B-C3B	-4.04	123.25	128.09
3	A	1082	CYC	CAA-CBA-CGA	-4.00	105.42	112.75
3	I	1082	CYC	OB-C4B-C3B	-4.00	123.30	128.09
3	H	1153	CYC	C1B-NB-C4B	-3.99	104.89	110.73
3	K	1082	CYC	CBD-CAD-C3D	-3.99	105.38	112.53
3	D	1153	CYC	C1B-NB-C4B	-3.98	104.90	110.73
3	B	1153	CYC	C1B-NB-C4B	-3.95	104.95	110.73
3	B	1153	CYC	OC-C1C-C2C	-3.95	123.06	126.25
3	L	1153	CYC	OB-C4B-C3B	-3.95	123.36	128.09
3	F	1082	CYC	C1B-C2B-C3B	-3.92	103.63	107.81
3	E	1082	CYC	OB-C4B-C3B	-3.91	123.40	128.09
3	C	1082	CYC	OC-C1C-C2C	-3.89	123.11	126.25
3	I	1082	CYC	C2C-C1C-NC	-3.88	104.59	108.30
3	K	1082	CYC	CMC-C2C-C1C	-3.87	104.30	112.43
3	J	1082	CYC	C1B-C2B-C3B	-3.84	103.72	107.81
3	L	1082	CYC	C1B-C2B-C3B	-3.81	103.75	107.81
3	L	1082	CYC	CBD-CAD-C3D	-3.78	105.75	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1082	CYC	CBD-CAD-C3D	-3.76	105.79	112.53
3	F	1153	CYC	C1B-C2B-C3B	-3.75	103.81	107.81
3	L	1153	CYC	C1B-C2B-C3B	-3.74	103.82	107.81
3	F	1082	CYC	CHB-C4A-NA	-3.73	117.81	124.91
3	E	1082	CYC	C1B-C2B-C3B	-3.72	103.84	107.81
3	I	1082	CYC	C1B-C2B-C3B	-3.69	103.87	107.81
3	F	1153	CYC	C1B-NB-C4B	-3.69	105.33	110.73
3	K	1082	CYC	CAA-CBA-CGA	-3.68	106.00	112.75
3	E	1082	CYC	CAA-CBA-CGA	-3.68	106.00	112.75
3	L	1153	CYC	C4A-C3A-C2A	-3.67	102.11	106.50
3	E	1082	CYC	C4A-C3A-C2A	-3.60	102.19	106.50
3	B	1082	CYC	C1A-C2A-C3A	-3.57	102.83	106.81
3	C	1082	CYC	CAA-CBA-CGA	-3.56	106.22	112.75
3	B	1082	CYC	CHB-C4A-NA	-3.56	118.13	124.91
3	G	1082	CYC	CAA-CBA-CGA	-3.54	106.27	112.75
3	H	1153	CYC	OC-C1C-C2C	-3.53	123.40	126.25
3	B	1082	CYC	C1B-C2B-C3B	-3.53	104.05	107.81
3	A	1082	CYC	CMC-C2C-C1C	-3.52	105.04	112.43
3	J	1153	CYC	C1B-NB-C4B	-3.49	105.63	110.73
3	D	1082	CYC	C1B-C2B-C3B	-3.46	104.12	107.81
3	D	1082	CYC	C1A-C2A-C3A	-3.45	102.96	106.81
3	I	1082	CYC	CAA-CBA-CGA	-3.44	106.43	112.75
3	K	1082	CYC	OB-C4B-C3B	-3.44	123.97	128.09
3	J	1082	CYC	C1A-C2A-C3A	-3.44	102.97	106.81
3	J	1082	CYC	CHB-C4A-NA	-3.44	118.37	124.91
3	C	1082	CYC	C4A-C3A-C2A	-3.43	102.40	106.50
3	E	1082	CYC	CMC-C2C-C1C	-3.42	105.25	112.43
3	B	1082	CYC	CBD-CAD-C3D	-3.42	106.40	112.53
3	H	1082	CYC	C1B-C2B-C3B	-3.41	104.17	107.81
3	J	1153	CYC	OB-C4B-C3B	-3.41	124.01	128.09
3	K	1082	CYC	C1B-C2B-C3B	-3.40	104.19	107.81
3	F	1082	CYC	CBD-CAD-C3D	-3.39	106.45	112.53
3	I	1082	CYC	CAD-CBD-CGD	-3.38	106.56	112.75
3	I	1082	CYC	CBD-CAD-C3D	-3.36	106.50	112.53
3	F	1082	CYC	C1A-C2A-C3A	-3.36	103.06	106.81
3	D	1082	CYC	CBD-CAD-C3D	-3.34	106.55	112.53
3	L	1082	CYC	C1A-C2A-C3A	-3.33	103.10	106.81
3	A	1082	CYC	C2C-C1C-NC	-3.33	105.12	108.30
3	G	1082	CYC	C4A-C3A-C2A	-3.33	102.52	106.50
3	D	1082	CYC	C1B-NB-C4B	-3.30	105.90	110.73
3	C	1082	CYC	C1B-C2B-C3B	-3.30	104.29	107.81
3	B	1082	CYC	OB-C4B-C3B	-3.29	124.14	128.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1082	CYC	C1A-C2A-C3A	-3.29	103.14	106.81
3	L	1082	CYC	CHB-C4A-NA	-3.26	118.69	124.91
3	H	1082	CYC	C1A-C2A-C3A	-3.26	103.17	106.81
3	H	1153	CYC	CHB-C1B-C2B	-3.22	120.19	126.89
3	A	1082	CYC	C1B-C2B-C3B	-3.22	104.37	107.81
3	H	1082	CYC	CBD-CAD-C3D	-3.21	106.77	112.53
3	C	1082	CYC	CHB-C4A-NA	-3.20	118.81	124.91
3	E	1082	CYC	C1A-C2A-C3A	-3.19	103.25	106.81
3	J	1082	CYC	C3C-C2C-C1C	-3.18	100.74	103.41
3	D	1153	CYC	CHB-C1B-C2B	-3.18	120.28	126.89
3	F	1082	CYC	OC-C1C-C2C	-3.18	123.69	126.25
3	L	1153	CYC	C1B-NB-C4B	-3.17	106.09	110.73
3	H	1082	CYC	C1B-NB-C4B	-3.16	106.11	110.73
3	I	1082	CYC	C4A-C3A-C2A	-3.16	102.72	106.50
3	E	1082	CYC	CHA-C1A-NA	-3.12	123.09	128.67
3	F	1082	CYC	C1B-NB-C4B	-3.09	106.21	110.73
3	G	1082	CYC	C1B-C2B-C3B	-3.07	104.54	107.81
3	D	1082	CYC	CHB-C4A-NA	-3.07	119.07	124.91
3	B	1153	CYC	C4A-C3A-C2A	-3.04	102.86	106.50
3	K	1082	CYC	CHA-C1A-NA	-3.03	123.26	128.67
3	H	1082	CYC	CHB-C4A-NA	-3.02	119.15	124.91
3	A	1082	CYC	CHA-C1A-NA	-3.02	123.27	128.67
3	E	1082	CYC	CHB-C4A-NA	-2.99	119.21	124.91
3	B	1153	CYC	C1A-C2A-C3A	-2.96	103.50	106.81
3	J	1082	CYC	C1B-NB-C4B	-2.93	106.44	110.73
3	I	1082	CYC	CHB-C4A-NA	-2.88	119.42	124.91
3	B	1082	CYC	C1B-NB-C4B	-2.85	106.56	110.73
3	C	1082	CYC	C1B-NB-C4B	-2.83	106.59	110.73
3	G	1082	CYC	CHA-C1A-NA	-2.81	123.64	128.67
3	G	1082	CYC	CHB-C4A-NA	-2.81	119.56	124.91
3	I	1082	CYC	CHA-C1A-NA	-2.77	123.73	128.67
3	B	1082	CYC	C4A-C3A-C2A	-2.75	103.21	106.50
3	B	1153	CYC	CHB-C1B-C2B	-2.74	121.20	126.89
3	J	1082	CYC	CHA-C1A-NA	-2.71	123.82	128.67
3	I	1082	CYC	C1B-NB-C4B	-2.69	106.79	110.73
3	D	1082	CYC	CHA-C1A-NA	-2.68	123.88	128.67
3	B	1153	CYC	C3C-C2C-C1C	-2.68	101.17	103.41
3	J	1082	CYC	C4A-C3A-C2A	-2.67	103.31	106.50
3	C	1082	CYC	CMC-C2C-C1C	-2.66	106.83	112.43
3	E	1082	CYC	CAD-CBD-CGD	-2.64	107.92	112.75
3	L	1082	CYC	C1B-NB-C4B	-2.63	106.88	110.73
3	L	1082	CYC	C4A-C3A-C2A	-2.63	103.36	106.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1082	CYC	C4A-C3A-C2A	-2.62	103.36	106.50
3	K	1082	CYC	CHB-C4A-NA	-2.61	119.94	124.91
3	F	1082	CYC	CHA-C1A-NA	-2.58	124.07	128.67
3	E	1082	CYC	C1B-NB-C4B	-2.57	106.97	110.73
3	A	1082	CYC	CHB-C4A-NA	-2.57	120.02	124.91
3	I	1082	CYC	OC-C1C-C2C	-2.56	124.19	126.25
3	K	1082	CYC	C4A-C3A-C2A	-2.52	103.49	106.50
3	K	1082	CYC	C1A-C2A-C3A	-2.52	104.00	106.81
3	G	1082	CYC	CMC-C2C-C1C	-2.50	107.18	112.43
3	F	1153	CYC	CHB-C1B-C2B	-2.49	121.71	126.89
3	A	1082	CYC	C4A-C3A-C2A	-2.49	103.53	106.50
3	C	1082	CYC	OB-C4B-C3B	-2.49	125.11	128.09
3	J	1153	CYC	CHB-C1B-C2B	-2.49	121.72	126.89
3	F	1153	CYC	CAC-C3C-C4C	-2.47	106.34	112.67
3	C	1082	CYC	CHA-C1A-NA	-2.44	124.31	128.67
3	B	1082	CYC	CHA-C1A-NA	-2.43	124.32	128.67
3	L	1153	CYC	C3C-C2C-C1C	-2.43	101.37	103.41
3	L	1082	CYC	CHA-C1A-NA	-2.38	124.41	128.67
3	I	1082	CYC	C1A-C2A-C3A	-2.37	104.17	106.81
3	H	1082	CYC	C4A-C3A-C2A	-2.36	103.68	106.50
3	G	1082	CYC	C1B-NB-C4B	-2.36	107.28	110.73
3	J	1153	CYC	C3C-C2C-C1C	-2.35	101.44	103.41
3	A	1082	CYC	C1B-NB-C4B	-2.34	107.32	110.73
3	H	1082	CYC	CHA-C1A-NA	-2.33	124.51	128.67
3	C	1082	CYC	C1A-C2A-C3A	-2.32	104.22	106.81
3	A	1082	CYC	CBC-CAC-C3C	-2.25	108.07	113.57
3	K	1082	CYC	CAD-CBD-CGD	-2.25	108.63	112.75
3	L	1153	CYC	CHB-C1B-C2B	-2.21	122.29	126.89
3	C	1082	CYC	CAD-CBD-CGD	-2.17	108.76	112.75
3	D	1153	CYC	CHA-C1A-NA	-2.16	124.80	128.67
3	E	1082	CYC	CBC-CAC-C3C	-2.16	108.28	113.57
3	K	1082	CYC	OC-C1C-C2C	-2.14	124.52	126.25
3	G	1082	CYC	CAD-CBD-CGD	-2.14	108.82	112.75
3	A	1082	CYC	OB-C4B-NB	-2.14	119.45	125.14
3	G	1082	CYC	C2C-C1C-NC	-2.13	106.26	108.30
3	A	1082	CYC	OB-C4B-C3B	-2.11	125.56	128.09
3	D	1153	CYC	CAC-C3C-C2C	-2.11	108.82	114.13
3	F	1153	CYC	CHA-C1A-C2A	-2.11	120.61	125.55
3	B	1153	CYC	CHA-C1A-C2A	-2.10	120.62	125.55
3	J	1153	CYC	CBD-CAD-C3D	-2.09	108.79	112.53
3	G	1082	CYC	C1A-C2A-C3A	-2.08	104.49	106.81
3	K	1082	CYC	C1B-NB-C4B	-2.08	107.69	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1082	CYC	C2C-C1C-NC	-2.05	106.34	108.30
3	C	1082	CYC	OB-C4B-NB	-2.03	119.75	125.14
3	K	1082	CYC	C2C-C1C-NC	-2.03	106.36	108.30
3	D	1082	CYC	C4A-C3A-C2A	-2.03	104.08	106.50
3	E	1082	CYC	C2C-C1C-NC	-2.02	106.37	108.30
3	J	1082	CYC	CAD-CBD-CGD	-2.01	109.07	112.75
3	B	1153	CYC	CAC-C3C-C4C	-2.00	107.53	112.67
3	L	1153	CYC	C2C-C3C-C4C	2.00	104.89	101.50
3	B	1082	CYC	C2C-C1C-NC	2.00	110.21	108.30
3	F	1082	CYC	CMB-C2B-C1B	2.01	126.87	124.20
3	D	1082	CYC	CAA-C2A-C1A	2.01	128.66	125.06
3	I	1082	CYC	CAA-C2A-C1A	2.02	128.67	125.06
3	A	1082	CYC	CAB-C3B-C2B	2.05	131.10	127.51
3	H	1153	CYC	CAD-C3D-C4D	2.06	129.25	127.01
3	G	1082	CYC	C3C-C4C-NC	2.07	110.00	107.93
3	H	1082	CYC	CAA-C2A-C1A	2.07	128.76	125.06
3	G	1082	CYC	C2A-C1A-NA	2.07	113.08	109.86
3	E	1082	CYC	CAB-C3B-C2B	2.07	131.14	127.51
3	I	1082	CYC	CAB-C3B-C2B	2.08	131.16	127.51
3	A	1082	CYC	C3C-C2C-C1C	2.09	105.16	103.41
3	J	1082	CYC	CAA-C2A-C1A	2.09	128.80	125.06
3	L	1082	CYC	CAA-C2A-C1A	2.09	128.80	125.06
3	B	1082	CYC	C2C-C3C-C4C	2.10	105.06	101.50
3	A	1082	CYC	C3C-C4C-NC	2.10	110.03	107.93
3	B	1082	CYC	CAA-C2A-C1A	2.14	128.89	125.06
3	E	1082	CYC	CAA-C2A-C1A	2.15	128.91	125.06
3	K	1082	CYC	C3C-C4C-NC	2.16	110.09	107.93
3	D	1153	CYC	CHB-C4A-C3A	2.16	130.15	124.88
3	J	1082	CYC	C2C-C3C-C4C	2.21	105.25	101.50
3	H	1153	CYC	C2C-C1C-NC	2.22	110.42	108.30
3	A	1082	CYC	CAA-C2A-C1A	2.25	129.08	125.06
3	K	1082	CYC	CAA-C2A-C1A	2.26	129.10	125.06
3	H	1153	CYC	CMB-C2B-C1B	2.26	127.21	124.20
3	F	1082	CYC	CAA-C2A-C1A	2.27	129.12	125.06
3	H	1082	CYC	CMB-C2B-C1B	2.28	127.23	124.20
3	D	1082	CYC	CMB-C2B-C1B	2.34	127.31	124.20
3	K	1082	CYC	C2A-C1A-NA	2.34	113.50	109.86
3	I	1082	CYC	C2A-C1A-NA	2.34	113.50	109.86
3	B	1082	CYC	CAB-C3B-C2B	2.35	131.62	127.51
3	I	1082	CYC	C3C-C4C-NC	2.38	110.31	107.93
3	E	1082	CYC	C3C-C4C-NC	2.41	110.34	107.93
3	L	1082	CYC	CMB-C2B-C1B	2.43	127.43	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	1082	CYC	C2C-C1C-NC	2.43	110.62	108.30
3	B	1153	CYC	CHB-C4A-C3A	2.44	130.85	124.88
3	L	1082	CYC	CAB-C3B-C2B	2.45	131.81	127.51
3	J	1082	CYC	OC-C1C-NC	2.46	127.81	124.83
3	D	1153	CYC	CAD-CBD-CGD	2.47	117.27	112.75
3	A	1082	CYC	OC-C1C-C2C	2.49	128.26	126.25
3	A	1082	CYC	C2A-C1A-NA	2.51	113.76	109.86
3	B	1153	CYC	CAA-CBA-CGA	2.52	117.37	112.75
3	B	1153	CYC	CMB-C2B-C1B	2.54	127.58	124.20
3	D	1082	CYC	C2A-C1A-NA	2.54	113.81	109.86
3	D	1082	CYC	CAB-C3B-C2B	2.55	131.97	127.51
3	H	1153	CYC	CHB-C4A-C3A	2.59	131.20	124.88
3	E	1082	CYC	OC-C1C-NC	2.60	127.97	124.83
3	B	1153	CYC	C2C-C1C-NC	2.60	110.78	108.30
3	H	1082	CYC	C2A-C1A-NA	2.62	113.92	109.86
3	E	1082	CYC	CMB-C2B-C1B	2.63	127.69	124.20
3	F	1153	CYC	OC-C1C-NC	2.65	128.04	124.83
3	J	1082	CYC	C2A-C1A-NA	2.67	114.00	109.86
3	H	1082	CYC	CAB-C3B-C2B	2.68	132.21	127.51
3	I	1082	CYC	C3C-C2C-C1C	2.68	105.66	103.41
3	J	1082	CYC	CAB-C3B-C2B	2.70	132.24	127.51
3	F	1082	CYC	CAB-C3B-C2B	2.73	132.29	127.51
3	D	1153	CYC	C2C-C1C-NC	2.73	110.91	108.30
3	F	1153	CYC	C2A-C1A-NA	2.74	114.11	109.86
3	L	1153	CYC	CMB-C2B-C1B	2.76	127.88	124.20
3	L	1082	CYC	C2A-C1A-NA	2.77	114.17	109.86
3	F	1082	CYC	C2A-C1A-NA	2.79	114.20	109.86
3	F	1153	CYC	CHB-C4A-C3A	2.80	131.72	124.88
3	B	1082	CYC	C2A-C1A-NA	2.80	114.21	109.86
3	J	1153	CYC	CHB-C4A-C3A	2.82	131.77	124.88
3	B	1153	CYC	C2A-C1A-NA	2.83	114.25	109.86
3	G	1082	CYC	OC-C1C-NC	2.86	128.28	124.83
3	A	1082	CYC	CMA-C3A-C4A	2.93	129.83	125.06
3	F	1153	CYC	C2C-C1C-NC	2.93	111.10	108.30
3	L	1153	CYC	CHB-C4A-C3A	3.00	132.21	124.88
3	B	1082	CYC	OC-C1C-NC	3.10	128.57	124.83
3	F	1082	CYC	C2C-C1C-NC	3.12	111.28	108.30
3	J	1153	CYC	CMB-C2B-C1B	3.14	128.38	124.20
3	G	1082	CYC	C2B-C1B-NB	3.15	111.56	107.00
3	J	1082	CYC	CMA-C3A-C4A	3.21	130.29	125.06
3	K	1082	CYC	OC-C1C-NC	3.22	128.72	124.83
3	E	1082	CYC	C2A-C1A-NA	3.31	115.00	109.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1082	CYC	C2C-C1C-NC	3.33	111.48	108.30
3	D	1082	CYC	CMA-C3A-C4A	3.51	130.77	125.06
3	K	1082	CYC	C2B-C1B-NB	3.53	112.11	107.00
3	H	1082	CYC	CMA-C3A-C4A	3.56	130.85	125.06
3	K	1082	CYC	CMA-C3A-C4A	3.56	130.86	125.06
3	D	1082	CYC	C2C-C1C-NC	3.58	111.72	108.30
3	E	1082	CYC	CAC-C3C-C4C	3.59	121.89	112.67
3	A	1082	CYC	CAC-C3C-C4C	3.60	121.92	112.67
3	A	1082	CYC	C2B-C1B-NB	3.66	112.31	107.00
3	G	1082	CYC	CAC-C3C-C4C	3.66	122.08	112.67
3	D	1153	CYC	CMB-C2B-C1B	3.71	129.14	124.20
3	H	1082	CYC	C2B-C1B-NB	3.72	112.39	107.00
3	D	1082	CYC	C2B-C1B-NB	3.73	112.40	107.00
3	C	1082	CYC	CMA-C3A-C4A	3.75	131.16	125.06
3	C	1082	CYC	CAC-C3C-C4C	3.77	122.35	112.67
3	F	1082	CYC	CMA-C3A-C4A	3.83	131.30	125.06
3	B	1082	CYC	CMA-C3A-C4A	3.84	131.31	125.06
3	I	1082	CYC	CAC-C3C-C4C	3.85	122.55	112.67
3	G	1082	CYC	CMA-C3A-C4A	3.85	131.33	125.06
3	L	1082	CYC	C2B-C1B-NB	3.86	112.59	107.00
3	E	1082	CYC	CMA-C3A-C4A	3.91	131.43	125.06
3	C	1082	CYC	C2B-C1B-NB	3.93	112.69	107.00
3	B	1082	CYC	C2B-C1B-NB	3.94	112.72	107.00
3	I	1082	CYC	CMA-C3A-C4A	3.97	131.52	125.06
3	H	1082	CYC	OC-C1C-NC	3.98	129.64	124.83
3	I	1082	CYC	C2B-C1B-NB	4.02	112.82	107.00
3	K	1082	CYC	CAC-C3C-C4C	4.04	123.06	112.67
3	J	1082	CYC	C2B-C1B-NB	4.05	112.87	107.00
3	E	1082	CYC	C2B-C1B-NB	4.05	112.87	107.00
3	L	1082	CYC	CMA-C3A-C4A	4.06	131.66	125.06
3	B	1153	CYC	CMA-C3A-C4A	4.12	131.76	125.06
3	C	1082	CYC	OC-C1C-NC	4.18	129.88	124.83
3	F	1082	CYC	C2B-C1B-NB	4.29	113.21	107.00
3	L	1153	CYC	C2B-C1B-NB	4.36	113.31	107.00
3	F	1153	CYC	C2B-C1B-NB	4.59	113.64	107.00
3	J	1153	CYC	CMA-C3A-C4A	4.60	132.55	125.06
3	F	1082	CYC	CAB-C3B-C4B	4.76	125.67	121.51
3	J	1082	CYC	C2C-C1C-NC	4.80	112.88	108.30
3	F	1153	CYC	CMB-C2B-C1B	4.88	130.69	124.20
3	B	1153	CYC	C2B-C1B-NB	4.90	114.10	107.00
3	J	1153	CYC	C2B-C1B-NB	4.92	114.13	107.00
3	L	1153	CYC	CMA-C3A-C4A	5.00	133.19	125.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1082	CYC	OC-C1C-NC	5.01	130.90	124.83
3	D	1153	CYC	C2B-C1B-NB	5.02	114.27	107.00
3	H	1153	CYC	C2B-C1B-NB	5.06	114.33	107.00
3	H	1082	CYC	CAB-C3B-C4B	5.07	125.93	121.51
3	F	1153	CYC	CMA-C3A-C4A	5.27	133.64	125.06
3	D	1153	CYC	CMA-C3A-C4A	5.49	133.99	125.06
3	J	1082	CYC	CAB-C3B-C4B	5.68	126.47	121.51
3	L	1082	CYC	CAB-C3B-C4B	5.73	126.51	121.51
3	D	1082	CYC	CAB-C3B-C4B	5.81	126.58	121.51
3	I	1082	CYC	CAB-C3B-C4B	6.08	126.82	121.51
3	B	1082	CYC	CAB-C3B-C4B	6.11	126.84	121.51
3	H	1153	CYC	CMA-C3A-C4A	6.41	135.50	125.06
3	E	1082	CYC	CAB-C3B-C4B	6.48	127.17	121.51
3	B	1153	CYC	CAB-C3B-C4B	6.56	127.24	121.51
3	G	1082	CYC	CAB-C3B-C4B	6.99	127.61	121.51
3	A	1082	CYC	CAB-C3B-C4B	7.29	127.88	121.51
3	K	1082	CYC	CAB-C3B-C4B	7.31	127.89	121.51
3	H	1153	CYC	CAB-C3B-C4B	7.38	127.95	121.51
3	D	1153	CYC	CAB-C3B-C4B	7.93	128.44	121.51
3	K	1082	CYC	C3B-C4B-NB	8.19	114.19	106.74
3	C	1082	CYC	CAB-C3B-C4B	8.28	128.74	121.51
3	F	1153	CYC	CAB-C3B-C4B	8.34	128.79	121.51
3	I	1082	CYC	C3B-C4B-NB	8.57	114.53	106.74
3	D	1153	CYC	C3B-C4B-NB	8.65	114.60	106.74
3	F	1153	CYC	C3B-C4B-NB	8.66	114.61	106.74
3	E	1082	CYC	C3B-C4B-NB	8.67	114.62	106.74
3	J	1153	CYC	C3B-C4B-NB	8.87	114.80	106.74
3	F	1082	CYC	C3B-C4B-NB	8.99	114.92	106.74
3	A	1082	CYC	C3B-C4B-NB	9.06	114.98	106.74
3	C	1082	CYC	C3B-C4B-NB	9.23	115.13	106.74
3	L	1082	CYC	C3B-C4B-NB	9.23	115.13	106.74
3	B	1082	CYC	C3B-C4B-NB	9.23	115.13	106.74
3	G	1082	CYC	C3B-C4B-NB	9.28	115.17	106.74
3	L	1153	CYC	CAB-C3B-C4B	9.29	129.62	121.51
3	H	1082	CYC	C3B-C4B-NB	9.62	115.48	106.74
3	L	1153	CYC	C3B-C4B-NB	9.66	115.52	106.74
3	H	1153	CYC	C3B-C4B-NB	9.75	115.60	106.74
3	J	1082	CYC	C3B-C4B-NB	9.82	115.66	106.74
3	J	1153	CYC	CAB-C3B-C4B	9.83	130.10	121.51
3	B	1153	CYC	C3B-C4B-NB	9.92	115.76	106.74
3	D	1082	CYC	C3B-C4B-NB	10.34	116.14	106.74

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1082	CYC	C1B-CHB-C4A-C3A
3	D	1082	CYC	C1B-CHB-C4A-C3A
3	F	1082	CYC	C1B-CHB-C4A-C3A
3	L	1082	CYC	C1B-CHB-C4A-C3A
3	K	1082	CYC	C1B-CHB-C4A-C3A
3	G	1082	CYC	C1B-CHB-C4A-C3A
3	E	1082	CYC	C1B-CHB-C4A-C3A
3	A	1082	CYC	C1B-CHB-C4A-C3A
3	B	1082	CYC	C1B-CHB-C4A-C3A
3	C	1082	CYC	C1B-CHB-C4A-C3A
3	H	1082	CYC	C1B-CHB-C4A-C3A
3	J	1082	CYC	C1B-CHB-C4A-C3A
3	D	1082	CYC	C1B-CHB-C4A-NA
3	F	1082	CYC	C1B-CHB-C4A-NA
3	L	1082	CYC	C1B-CHB-C4A-NA
3	H	1082	CYC	C1B-CHB-C4A-NA
3	B	1082	CYC	C1B-CHB-C4A-NA
3	A	1082	CYC	C1B-CHB-C4A-NA
3	D	1153	CYC	C1B-CHB-C4A-C3A
3	I	1082	CYC	C1B-CHB-C4A-NA
3	G	1082	CYC	C1B-CHB-C4A-NA
3	J	1082	CYC	C1B-CHB-C4A-NA
3	H	1153	CYC	C1B-CHB-C4A-C3A
3	K	1082	CYC	C1B-CHB-C4A-NA
3	B	1153	CYC	C1B-CHB-C4A-C3A
3	E	1082	CYC	C1B-CHB-C4A-NA
3	C	1082	CYC	C1B-CHB-C4A-NA
3	L	1153	CYC	C1B-CHB-C4A-C3A
3	F	1153	CYC	C1B-CHB-C4A-C3A
3	J	1153	CYC	C1B-CHB-C4A-C3A
3	L	1153	CYC	C1B-CHB-C4A-NA
3	D	1153	CYC	C1B-CHB-C4A-NA
3	B	1153	CYC	C1B-CHB-C4A-NA
3	H	1153	CYC	C1B-CHB-C4A-NA
3	F	1153	CYC	C1B-CHB-C4A-NA
3	J	1153	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

18 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1082	CYC	6	0
3	B	1082	CYC	6	0
3	B	1153	CYC	6	0
3	C	1082	CYC	6	0
3	D	1082	CYC	7	0
3	D	1153	CYC	7	0
3	E	1082	CYC	7	0
3	F	1082	CYC	7	0
3	F	1153	CYC	7	0
3	G	1082	CYC	6	0
3	H	1082	CYC	6	0
3	H	1153	CYC	4	0
3	I	1082	CYC	5	0
3	J	1082	CYC	8	0
3	J	1153	CYC	5	0
3	K	1082	CYC	6	0
3	L	1082	CYC	6	0
3	L	1153	CYC	6	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, 95^{th} 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%)	-0.22	0	100	100	30, 34, 39, 41	0
1	C	162/162 (100%)	0.06	0	100	100	30, 34, 39, 43	0
1	E	162/162 (100%)	-0.11	0	100	100	30, 34, 39, 41	0
1	G	162/162 (100%)	-0.04	0	100	100	30, 34, 39, 41	0
1	I	162/162 (100%)	-0.21	0	100	100	30, 34, 40, 41	0
1	K	162/162 (100%)	-0.13	0	100	100	30, 34, 40, 41	0
2	B	172/172 (100%)	-0.19	2 (1%)	81	81	26, 34, 45, 53	0
2	D	172/172 (100%)	-0.13	1 (0%)	90	90	26, 34, 44, 53	0
2	F	172/172 (100%)	-0.15	2 (1%)	81	81	26, 34, 45, 53	0
2	H	172/172 (100%)	-0.20	1 (0%)	90	90	26, 34, 45, 53	0
2	J	172/172 (100%)	-0.14	4 (2%)	64	63	26, 34, 45, 53	0
2	L	172/172 (100%)	-0.02	5 (2%)	55	54	26, 34, 45, 53	0
All	All	2004/2004 (100%)	-0.12	15 (0%)	89	88	26, 34, 44, 53	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	22	GLN	2.9
2	L	145	PRO	2.8
2	J	22	GLN	2.4
2	L	21	GLU	2.4
2	D	172	ALA	2.3
2	L	146	SER	2.2
2	J	145	PRO	2.2
2	F	22	GLN	2.2
2	B	118	VAL	2.1
2	B	120	LEU	2.1
2	J	150	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	25	ASN	2.0
2	L	150	ARG	2.0
2	J	21	GLU	2.0
2	F	21	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	J	1082	43/43	0.91	0.25	3.08	30,38,46,52	0
3	CYC	D	1082	43/43	0.88	0.22	2.40	30,38,46,52	0
3	CYC	F	1082	43/43	0.89	0.22	1.93	30,38,46,52	0
3	CYC	I	1082	43/43	0.94	0.15	1.60	27,32,36,45	0
3	CYC	H	1082	43/43	0.94	0.18	1.49	30,38,46,52	0
3	CYC	B	1082	43/43	0.94	0.20	1.41	30,38,45,52	0
3	CYC	L	1082	43/43	0.92	0.20	1.12	30,39,46,52	0
3	CYC	E	1082	43/43	0.93	0.15	0.97	27,32,36,45	0
3	CYC	G	1082	43/43	0.93	0.15	0.78	26,32,36,45	0
3	CYC	A	1082	43/43	0.94	0.14	0.65	27,32,36,45	0
3	CYC	C	1082	43/43	0.94	0.15	0.60	27,32,36,45	0
3	CYC	K	1082	43/43	0.95	0.14	0.36	27,32,36,45	0
3	CYC	J	1153	43/43	0.93	0.15	-0.21	27,31,36,40	0
3	CYC	F	1153	43/43	0.93	0.14	-0.31	21,26,32,36	0
3	CYC	H	1153	43/43	0.93	0.14	-0.37	27,30,32,33	0
3	CYC	D	1153	43/43	0.93	0.14	-0.47	29,33,35,37	0
3	CYC	L	1153	43/43	0.92	0.13	-0.53	32,35,39,43	0
3	CYC	B	1153	43/43	0.95	0.11	-0.89	26,33,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.