Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:51 PM GMT

PDB ID	:	1HA7
Title	:	STRUCTURE OF A LIGHT-HARVESTING PHYCOBILIPROTEIN, C-PHYCOCYANIN FROM SPIRULINA PLATENSIS AT 2.2A RESOLUTION
Authors	:	Padyana, A.K.; Rajashankar, K.R.; Ramakumar, S.
Deposited on	:	2001-03-29
Resolution	:	2.20 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:

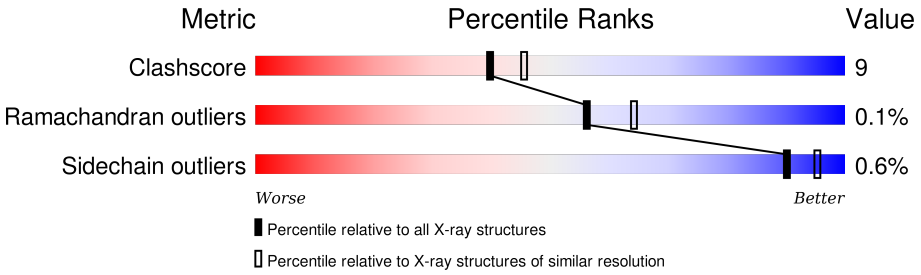
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	86% 14%
1	C	162	82% 17%
1	E	162	84% 15%
1	G	162	86% 14%
1	I	162	86% 14%
1	K	162	86% 14%
1	M	162	84% 16%

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Mol	Chain	Length	Quality of chain
1	O	162	88% 12%
1	Q	162	85% 15%
1	S	162	83% 17%
1	U	162	83% 17%
1	W	162	81% 19%
2	B	172	82% 18%
2	D	172	88% 10%
2	F	172	85% 15%
2	H	172	93% 7%
2	J	172	87% 13%
2	L	172	90% 9%
2	N	172	83% 17%
2	P	172	88% 12%
2	R	172	84% 16%
2	T	172	80% 20%
2	V	172	88% 11%
2	X	172	88% 12%

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	E	184	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33855 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 C-PHYCOCYANIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	C	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	E	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	G	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	I	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	K	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	M	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	O	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	Q	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	S	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	U	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			
1	W	162	Total	C	N	O	S	0	0	0
			1238	781	208	243	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LEU	ARG	CONFLICT	UNP P72509
A	160	THR	GLY	CONFLICT	UNP P72509
C	51	LEU	ARG	CONFLICT	UNP P72509
C	160	THR	GLY	CONFLICT	UNP P72509
E	51	LEU	ARG	CONFLICT	UNP P72509

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	THR	GLY	CONFLICT	UNP P72509
G	51	LEU	ARG	CONFLICT	UNP P72509
G	160	THR	GLY	CONFLICT	UNP P72509
I	51	LEU	ARG	CONFLICT	UNP P72509
I	160	THR	GLY	CONFLICT	UNP P72509
K	51	LEU	ARG	CONFLICT	UNP P72509
K	160	THR	GLY	CONFLICT	UNP P72509
M	51	LEU	ARG	CONFLICT	UNP P72509
M	160	THR	GLY	CONFLICT	UNP P72509
O	51	LEU	ARG	CONFLICT	UNP P72509
O	160	THR	GLY	CONFLICT	UNP P72509
Q	51	LEU	ARG	CONFLICT	UNP P72509
Q	160	THR	GLY	CONFLICT	UNP P72509
S	51	LEU	ARG	CONFLICT	UNP P72509
S	160	THR	GLY	CONFLICT	UNP P72509
U	51	LEU	ARG	CONFLICT	UNP P72509
U	160	THR	GLY	CONFLICT	UNP P72509
W	51	LEU	ARG	CONFLICT	UNP P72509
W	160	THR	GLY	CONFLICT	UNP P72509

- Molecule 2 is a protein called C-PHYCOCYANIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	D	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	F	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	H	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	J	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	L	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	N	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	P	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	R	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	T	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			

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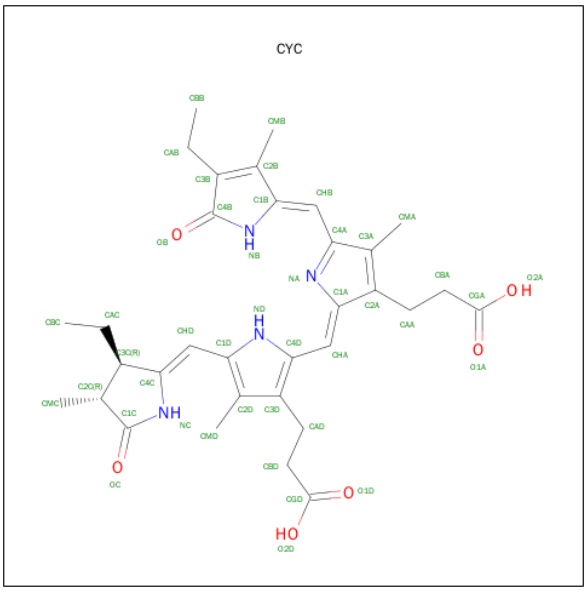
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			
2	X	172	Total	C	N	O	S	0	0	0
			1264	781	221	252	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	78	SER	ASN	CONFLICT	UNP P72508
D	78	SER	ASN	CONFLICT	UNP P72508
F	78	SER	ASN	CONFLICT	UNP P72508
H	78	SER	ASN	CONFLICT	UNP P72508
J	78	SER	ASN	CONFLICT	UNP P72508
L	78	SER	ASN	CONFLICT	UNP P72508
N	78	SER	ASN	CONFLICT	UNP P72508
P	78	SER	ASN	CONFLICT	UNP P72508
R	78	SER	ASN	CONFLICT	UNP P72508
T	78	SER	ASN	CONFLICT	UNP P72508
V	78	SER	ASN	CONFLICT	UNP P72508
X	78	SER	ASN	CONFLICT	UNP P72508

- 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		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	P	1	Total	C	N	O	0	0
			43	33	4	6		
3	Q	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	R	1	Total	C	N	O	0	0
			43	33	4	6		
3	S	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	T	1	Total	C	N	O	0	0
			43	33	4	6		
3	U	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	V	1	Total	C	N	O	0	0
			43	33	4	6		
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	102	Total	O	0	0
			102	102		
4	C	77	Total	O	0	0
			77	77		
4	D	95	Total	O	0	0
			95	95		
4	E	111	Total	O	0	0
			111	111		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	115	Total O 115 115	0	0
4	G	79	Total O 79 79	0	0
4	H	113	Total O 113 113	0	0
4	I	120	Total O 120 120	0	0
4	J	102	Total O 102 102	0	0
4	K	98	Total O 98 98	0	0
4	L	107	Total O 107 107	0	0
4	M	73	Total O 73 73	0	0
4	N	94	Total O 94 94	0	0
4	O	102	Total O 102 102	0	0
4	P	83	Total O 83 83	0	0
4	Q	93	Total O 93 93	0	0
4	R	72	Total O 72 72	0	0
4	S	104	Total O 104 104	0	0
4	T	58	Total O 58 58	0	0
4	U	62	Total O 62 62	0	0
4	V	90	Total O 90 90	0	0
4	W	111	Total O 111 111	0	0
4	X	102	Total O 102 102	0	0

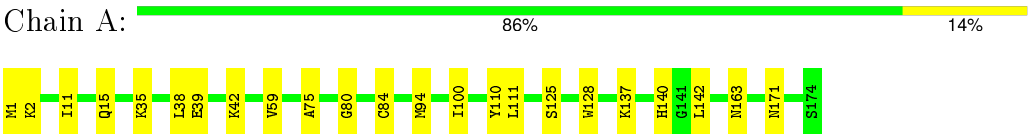
3 Residue-property plots (i)

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

Note EDS was not executed.

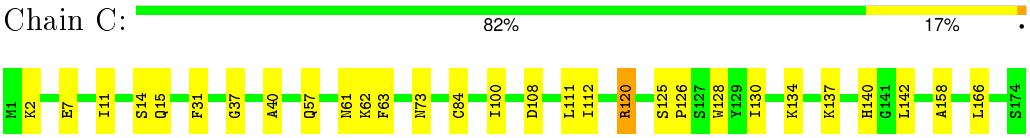
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain A:



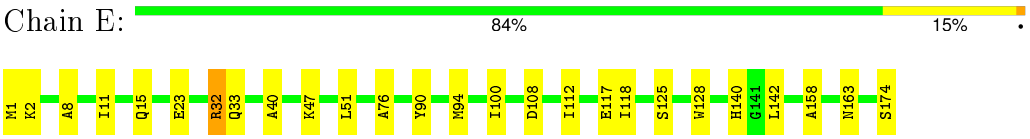
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain C:



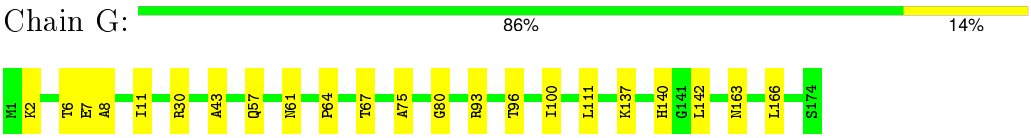
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain E:



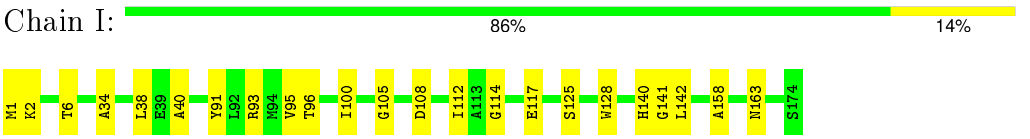
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain G:



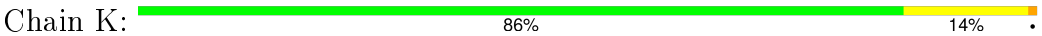
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain I:



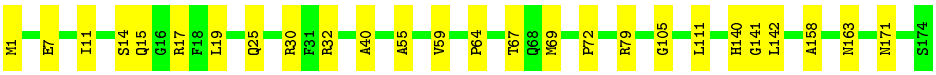
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain K:



• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain M:

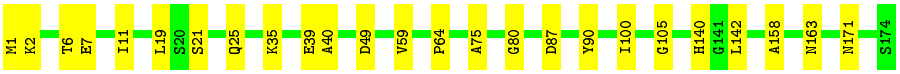


• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain O:

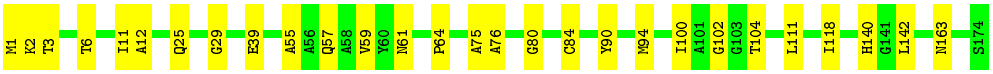
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain Q:



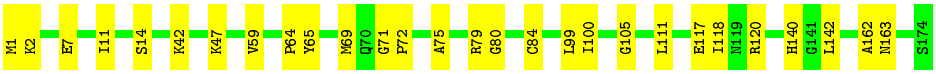
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain S:



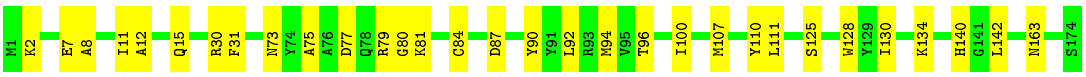
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain U:



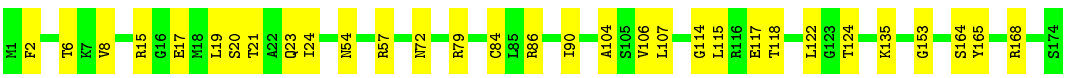
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain W:



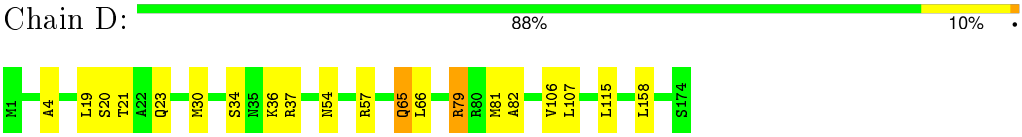
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain B:



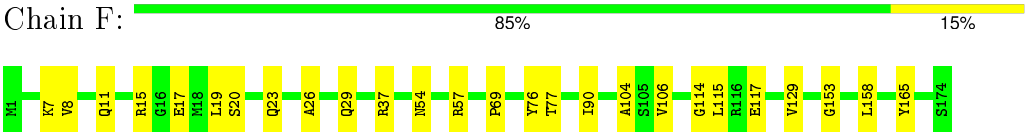
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain D:



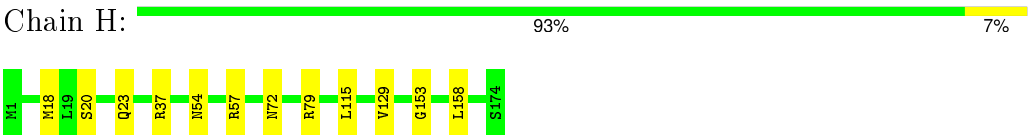
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain F:



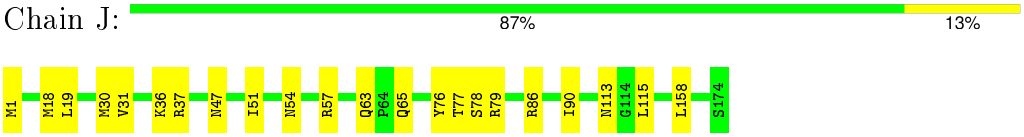
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain H:



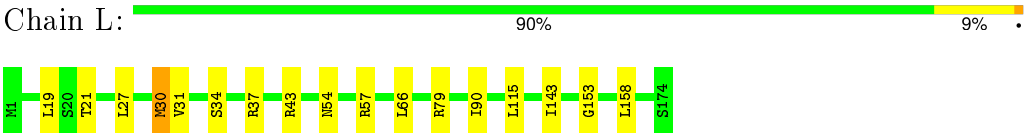
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain J:



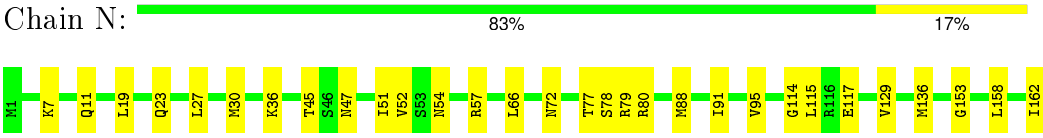
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain L:



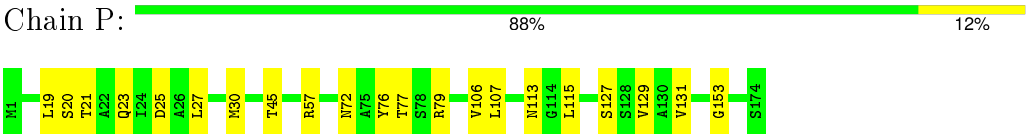
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain N:



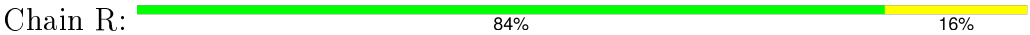
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain P:



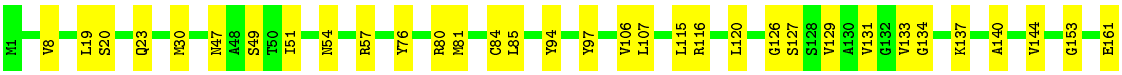
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain R:



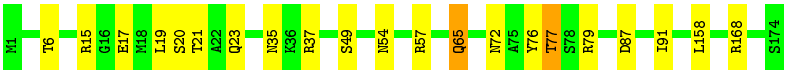
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain T:



• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain V:



• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain X:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.20Å 115.40Å 183.04Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	22.90 – 2.20	Depositor
% Data completeness (in resolution range)	92.4 (22.90-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33855	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1261	0.54	0/1704
1	C	0.33	0/1261	0.53	0/1704
1	E	0.34	0/1261	0.54	0/1704
1	G	0.32	0/1261	0.52	0/1704
1	I	0.34	0/1261	0.55	0/1704
1	K	0.33	0/1261	0.54	0/1704
1	M	0.32	0/1261	0.52	0/1704
1	O	0.35	0/1261	0.53	0/1704
1	Q	0.32	0/1261	0.53	0/1704
1	S	0.34	0/1261	0.54	0/1704
1	U	0.31	0/1261	0.52	0/1704
1	W	0.34	0/1261	0.53	0/1704
2	B	0.31	0/1268	0.55	0/1715
2	D	0.32	0/1268	0.54	0/1715
2	F	0.33	0/1268	0.54	0/1715
2	H	0.34	0/1268	0.56	0/1715
2	J	0.32	0/1268	0.55	0/1715
2	L	0.31	0/1268	0.54	0/1715
2	N	0.32	0/1268	0.54	0/1715
2	P	0.30	0/1268	0.53	0/1715
2	R	0.31	0/1268	0.54	0/1715
2	T	0.31	0/1268	0.54	0/1715
2	V	0.32	0/1268	0.55	0/1715
2	X	0.33	0/1268	0.55	0/1715
All	All	0.32	0/30348	0.54	0/41028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1238	0	1216	23	0
1	C	1238	0	1216	29	0
1	E	1238	0	1216	21	0
1	G	1238	0	1216	21	0
1	I	1238	0	1216	18	0
1	K	1238	0	1216	24	0
1	M	1238	0	1216	27	0
1	O	1238	0	1216	20	0
1	Q	1238	0	1216	26	0
1	S	1238	0	1216	29	0
1	U	1238	0	1216	30	0
1	W	1238	0	1216	31	0
2	B	1264	0	1263	31	0
2	D	1264	0	1263	21	0
2	F	1264	0	1263	20	0
2	H	1264	0	1263	13	0
2	J	1264	0	1263	20	0
2	L	1264	0	1263	15	0
2	N	1264	0	1263	30	0
2	P	1264	0	1263	15	0
2	R	1264	0	1263	19	0
2	T	1264	0	1263	33	0
2	V	1264	0	1263	21	0
2	X	1264	0	1263	19	0
3	A	43	0	36	4	0
3	B	86	0	72	9	0
3	C	43	0	36	4	0
3	D	86	0	72	6	0
3	E	43	0	36	2	0
3	F	86	0	72	8	0
3	G	43	0	35	1	0
3	H	86	0	72	8	0
3	I	43	0	36	1	0
3	J	86	0	72	5	0
3	K	43	0	36	2	0
3	L	86	0	72	9	0
3	M	43	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	86	0	72	11	0
3	O	43	0	36	4	0
3	P	86	0	72	8	0
3	Q	43	0	36	3	0
3	R	86	0	72	7	0
3	S	43	0	36	5	0
3	T	86	0	72	7	0
3	U	43	0	36	5	0
3	V	86	0	72	5	0
3	W	43	0	36	3	0
3	X	86	0	72	6	0
4	A	120	0	0	2	0
4	B	102	0	0	3	0
4	C	77	0	0	4	0
4	D	95	0	0	1	0
4	E	111	0	0	1	0
4	F	115	0	0	2	0
4	G	79	0	0	3	0
4	H	113	0	0	1	0
4	I	120	0	0	1	0
4	J	102	0	0	1	0
4	K	98	0	0	1	0
4	L	107	0	0	0	0
4	M	73	0	0	3	0
4	N	94	0	0	1	0
4	O	102	0	0	2	0
4	P	83	0	0	1	0
4	Q	93	0	0	3	0
4	R	72	0	0	2	0
4	S	104	0	0	3	0
4	T	58	0	0	1	0
4	U	62	0	0	3	0
4	V	90	0	0	1	0
4	W	111	0	0	1	0
4	X	102	0	0	3	0
All	All	33855	0	31043	553	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 9.

All (553) 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:D:20:SER:H	2:D:23:GLN:HE21	1.09	0.97
1:Q:11:ILE:HD11	1:U:11:ILE:HD11	1.50	0.94
1:O:140:HIS:HD2	1:O:142:LEU:H	1.12	0.93
1:K:42:LYS:HE3	2:L:21:THR:HG23	1.51	0.93
1:K:73:ASN:H	1:K:73:ASN:HD22	1.10	0.92
1:C:140:HIS:HD2	1:C:142:LEU:H	1.17	0.89
1:G:140:HIS:HD2	1:G:142:LEU:H	1.21	0.89
1:O:11:ILE:HD11	1:W:11:ILE:HG21	1.57	0.86
2:H:54:ASN:HD22	2:H:57:ARG:NH2	1.74	0.86
2:J:63:GLN:HB3	2:J:65:GLN:NE2	1.91	0.84
1:E:140:HIS:HD2	1:E:142:LEU:H	1.26	0.82
1:W:140:HIS:HD2	1:W:142:LEU:H	1.28	0.81
2:T:20:SER:H	2:T:23:GLN:NE2	1.79	0.80
2:J:63:GLN:HB3	2:J:65:GLN:HE22	1.44	0.80
1:U:1:MET:HG2	2:V:6:THR:HG21	1.62	0.80
1:Q:11:ILE:CD1	1:U:11:ILE:HD11	2.11	0.79
1:C:140:HIS:CD2	1:C:142:LEU:H	1.98	0.79
2:V:54:ASN:HD22	2:V:57:ARG:NH2	1.78	0.79
1:M:11:ILE:CD1	1:S:11:ILE:HG21	2.12	0.79
1:U:100:ILE:HD13	2:V:19:LEU:HD22	1.63	0.79
1:O:140:HIS:CD2	1:O:142:LEU:H	2.01	0.79
2:N:52:VAL:HA	2:N:136:MET:HE2	1.65	0.78
2:X:15:ARG:HD2	4:X:2010:HOH:O	1.83	0.78
2:D:65:GLN:H	2:D:65:GLN:NE2	1.83	0.77
2:T:54:ASN:HD22	2:T:57:ARG:NH2	1.84	0.76
2:H:54:ASN:ND2	2:H:57:ARG:NH2	2.33	0.76
1:C:7:GLU:O	1:C:11:ILE:HG13	1.86	0.75
1:E:140:HIS:CD2	1:E:142:LEU:H	2.03	0.75
1:Q:140:HIS:HD2	1:Q:142:LEU:H	1.34	0.75
1:W:140:HIS:CD2	1:W:142:LEU:H	2.04	0.75
2:X:54:ASN:HD22	2:X:57:ARG:HH21	1.31	0.74
1:W:94:MET:HE3	1:W:107:MET:HA	1.70	0.74
2:N:88:MET:HB3	2:N:136:MET:HE1	1.69	0.74
2:X:54:ASN:ND2	2:X:57:ARG:HH21	1.86	0.74
2:V:20:SER:H	2:V:23:GLN:HE21	1.35	0.73
1:U:120:ARG:HB3	1:U:120:ARG:NH1	2.04	0.73
1:U:140:HIS:HD2	1:U:142:LEU:H	1.37	0.73
2:H:54:ASN:ND2	2:H:57:ARG:HH21	1.87	0.72
1:G:8:ALA:HA	1:G:11:ILE:HD12	1.71	0.72
2:H:54:ASN:HD22	2:H:57:ARG:HH21	1.35	0.72
2:V:20:SER:OG	2:V:23:GLN:HG3	1.90	0.72
1:O:11:ILE:CD1	1:W:11:ILE:HG21	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:54:ASN:ND2	2:V:57:ARG:NH2	2.38	0.72
2:B:54:ASN:HD22	2:B:57:ARG:NH2	1.88	0.71
1:S:140:HIS:HD2	1:S:142:LEU:H	1.35	0.71
1:A:140:HIS:HD2	1:A:142:LEU:H	1.34	0.71
2:T:20:SER:H	2:T:23:GLN:HE21	1.38	0.71
2:N:52:VAL:HG22	2:N:136:MET:CE	2.21	0.71
1:Q:11:ILE:HD11	1:U:11:ILE:CD1	2.19	0.71
1:E:2:LYS:HE2	4:I:2013:HOH:O	1.91	0.71
1:K:140:HIS:HD2	1:K:142:LEU:H	1.37	0.71
2:T:115:LEU:HD13	3:T:184:CYC:HMB3	1.71	0.70
1:S:11:ILE:HD12	1:S:12:ALA:N	2.06	0.70
2:B:54:ASN:ND2	2:B:57:ARG:HH21	1.90	0.70
1:K:140:HIS:CD2	1:K:142:LEU:H	2.09	0.70
1:S:100:ILE:HD13	2:T:19:LEU:HD12	1.72	0.70
1:Q:140:HIS:CD2	1:Q:142:LEU:H	2.10	0.70
2:T:54:ASN:HD22	2:T:57:ARG:HH21	1.38	0.70
2:B:54:ASN:HD22	2:B:57:ARG:HH21	1.37	0.69
1:I:6:THR:HG23	2:J:1:MET:HE2	1.74	0.69
1:S:140:HIS:CD2	1:S:142:LEU:H	2.10	0.69
2:X:54:ASN:HD22	2:X:57:ARG:NH2	1.90	0.69
3:L:255:CYC:HMA1	3:L:255:CYC:HB	1.58	0.68
1:M:64:PRO:O	1:M:67:THR:HG22	1.94	0.68
1:M:140:HIS:CD2	1:M:142:LEU:H	2.11	0.68
3:R:255:CYC:HB	3:R:255:CYC:HMA1	1.58	0.67
2:X:54:ASN:ND2	2:X:57:ARG:NH2	2.43	0.67
1:M:171:ASN:ND2	2:T:49:SER:H	1.93	0.67
3:B:255:CYC:HB	3:B:255:CYC:HMA1	1.60	0.66
1:C:11:ILE:CD1	1:K:11:ILE:HD11	2.25	0.66
2:B:2:PHE:HD2	2:B:6:THR:HG22	1.60	0.66
1:A:140:HIS:CD2	1:A:142:LEU:H	2.13	0.66
2:D:20:SER:H	2:D:23:GLN:NE2	1.88	0.66
1:A:94:MET:HE1	1:A:110:TYR:HD2	1.60	0.66
2:B:20:SER:H	2:B:23:GLN:NE2	1.93	0.66
1:G:64:PRO:O	1:G:67:THR:HG22	1.96	0.65
3:T:255:CYC:HB	3:T:255:CYC:HMA1	1.62	0.65
2:V:65:GLN:H	2:V:65:GLN:NE2	1.94	0.65
1:S:6:THR:HG21	4:T:2001:HOH:O	1.94	0.65
3:N:255:CYC:HB	3:N:255:CYC:HMA1	1.61	0.65
2:N:66:LEU:HD13	3:N:184:CYC:HMC2	1.79	0.65
2:V:54:ASN:HD22	2:V:57:ARG:HH21	1.45	0.64
1:A:2:LYS:HE2	4:G:2006:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:ASN:H	1:K:73:ASN:ND2	1.89	0.64
1:Q:1:MET:HG2	1:Q:105:GLY:HA3	1.80	0.64
3:F:255:CYC:HMA1	3:F:255:CYC:HB	1.62	0.64
1:G:7:GLU:O	1:G:11:ILE:HG13	1.98	0.64
1:Q:171:ASN:HD21	2:V:49:SER:H	1.45	0.64
2:B:54:ASN:ND2	2:B:57:ARG:NH2	2.45	0.63
1:I:140:HIS:CD2	1:I:142:LEU:H	2.16	0.63
2:B:20:SER:H	2:B:23:GLN:HE21	1.44	0.63
1:M:171:ASN:HD21	2:T:49:SER:H	1.47	0.63
2:T:54:ASN:ND2	2:T:57:ARG:NH2	2.46	0.63
2:N:52:VAL:HG22	2:N:136:MET:HE2	1.80	0.63
1:M:11:ILE:HD11	1:S:11:ILE:HG21	1.80	0.63
2:D:20:SER:OG	2:D:23:GLN:HG3	1.98	0.63
2:V:65:GLN:H	2:V:65:GLN:HE21	1.46	0.63
1:Q:6:THR:HG21	4:R:2003:HOH:O	1.98	0.63
1:W:94:MET:HE1	1:W:110:TYR:HB2	1.80	0.62
1:Q:171:ASN:ND2	2:V:49:SER:H	1.96	0.62
2:R:115:LEU:HD13	3:R:184:CYC:HMB3	1.81	0.62
3:P:255:CYC:HB	3:P:255:CYC:HMA1	1.63	0.62
1:M:140:HIS:HD2	1:M:142:LEU:H	1.47	0.62
2:F:8:VAL:HG12	2:F:19:LEU:HD21	1.81	0.62
2:N:54:ASN:HD22	2:N:57:ARG:NH2	1.97	0.62
1:W:94:MET:CE	1:W:107:MET:HA	2.30	0.62
2:N:54:ASN:ND2	2:N:57:ARG:NH2	2.47	0.62
1:Q:64:PRO:HG2	4:Q:2037:HOH:O	1.99	0.62
2:N:88:MET:HB3	2:N:136:MET:CE	2.29	0.61
1:C:2:LYS:HE2	4:K:2006:HOH:O	2.00	0.61
1:G:140:HIS:CD2	1:G:142:LEU:H	2.11	0.61
3:X:255:CYC:HMA1	3:X:255:CYC:HB	1.65	0.61
1:C:40:ALA:HB2	1:C:158:ALA:HB1	1.83	0.61
1:E:1:MET:HG2	4:F:2001:HOH:O	2.00	0.61
1:C:11:ILE:HD11	4:C:2004:HOH:O	2.00	0.61
1:U:64:PRO:HG2	4:U:2024:HOH:O	2.00	0.60
1:Q:7:GLU:O	1:Q:11:ILE:HG13	2.01	0.60
1:U:140:HIS:CD2	1:U:142:LEU:H	2.20	0.60
1:I:6:THR:HG23	2:J:1:MET:CE	2.31	0.60
1:U:1:MET:HG2	2:V:6:THR:CG2	2.30	0.60
2:V:72:MEN:HE22	3:V:184:CYC:HBD2	1.83	0.60
1:O:59:VAL:HG11	3:O:184:CYC:HMC1	1.84	0.60
1:Q:2:LYS:HE2	4:U:2006:HOH:O	2.00	0.60
1:Q:21:SER:O	1:Q:25:GLN:HG3	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:ND2	2:D:57:ARG:NH2	2.50	0.59
2:B:135:LYS:HG2	4:B:2083:HOH:O	2.02	0.59
1:A:38:LEU:HD22	2:B:24:ILE:HG23	1.84	0.59
2:D:54:ASN:HD22	2:D:57:ARG:NH2	1.99	0.59
1:U:120:ARG:HB3	1:U:120:ARG:HH11	1.66	0.59
1:E:32:ARG:HD3	1:E:33:GLN:N	2.18	0.59
2:T:161:GLU:O	2:T:164:SER:HB3	2.02	0.59
1:S:57:GLN:HE21	1:S:61:ASN:ND2	2.01	0.58
1:G:96:THR:O	1:G:100:ILE:HG12	2.03	0.58
2:L:37:ARG:HA	2:L:158:LEU:HD21	1.85	0.58
1:C:37:GLY:HA3	4:C:2044:HOH:O	2.03	0.58
1:K:100:ILE:HD13	2:L:19:LEU:CD1	2.33	0.58
2:T:54:ASN:ND2	2:T:57:ARG:HH21	1.99	0.58
2:R:66:LEU:HD13	3:R:184:CYC:HMC2	1.86	0.58
1:S:39:GLU:HG2	4:S:2023:HOH:O	2.04	0.58
1:K:140:HIS:HE1	1:K:163:ASN:OD1	1.86	0.58
3:D:255:CYC:HB	3:D:255:CYC:HMA1	1.69	0.57
1:S:100:ILE:HD13	2:T:19:LEU:CD1	2.34	0.57
2:X:115:LEU:HD13	3:X:184:CYC:HMB3	1.85	0.57
3:S:184:CYC:HMD2	3:S:184:CYC:HC	1.70	0.57
1:S:118:ILE:HD11	2:X:78:SER:HA	1.87	0.57
1:Q:35:LYS:HB2	4:Q:2014:HOH:O	2.03	0.57
1:K:40:ALA:HB2	1:K:158:ALA:HB1	1.86	0.57
1:W:7:GLU:O	1:W:11:ILE:HG23	2.04	0.57
1:A:35:LYS:O	1:A:39:GLU:HG3	2.05	0.57
3:T:255:CYC:NB	3:T:255:CYC:HMA1	2.20	0.57
1:I:125:SER:HB3	1:I:128:TRP:CE2	2.39	0.57
1:C:73:ASN:HA	3:C:184:CYC:HBD2	1.86	0.57
1:K:1:MET:HG2	1:K:105:GLY:HA3	1.86	0.57
1:K:73:ASN:N	1:K:73:ASN:HD22	1.90	0.57
2:T:8:VAL:HG12	2:T:19:LEU:HD21	1.85	0.57
3:M:184:CYC:HC	3:M:184:CYC:HMD2	1.69	0.56
3:N:255:CYC:NB	3:N:255:CYC:HMA1	2.19	0.56
4:A:2015:HOH:O	1:G:2:LYS:HE2	2.04	0.56
3:J:255:CYC:HB	3:J:255:CYC:HMA1	1.69	0.56
2:X:1:MET:HG3	2:X:106:VAL:HB	1.87	0.56
1:W:130:ILE:O	1:W:134:LYS:HG2	2.05	0.56
1:U:42:LYS:NZ	2:V:21:THR:HG23	2.21	0.56
2:N:54:ASN:ND2	2:N:57:ARG:HH21	2.03	0.56
1:A:11:ILE:HD11	1:G:11:ILE:HG12	1.87	0.56
2:F:54:ASN:ND2	2:F:57:ARG:NH2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:27:LEU:O	2:N:30:MET:HG3	2.06	0.56
2:N:52:VAL:HG22	2:N:136:MET:HE1	1.87	0.56
3:C:184:CYC:HMD2	3:C:184:CYC:HC	1.71	0.56
3:L:255:CYC:HMA1	3:L:255:CYC:NB	2.18	0.55
1:M:32:ARG:HB3	4:M:2014:HOH:O	2.07	0.55
3:D:184:CYC:HC	3:D:184:CYC:HMD2	1.71	0.55
2:L:115:LEU:HD13	3:L:184:CYC:HMB3	1.88	0.55
3:F:255:CYC:NB	3:F:255:CYC:HMA1	2.21	0.55
1:E:100:ILE:HD13	2:F:19:LEU:HD12	1.87	0.55
2:T:127:SER:O	2:T:131:VAL:HG23	2.06	0.55
2:J:30:MET:HG3	2:J:31:VAL:N	2.22	0.55
2:T:129:VAL:O	2:T:133:VAL:HG23	2.07	0.55
3:V:255:CYC:HB	3:V:255:CYC:HMA1	1.72	0.55
1:A:11:ILE:HD11	1:G:11:ILE:CD1	2.37	0.55
3:A:184:CYC:HC	3:A:184:CYC:HMD2	1.70	0.55
1:E:140:HIS:HE1	1:E:163:ASN:OD1	1.89	0.55
2:F:114:GLY:HA2	2:F:117:GLU:OE1	2.07	0.55
2:J:54:ASN:ND2	2:J:57:ARG:NH2	2.55	0.55
1:M:7:GLU:O	1:M:11:ILE:HG13	2.07	0.55
3:B:255:CYC:NB	3:B:255:CYC:HMA1	2.22	0.55
2:H:37:ARG:HA	2:H:158:LEU:HD21	1.89	0.55
2:T:47:ASN:O	2:T:51:ILE:HG13	2.07	0.55
2:D:115:LEU:HD13	3:D:184:CYC:HMB3	1.89	0.54
3:G:184:CYC:HMD2	3:G:184:CYC:HC	1.72	0.54
2:B:2:PHE:CD2	2:B:6:THR:HG22	2.42	0.54
2:V:54:ASN:ND2	2:V:57:ARG:HH21	2.00	0.54
2:L:153:GLY:HA3	3:L:255:CYC:CMD	2.38	0.54
1:C:137:LYS:HG3	1:C:166:LEU:HD13	1.89	0.54
1:I:140:HIS:HE1	1:I:163:ASN:OD1	1.91	0.54
3:P:255:CYC:NB	3:P:255:CYC:HMA1	2.22	0.54
3:H:184:CYC:HC	3:H:184:CYC:HMD2	1.72	0.54
2:J:63:GLN:CB	2:J:65:GLN:HE22	2.16	0.54
1:W:90:TYR:O	1:W:94:MET:HG2	2.08	0.54
1:Q:6:THR:HG23	2:R:3:ASP:OD2	2.07	0.54
1:S:57:GLN:HE21	1:S:61:ASN:HD21	1.54	0.54
1:W:100:ILE:HD13	2:X:19:LEU:CD1	2.38	0.54
2:P:57:ARG:NH1	3:Q:184:CYC:O1D	2.40	0.54
1:G:30:ARG:NH1	4:G:2015:HOH:O	2.41	0.54
2:T:140:ALA:O	2:T:144:VAL:HG23	2.08	0.54
3:H:255:CYC:HMA1	3:H:255:CYC:HB	1.73	0.54
2:F:115:LEU:HD13	3:F:184:CYC:HMB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:GLY:HA2	1:I:117:GLU:OE1	2.08	0.54
2:N:52:VAL:HA	2:N:136:MET:CE	2.38	0.53
3:R:255:CYC:NB	3:R:255:CYC:HMA1	2.21	0.53
2:F:54:ASN:HD22	2:F:57:ARG:NH2	2.07	0.53
3:I:184:CYC:HMD2	3:I:184:CYC:HC	1.73	0.53
2:V:15:ARG:NH1	2:V:17:GLU:OE1	2.40	0.53
1:W:94:MET:CE	1:W:110:TYR:HB2	2.38	0.53
1:A:140:HIS:HE1	1:A:163:ASN:OD1	1.92	0.53
3:X:255:CYC:HMA1	3:X:255:CYC:NB	2.23	0.53
1:S:111:LEU:C	1:S:111:LEU:HD23	2.29	0.53
1:U:7:GLU:O	1:U:11:ILE:HG13	2.09	0.52
2:H:79:ARG:HH11	2:H:79:ARG:HG2	1.73	0.52
2:B:115:LEU:HD13	3:B:184:CYC:HMB3	1.90	0.52
3:O:184:CYC:HMD2	3:O:184:CYC:HC	1.73	0.52
1:K:100:ILE:HD13	2:L:19:LEU:HD12	1.92	0.52
1:K:59:VAL:HG11	3:K:184:CYC:HMC1	1.92	0.52
2:T:20:SER:N	2:T:23:GLN:HE21	2.06	0.52
3:N:184:CYC:HMD2	3:N:184:CYC:HC	1.75	0.52
1:E:40:ALA:HB2	1:E:158:ALA:HB1	1.92	0.52
1:G:6:THR:HG21	4:H:2003:HOH:O	2.08	0.52
1:U:117:GLU:HA	1:U:120:ARG:HH12	1.74	0.52
1:O:140:HIS:HE1	1:O:163:ASN:OD1	1.93	0.52
4:Q:2004:HOH:O	1:U:2:LYS:HE2	2.10	0.52
1:A:42:LYS:HE2	2:B:21:THR:HG23	1.91	0.52
2:B:72:MEN:HB2	3:B:184:CYC:OC	2.10	0.52
1:A:100:ILE:HD13	2:B:19:LEU:HD12	1.92	0.51
1:G:140:HIS:HE1	1:G:163:ASN:OD1	1.93	0.51
1:I:34:ALA:O	1:I:38:LEU:HG	2.10	0.51
2:D:4:ALA:HB2	2:D:30:MET:HE1	1.92	0.51
1:I:96:THR:O	1:I:100:ILE:HG12	2.10	0.51
1:G:137:LYS:HG3	1:G:166:LEU:HD13	1.93	0.51
1:Q:100:ILE:HD13	2:R:19:LEU:HD12	1.92	0.51
2:R:7:LYS:O	2:R:11:GLN:HG3	2.11	0.51
3:W:184:CYC:HMD2	3:W:184:CYC:HC	1.74	0.51
1:C:57:GLN:HE21	1:C:61:ASN:ND2	2.09	0.51
1:S:55:ALA:O	1:S:59:VAL:HG23	2.11	0.50
1:C:57:GLN:HE21	1:C:61:ASN:HD21	1.59	0.50
3:D:255:CYC:NB	3:D:255:CYC:HMA1	2.27	0.50
1:M:59:VAL:HG11	3:M:184:CYC:HMC1	1.93	0.50
2:P:115:LEU:HD13	3:P:184:CYC:HMB3	1.93	0.50
1:W:2:LYS:HD2	1:W:7:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:140:HIS:HE1	1:S:163:ASN:OD1	1.94	0.50
4:O:2016:HOH:O	1:W:2:LYS:HE2	2.11	0.50
1:M:11:ILE:HD13	1:S:11:ILE:HG21	1.93	0.50
1:W:79:ARG:HD2	4:W:2053:HOH:O	2.11	0.50
1:M:140:HIS:HE1	1:M:163:ASN:OD1	1.94	0.50
2:J:54:ASN:HD22	2:J:57:ARG:NH2	2.09	0.50
2:D:82:ALA:HB1	1:E:117:GLU:OE1	2.12	0.50
1:M:1:MET:HG2	1:M:105:GLY:HA3	1.94	0.50
1:I:140:HIS:HD2	1:I:142:LEU:H	1.59	0.50
2:B:106:VAL:HG13	2:B:107:LEU:N	2.27	0.50
2:D:54:ASN:ND2	2:D:57:ARG:HH21	2.09	0.49
3:K:184:CYC:HMD2	3:K:184:CYC:HC	1.77	0.49
1:Q:35:LYS:O	1:Q:39:GLU:HG3	2.12	0.49
1:G:43:ALA:HB3	1:G:142:LEU:HD21	1.94	0.49
3:E:184:CYC:HC	3:E:184:CYC:HMD2	1.77	0.49
2:X:153:GLY:HA3	3:X:255:CYC:CMD	2.42	0.49
3:Q:184:CYC:HC	3:Q:184:CYC:HMD2	1.78	0.49
1:U:79:ARG:HD2	4:U:2028:HOH:O	2.10	0.49
2:X:29:GLN:HB2	4:X:2020:HOH:O	2.12	0.49
1:Q:40:ALA:HB2	1:Q:158:ALA:HB1	1.93	0.49
2:T:106:VAL:HG13	2:T:107:LEU:N	2.28	0.49
3:V:255:CYC:NB	3:V:255:CYC:HMA1	2.27	0.49
1:A:1:MET:HG2	4:B:2001:HOH:O	2.13	0.49
2:N:115:LEU:HD13	3:N:184:CYC:HMB3	1.95	0.49
2:R:125:PRO:HG2	2:R:128:SER:HB2	1.95	0.49
2:F:8:VAL:HG12	2:F:19:LEU:CD2	2.41	0.49
1:M:17:ARG:HB2	4:M:2007:HOH:O	2.12	0.49
2:F:15:ARG:NH1	2:F:17:GLU:OE2	2.45	0.49
2:L:90:ILE:HG21	3:L:184:CYC:HAB1	1.93	0.49
1:E:100:ILE:HD13	2:F:19:LEU:CD1	2.43	0.49
3:L:184:CYC:HMD2	3:L:184:CYC:HC	1.77	0.49
2:J:115:LEU:HD13	3:J:184:CYC:HMB3	1.95	0.49
2:J:86:ARG:O	2:J:90:ILE:HG13	2.13	0.48
2:D:106:VAL:HG13	2:D:107:LEU:N	2.28	0.48
1:I:140:HIS:HD2	1:I:141:GLY:N	2.11	0.48
2:X:114:GLY:HA2	2:X:117:GLU:OE1	2.13	0.48
2:T:19:LEU:HA	2:T:23:GLN:NE2	2.28	0.48
1:Q:19:LEU:O	2:R:45:THR:HG21	2.13	0.48
1:W:11:ILE:HG13	1:W:12:ALA:N	2.28	0.48
1:A:59:VAL:HG11	3:A:184:CYC:HMC1	1.96	0.48
3:X:184:CYC:HMD2	3:X:184:CYC:HC	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:184:CYC:HMD2	3:J:184:CYC:HC	1.79	0.48
1:A:125:SER:HB3	1:A:128:TRP:CE2	2.48	0.48
2:X:7:LYS:O	2:X:11:GLN:HG3	2.14	0.48
1:C:100:ILE:HD13	2:D:19:LEU:HD12	1.95	0.48
1:U:59:VAL:HG11	3:U:184:CYC:HMC1	1.96	0.48
2:B:15:ARG:HD2	4:B:2019:HOH:O	2.14	0.48
2:T:134:GLY:O	2:T:137:LYS:HB3	2.14	0.48
3:H:255:CYC:HMA1	3:H:255:CYC:NB	2.28	0.47
2:T:116:ARG:HG2	2:T:120:LEU:HD23	1.95	0.47
2:T:116:ARG:O	2:T:120:LEU:HD23	2.13	0.47
2:N:114:GLY:HA2	2:N:117:GLU:OE1	2.14	0.47
2:N:47:ASN:O	2:N:51:ILE:HG13	2.14	0.47
1:U:111:LEU:C	1:U:111:LEU:HD23	2.34	0.47
3:U:184:CYC:HC	3:U:184:CYC:HMD2	1.78	0.47
1:O:11:ILE:O	1:O:15:GLN:HG3	2.13	0.47
2:N:79:ARG:NH1	3:N:184:CYC:O2D	2.47	0.47
1:U:2:LYS:O	1:U:2:LYS:HG2	2.13	0.47
1:G:111:LEU:C	1:G:111:LEU:HD23	2.35	0.47
2:N:91:ILE:O	2:N:95:VAL:HG23	2.14	0.47
2:B:20:SER:N	2:B:23:GLN:HE21	2.13	0.47
1:W:84:CYS:HA	3:W:184:CYC:HAC1	1.93	0.47
1:G:75:ALA:HA	1:G:80:GLY:HA3	1.96	0.47
2:T:8:VAL:HG12	2:T:19:LEU:CD2	2.44	0.47
1:A:137:LYS:HG3	1:A:163:ASN:OD1	2.15	0.47
2:H:129:VAL:HG22	3:H:184:CYC:H3C	1.97	0.47
3:J:255:CYC:HMA1	3:J:255:CYC:NB	2.30	0.47
1:Q:100:ILE:HD13	2:R:19:LEU:CD1	2.44	0.47
2:P:72:MEN:HE22	3:P:184:CYC:HBD2	1.96	0.47
1:C:125:SER:HB3	1:C:128:TRP:CE2	2.50	0.47
2:F:26:ALA:O	2:F:29:GLN:HB3	2.15	0.46
1:S:75:ALA:HA	1:S:80:GLY:HA3	1.95	0.46
1:K:42:LYS:CE	2:L:21:THR:HG23	2.35	0.46
2:H:72:MEN:HB2	3:H:184:CYC:OC	2.15	0.46
2:L:54:ASN:OD1	2:L:57:ARG:NH2	2.47	0.46
2:T:76:TYR:O	2:T:80:ARG:HB2	2.16	0.46
2:B:8:VAL:HG12	2:B:19:LEU:HD21	1.97	0.46
1:W:75:ALA:HA	1:W:80:GLY:HA3	1.96	0.46
1:E:125:SER:HB3	1:E:128:TRP:CE2	2.50	0.46
2:F:104:ALA:HB2	2:F:165:TYR:CE1	2.50	0.46
1:U:140:HIS:HE1	1:U:163:ASN:OD1	1.98	0.46
3:T:255:CYC:CMA	3:T:255:CYC:HB	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ALA:O	1:E:11:ILE:HG22	2.14	0.46
1:W:140:HIS:HE1	1:W:163:ASN:OD1	1.98	0.46
1:M:30:ARG:HD2	1:S:25:GLN:OE1	2.16	0.46
1:K:7:GLU:O	1:K:11:ILE:HG13	2.15	0.46
1:O:18:PHE:HB3	2:P:45:THR:HG23	1.97	0.46
2:R:153:GLY:HA3	3:R:255:CYC:CMD	2.46	0.46
2:N:153:GLY:HA3	3:N:255:CYC:CMD	2.46	0.46
2:P:20:SER:OG	2:P:23:GLN:HG3	2.16	0.46
1:E:174:SER:O	1:K:120:ARG:NH1	2.48	0.46
2:X:72:MEN:HE22	3:X:184:CYC:HBD2	1.98	0.46
2:F:20:SER:H	2:F:23:GLN:NE2	2.14	0.46
1:K:137:LYS:HG3	1:K:166:LEU:HD13	1.98	0.46
3:M:184:CYC:HC	3:M:184:CYC:CMD	2.29	0.46
1:K:48:ALA:O	1:K:52:ILE:HG13	2.15	0.46
2:L:27:LEU:O	2:L:31:VAL:HG23	2.16	0.46
2:V:37:ARG:HA	2:V:158:LEU:HD21	1.97	0.46
1:O:111:LEU:HD23	1:O:111:LEU:C	2.37	0.46
2:T:94:TYR:O	2:T:97:TYR:HB2	2.16	0.46
1:W:11:ILE:O	1:W:15:GLN:HG3	2.17	0.45
1:Q:140:HIS:HD2	1:Q:142:LEU:N	2.10	0.45
1:Q:1:MET:HG2	1:Q:105:GLY:CA	2.46	0.45
3:V:184:CYC:HMD2	3:V:184:CYC:HC	1.81	0.45
1:O:1:MET:HG2	4:P:2004:HOH:O	2.15	0.45
1:I:108:ASP:HA	1:I:112:ILE:HB	1.99	0.45
1:W:8:ALA:O	1:W:11:ILE:HG12	2.17	0.45
2:F:7:LYS:O	2:F:11:GLN:HG3	2.17	0.45
3:V:255:CYC:HMD2	3:V:255:CYC:HC	1.81	0.45
1:A:11:ILE:O	1:A:15:GLN:HG3	2.16	0.45
1:A:11:ILE:CD1	1:G:11:ILE:HG12	2.45	0.45
2:H:115:LEU:HD13	3:H:184:CYC:HMB3	1.99	0.45
2:P:76:TYR:CD2	2:P:77:THR:HG23	2.52	0.45
2:J:36:LYS:HE3	4:J:2101:HOH:O	2.15	0.45
1:Q:59:VAL:HG11	3:Q:184:CYC:HMC1	1.99	0.45
2:B:90:ILE:HG21	3:B:184:CYC:HAB1	1.99	0.45
1:C:62:LYS:HD2	1:C:63:PHE:CZ	2.52	0.45
1:W:100:ILE:HD13	2:X:19:LEU:HD12	1.98	0.45
2:R:91:ILE:O	2:R:95:VAL:HG23	2.16	0.45
1:W:111:LEU:C	1:W:111:LEU:HD23	2.36	0.45
1:C:108:ASP:HA	1:C:112:ILE:HB	1.98	0.45
1:M:11:ILE:O	1:M:14:SER:HB3	2.17	0.45
2:N:72:MEN:HE22	3:N:184:CYC:HBD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:255:CYC:HB	3:P:255:CYC:CMA	2.30	0.45
2:R:49:SER:O	2:R:53:SER:HB2	2.16	0.45
1:M:111:LEU:C	1:M:111:LEU:HD23	2.37	0.45
3:N:255:CYC:HMD2	3:N:255:CYC:HC	1.82	0.45
2:H:20:SER:H	2:H:23:GLN:NE2	2.15	0.45
1:E:90:TYR:O	1:E:94:MET:HG2	2.16	0.45
1:C:111:LEU:C	1:C:111:LEU:HD23	2.36	0.45
3:N:255:CYC:CMA	3:N:255:CYC:HB	2.27	0.45
2:J:76:TYR:CD2	2:J:77:THR:HG23	2.52	0.44
1:G:57:GLN:HE21	1:G:61:ASN:ND2	2.16	0.44
1:O:100:ILE:HD13	2:P:19:LEU:CD1	2.47	0.44
3:U:184:CYC:HC	3:U:184:CYC:CMD	2.30	0.44
2:T:126:GLY:HA3	2:T:173:VAL:O	2.16	0.44
2:D:37:ARG:HA	2:D:158:LEU:HD21	2.00	0.44
2:J:47:ASN:O	2:J:51:ILE:HG13	2.17	0.44
1:O:7:GLU:O	1:O:11:ILE:HG13	2.17	0.44
3:J:255:CYC:HMD2	3:J:255:CYC:HC	1.82	0.44
3:F:184:CYC:HC	3:F:184:CYC:HMD2	1.81	0.44
1:S:90:TYR:O	1:S:94:MET:HG2	2.17	0.44
1:M:55:ALA:O	1:M:59:VAL:HG23	2.18	0.44
2:V:76:TYR:CD2	2:V:77:THR:HG23	2.53	0.44
2:V:35:ASN:HB2	4:V:2089:HOH:O	2.18	0.44
2:P:127:SER:O	2:P:131:VAL:HG23	2.18	0.44
1:I:91:TYR:O	1:I:95:VAL:HG23	2.17	0.44
2:R:54:ASN:OD1	2:R:57:ARG:NH2	2.51	0.44
2:V:87:ASP:O	2:V:91:ILE:HG13	2.17	0.44
1:Q:75:ALA:HA	1:Q:80:GLY:HA3	1.98	0.44
1:U:72:PRO:HA	1:U:79:ARG:NH2	2.32	0.44
2:F:69:PRO:HA	2:F:76:TYR:CG	2.53	0.44
1:W:87:ASP:O	1:W:90:TYR:HB2	2.18	0.44
2:F:153:GLY:HA3	3:F:255:CYC:CMD	2.48	0.44
3:S:184:CYC:HC	3:S:184:CYC:CMD	2.29	0.44
2:J:78:SER:HA	1:K:118:ILE:HD11	2.00	0.44
1:Q:87:ASP:O	1:Q:90:TYR:HB2	2.18	0.44
1:I:1:MET:HG2	1:I:105:GLY:HA3	1.99	0.44
1:A:75:ALA:HA	1:A:80:GLY:HA3	1.98	0.44
2:N:52:VAL:CA	2:N:136:MET:HE2	2.43	0.44
2:X:26:ALA:O	2:X:29:GLN:HG2	2.17	0.44
2:R:51:ILE:HD11	2:R:143:ILE:HD12	2.00	0.44
1:U:117:GLU:HA	1:U:120:ARG:NH1	2.32	0.44
2:F:90:ILE:HG21	3:F:184:CYC:HAB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:MEN:OD1	2:B:124:THR:HA	2.18	0.44
1:E:47:LYS:HG2	1:E:51:LEU:HG	2.00	0.44
1:U:47:LYS:HB3	1:U:47:LYS:HE2	1.83	0.44
2:F:37:ARG:HA	2:F:158:LEU:HD21	1.99	0.44
2:B:153:GLY:HA3	3:B:255:CYC:CMD	2.48	0.43
2:N:72:MEN:O	2:N:80:ARG:HD2	2.18	0.43
1:C:84:CYS:HA	3:C:184:CYC:HAC1	1.94	0.43
3:H:255:CYC:HC	3:H:255:CYC:HMD2	1.83	0.43
1:W:30:ARG:HD2	1:W:30:ARG:HA	1.92	0.43
2:J:79:ARG:HG2	2:J:79:ARG:HH11	1.83	0.43
1:I:40:ALA:HB2	1:I:158:ALA:HB1	1.99	0.43
2:B:19:LEU:HA	2:B:23:GLN:NE2	2.32	0.43
2:B:86:ARG:O	2:B:90:ILE:HG13	2.17	0.43
2:L:43:ARG:HB3	2:L:143:ILE:HG22	2.00	0.43
2:N:7:LYS:O	2:N:11:GLN:HG2	2.19	0.43
3:T:184:CYC:HMD2	3:T:184:CYC:HC	1.84	0.43
1:A:84:CYS:HA	3:A:184:CYC:HAC1	1.93	0.43
1:W:31:PHE:CE1	2:X:30:MET:HE1	2.53	0.43
1:A:11:ILE:HD11	1:G:11:ILE:CG1	2.48	0.43
2:J:76:TYR:O	2:J:77:THR:OG1	2.26	0.43
1:W:77:ASP:O	1:W:81:LYS:HG3	2.18	0.43
2:F:106:VAL:HG12	4:F:2075:HOH:O	2.18	0.43
2:D:21:THR:HG23	4:D:2015:HOH:O	2.17	0.43
3:F:255:CYC:HMD2	3:F:255:CYC:HC	1.84	0.43
2:L:79:ARG:HG2	2:L:79:ARG:HH21	1.83	0.43
3:C:184:CYC:CMD	3:C:184:CYC:HC	2.31	0.43
1:U:75:ALA:HA	1:U:80:GLY:HA3	2.00	0.43
1:Q:140:HIS:HE1	1:Q:163:ASN:OD1	2.01	0.43
1:E:32:ARG:HD3	1:E:32:ARG:C	2.39	0.43
1:I:117:GLU:CD	1:I:117:GLU:H	2.21	0.43
1:M:15:GLN:HB2	1:M:17:ARG:HG2	2.00	0.43
2:T:81:MET:HG2	3:U:184:CYC:HMA2	2.01	0.43
1:M:30:ARG:HA	1:S:25:GLN:OE1	2.19	0.43
2:T:94:TYR:HA	2:T:97:TYR:CD2	2.54	0.43
2:N:19:LEU:HD22	2:N:23:GLN:NE2	2.34	0.43
2:R:117:GLU:CD	2:R:117:GLU:H	2.21	0.43
2:R:84:CYS:HA	3:R:184:CYC:HAC1	1.98	0.43
2:N:158:LEU:O	2:N:162:ILE:HG13	2.19	0.43
2:B:79:ARG:HG2	2:B:79:ARG:HH11	1.84	0.43
3:B:184:CYC:HMD2	3:B:184:CYC:HC	1.84	0.42
1:S:84:CYS:HA	3:S:184:CYC:HAC1	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:79:ARG:NH1	2:H:79:ARG:HG2	2.34	0.42
1:O:11:ILE:HD12	4:O:2004:HOH:O	2.19	0.42
3:L:255:CYC:HMD2	3:L:255:CYC:HC	1.85	0.42
1:U:84:CYS:HA	3:U:184:CYC:HAC1	1.91	0.42
1:O:87:ASP:O	1:O:90:TYR:HB2	2.20	0.42
1:K:31:PHE:CE1	2:L:30:MET:HE1	2.55	0.42
1:W:125:SER:HB3	1:W:128:TRP:CE2	2.54	0.42
1:S:64:PRO:HG2	4:S:2044:HOH:O	2.18	0.42
1:O:47:LYS:HG2	1:O:51:LEU:HG	2.01	0.42
1:O:60:TYR:HB3	1:O:67:THR:CG2	2.50	0.42
1:M:7:GLU:OE1	1:S:11:ILE:HD13	2.19	0.42
1:A:1:MET:HG2	2:B:6:THR:HG21	2.01	0.42
1:M:19:LEU:O	2:N:45:THR:HG21	2.20	0.42
2:R:137:LYS:NZ	2:R:137:LYS:HB3	2.35	0.42
2:N:129:VAL:HG22	3:N:184:CYC:H3C	2.00	0.42
1:E:11:ILE:O	1:E:15:GLN:HG3	2.20	0.42
1:M:25:GLN:NE2	1:S:102:GLY:O	2.52	0.42
2:J:37:ARG:HA	2:J:158:LEU:HD21	2.01	0.42
1:O:2:LYS:O	1:O:2:LYS:HG3	2.20	0.42
2:H:153:GLY:HA3	3:H:255:CYC:CMD	2.50	0.42
3:E:184:CYC:NB	3:E:184:CYC:HMA1	2.35	0.42
1:I:93:ARG:HG3	2:J:18:MET:HG2	2.02	0.42
2:V:79:ARG:HH11	2:V:79:ARG:HG2	1.84	0.42
2:P:79:ARG:HG2	2:P:79:ARG:HH11	1.84	0.42
1:U:65:TYR:HB2	1:U:69:MET:CE	2.48	0.42
2:P:106:VAL:HG13	2:P:107:LEU:N	2.34	0.42
2:F:129:VAL:HG22	3:F:184:CYC:H3C	2.02	0.42
1:U:99:LEU:HD21	1:U:162:ALA:HA	2.02	0.42
2:X:63:GLN:NE2	4:X:2054:HOH:O	2.52	0.42
1:C:31:PHE:CE2	2:D:34:SER:HB2	2.54	0.42
1:G:93:ARG:HG3	2:H:18:MET:HG2	2.01	0.42
2:T:81:MET:HB3	1:U:118:ILE:HD11	2.02	0.42
2:N:19:LEU:HA	2:N:23:GLN:NE2	2.35	0.42
2:P:27:LEU:O	2:P:30:MET:HG3	2.20	0.42
2:D:81:MET:HG3	1:E:118:ILE:HD12	2.00	0.42
2:R:69:PRO:HA	2:R:76:TYR:CD2	2.55	0.42
2:T:84:CYS:HA	3:T:184:CYC:HAC1	1.93	0.42
3:R:184:CYC:HC	3:R:184:CYC:HMD2	1.84	0.42
1:E:108:ASP:HA	1:E:112:ILE:HB	2.00	0.42
1:A:111:LEU:HD23	1:A:111:LEU:C	2.40	0.42
2:D:66:LEU:HD13	3:D:184:CYC:HMC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1:MET:HG3	1:S:3:THR:HG23	2.02	0.41
1:W:92:LEU:O	1:W:96:THR:HG23	2.20	0.41
1:C:11:ILE:O	1:C:14:SER:HB3	2.19	0.41
1:G:67:THR:HB	4:G:2031:HOH:O	2.20	0.41
2:B:118:THR:O	2:B:122:LEU:HG	2.20	0.41
3:L:255:CYC:CMA	3:L:255:CYC:HB	2.28	0.41
3:B:255:CYC:HMD2	3:B:255:CYC:HC	1.84	0.41
3:A:184:CYC:CMD	3:A:184:CYC:HC	2.33	0.41
2:J:54:ASN:ND2	2:J:57:ARG:HH22	2.18	0.41
2:T:81:MET:O	2:T:85:LEU:HG	2.20	0.41
1:A:171:ASN:ND2	4:A:2111:HOH:O	2.51	0.41
2:N:78:SER:HA	1:O:118:ILE:HD11	2.03	0.41
2:N:36:LYS:HE3	4:N:2091:HOH:O	2.21	0.41
1:C:11:ILE:O	1:C:15:GLN:HG3	2.20	0.41
2:T:153:GLY:HA3	3:T:255:CYC:CMD	2.50	0.41
2:B:104:ALA:HB2	2:B:165:TYR:CE1	2.55	0.41
1:C:120:ARG:NH2	4:C:2050:HOH:O	2.53	0.41
1:E:76:ALA:HB3	4:E:2051:HOH:O	2.20	0.41
1:O:100:ILE:HD13	2:P:19:LEU:HD12	2.02	0.41
1:M:25:GLN:O	1:S:29:GLY:HA3	2.21	0.41
2:X:51:ILE:HD11	2:X:143:ILE:HD12	2.02	0.41
2:B:114:GLY:HA2	2:B:117:GLU:OE1	2.20	0.41
1:U:11:ILE:O	1:U:14:SER:HB2	2.21	0.41
1:C:11:ILE:H	1:C:11:ILE:HG13	1.61	0.41
1:M:140:HIS:HD2	1:M:141:GLY:N	2.18	0.41
1:I:100:ILE:HG21	2:J:19:LEU:HD11	2.03	0.41
1:W:73:ASN:HA	3:W:184:CYC:HBD2	2.03	0.41
3:P:184:CYC:HC	3:P:184:CYC:HMD2	1.86	0.41
2:B:15:ARG:O	2:B:17:GLU:HG3	2.21	0.41
2:B:164:SER:O	2:B:168:ARG:HG3	2.21	0.41
1:C:11:ILE:HD11	1:K:11:ILE:HD11	2.01	0.41
2:P:153:GLY:HA3	3:P:255:CYC:CMD	2.51	0.41
3:S:184:CYC:NB	3:S:184:CYC:HMA1	2.36	0.41
1:K:125:SER:HA	1:K:126:PRO:HD3	1.97	0.41
1:K:11:ILE:O	1:K:15:GLN:HG3	2.21	0.40
3:O:184:CYC:CMD	3:O:184:CYC:HC	2.33	0.40
2:N:57:ARG:HD3	3:O:184:CYC:O1D	2.21	0.40
2:D:36:LYS:HG2	3:D:255:CYC:C1D	2.51	0.40
1:S:59:VAL:HG11	3:S:184:CYC:HMC1	2.03	0.40
2:L:66:LEU:HD13	3:L:184:CYC:HMC2	2.02	0.40
2:B:84:CYS:HA	3:B:184:CYC:HAC1	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:2:LYS:H	1:U:105:GLY:HA3	1.85	0.40
4:M:2010:HOH:O	1:S:104:THR:HG23	2.21	0.40
1:S:76:ALA:HB3	4:S:2046:HOH:O	2.21	0.40
1:M:72:PRO:HA	1:M:79:ARG:NH2	2.36	0.40
2:P:21:THR:HG22	2:P:25:ASP:OD2	2.20	0.40
2:D:79:ARG:HB3	2:D:79:ARG:HE	1.54	0.40
1:C:73:ASN:HB3	4:C:2077:HOH:O	2.21	0.40
2:R:95:VAL:O	2:R:99:VAL:HG23	2.22	0.40
1:O:25:GLN:OE1	1:W:30:ARG:HD2	2.21	0.40
1:C:31:PHE:CD2	2:D:34:SER:HB2	2.56	0.40
2:F:54:ASN:ND2	2:F:57:ARG:HH21	2.18	0.40
1:C:125:SER:HA	1:C:126:PRO:HD3	1.93	0.40
1:E:23:GLU:OE1	1:I:2:LYS:NZ	2.52	0.40
2:P:129:VAL:HG22	3:P:184:CYC:H3C	2.03	0.40
1:C:100:ILE:HD13	2:D:19:LEU:CD1	2.52	0.40
1:K:31:PHE:CD2	2:L:34:SER:HB2	2.56	0.40
1:C:130:ILE:HG22	1:C:134:LYS:HE2	2.03	0.40
1:M:40:ALA:HB2	1:M:158:ALA:HB1	2.03	0.40
2:R:29:GLN:NE2	4:R:2013:HOH:O	2.54	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%)	155 (97%)	5 (3%)	0	100	100
1	C	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	E	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	G	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	I	160/162 (99%)	156 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
1	M	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	O	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	Q	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	S	160/162 (99%)	154 (96%)	5 (3%)	1 (1%)	30	29
1	U	160/162 (99%)	151 (94%)	8 (5%)	1 (1%)	30	29
1	W	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
2	B	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	D	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	F	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	30	29
2	H	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
2	J	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	L	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
2	N	169/172 (98%)	166 (98%)	2 (1%)	1 (1%)	30	29
2	P	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	R	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	T	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	V	169/172 (98%)	166 (98%)	2 (1%)	1 (1%)	30	29
2	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
All	All	3948/4008 (98%)	3842 (97%)	101 (3%)	5 (0%)	56	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	2	LYS
1	U	71	GLY
2	N	77	THR
2	F	77	THR
2	V	77	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	125/125 (100%)	125 (100%)	0	100 100
1	C	125/125 (100%)	124 (99%)	1 (1%)	86 93
1	E	125/125 (100%)	124 (99%)	1 (1%)	86 93
1	G	125/125 (100%)	125 (100%)	0	100 100
1	I	125/125 (100%)	125 (100%)	0	100 100
1	K	125/125 (100%)	124 (99%)	1 (1%)	86 93
1	M	125/125 (100%)	124 (99%)	1 (1%)	86 93
1	O	125/125 (100%)	125 (100%)	0	100 100
1	Q	125/125 (100%)	124 (99%)	1 (1%)	86 93
1	S	125/125 (100%)	125 (100%)	0	100 100
1	U	125/125 (100%)	125 (100%)	0	100 100
1	W	125/125 (100%)	125 (100%)	0	100 100
2	B	131/131 (100%)	131 (100%)	0	100 100
2	D	131/131 (100%)	129 (98%)	2 (2%)	72 84
2	F	131/131 (100%)	131 (100%)	0	100 100
2	H	131/131 (100%)	131 (100%)	0	100 100
2	J	131/131 (100%)	130 (99%)	1 (1%)	86 93
2	L	131/131 (100%)	130 (99%)	1 (1%)	86 93
2	N	131/131 (100%)	131 (100%)	0	100 100
2	P	131/131 (100%)	130 (99%)	1 (1%)	86 93
2	R	131/131 (100%)	129 (98%)	2 (2%)	72 84
2	T	131/131 (100%)	130 (99%)	1 (1%)	86 93
2	V	131/131 (100%)	129 (98%)	2 (2%)	72 84
2	X	131/131 (100%)	129 (98%)	2 (2%)	72 84
All	All	3072/3072 (100%)	3055 (99%)	17 (1%)	90 95

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	120	ARG
2	D	65	GLN
2	D	79	ARG

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Mol	Chain	Res	Type
1	E	32	ARG
2	J	113	ASN
1	K	73	ASN
2	L	30	MET
1	M	69	MET
2	P	113	ASN
1	Q	49	ASP
2	R	79	ARG
2	R	113	ASN
2	T	30	MET
2	V	65	GLN
2	V	168	ARG
2	X	30	MET
2	X	113	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	119	ASN
1	A	140	HIS
2	B	23	GLN
2	B	35	ASN
2	B	54	ASN
2	B	113	ASN
2	B	145	ASN
1	C	61	ASN
1	C	68	GLN
1	C	70	GLN
1	C	119	ASN
1	C	140	HIS
2	D	23	GLN
2	D	35	ASN
2	D	47	ASN
2	D	54	ASN
2	D	65	GLN
1	E	61	ASN
1	E	119	ASN
1	E	140	HIS
2	F	23	GLN
2	F	35	ASN
2	F	42	ASN

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Mol	Chain	Res	Type
2	F	47	ASN
2	F	54	ASN
2	F	63	GLN
1	G	61	ASN
1	G	119	ASN
1	G	140	HIS
2	H	23	GLN
2	H	29	GLN
2	H	35	ASN
2	H	47	ASN
2	H	54	ASN
2	H	63	GLN
2	H	113	ASN
1	I	119	ASN
1	I	140	HIS
2	J	35	ASN
2	J	47	ASN
2	J	54	ASN
2	J	63	GLN
2	J	65	GLN
2	J	113	ASN
1	K	73	ASN
1	K	78	GLN
1	K	119	ASN
1	K	140	HIS
2	L	35	ASN
2	L	47	ASN
2	L	63	GLN
2	L	113	ASN
1	M	119	ASN
1	M	139	ASN
1	M	140	HIS
1	M	171	ASN
2	N	23	GLN
2	N	35	ASN
2	N	47	ASN
2	N	54	ASN
2	N	63	GLN
1	O	61	ASN
1	O	78	GLN
1	O	119	ASN
1	O	139	ASN

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Mol	Chain	Res	Type
1	O	140	HIS
2	P	35	ASN
2	P	47	ASN
2	P	54	ASN
2	P	63	GLN
2	P	113	ASN
1	Q	119	ASN
1	Q	140	HIS
1	Q	171	ASN
2	R	29	GLN
2	R	35	ASN
2	R	42	ASN
2	R	47	ASN
2	R	63	GLN
2	R	113	ASN
1	S	61	ASN
1	S	78	GLN
1	S	119	ASN
1	S	140	HIS
2	T	23	GLN
2	T	35	ASN
2	T	47	ASN
2	T	54	ASN
2	T	63	GLN
2	T	113	ASN
2	T	145	ASN
1	U	57	GLN
1	U	61	ASN
1	U	68	GLN
1	U	119	ASN
1	U	139	ASN
1	U	140	HIS
2	V	23	GLN
2	V	35	ASN
2	V	47	ASN
2	V	54	ASN
2	V	63	GLN
2	V	65	GLN
2	V	113	ASN
1	W	119	ASN
1	W	140	HIS
2	X	35	ASN

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Mol	Chain	Res	Type
2	X	47	ASN
2	X	54	ASN
2	X	63	GLN
2	X	113	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MEN	B	72	2	7,8,9	0.44	0	5,9,11	0.88	0
2	MEN	D	72	2	7,8,9	0.42	0	5,9,11	0.97	1 (20%)
2	MEN	F	72	2	7,8,9	0.44	0	5,9,11	1.01	1 (20%)
2	MEN	H	72	2	7,8,9	0.51	0	5,9,11	0.94	1 (20%)
2	MEN	J	72	2	7,8,9	0.43	0	5,9,11	0.90	0
2	MEN	L	72	2	7,8,9	0.45	0	5,9,11	0.92	1 (20%)
2	MEN	N	72	2	7,8,9	0.47	0	5,9,11	0.97	1 (20%)
2	MEN	P	72	2	7,8,9	0.44	0	5,9,11	0.95	1 (20%)
2	MEN	R	72	2	7,8,9	0.48	0	5,9,11	0.96	1 (20%)
2	MEN	T	72	2	7,8,9	0.48	0	5,9,11	0.92	1 (20%)
2	MEN	V	72	2	7,8,9	0.48	0	5,9,11	0.89	0
2	MEN	X	72	2	7,8,9	0.41	0	5,9,11	0.94	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	B	72	2	-	0/6/8/10	0/0/0/0
2	MEN	D	72	2	-	0/6/8/10	0/0/0/0
2	MEN	F	72	2	-	0/6/8/10	0/0/0/0
2	MEN	H	72	2	-	0/6/8/10	0/0/0/0
2	MEN	J	72	2	-	0/6/8/10	0/0/0/0
2	MEN	L	72	2	-	0/6/8/10	0/0/0/0
2	MEN	N	72	2	-	0/6/8/10	0/0/0/0
2	MEN	P	72	2	-	0/6/8/10	0/0/0/0
2	MEN	R	72	2	-	0/6/8/10	0/0/0/0
2	MEN	T	72	2	-	0/6/8/10	0/0/0/0
2	MEN	V	72	2	-	0/6/8/10	0/0/0/0
2	MEN	X	72	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	72	MEN	O-C-CA	-2.22	119.71	125.49
2	D	72	MEN	O-C-CA	-2.15	119.89	125.49
2	R	72	MEN	O-C-CA	-2.15	119.90	125.49
2	N	72	MEN	O-C-CA	-2.14	119.90	125.49
2	P	72	MEN	O-C-CA	-2.12	119.96	125.49
2	H	72	MEN	O-C-CA	-2.09	120.04	125.49
2	X	72	MEN	O-C-CA	-2.08	120.07	125.49
2	T	72	MEN	O-C-CA	-2.04	120.19	125.49
2	L	72	MEN	O-C-CA	-2.03	120.19	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	2	0
2	H	72	MEN	1	0
2	N	72	MEN	2	0
2	P	72	MEN	1	0
2	V	72	MEN	1	0
2	X	72	MEN	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

36 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	184	1	35,46,46	1.94	11 (31%)	47,67,67	3.01	16 (34%)
3	CYC	B	184	2	35,46,46	2.01	8 (22%)	47,67,67	2.97	15 (31%)
3	CYC	B	255	2	35,46,46	1.97	10 (28%)	47,67,67	2.95	16 (34%)
3	CYC	C	184	1	35,46,46	1.96	9 (25%)	47,67,67	3.05	14 (29%)
3	CYC	D	184	2	35,46,46	1.93	10 (28%)	47,67,67	3.03	13 (27%)
3	CYC	D	255	2	35,46,46	2.04	8 (22%)	47,67,67	2.87	13 (27%)
3	CYC	E	184	1	35,46,46	1.83	9 (25%)	47,67,67	3.04	16 (34%)
3	CYC	F	184	2	35,46,46	1.98	9 (25%)	47,67,67	3.06	14 (29%)
3	CYC	F	255	2	35,46,46	2.02	8 (22%)	47,67,67	2.92	14 (29%)
3	CYC	G	184	1	35,46,46	1.87	9 (25%)	47,67,67	3.01	17 (36%)
3	CYC	H	184	2	35,46,46	1.94	10 (28%)	47,67,67	2.96	14 (29%)
3	CYC	H	255	2	35,46,46	2.17	8 (22%)	47,67,67	2.92	13 (27%)
3	CYC	I	184	1	35,46,46	1.92	10 (28%)	47,67,67	3.05	14 (29%)
3	CYC	J	184	2	35,46,46	2.15	8 (22%)	47,67,67	2.94	15 (31%)
3	CYC	J	255	2	35,46,46	1.94	8 (22%)	47,67,67	3.02	15 (31%)
3	CYC	K	184	1	35,46,46	1.99	10 (28%)	47,67,67	3.10	17 (36%)
3	CYC	L	184	2	35,46,46	1.97	10 (28%)	47,67,67	3.04	14 (29%)
3	CYC	L	255	2	35,46,46	2.03	8 (22%)	47,67,67	2.91	14 (29%)
3	CYC	M	184	1	35,46,46	1.89	11 (31%)	47,67,67	3.03	14 (29%)
3	CYC	N	184	2	35,46,46	1.96	8 (22%)	47,67,67	2.94	14 (29%)
3	CYC	N	255	2	35,46,46	2.13	9 (25%)	47,67,67	2.93	13 (27%)
3	CYC	O	184	1	35,46,46	1.91	10 (28%)	47,67,67	2.95	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CYC	P	184	2	35,46,46	1.99	9 (25%)	47,67,67	3.00	14 (29%)
3	CYC	P	255	2	35,46,46	2.05	8 (22%)	47,67,67	2.92	14 (29%)
3	CYC	Q	184	1	35,46,46	1.89	10 (28%)	47,67,67	3.07	15 (31%)
3	CYC	R	184	2	35,46,46	2.02	10 (28%)	47,67,67	3.10	16 (34%)
3	CYC	R	255	2	35,46,46	1.98	10 (28%)	47,67,67	2.98	15 (31%)
3	CYC	S	184	1	35,46,46	1.88	10 (28%)	47,67,67	3.02	16 (34%)
3	CYC	T	184	2	35,46,46	1.98	12 (34%)	47,67,67	3.01	14 (29%)
3	CYC	T	255	2	35,46,46	2.04	10 (28%)	47,67,67	2.94	16 (34%)
3	CYC	U	184	1	35,46,46	2.02	10 (28%)	47,67,67	3.05	16 (34%)
3	CYC	V	184	2	35,46,46	1.96	9 (25%)	47,67,67	3.01	15 (31%)
3	CYC	V	255	2	35,46,46	2.00	9 (25%)	47,67,67	2.91	14 (29%)
3	CYC	W	184	1	35,46,46	1.85	11 (31%)	47,67,67	3.05	15 (31%)
3	CYC	X	184	2	35,46,46	1.96	10 (28%)	47,67,67	3.00	13 (27%)
3	CYC	X	255	2	35,46,46	2.00	10 (28%)	47,67,67	2.90	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	184	1	-	2/21/74/74	0/4/4/4
3	CYC	B	184	2	-	2/21/74/74	0/4/4/4
3	CYC	B	255	2	-	2/21/74/74	0/4/4/4
3	CYC	C	184	1	-	2/21/74/74	0/4/4/4
3	CYC	D	184	2	-	2/21/74/74	0/4/4/4
3	CYC	D	255	2	-	2/21/74/74	0/4/4/4
3	CYC	E	184	1	1/1/14/19	2/21/74/74	0/4/4/4
3	CYC	F	184	2	-	2/21/74/74	0/4/4/4
3	CYC	F	255	2	-	2/21/74/74	0/4/4/4
3	CYC	G	184	1	-	2/21/74/74	0/4/4/4
3	CYC	H	184	2	-	2/21/74/74	0/4/4/4
3	CYC	H	255	2	-	2/21/74/74	0/4/4/4
3	CYC	I	184	1	-	2/21/74/74	0/4/4/4
3	CYC	J	184	2	-	2/21/74/74	0/4/4/4
3	CYC	J	255	2	-	2/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	K	184	1	-	2/21/74/74	0/4/4/4
3	CYC	L	184	2	-	2/21/74/74	0/4/4/4
3	CYC	L	255	2	-	2/21/74/74	0/4/4/4
3	CYC	M	184	1	-	2/21/74/74	0/4/4/4
3	CYC	N	184	2	-	2/21/74/74	0/4/4/4
3	CYC	N	255	2	-	2/21/74/74	0/4/4/4
3	CYC	O	184	1	-	2/21/74/74	0/4/4/4
3	CYC	P	184	2	-	2/21/74/74	0/4/4/4
3	CYC	P	255	2	-	2/21/74/74	0/4/4/4
3	CYC	Q	184	1	-	2/21/74/74	0/4/4/4
3	CYC	R	184	2	-	2/21/74/74	0/4/4/4
3	CYC	R	255	2	-	2/21/74/74	0/4/4/4
3	CYC	S	184	1	-	2/21/74/74	0/4/4/4
3	CYC	T	184	2	-	2/21/74/74	0/4/4/4
3	CYC	T	255	2	-	2/21/74/74	0/4/4/4
3	CYC	U	184	1	-	2/21/74/74	0/4/4/4
3	CYC	V	184	2	-	2/21/74/74	0/4/4/4
3	CYC	V	255	2	-	2/21/74/74	0/4/4/4
3	CYC	W	184	1	-	2/21/74/74	0/4/4/4
3	CYC	X	184	2	-	2/21/74/74	0/4/4/4
3	CYC	X	255	2	-	2/21/74/74	0/4/4/4

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	255	CYC	C1C-NC	-5.09	1.31	1.37
3	V	255	CYC	C1C-NC	-4.88	1.31	1.37
3	F	255	CYC	C1C-NC	-4.69	1.31	1.37
3	P	255	CYC	C1C-NC	-4.68	1.31	1.37
3	H	255	CYC	C1C-NC	-4.58	1.31	1.37
3	D	255	CYC	C1C-NC	-4.53	1.31	1.37
3	X	255	CYC	C1C-NC	-4.43	1.32	1.37
3	L	255	CYC	C1C-NC	-4.42	1.32	1.37
3	J	184	CYC	C1C-NC	-4.42	1.32	1.37
3	R	255	CYC	C1C-NC	-4.26	1.32	1.37
3	T	255	CYC	C1C-NC	-4.13	1.32	1.37
3	T	184	CYC	C1C-NC	-4.07	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	255	CYC	C1C-NC	-4.07	1.32	1.37
3	D	184	CYC	C1C-NC	-3.92	1.32	1.37
3	M	184	CYC	C1C-NC	-3.90	1.32	1.37
3	F	184	CYC	C1C-NC	-3.88	1.32	1.37
3	N	184	CYC	C1C-NC	-3.87	1.32	1.37
3	X	184	CYC	C1C-NC	-3.86	1.32	1.37
3	B	255	CYC	C1C-NC	-3.81	1.32	1.37
3	S	184	CYC	C1C-NC	-3.74	1.32	1.37
3	R	184	CYC	C1C-NC	-3.67	1.33	1.37
3	H	184	CYC	C1C-NC	-3.64	1.33	1.37
3	C	184	CYC	C1C-NC	-3.58	1.33	1.37
3	P	184	CYC	C1C-NC	-3.57	1.33	1.37
3	L	184	CYC	C1C-NC	-3.53	1.33	1.37
3	A	184	CYC	C1C-NC	-3.53	1.33	1.37
3	B	184	CYC	C1C-NC	-3.52	1.33	1.37
3	V	184	CYC	C1C-NC	-3.38	1.33	1.37
3	E	184	CYC	C1C-NC	-3.35	1.33	1.37
3	Q	184	CYC	C1C-NC	-3.34	1.33	1.37
3	U	184	CYC	C1C-NC	-3.33	1.33	1.37
3	K	184	CYC	C1C-NC	-3.32	1.33	1.37
3	I	184	CYC	C1C-NC	-3.27	1.33	1.37
3	W	184	CYC	C1C-NC	-3.24	1.33	1.37
3	P	184	CYC	C2C-C1C	-3.15	1.49	1.52
3	J	255	CYC	C2C-C1C	-3.09	1.49	1.52
3	O	184	CYC	C2C-C1C	-3.07	1.49	1.52
3	O	184	CYC	C1C-NC	-3.01	1.33	1.37
3	G	184	CYC	C1C-NC	-2.89	1.34	1.37
3	H	184	CYC	C2C-C1C	-2.81	1.49	1.52
3	V	184	CYC	C2C-C1C	-2.76	1.49	1.52
3	U	184	CYC	C4B-C3B	-2.67	1.42	1.48
3	W	184	CYC	C2C-C1C	-2.57	1.49	1.52
3	D	255	CYC	C4B-C3B	-2.56	1.42	1.48
3	P	255	CYC	C4B-C3B	-2.53	1.42	1.48
3	L	184	CYC	C2C-C1C	-2.52	1.49	1.52
3	A	184	CYC	C2C-C1C	-2.52	1.49	1.52
3	U	184	CYC	C2C-C1C	-2.51	1.49	1.52
3	N	184	CYC	C2C-C1C	-2.49	1.49	1.52
3	Q	184	CYC	C2C-C1C	-2.48	1.49	1.52
3	F	184	CYC	C2C-C1C	-2.47	1.49	1.52
3	J	184	CYC	C2C-C1C	-2.47	1.49	1.52
3	K	184	CYC	C2C-C1C	-2.46	1.49	1.52
3	X	255	CYC	C2C-C1C	-2.46	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	255	CYC	C2C-C1C	-2.43	1.49	1.52
3	R	184	CYC	C2C-C1C	-2.42	1.49	1.52
3	I	184	CYC	C4B-C3B	-2.41	1.43	1.48
3	X	255	CYC	C4B-C3B	-2.39	1.43	1.48
3	J	184	CYC	C4B-C3B	-2.39	1.43	1.48
3	N	255	CYC	C4B-C3B	-2.38	1.43	1.48
3	H	255	CYC	C4B-C3B	-2.37	1.43	1.48
3	B	255	CYC	C4B-C3B	-2.35	1.43	1.48
3	O	184	CYC	C4B-C3B	-2.34	1.43	1.48
3	V	255	CYC	C4B-C3B	-2.33	1.43	1.48
3	M	184	CYC	C2C-C1C	-2.31	1.49	1.52
3	P	255	CYC	C2C-C1C	-2.31	1.49	1.52
3	E	184	CYC	C2C-C1C	-2.30	1.49	1.52
3	W	184	CYC	C4B-C3B	-2.29	1.43	1.48
3	H	184	CYC	C4B-C3B	-2.29	1.43	1.48
3	A	184	CYC	C4B-C3B	-2.28	1.43	1.48
3	T	184	CYC	C4B-C3B	-2.27	1.43	1.48
3	C	184	CYC	C2C-C1C	-2.27	1.49	1.52
3	N	255	CYC	C2C-C1C	-2.26	1.49	1.52
3	X	184	CYC	C2C-C1C	-2.25	1.49	1.52
3	P	184	CYC	C4B-C3B	-2.23	1.43	1.48
3	F	255	CYC	C4B-C3B	-2.23	1.43	1.48
3	R	255	CYC	C4B-C3B	-2.21	1.43	1.48
3	V	184	CYC	C4B-C3B	-2.19	1.43	1.48
3	E	184	CYC	C4B-C3B	-2.18	1.43	1.48
3	T	255	CYC	C2C-C1C	-2.15	1.50	1.52
3	D	184	CYC	C2C-C1C	-2.15	1.50	1.52
3	M	184	CYC	C4B-C3B	-2.14	1.43	1.48
3	B	255	CYC	C2C-C1C	-2.13	1.50	1.52
3	X	184	CYC	C4B-C3B	-2.12	1.43	1.48
3	L	184	CYC	C4B-C3B	-2.12	1.43	1.48
3	T	255	CYC	C4B-C3B	-2.12	1.43	1.48
3	N	184	CYC	C4B-C3B	-2.11	1.43	1.48
3	G	184	CYC	C4B-C3B	-2.10	1.43	1.48
3	B	184	CYC	C4B-C3B	-2.09	1.43	1.48
3	J	255	CYC	C4B-C3B	-2.09	1.43	1.48
3	L	255	CYC	C4B-C3B	-2.09	1.43	1.48
3	Q	184	CYC	C4B-C3B	-2.09	1.43	1.48
3	T	184	CYC	C2C-C1C	-2.08	1.50	1.52
3	S	184	CYC	C4B-C3B	-2.06	1.43	1.48
3	C	184	CYC	C4B-C3B	-2.06	1.43	1.48
3	K	184	CYC	C4B-C3B	-2.05	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	184	CYC	CAB-C3B	2.00	1.56	1.51
3	I	184	CYC	CHD-C4C	2.01	1.43	1.38
3	H	184	CYC	CHD-C4C	2.01	1.43	1.38
3	X	184	CYC	CMD-C2D	2.01	1.55	1.51
3	J	184	CYC	CMD-C2D	2.01	1.55	1.51
3	W	184	CYC	CMD-C2D	2.01	1.55	1.51
3	N	184	CYC	CMD-C2D	2.01	1.55	1.51
3	D	255	CYC	CHD-C4C	2.02	1.43	1.38
3	T	184	CYC	C4A-C3A	2.02	1.50	1.45
3	F	255	CYC	C4C-NC	2.02	1.41	1.37
3	S	184	CYC	C4A-C3A	2.02	1.50	1.45
3	H	184	CYC	CMD-C2D	2.03	1.55	1.51
3	I	184	CYC	C4A-C3A	2.03	1.50	1.45
3	E	184	CYC	CHD-C4C	2.04	1.43	1.38
3	U	184	CYC	C4C-NC	2.04	1.42	1.37
3	P	255	CYC	CHD-C4C	2.05	1.43	1.38
3	B	255	CYC	C4A-C3A	2.05	1.50	1.45
3	J	184	CYC	OC-C1C	2.06	1.27	1.23
3	H	255	CYC	CAC-C3C	2.06	1.58	1.54
3	R	255	CYC	C4C-NC	2.06	1.42	1.37
3	A	184	CYC	C4C-NC	2.07	1.42	1.37
3	T	184	CYC	CHD-C4C	2.07	1.43	1.38
3	D	184	CYC	CMD-C2D	2.07	1.55	1.51
3	F	184	CYC	CMD-C2D	2.07	1.55	1.51
3	X	184	CYC	CHD-C4C	2.07	1.43	1.38
3	X	255	CYC	OC-C1C	2.07	1.27	1.23
3	P	184	CYC	C4A-C3A	2.07	1.50	1.45
3	W	184	CYC	C4A-C3A	2.08	1.50	1.45
3	L	184	CYC	CAB-C3B	2.08	1.56	1.51
3	X	255	CYC	C4A-C3A	2.08	1.50	1.45
3	N	255	CYC	C4A-C3A	2.09	1.50	1.45
3	L	255	CYC	C4C-NC	2.10	1.42	1.37
3	O	184	CYC	C4C-NC	2.10	1.42	1.37
3	R	255	CYC	CHD-C4C	2.10	1.43	1.38
3	T	184	CYC	OC-C1C	2.10	1.27	1.23
3	T	184	CYC	C4C-NC	2.10	1.42	1.37
3	C	184	CYC	CMD-C2D	2.10	1.56	1.51
3	G	184	CYC	CMD-C2D	2.11	1.56	1.51
3	J	255	CYC	C4C-NC	2.12	1.42	1.37
3	R	184	CYC	C4A-C3A	2.12	1.50	1.45
3	F	184	CYC	CAC-C3C	2.13	1.58	1.54
3	A	184	CYC	CHD-C4C	2.13	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	255	CYC	OC-C1C	2.13	1.27	1.23
3	U	184	CYC	CMD-C2D	2.15	1.56	1.51
3	L	184	CYC	CHD-C4C	2.16	1.43	1.38
3	V	255	CYC	CHD-C4C	2.16	1.43	1.38
3	L	184	CYC	C4C-NC	2.16	1.42	1.37
3	T	255	CYC	CMD-C2D	2.16	1.56	1.51
3	Q	184	CYC	C4C-NC	2.16	1.42	1.37
3	W	184	CYC	C4C-NC	2.17	1.42	1.37
3	M	184	CYC	C4C-NC	2.17	1.42	1.37
3	T	184	CYC	CAB-C3B	2.17	1.57	1.51
3	H	184	CYC	OC-C1C	2.17	1.27	1.23
3	D	255	CYC	C4C-NC	2.18	1.42	1.37
3	C	184	CYC	CHD-C4C	2.18	1.43	1.38
3	V	255	CYC	C4A-C3A	2.18	1.50	1.45
3	N	255	CYC	CHD-C4C	2.19	1.43	1.38
3	M	184	CYC	CMD-C2D	2.19	1.56	1.51
3	S	184	CYC	CHD-C4C	2.19	1.43	1.38
3	A	184	CYC	C4A-C3A	2.19	1.50	1.45
3	T	184	CYC	CHB-C4A	2.19	1.45	1.40
3	X	184	CYC	OC-C1C	2.19	1.27	1.23
3	O	184	CYC	CMD-C2D	2.19	1.56	1.51
3	E	184	CYC	CMD-C2D	2.20	1.56	1.51
3	X	255	CYC	CHD-C4C	2.20	1.43	1.38
3	C	184	CYC	OC-C1C	2.20	1.27	1.23
3	I	184	CYC	C4C-NC	2.20	1.42	1.37
3	D	184	CYC	CHD-C4C	2.20	1.43	1.38
3	Q	184	CYC	CMD-C2D	2.21	1.56	1.51
3	G	184	CYC	CMA-C3A	2.21	1.55	1.50
3	I	184	CYC	OC-C1C	2.21	1.27	1.23
3	Q	184	CYC	OC-C1C	2.21	1.27	1.23
3	D	255	CYC	OC-C1C	2.22	1.27	1.23
3	B	184	CYC	CHD-C4C	2.22	1.43	1.38
3	L	255	CYC	CHD-C4C	2.22	1.43	1.38
3	B	184	CYC	C4C-NC	2.22	1.42	1.37
3	H	255	CYC	CHD-C4C	2.23	1.43	1.38
3	K	184	CYC	C4C-NC	2.23	1.42	1.37
3	S	184	CYC	C4C-NC	2.23	1.42	1.37
3	X	255	CYC	CMD-C2D	2.24	1.56	1.51
3	M	184	CYC	OC-C1C	2.25	1.27	1.23
3	W	184	CYC	CHD-C4C	2.25	1.43	1.38
3	S	184	CYC	OC-C1C	2.25	1.27	1.23
3	V	184	CYC	CHD-C4C	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	184	CYC	CHD-C4C	2.26	1.43	1.38
3	F	255	CYC	C4A-C3A	2.26	1.50	1.45
3	V	255	CYC	CHB-C4A	2.26	1.46	1.40
3	X	184	CYC	C4C-NC	2.26	1.42	1.37
3	G	184	CYC	OC-C1C	2.27	1.27	1.23
3	A	184	CYC	CMD-C2D	2.28	1.56	1.51
3	R	255	CYC	C4A-C3A	2.28	1.50	1.45
3	L	184	CYC	OC-C1C	2.28	1.27	1.23
3	Q	184	CYC	CHD-C4C	2.29	1.44	1.38
3	P	184	CYC	CHD-C4C	2.29	1.44	1.38
3	I	184	CYC	CMD-C2D	2.29	1.56	1.51
3	J	255	CYC	C4A-C3A	2.29	1.50	1.45
3	P	184	CYC	OC-C1C	2.30	1.27	1.23
3	K	184	CYC	CHD-C4C	2.30	1.44	1.38
3	R	184	CYC	CAB-C3B	2.30	1.57	1.51
3	F	184	CYC	CAB-C3B	2.32	1.57	1.51
3	T	255	CYC	C4C-NC	2.34	1.42	1.37
3	M	184	CYC	CHD-C4C	2.35	1.44	1.38
3	D	184	CYC	CMA-C3A	2.36	1.55	1.50
3	A	184	CYC	OC-C1C	2.36	1.28	1.23
3	G	184	CYC	CHD-C4C	2.36	1.44	1.38
3	I	184	CYC	CAD-C3D	2.37	1.56	1.52
3	S	184	CYC	CMD-C2D	2.38	1.56	1.51
3	H	184	CYC	C4C-NC	2.38	1.42	1.37
3	D	184	CYC	CAC-C3C	2.38	1.58	1.54
3	D	184	CYC	C4C-NC	2.38	1.42	1.37
3	V	184	CYC	C4C-NC	2.38	1.42	1.37
3	R	184	CYC	CHD-C4C	2.39	1.44	1.38
3	T	184	CYC	CMA-C3A	2.40	1.55	1.50
3	X	255	CYC	CMA-C3A	2.40	1.55	1.50
3	V	184	CYC	OC-C1C	2.41	1.28	1.23
3	F	184	CYC	CMA-C3A	2.41	1.55	1.50
3	R	184	CYC	OC-C1C	2.41	1.28	1.23
3	T	255	CYC	OC-C1C	2.41	1.28	1.23
3	L	255	CYC	OC-C1C	2.42	1.28	1.23
3	P	255	CYC	OC-C1C	2.42	1.28	1.23
3	K	184	CYC	CMA-C3A	2.42	1.56	1.50
3	E	184	CYC	CAD-C3D	2.43	1.56	1.52
3	T	255	CYC	CMA-C3A	2.43	1.56	1.50
3	B	255	CYC	C4C-NC	2.43	1.42	1.37
3	B	184	CYC	OC-C1C	2.43	1.28	1.23
3	E	184	CYC	CMA-C3A	2.44	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	184	CYC	CAD-C3D	2.44	1.56	1.52
3	U	184	CYC	CMA-C3A	2.44	1.56	1.50
3	D	184	CYC	OC-C1C	2.44	1.28	1.23
3	K	184	CYC	CMD-C2D	2.44	1.56	1.51
3	F	184	CYC	OC-C1C	2.44	1.28	1.23
3	B	255	CYC	CHD-C4C	2.45	1.44	1.38
3	R	184	CYC	CMA-C3A	2.46	1.56	1.50
3	U	184	CYC	OC-C1C	2.46	1.28	1.23
3	R	184	CYC	C4C-NC	2.46	1.42	1.37
3	K	184	CYC	OC-C1C	2.46	1.28	1.23
3	W	184	CYC	CMA-C3A	2.47	1.56	1.50
3	B	255	CYC	OC-C1C	2.47	1.28	1.23
3	F	255	CYC	OC-C1C	2.47	1.28	1.23
3	R	255	CYC	OC-C1C	2.47	1.28	1.23
3	D	184	CYC	CAD-C3D	2.47	1.56	1.52
3	I	184	CYC	CMA-C3A	2.48	1.56	1.50
3	T	255	CYC	CHD-C4C	2.48	1.44	1.38
3	O	184	CYC	OC-C1C	2.48	1.28	1.23
3	O	184	CYC	CMA-C3A	2.48	1.56	1.50
3	W	184	CYC	OC-C1C	2.48	1.28	1.23
3	R	255	CYC	CMA-C3A	2.49	1.56	1.50
3	H	255	CYC	CMA-C3A	2.50	1.56	1.50
3	N	184	CYC	OC-C1C	2.50	1.28	1.23
3	N	184	CYC	CMA-C3A	2.50	1.56	1.50
3	G	184	CYC	C4C-NC	2.51	1.43	1.37
3	L	184	CYC	CMA-C3A	2.51	1.56	1.50
3	D	255	CYC	CMA-C3A	2.53	1.56	1.50
3	F	255	CYC	CMA-C3A	2.53	1.56	1.50
3	N	255	CYC	OC-C1C	2.54	1.28	1.23
3	B	255	CYC	CMA-C3A	2.54	1.56	1.50
3	V	255	CYC	CMA-C3A	2.58	1.56	1.50
3	J	255	CYC	CMA-C3A	2.60	1.56	1.50
3	S	184	CYC	CMA-C3A	2.60	1.56	1.50
3	J	184	CYC	CMA-C3A	2.60	1.56	1.50
3	H	184	CYC	CMA-C3A	2.61	1.56	1.50
3	B	184	CYC	CMA-C3A	2.62	1.56	1.50
3	L	255	CYC	CMA-C3A	2.63	1.56	1.50
3	X	184	CYC	CMA-C3A	2.63	1.56	1.50
3	G	184	CYC	CAD-C3D	2.63	1.56	1.52
3	Q	184	CYC	CAD-C3D	2.64	1.56	1.52
3	T	184	CYC	CAD-C3D	2.65	1.56	1.52
3	A	184	CYC	CMA-C3A	2.65	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	184	CYC	CMA-C3A	2.66	1.56	1.50
3	S	184	CYC	CAD-C3D	2.66	1.56	1.52
3	Q	184	CYC	CMA-C3A	2.67	1.56	1.50
3	P	184	CYC	CMA-C3A	2.67	1.56	1.50
3	M	184	CYC	CMA-C3A	2.68	1.56	1.50
3	H	255	CYC	OC-C1C	2.68	1.28	1.23
3	P	255	CYC	CMA-C3A	2.69	1.56	1.50
3	E	184	CYC	OC-C1C	2.71	1.28	1.23
3	N	255	CYC	CAD-C3D	2.72	1.56	1.52
3	F	184	CYC	CAD-C3D	2.75	1.56	1.52
3	O	184	CYC	CHD-C4C	2.77	1.45	1.38
3	N	255	CYC	CMA-C3A	2.78	1.56	1.50
3	P	184	CYC	CAD-C3D	2.78	1.56	1.52
3	W	184	CYC	CAD-C3D	2.80	1.56	1.52
3	C	184	CYC	CMA-C3A	2.83	1.56	1.50
3	K	184	CYC	CAD-C3D	2.86	1.56	1.52
3	C	184	CYC	CAD-C3D	2.89	1.57	1.52
3	U	184	CYC	CAD-C3D	2.91	1.57	1.52
3	B	184	CYC	CAD-C3D	2.93	1.57	1.52
3	X	184	CYC	CAD-C3D	2.97	1.57	1.52
3	L	255	CYC	CAD-C3D	2.99	1.57	1.52
3	H	184	CYC	CAD-C3D	3.01	1.57	1.52
3	L	184	CYC	CAD-C3D	3.02	1.57	1.52
3	N	184	CYC	CAD-C3D	3.05	1.57	1.52
3	X	255	CYC	CAD-C3D	3.05	1.57	1.52
3	P	255	CYC	CAD-C3D	3.09	1.57	1.52
3	A	184	CYC	CAD-C3D	3.10	1.57	1.52
3	M	184	CYC	CAD-C3D	3.10	1.57	1.52
3	V	184	CYC	CAD-C3D	3.11	1.57	1.52
3	F	255	CYC	CAD-C3D	3.13	1.57	1.52
3	J	255	CYC	CAD-C3D	3.21	1.57	1.52
3	J	184	CYC	CAD-C3D	3.23	1.57	1.52
3	H	255	CYC	CAD-C3D	3.28	1.57	1.52
3	B	255	CYC	CAD-C3D	3.29	1.57	1.52
3	T	255	CYC	CAD-C3D	3.29	1.57	1.52
3	R	255	CYC	CAD-C3D	3.35	1.57	1.52
3	R	184	CYC	CAD-C3D	3.38	1.57	1.52
3	D	255	CYC	CAD-C3D	3.40	1.57	1.52
3	V	255	CYC	CAD-C3D	3.50	1.58	1.52
3	M	184	CYC	CHA-C1A	6.00	1.40	1.35
3	E	184	CYC	CHA-C1A	6.16	1.40	1.35
3	R	255	CYC	CHA-C1A	6.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	255	CYC	CHA-C1A	6.21	1.40	1.35
3	W	184	CYC	CHA-C1A	6.26	1.40	1.35
3	V	255	CYC	CHA-C1A	6.34	1.40	1.35
3	D	184	CYC	CHA-C1A	6.42	1.40	1.35
3	B	255	CYC	CHA-C1A	6.46	1.40	1.35
3	S	184	CYC	CHA-C1A	6.54	1.40	1.35
3	Q	184	CYC	CHA-C1A	6.64	1.41	1.35
3	H	184	CYC	CHA-C1A	6.66	1.41	1.35
3	V	184	CYC	CHA-C1A	6.68	1.41	1.35
3	X	255	CYC	CHA-C1A	6.69	1.41	1.35
3	O	184	CYC	CHA-C1A	6.74	1.41	1.35
3	N	184	CYC	CHA-C1A	6.74	1.41	1.35
3	A	184	CYC	CHA-C1A	6.75	1.41	1.35
3	T	184	CYC	CHA-C1A	6.80	1.41	1.35
3	P	184	CYC	CHA-C1A	6.87	1.41	1.35
3	F	255	CYC	CHA-C1A	6.88	1.41	1.35
3	G	184	CYC	CHA-C1A	6.89	1.41	1.35
3	T	255	CYC	CHA-C1A	6.97	1.41	1.35
3	C	184	CYC	CHA-C1A	6.97	1.41	1.35
3	F	184	CYC	CHA-C1A	7.01	1.41	1.35
3	R	184	CYC	CHA-C1A	7.05	1.41	1.35
3	P	255	CYC	CHA-C1A	7.07	1.41	1.35
3	X	184	CYC	CHA-C1A	7.11	1.41	1.35
3	I	184	CYC	CHA-C1A	7.12	1.41	1.35
3	D	255	CYC	CHA-C1A	7.17	1.41	1.35
3	L	184	CYC	CHA-C1A	7.23	1.41	1.35
3	U	184	CYC	CHA-C1A	7.37	1.41	1.35
3	B	184	CYC	CHA-C1A	7.42	1.41	1.35
3	K	184	CYC	CHA-C1A	7.46	1.41	1.35
3	L	255	CYC	CHA-C1A	7.49	1.41	1.35
3	N	255	CYC	CHA-C1A	7.50	1.41	1.35
3	H	255	CYC	CHA-C1A	8.05	1.42	1.35
3	J	184	CYC	CHA-C1A	8.14	1.42	1.35

All (528) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	184	CYC	C4B-C3B-C2B	-7.56	103.73	108.05
3	F	184	CYC	C4B-C3B-C2B	-7.54	103.74	108.05
3	L	184	CYC	C4B-C3B-C2B	-7.40	103.82	108.05
3	T	184	CYC	C4B-C3B-C2B	-7.34	103.86	108.05
3	D	184	CYC	C4B-C3B-C2B	-7.33	103.86	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	184	CYC	C4B-C3B-C2B	-7.31	103.88	108.05
3	N	255	CYC	C4B-C3B-C2B	-7.29	103.89	108.05
3	K	184	CYC	C4B-C3B-C2B	-7.28	103.89	108.05
3	W	184	CYC	C4B-C3B-C2B	-7.28	103.89	108.05
3	H	255	CYC	C4B-C3B-C2B	-7.22	103.93	108.05
3	E	184	CYC	C4B-C3B-C2B	-7.20	103.94	108.05
3	P	184	CYC	C4B-C3B-C2B	-7.17	103.96	108.05
3	Q	184	CYC	C4B-C3B-C2B	-7.17	103.96	108.05
3	A	184	CYC	C4B-C3B-C2B	-7.17	103.96	108.05
3	X	184	CYC	C4B-C3B-C2B	-7.16	103.96	108.05
3	V	184	CYC	C4B-C3B-C2B	-7.14	103.97	108.05
3	P	255	CYC	C4B-C3B-C2B	-7.10	104.00	108.05
3	J	255	CYC	C4B-C3B-C2B	-7.09	104.00	108.05
3	I	184	CYC	C4B-C3B-C2B	-7.08	104.01	108.05
3	B	184	CYC	C4B-C3B-C2B	-7.06	104.02	108.05
3	V	255	CYC	C4B-C3B-C2B	-7.06	104.02	108.05
3	M	184	CYC	C4B-C3B-C2B	-7.04	104.03	108.05
3	R	255	CYC	C4B-C3B-C2B	-7.04	104.03	108.05
3	F	255	CYC	C4B-C3B-C2B	-7.03	104.04	108.05
3	N	184	CYC	C4B-C3B-C2B	-7.01	104.05	108.05
3	J	184	CYC	C4B-C3B-C2B	-7.01	104.05	108.05
3	O	184	CYC	C4B-C3B-C2B	-7.00	104.06	108.05
3	S	184	CYC	C4B-C3B-C2B	-6.96	104.07	108.05
3	H	184	CYC	C4B-C3B-C2B	-6.94	104.09	108.05
3	T	255	CYC	C4B-C3B-C2B	-6.93	104.09	108.05
3	C	184	CYC	C4B-C3B-C2B	-6.92	104.10	108.05
3	L	255	CYC	C4B-C3B-C2B	-6.91	104.10	108.05
3	B	255	CYC	C4B-C3B-C2B	-6.91	104.10	108.05
3	G	184	CYC	C4B-C3B-C2B	-6.85	104.14	108.05
3	L	184	CYC	OC-C1C-C2C	-6.85	120.72	126.25
3	V	184	CYC	OC-C1C-C2C	-6.83	120.73	126.25
3	D	255	CYC	C4B-C3B-C2B	-6.69	104.23	108.05
3	H	184	CYC	OC-C1C-C2C	-6.66	120.87	126.25
3	P	184	CYC	OC-C1C-C2C	-6.61	120.91	126.25
3	O	184	CYC	OC-C1C-C2C	-6.59	120.93	126.25
3	X	255	CYC	C4B-C3B-C2B	-6.48	104.35	108.05
3	U	184	CYC	OC-C1C-C2C	-6.44	121.05	126.25
3	D	184	CYC	OC-C1C-C2C	-6.42	121.07	126.25
3	K	184	CYC	OC-C1C-C2C	-6.40	121.08	126.25
3	J	255	CYC	OC-C1C-C2C	-6.39	121.09	126.25
3	W	184	CYC	OC-C1C-C2C	-6.39	121.09	126.25
3	R	184	CYC	OC-C1C-C2C	-6.39	121.09	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	184	CYC	OC-C1C-C2C	-6.38	121.10	126.25
3	B	184	CYC	OC-C1C-C2C	-6.37	121.10	126.25
3	Q	184	CYC	OC-C1C-C2C	-6.37	121.10	126.25
3	G	184	CYC	OC-C1C-C2C	-6.34	121.13	126.25
3	X	184	CYC	OC-C1C-C2C	-6.32	121.14	126.25
3	A	184	CYC	OC-C1C-C2C	-6.24	121.21	126.25
3	T	184	CYC	OC-C1C-C2C	-6.22	121.22	126.25
3	F	184	CYC	OC-C1C-C2C	-6.15	121.28	126.25
3	M	184	CYC	OC-C1C-C2C	-6.11	121.32	126.25
3	C	184	CYC	OC-C1C-C2C	-6.11	121.32	126.25
3	B	255	CYC	OC-C1C-C2C	-6.09	121.33	126.25
3	R	255	CYC	OC-C1C-C2C	-6.09	121.33	126.25
3	J	184	CYC	OC-C1C-C2C	-6.08	121.34	126.25
3	E	184	CYC	OC-C1C-C2C	-5.99	121.42	126.25
3	N	184	CYC	OC-C1C-C2C	-5.96	121.44	126.25
3	S	184	CYC	OC-C1C-C2C	-5.93	121.47	126.25
3	T	255	CYC	OC-C1C-C2C	-5.89	121.50	126.25
3	X	255	CYC	OC-C1C-C2C	-5.80	121.57	126.25
3	P	255	CYC	OC-C1C-C2C	-5.79	121.57	126.25
3	F	255	CYC	OC-C1C-C2C	-5.66	121.68	126.25
3	L	255	CYC	OC-C1C-C2C	-5.65	121.69	126.25
3	D	255	CYC	OC-C1C-C2C	-5.58	121.74	126.25
3	H	255	CYC	OC-C1C-C2C	-5.53	121.78	126.25
3	N	255	CYC	OC-C1C-C2C	-5.47	121.83	126.25
3	V	255	CYC	OC-C1C-C2C	-5.43	121.87	126.25
3	D	255	CYC	OB-C4B-C3B	-3.80	123.53	128.09
3	X	255	CYC	OB-C4B-C3B	-3.77	123.57	128.09
3	M	184	CYC	CHA-C1A-NA	-3.73	122.00	128.67
3	S	184	CYC	CHA-C1A-NA	-3.73	122.01	128.67
3	U	184	CYC	OB-C4B-C3B	-3.72	123.64	128.09
3	D	184	CYC	CHA-C1A-NA	-3.71	122.03	128.67
3	B	255	CYC	OB-C4B-C3B	-3.70	123.65	128.09
3	P	255	CYC	OB-C4B-C3B	-3.69	123.67	128.09
3	A	184	CYC	CHA-C1A-NA	-3.67	122.11	128.67
3	H	255	CYC	OB-C4B-C3B	-3.65	123.72	128.09
3	N	184	CYC	CHA-C1A-NA	-3.63	122.19	128.67
3	L	255	CYC	OB-C4B-C3B	-3.60	123.78	128.09
3	E	184	CYC	CHA-C1A-NA	-3.59	122.25	128.67
3	O	184	CYC	CHA-C1A-NA	-3.59	122.26	128.67
3	X	184	CYC	OB-C4B-C3B	-3.56	123.82	128.09
3	I	184	CYC	CHA-C1A-NA	-3.55	122.33	128.67
3	I	184	CYC	OB-C4B-C3B	-3.54	123.85	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	184	CYC	CHA-C1A-NA	-3.53	122.37	128.67
3	Q	184	CYC	CHA-C1A-NA	-3.52	122.37	128.67
3	R	255	CYC	OB-C4B-C3B	-3.50	123.90	128.09
3	U	184	CYC	CHA-C1A-NA	-3.50	122.42	128.67
3	W	184	CYC	CHA-C1A-NA	-3.49	122.43	128.67
3	B	184	CYC	OB-C4B-C3B	-3.48	123.92	128.09
3	J	184	CYC	OB-C4B-C3B	-3.47	123.94	128.09
3	V	184	CYC	CHA-C1A-NA	-3.46	122.48	128.67
3	H	184	CYC	OB-C4B-C3B	-3.46	123.94	128.09
3	K	184	CYC	CHA-C1A-NA	-3.45	122.50	128.67
3	G	184	CYC	OB-C4B-C3B	-3.44	123.96	128.09
3	J	255	CYC	C1B-NB-C4B	-3.44	105.69	110.73
3	P	184	CYC	CHA-C1A-NA	-3.44	122.51	128.67
3	J	255	CYC	OB-C4B-C3B	-3.43	123.98	128.09
3	N	255	CYC	OB-C4B-C3B	-3.43	123.98	128.09
3	T	184	CYC	OB-C4B-C3B	-3.43	123.98	128.09
3	H	184	CYC	CHA-C1A-NA	-3.43	122.54	128.67
3	T	255	CYC	OB-C4B-C3B	-3.41	124.00	128.09
3	X	184	CYC	CHA-C1A-NA	-3.41	122.57	128.67
3	G	184	CYC	CHA-C1A-NA	-3.41	122.58	128.67
3	X	255	CYC	CHA-C1A-NA	-3.40	122.60	128.67
3	C	184	CYC	CHA-C1A-NA	-3.39	122.61	128.67
3	P	184	CYC	OB-C4B-C3B	-3.38	124.03	128.09
3	B	184	CYC	CHA-C1A-NA	-3.38	122.62	128.67
3	X	184	CYC	C1B-NB-C4B	-3.38	105.78	110.73
3	V	255	CYC	OB-C4B-C3B	-3.35	124.07	128.09
3	O	184	CYC	OB-C4B-C3B	-3.35	124.07	128.09
3	L	255	CYC	C1B-NB-C4B	-3.34	105.84	110.73
3	N	184	CYC	OB-C4B-C3B	-3.34	124.09	128.09
3	L	184	CYC	OB-C4B-C3B	-3.33	124.10	128.09
3	V	184	CYC	OB-C4B-C3B	-3.32	124.11	128.09
3	F	255	CYC	OB-C4B-C3B	-3.31	124.13	128.09
3	B	255	CYC	C1B-NB-C4B	-3.30	105.90	110.73
3	D	184	CYC	OB-C4B-C3B	-3.30	124.14	128.09
3	F	184	CYC	CHA-C1A-NA	-3.29	122.78	128.67
3	X	255	CYC	C1B-NB-C4B	-3.28	105.93	110.73
3	N	255	CYC	CHA-C1A-NA	-3.26	122.84	128.67
3	K	184	CYC	OB-C4B-C3B	-3.25	124.20	128.09
3	V	255	CYC	CHA-C1A-NA	-3.25	122.87	128.67
3	L	184	CYC	CHA-C1A-NA	-3.24	122.87	128.67
3	A	184	CYC	OB-C4B-C3B	-3.24	124.21	128.09
3	K	184	CYC	C1B-NB-C4B	-3.24	106.00	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	184	CYC	OB-C4B-C3B	-3.23	124.22	128.09
3	D	184	CYC	C1B-NB-C4B	-3.23	106.01	110.73
3	N	184	CYC	C1B-NB-C4B	-3.23	106.01	110.73
3	L	184	CYC	C1B-NB-C4B	-3.22	106.02	110.73
3	H	255	CYC	C1B-NB-C4B	-3.22	106.03	110.73
3	G	184	CYC	C1B-NB-C4B	-3.21	106.03	110.73
3	R	255	CYC	CHA-C1A-NA	-3.21	122.93	128.67
3	F	255	CYC	CHA-C1A-NA	-3.21	122.93	128.67
3	F	255	CYC	C1B-NB-C4B	-3.20	106.05	110.73
3	D	255	CYC	C1B-NB-C4B	-3.20	106.05	110.73
3	M	184	CYC	C1B-NB-C4B	-3.20	106.05	110.73
3	T	184	CYC	CHA-C1A-NA	-3.19	122.97	128.67
3	E	184	CYC	OB-C4B-C3B	-3.19	124.27	128.09
3	H	184	CYC	C1B-NB-C4B	-3.18	106.08	110.73
3	T	255	CYC	C1B-NB-C4B	-3.18	106.08	110.73
3	Q	184	CYC	OB-C4B-C3B	-3.17	124.29	128.09
3	P	255	CYC	CHA-C1A-NA	-3.17	123.01	128.67
3	S	184	CYC	C1B-NB-C4B	-3.16	106.10	110.73
3	I	184	CYC	C1B-NB-C4B	-3.16	106.11	110.73
3	L	255	CYC	CHA-C1A-NA	-3.16	123.02	128.67
3	E	184	CYC	C1B-NB-C4B	-3.16	106.11	110.73
3	M	184	CYC	OB-C4B-C3B	-3.15	124.31	128.09
3	J	255	CYC	CHA-C1A-NA	-3.15	123.03	128.67
3	A	184	CYC	C1B-NB-C4B	-3.15	106.12	110.73
3	B	255	CYC	CHA-C1A-NA	-3.14	123.05	128.67
3	U	184	CYC	C1B-NB-C4B	-3.14	106.14	110.73
3	P	255	CYC	C1B-NB-C4B	-3.13	106.15	110.73
3	R	255	CYC	C1B-NB-C4B	-3.12	106.16	110.73
3	N	255	CYC	C1B-NB-C4B	-3.12	106.17	110.73
3	W	184	CYC	C1B-NB-C4B	-3.11	106.18	110.73
3	Q	184	CYC	C1B-NB-C4B	-3.11	106.18	110.73
3	S	184	CYC	OB-C4B-C3B	-3.11	124.36	128.09
3	D	255	CYC	CHA-C1A-NA	-3.10	123.14	128.67
3	V	184	CYC	C1B-NB-C4B	-3.09	106.21	110.73
3	B	184	CYC	C1B-NB-C4B	-3.09	106.21	110.73
3	J	184	CYC	CHA-C1A-NA	-3.09	123.15	128.67
3	T	255	CYC	CHA-C1A-NA	-3.07	123.19	128.67
3	V	255	CYC	C1B-NB-C4B	-3.07	106.25	110.73
3	J	184	CYC	C1B-NB-C4B	-3.06	106.25	110.73
3	O	184	CYC	C1B-NB-C4B	-3.05	106.27	110.73
3	F	184	CYC	C1B-NB-C4B	-3.05	106.27	110.73
3	C	184	CYC	OB-C4B-C3B	-3.01	124.48	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	184	CYC	C1B-NB-C4B	-3.01	106.33	110.73
3	F	184	CYC	OB-C4B-C3B	-3.01	124.48	128.09
3	C	184	CYC	CAD-C3D-C4D	-3.00	123.75	127.01
3	T	184	CYC	C1B-NB-C4B	-3.00	106.35	110.73
3	R	184	CYC	C1B-NB-C4B	-2.99	106.36	110.73
3	C	184	CYC	C1B-NB-C4B	-2.98	106.37	110.73
3	R	184	CYC	OB-C4B-C3B	-2.96	124.54	128.09
3	J	255	CYC	CHB-C4A-NA	-2.91	119.36	124.91
3	D	184	CYC	CAD-C3D-C4D	-2.88	123.88	127.01
3	H	255	CYC	CHA-C1A-NA	-2.88	123.52	128.67
3	G	184	CYC	CAD-C3D-C4D	-2.82	123.94	127.01
3	M	184	CYC	CAD-C3D-C4D	-2.77	124.00	127.01
3	Q	184	CYC	CAD-C3D-C4D	-2.76	124.02	127.01
3	S	184	CYC	CAD-C3D-C4D	-2.67	124.11	127.01
3	B	255	CYC	CHB-C4A-NA	-2.66	119.84	124.91
3	E	184	CYC	CAD-C3D-C4D	-2.66	124.12	127.01
3	D	255	CYC	CHB-C4A-NA	-2.66	119.85	124.91
3	A	184	CYC	CAD-C3D-C4D	-2.64	124.14	127.01
3	X	184	CYC	CAD-C3D-C4D	-2.64	124.14	127.01
3	R	255	CYC	CHB-C4A-NA	-2.63	119.89	124.91
3	W	184	CYC	CAD-C3D-C4D	-2.62	124.16	127.01
3	P	255	CYC	CHB-C4A-NA	-2.61	119.95	124.91
3	X	255	CYC	CHB-C4A-NA	-2.58	120.00	124.91
3	F	184	CYC	CAD-C3D-C4D	-2.47	124.33	127.01
3	K	184	CYC	CAD-C3D-C4D	-2.46	124.33	127.01
3	T	184	CYC	CAD-C3D-C4D	-2.46	124.33	127.01
3	F	255	CYC	CHB-C4A-NA	-2.45	120.24	124.91
3	L	184	CYC	CAD-C3D-C4D	-2.44	124.36	127.01
3	H	184	CYC	CAD-C3D-C4D	-2.41	124.39	127.01
3	L	255	CYC	CHB-C4A-NA	-2.40	120.33	124.91
3	O	184	CYC	CAD-C3D-C4D	-2.39	124.42	127.01
3	T	255	CYC	CHB-C4A-NA	-2.38	120.38	124.91
3	N	255	CYC	CHB-C4A-NA	-2.37	120.39	124.91
3	U	184	CYC	CAD-C3D-C4D	-2.36	124.44	127.01
3	V	255	CYC	CHB-C4A-NA	-2.33	120.47	124.91
3	P	184	CYC	CAD-C3D-C4D	-2.31	124.50	127.01
3	I	184	CYC	CAD-C3D-C4D	-2.28	124.53	127.01
3	P	184	CYC	CHB-C1B-NB	-2.27	121.24	126.16
3	B	255	CYC	CAD-C3D-C4D	-2.27	124.54	127.01
3	R	184	CYC	CHB-C4A-NA	-2.27	120.59	124.91
3	U	184	CYC	CHB-C4A-NA	-2.26	120.60	124.91
3	B	184	CYC	CAD-C3D-C4D	-2.26	124.55	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	255	CYC	CHB-C4A-NA	-2.23	120.67	124.91
3	J	184	CYC	CAD-C3D-C4D	-2.20	124.62	127.01
3	V	184	CYC	CAD-C3D-C4D	-2.18	124.64	127.01
3	G	184	CYC	CHB-C4A-NA	-2.18	120.76	124.91
3	T	255	CYC	CAD-C3D-C4D	-2.16	124.67	127.01
3	R	255	CYC	CAD-C3D-C4D	-2.15	124.67	127.01
3	Q	184	CYC	CHB-C4A-NA	-2.15	120.81	124.91
3	S	184	CYC	CHB-C4A-NA	-2.14	120.84	124.91
3	J	255	CYC	CAD-C3D-C4D	-2.13	124.69	127.01
3	N	184	CYC	CAD-C3D-C4D	-2.13	124.69	127.01
3	X	255	CYC	CAD-C3D-C4D	-2.10	124.73	127.01
3	E	184	CYC	CHB-C4A-NA	-2.08	120.95	124.91
3	B	184	CYC	CHB-C1B-NB	-2.08	121.67	126.16
3	R	184	CYC	CAD-C3D-C4D	-2.07	124.76	127.01
3	F	184	CYC	CHB-C1B-NB	-2.06	121.70	126.16
3	O	184	CYC	CHB-C4A-NA	-2.06	120.99	124.91
3	T	184	CYC	CHB-C1B-NB	-2.05	121.71	126.16
3	J	184	CYC	CHB-C1B-NB	-2.05	121.72	126.16
3	R	184	CYC	CHB-C1B-NB	-2.05	121.72	126.16
3	N	184	CYC	CHB-C1B-NB	-2.03	121.77	126.16
3	K	184	CYC	CHB-C4A-NA	-2.02	121.07	124.91
3	A	184	CYC	CHB-C4A-NA	-2.00	121.09	124.91
3	M	184	CYC	CHB-C4A-NA	-2.00	121.10	124.91
3	H	184	CYC	CAD-CBD-CGD	2.01	116.42	112.75
3	T	184	CYC	CBD-CAD-C3D	2.01	116.13	112.53
3	A	184	CYC	CHB-C4A-C3A	2.02	129.81	124.88
3	K	184	CYC	CHB-C4A-C3A	2.02	129.82	124.88
3	J	255	CYC	CAD-CBD-CGD	2.03	116.47	112.75
3	K	184	CYC	C2C-C3C-C4C	2.04	104.95	101.50
3	L	184	CYC	CAD-CBD-CGD	2.04	116.49	112.75
3	G	184	CYC	CAC-C3C-C2C	2.05	119.29	114.13
3	V	184	CYC	C1D-CHD-C4C	2.05	134.70	127.23
3	O	184	CYC	CHB-C4A-C3A	2.05	129.89	124.88
3	E	184	CYC	CHB-C4A-C3A	2.06	129.91	124.88
3	B	255	CYC	CBD-CAD-C3D	2.07	116.24	112.53
3	P	255	CYC	CAD-CBD-CGD	2.07	116.55	112.75
3	U	184	CYC	C1D-CHD-C4C	2.08	134.81	127.23
3	V	184	CYC	CAD-CBD-CGD	2.08	116.57	112.75
3	S	184	CYC	CAC-C3C-C2C	2.09	119.39	114.13
3	B	184	CYC	C1D-CHD-C4C	2.12	134.93	127.23
3	C	184	CYC	CAC-C3C-C2C	2.12	119.46	114.13
3	S	184	CYC	CHB-C4A-C3A	2.12	130.06	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	184	CYC	CHB-C4A-C3A	2.12	130.06	124.88
3	G	184	CYC	C2C-C3C-C4C	2.14	105.12	101.50
3	T	255	CYC	CBD-CAD-C3D	2.14	116.36	112.53
3	V	255	CYC	CAD-CBD-CGD	2.14	116.67	112.75
3	X	255	CYC	CAD-CBD-CGD	2.16	116.71	112.75
3	L	184	CYC	CBD-CAD-C3D	2.17	116.42	112.53
3	W	184	CYC	C2C-C3C-C4C	2.18	105.19	101.50
3	B	184	CYC	CBD-CAD-C3D	2.21	116.49	112.53
3	J	184	CYC	CAD-CBD-CGD	2.21	116.80	112.75
3	G	184	CYC	CHB-C4A-C3A	2.21	130.28	124.88
3	F	184	CYC	CMC-C2C-C3C	2.23	124.19	114.35
3	L	255	CYC	CAD-CBD-CGD	2.25	116.86	112.75
3	U	184	CYC	CHB-C4A-C3A	2.26	130.39	124.88
3	N	184	CYC	CMC-C2C-C3C	2.28	124.42	114.35
3	J	184	CYC	CMC-C2C-C3C	2.28	124.45	114.35
3	P	184	CYC	CAD-CBD-CGD	2.29	116.94	112.75
3	H	255	CYC	CHB-C4A-C3A	2.29	130.48	124.88
3	F	255	CYC	CAD-CBD-CGD	2.30	116.96	112.75
3	X	184	CYC	CMC-C2C-C3C	2.33	124.66	114.35
3	X	184	CYC	CBD-CAD-C3D	2.34	116.72	112.53
3	B	184	CYC	CMC-C2C-C3C	2.34	124.70	114.35
3	R	184	CYC	CHB-C4A-C3A	2.36	130.64	124.88
3	E	184	CYC	CAC-C3C-C2C	2.36	120.07	114.13
3	T	184	CYC	CMC-C2C-C3C	2.37	124.83	114.35
3	F	255	CYC	CMC-C2C-C3C	2.37	124.85	114.35
3	I	184	CYC	CAC-C3C-C2C	2.38	120.11	114.13
3	L	255	CYC	CHB-C4A-C3A	2.39	130.71	124.88
3	K	184	CYC	CAC-C3C-C2C	2.39	120.14	114.13
3	B	255	CYC	CAD-CBD-CGD	2.39	117.13	112.75
3	A	184	CYC	CAC-C3C-C2C	2.39	120.14	114.13
3	T	255	CYC	CAD-CBD-CGD	2.40	117.14	112.75
3	W	184	CYC	CAC-C3C-C2C	2.40	120.16	114.13
3	P	184	CYC	CMC-C2C-C3C	2.41	125.02	114.35
3	L	184	CYC	CMC-C2C-C3C	2.42	125.04	114.35
3	D	184	CYC	CMC-C2C-C3C	2.42	125.05	114.35
3	V	255	CYC	CHB-C4A-C3A	2.42	130.79	124.88
3	N	255	CYC	CHB-C4A-C3A	2.43	130.80	124.88
3	L	255	CYC	CMC-C2C-C3C	2.43	125.11	114.35
3	T	255	CYC	CHB-C4A-C3A	2.44	130.83	124.88
3	H	255	CYC	CMC-C2C-C3C	2.44	125.15	114.35
3	H	184	CYC	CBD-CAD-C3D	2.44	116.91	112.53
3	H	184	CYC	CMC-C2C-C3C	2.45	125.18	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	184	CYC	CMC-C2C-C3C	2.45	125.20	114.35
3	J	184	CYC	CBD-CAD-C3D	2.45	116.93	112.53
3	P	255	CYC	CMC-C2C-C3C	2.46	125.22	114.35
3	F	255	CYC	CHB-C4A-C3A	2.47	130.91	124.88
3	B	255	CYC	CMC-C2C-C3C	2.48	125.34	114.35
3	X	255	CYC	CMC-C2C-C3C	2.50	125.39	114.35
3	V	184	CYC	CMC-C2C-C3C	2.50	125.40	114.35
3	V	255	CYC	CMC-C2C-C3C	2.50	125.41	114.35
3	J	255	CYC	CMC-C2C-C3C	2.53	125.55	114.35
3	P	255	CYC	CHB-C4A-C3A	2.54	131.07	124.88
3	N	255	CYC	CMC-C2C-C3C	2.54	125.59	114.35
3	T	255	CYC	CMC-C2C-C3C	2.55	125.62	114.35
3	R	255	CYC	CMC-C2C-C3C	2.56	125.66	114.35
3	R	184	CYC	CAD-CBD-CGD	2.58	117.47	112.75
3	D	255	CYC	CMC-C2C-C3C	2.59	125.81	114.35
3	B	255	CYC	CHB-C4A-C3A	2.60	131.24	124.88
3	X	255	CYC	CHB-C4A-C3A	2.62	131.27	124.88
3	G	184	CYC	CMC-C2C-C3C	2.62	125.94	114.35
3	M	184	CYC	CMC-C2C-C3C	2.62	125.94	114.35
3	U	184	CYC	CMC-C2C-C3C	2.62	125.96	114.35
3	N	184	CYC	CAD-CBD-CGD	2.63	117.57	112.75
3	C	184	CYC	CMC-C2C-C3C	2.64	126.01	114.35
3	Q	184	CYC	CMC-C2C-C3C	2.64	126.04	114.35
3	R	255	CYC	CAD-CBD-CGD	2.65	117.60	112.75
3	S	184	CYC	CMC-C2C-C3C	2.66	126.11	114.35
3	D	255	CYC	CHB-C4A-C3A	2.68	131.43	124.88
3	R	255	CYC	CHB-C4A-C3A	2.68	131.43	124.88
3	O	184	CYC	CMC-C2C-C3C	2.70	126.30	114.35
3	W	184	CYC	CMC-C2C-C3C	2.75	126.52	114.35
3	K	184	CYC	CMC-C2C-C3C	2.75	126.53	114.35
3	I	184	CYC	CMC-C2C-C3C	2.75	126.53	114.35
3	J	255	CYC	CHB-C4A-C3A	2.76	131.62	124.88
3	D	184	CYC	CBD-CAD-C3D	2.78	117.52	112.53
3	A	184	CYC	CMC-C2C-C3C	2.80	126.72	114.35
3	E	184	CYC	CMC-C2C-C3C	2.80	126.75	114.35
3	V	184	CYC	CBD-CAD-C3D	2.84	117.61	112.53
3	F	184	CYC	CBD-CAD-C3D	2.84	117.62	112.53
3	O	184	CYC	CAD-CBD-CGD	2.93	118.11	112.75
3	V	184	CYC	CMA-C3A-C4A	3.07	130.06	125.06
3	L	184	CYC	CMA-C3A-C4A	3.12	130.14	125.06
3	B	184	CYC	CMA-C3A-C4A	3.15	130.18	125.06
3	G	184	CYC	CAD-CBD-CGD	3.16	118.53	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	184	CYC	CMA-C3A-C4A	3.17	130.22	125.06
3	J	184	CYC	CMA-C3A-C4A	3.20	130.26	125.06
3	N	184	CYC	CMA-C3A-C4A	3.20	130.26	125.06
3	T	184	CYC	CMA-C3A-C4A	3.22	130.30	125.06
3	X	184	CYC	CMA-C3A-C4A	3.26	130.36	125.06
3	H	184	CYC	CMA-C3A-C4A	3.26	130.37	125.06
3	F	184	CYC	CMA-C3A-C4A	3.27	130.38	125.06
3	O	184	CYC	CMA-C3A-C4A	3.28	130.40	125.06
3	W	184	CYC	CMA-C3A-C4A	3.31	130.45	125.06
3	E	184	CYC	CMA-C3A-C4A	3.32	130.46	125.06
3	G	184	CYC	CMA-C3A-C4A	3.32	130.47	125.06
3	I	184	CYC	CMA-C3A-C4A	3.33	130.47	125.06
3	P	184	CYC	CMA-C3A-C4A	3.35	130.51	125.06
3	K	184	CYC	CMA-C3A-C4A	3.37	130.54	125.06
3	A	184	CYC	CAD-CBD-CGD	3.40	118.98	112.75
3	M	184	CYC	CAD-CBD-CGD	3.42	119.01	112.75
3	R	184	CYC	CMA-C3A-C4A	3.45	130.67	125.06
3	M	184	CYC	CMA-C3A-C4A	3.48	130.73	125.06
3	U	184	CYC	CMA-C3A-C4A	3.49	130.74	125.06
3	U	184	CYC	CAD-CBD-CGD	3.51	119.19	112.75
3	Q	184	CYC	CMA-C3A-C4A	3.54	130.81	125.06
3	H	255	CYC	CMA-C3A-C4A	3.57	130.86	125.06
3	C	184	CYC	CMA-C3A-C4A	3.57	130.87	125.06
3	E	184	CYC	CAD-CBD-CGD	3.57	119.29	112.75
3	Q	184	CYC	CAD-CBD-CGD	3.59	119.33	112.75
3	A	184	CYC	CMA-C3A-C4A	3.62	130.94	125.06
3	S	184	CYC	CAD-CBD-CGD	3.63	119.39	112.75
3	I	184	CYC	CAD-CBD-CGD	3.65	119.43	112.75
3	L	255	CYC	CMA-C3A-C4A	3.66	131.02	125.06
3	S	184	CYC	CMA-C3A-C4A	3.68	131.05	125.06
3	T	255	CYC	CMA-C3A-C4A	3.68	131.05	125.06
3	D	255	CYC	CMA-C3A-C4A	3.69	131.07	125.06
3	B	255	CYC	CMA-C3A-C4A	3.72	131.12	125.06
3	W	184	CYC	CAD-CBD-CGD	3.78	119.67	112.75
3	N	255	CYC	CMA-C3A-C4A	3.84	131.30	125.06
3	V	255	CYC	CMA-C3A-C4A	3.84	131.31	125.06
3	P	255	CYC	CMA-C3A-C4A	3.87	131.36	125.06
3	R	255	CYC	CMA-C3A-C4A	3.88	131.37	125.06
3	F	255	CYC	CMA-C3A-C4A	3.93	131.45	125.06
3	X	255	CYC	CMA-C3A-C4A	3.94	131.48	125.06
3	K	184	CYC	CAD-CBD-CGD	3.96	120.01	112.75
3	J	255	CYC	CMA-C3A-C4A	4.07	131.68	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	184	CYC	CAD-CBD-CGD	4.08	120.22	112.75
3	E	184	CYC	C2C-C1C-NC	6.03	114.06	108.30
3	O	184	CYC	C2C-C1C-NC	6.10	114.12	108.30
3	S	184	CYC	C2C-C1C-NC	6.13	114.15	108.30
3	A	184	CYC	C2C-C1C-NC	6.13	114.15	108.30
3	B	255	CYC	C2C-C1C-NC	6.14	114.16	108.30
3	N	255	CYC	C2C-C1C-NC	6.15	114.17	108.30
3	W	184	CYC	C2C-C1C-NC	6.17	114.20	108.30
3	D	255	CYC	C2C-C1C-NC	6.18	114.20	108.30
3	R	184	CYC	C2C-C1C-NC	6.18	114.21	108.30
3	H	255	CYC	C2C-C1C-NC	6.20	114.22	108.30
3	T	255	CYC	C2C-C1C-NC	6.21	114.23	108.30
3	N	184	CYC	C2C-C1C-NC	6.21	114.23	108.30
3	F	184	CYC	C2C-C1C-NC	6.21	114.24	108.30
3	L	255	CYC	C2C-C1C-NC	6.22	114.25	108.30
3	G	184	CYC	C2C-C1C-NC	6.22	114.25	108.30
3	R	255	CYC	C2C-C1C-NC	6.24	114.27	108.30
3	F	255	CYC	C2C-C1C-NC	6.26	114.28	108.30
3	Q	184	CYC	C2C-C1C-NC	6.30	114.31	108.30
3	V	255	CYC	C2C-C1C-NC	6.30	114.32	108.30
3	I	184	CYC	C2C-C1C-NC	6.30	114.32	108.30
3	X	184	CYC	C2C-C1C-NC	6.31	114.33	108.30
3	V	184	CYC	C2C-C1C-NC	6.32	114.34	108.30
3	M	184	CYC	C2C-C1C-NC	6.32	114.34	108.30
3	P	255	CYC	C2C-C1C-NC	6.34	114.35	108.30
3	K	184	CYC	C2C-C1C-NC	6.35	114.37	108.30
3	H	184	CYC	C2C-C1C-NC	6.36	114.37	108.30
3	B	184	CYC	C2C-C1C-NC	6.37	114.39	108.30
3	J	184	CYC	C2C-C1C-NC	6.38	114.39	108.30
3	D	184	CYC	C2C-C1C-NC	6.40	114.41	108.30
3	P	184	CYC	C2C-C1C-NC	6.40	114.42	108.30
3	X	255	CYC	C2C-C1C-NC	6.42	114.44	108.30
3	T	184	CYC	C2C-C1C-NC	6.44	114.45	108.30
3	C	184	CYC	C2C-C1C-NC	6.45	114.46	108.30
3	U	184	CYC	C2C-C1C-NC	6.47	114.48	108.30
3	J	255	CYC	C2C-C1C-NC	6.53	114.54	108.30
3	L	184	CYC	C2C-C1C-NC	6.54	114.54	108.30
3	W	184	CYC	C3B-C4B-NB	6.97	113.08	106.74
3	D	184	CYC	CMC-C2C-C1C	6.98	127.08	112.43
3	F	184	CYC	CMC-C2C-C1C	6.99	127.11	112.43
3	O	184	CYC	C3B-C4B-NB	6.99	113.09	106.74
3	N	255	CYC	CMC-C2C-C1C	7.05	127.23	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	184	CYC	C3B-C4B-NB	7.07	113.16	106.74
3	G	184	CYC	C3B-C4B-NB	7.07	113.16	106.74
3	S	184	CYC	C3B-C4B-NB	7.07	113.17	106.74
3	F	255	CYC	C3B-C4B-NB	7.08	113.18	106.74
3	M	184	CYC	C3B-C4B-NB	7.09	113.18	106.74
3	C	184	CYC	C3B-C4B-NB	7.09	113.19	106.74
3	T	255	CYC	C3B-C4B-NB	7.09	113.19	106.74
3	V	255	CYC	C3B-C4B-NB	7.11	113.20	106.74
3	L	255	CYC	C3B-C4B-NB	7.12	113.21	106.74
3	B	255	CYC	C3B-C4B-NB	7.14	113.23	106.74
3	P	184	CYC	CMC-C2C-C1C	7.14	127.44	112.43
3	F	255	CYC	CMC-C2C-C1C	7.19	127.54	112.43
3	V	255	CYC	CMC-C2C-C1C	7.20	127.55	112.43
3	X	184	CYC	CMC-C2C-C1C	7.20	127.56	112.43
3	Q	184	CYC	C3B-C4B-NB	7.20	113.29	106.74
3	H	184	CYC	CMC-C2C-C1C	7.20	127.56	112.43
3	J	184	CYC	CMC-C2C-C1C	7.25	127.66	112.43
3	H	184	CYC	C3B-C4B-NB	7.26	113.34	106.74
3	B	184	CYC	C3B-C4B-NB	7.27	113.35	106.74
3	J	255	CYC	CMC-C2C-C1C	7.27	127.70	112.43
3	V	184	CYC	CMC-C2C-C1C	7.27	127.70	112.43
3	I	184	CYC	C3B-C4B-NB	7.27	113.35	106.74
3	N	184	CYC	C3B-C4B-NB	7.28	113.36	106.74
3	T	255	CYC	CMC-C2C-C1C	7.28	127.72	112.43
3	V	184	CYC	C3B-C4B-NB	7.29	113.37	106.74
3	N	184	CYC	CMC-C2C-C1C	7.29	127.75	112.43
3	P	255	CYC	CMC-C2C-C1C	7.29	127.75	112.43
3	R	255	CYC	CMC-C2C-C1C	7.30	127.76	112.43
3	R	184	CYC	C3B-C4B-NB	7.30	113.38	106.74
3	L	184	CYC	CMC-C2C-C1C	7.31	127.78	112.43
3	X	255	CYC	C3B-C4B-NB	7.31	113.38	106.74
3	P	255	CYC	C3B-C4B-NB	7.31	113.39	106.74
3	D	184	CYC	C3B-C4B-NB	7.32	113.39	106.74
3	K	184	CYC	C3B-C4B-NB	7.32	113.40	106.74
3	R	184	CYC	CMC-C2C-C1C	7.33	127.82	112.43
3	L	184	CYC	C3B-C4B-NB	7.33	113.40	106.74
3	D	255	CYC	C3B-C4B-NB	7.34	113.41	106.74
3	D	255	CYC	CMC-C2C-C1C	7.34	127.84	112.43
3	E	184	CYC	C3B-C4B-NB	7.34	113.42	106.74
3	J	184	CYC	C3B-C4B-NB	7.35	113.42	106.74
3	F	184	CYC	C3B-C4B-NB	7.37	113.44	106.74
3	H	255	CYC	CMC-C2C-C1C	7.38	127.93	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	255	CYC	C3B-C4B-NB	7.38	113.45	106.74
3	X	255	CYC	CMC-C2C-C1C	7.40	127.97	112.43
3	J	255	CYC	C3B-C4B-NB	7.40	113.47	106.74
3	T	184	CYC	CMC-C2C-C1C	7.40	127.97	112.43
3	U	184	CYC	C3B-C4B-NB	7.41	113.47	106.74
3	B	184	CYC	CMC-C2C-C1C	7.41	127.99	112.43
3	X	184	CYC	C3B-C4B-NB	7.44	113.50	106.74
3	B	255	CYC	CMC-C2C-C1C	7.44	128.06	112.43
3	L	255	CYC	CMC-C2C-C1C	7.47	128.12	112.43
3	T	184	CYC	C3B-C4B-NB	7.48	113.54	106.74
3	H	255	CYC	C3B-C4B-NB	7.49	113.55	106.74
3	U	184	CYC	CMC-C2C-C1C	7.49	128.17	112.43
3	P	184	CYC	C3B-C4B-NB	7.52	113.58	106.74
3	N	255	CYC	C3B-C4B-NB	7.53	113.58	106.74
3	K	184	CYC	CMC-C2C-C1C	7.61	128.42	112.43
3	M	184	CYC	CMC-C2C-C1C	7.63	128.45	112.43
3	O	184	CYC	CMC-C2C-C1C	7.64	128.49	112.43
3	A	184	CYC	CMC-C2C-C1C	7.69	128.57	112.43
3	S	184	CYC	CMC-C2C-C1C	7.71	128.63	112.43
3	W	184	CYC	CMC-C2C-C1C	7.77	128.74	112.43
3	G	184	CYC	CMC-C2C-C1C	7.79	128.79	112.43
3	Q	184	CYC	CMC-C2C-C1C	7.79	128.79	112.43
3	E	184	CYC	CMC-C2C-C1C	7.80	128.81	112.43
3	I	184	CYC	CMC-C2C-C1C	7.85	128.92	112.43
3	X	255	CYC	CAB-C3B-C4B	7.86	128.38	121.51
3	C	184	CYC	CMC-C2C-C1C	7.90	129.03	112.43
3	D	255	CYC	CAB-C3B-C4B	8.05	128.54	121.51
3	P	255	CYC	CAB-C3B-C4B	8.15	128.62	121.51
3	O	184	CYC	CAB-C3B-C4B	8.22	128.69	121.51
3	H	184	CYC	CAB-C3B-C4B	8.49	128.92	121.51
3	H	255	CYC	CAB-C3B-C4B	8.51	128.94	121.51
3	J	184	CYC	CAB-C3B-C4B	8.53	128.96	121.51
3	B	255	CYC	CAB-C3B-C4B	8.55	128.98	121.51
3	U	184	CYC	CAB-C3B-C4B	8.58	129.00	121.51
3	A	184	CYC	CAB-C3B-C4B	8.61	129.03	121.51
3	L	255	CYC	CAB-C3B-C4B	8.62	129.04	121.51
3	V	255	CYC	CAB-C3B-C4B	8.64	129.05	121.51
3	N	255	CYC	CAB-C3B-C4B	8.67	129.08	121.51
3	P	184	CYC	CAB-C3B-C4B	8.68	129.09	121.51
3	R	255	CYC	CAB-C3B-C4B	8.70	129.11	121.51
3	G	184	CYC	CAB-C3B-C4B	8.73	129.13	121.51
3	N	184	CYC	CAB-C3B-C4B	8.75	129.15	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	184	CYC	CAB-C3B-C4B	8.76	129.16	121.51
3	I	184	CYC	CAB-C3B-C4B	8.77	129.17	121.51
3	F	255	CYC	CAB-C3B-C4B	8.81	129.21	121.51
3	J	255	CYC	CAB-C3B-C4B	8.85	129.24	121.51
3	V	184	CYC	CAB-C3B-C4B	8.87	129.26	121.51
3	T	255	CYC	CAB-C3B-C4B	8.88	129.27	121.51
3	X	184	CYC	CAB-C3B-C4B	8.88	129.27	121.51
3	E	184	CYC	CAB-C3B-C4B	8.95	129.32	121.51
3	S	184	CYC	CAB-C3B-C4B	8.98	129.35	121.51
3	C	184	CYC	CAB-C3B-C4B	9.04	129.41	121.51
3	M	184	CYC	CAB-C3B-C4B	9.06	129.43	121.51
3	W	184	CYC	CAB-C3B-C4B	9.07	129.43	121.51
3	Q	184	CYC	CAB-C3B-C4B	9.11	129.47	121.51
3	T	184	CYC	CAB-C3B-C4B	9.14	129.49	121.51
3	L	184	CYC	CAB-C3B-C4B	9.30	129.63	121.51
3	K	184	CYC	CAB-C3B-C4B	9.35	129.67	121.51
3	D	184	CYC	CAB-C3B-C4B	9.48	129.78	121.51
3	F	184	CYC	CAB-C3B-C4B	9.98	130.22	121.51
3	R	184	CYC	CAB-C3B-C4B	9.99	130.24	121.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	184	CYC	C2C

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	184	CYC	C1B-CHB-C4A-C3A
3	L	184	CYC	C1B-CHB-C4A-C3A
3	H	184	CYC	C1B-CHB-C4A-C3A
3	J	184	CYC	C1B-CHB-C4A-C3A
3	B	184	CYC	C1B-CHB-C4A-C3A
3	N	184	CYC	C1B-CHB-C4A-C3A
3	D	184	CYC	C1B-CHB-C4A-C3A
3	V	184	CYC	C1B-CHB-C4A-C3A
3	F	184	CYC	C1B-CHB-C4A-C3A
3	P	184	CYC	C1B-CHB-C4A-C3A
3	T	184	CYC	C1B-CHB-C4A-C3A
3	X	184	CYC	C1B-CHB-C4A-NA
3	L	184	CYC	C1B-CHB-C4A-NA
3	M	184	CYC	C1B-CHB-C4A-C3A

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Mol	Chain	Res	Type	Atoms
3	R	184	CYC	C1B-CHB-C4A-C3A
3	W	184	CYC	C1B-CHB-C4A-C3A
3	H	184	CYC	C1B-CHB-C4A-NA
3	I	184	CYC	C1B-CHB-C4A-C3A
3	Q	184	CYC	C1B-CHB-C4A-C3A
3	O	184	CYC	C1B-CHB-C4A-C3A
3	J	184	CYC	C1B-CHB-C4A-NA
3	C	184	CYC	C1B-CHB-C4A-C3A
3	G	184	CYC	C1B-CHB-C4A-C3A
3	B	184	CYC	C1B-CHB-C4A-NA
3	N	184	CYC	C1B-CHB-C4A-NA
3	A	184	CYC	C1B-CHB-C4A-C3A
3	K	184	CYC	C1B-CHB-C4A-C3A
3	E	184	CYC	C1B-CHB-C4A-C3A
3	S	184	CYC	C1B-CHB-C4A-C3A
3	U	184	CYC	C1B-CHB-C4A-C3A
3	V	184	CYC	C1B-CHB-C4A-NA
3	D	184	CYC	C1B-CHB-C4A-NA
3	F	184	CYC	C1B-CHB-C4A-NA
3	P	184	CYC	C1B-CHB-C4A-NA
3	T	184	CYC	C1B-CHB-C4A-NA
3	H	255	CYC	C1B-CHB-C4A-C3A
3	V	255	CYC	C1B-CHB-C4A-C3A
3	M	184	CYC	C1B-CHB-C4A-NA
3	R	184	CYC	C1B-CHB-C4A-NA
3	W	184	CYC	C1B-CHB-C4A-NA
3	O	184	CYC	C1B-CHB-C4A-NA
3	Q	184	CYC	C1B-CHB-C4A-NA
3	I	184	CYC	C1B-CHB-C4A-NA
3	C	184	CYC	C1B-CHB-C4A-NA
3	D	255	CYC	C1B-CHB-C4A-C3A
3	T	255	CYC	C1B-CHB-C4A-C3A
3	N	255	CYC	C1B-CHB-C4A-C3A
3	G	184	CYC	C1B-CHB-C4A-NA
3	P	255	CYC	C1B-CHB-C4A-C3A
3	J	255	CYC	C1B-CHB-C4A-C3A
3	X	255	CYC	C1B-CHB-C4A-C3A
3	K	184	CYC	C1B-CHB-C4A-NA
3	E	184	CYC	C1B-CHB-C4A-NA
3	A	184	CYC	C1B-CHB-C4A-NA
3	F	255	CYC	C1B-CHB-C4A-C3A
3	S	184	CYC	C1B-CHB-C4A-NA

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Mol	Chain	Res	Type	Atoms
3	U	184	CYC	C1B-CHB-C4A-NA
3	L	255	CYC	C1B-CHB-C4A-C3A
3	B	255	CYC	C1B-CHB-C4A-C3A
3	R	255	CYC	C1B-CHB-C4A-C3A
3	H	255	CYC	C1B-CHB-C4A-NA
3	V	255	CYC	C1B-CHB-C4A-NA
3	D	255	CYC	C1B-CHB-C4A-NA
3	T	255	CYC	C1B-CHB-C4A-NA
3	N	255	CYC	C1B-CHB-C4A-NA
3	P	255	CYC	C1B-CHB-C4A-NA
3	J	255	CYC	C1B-CHB-C4A-NA
3	X	255	CYC	C1B-CHB-C4A-NA
3	F	255	CYC	C1B-CHB-C4A-NA
3	L	255	CYC	C1B-CHB-C4A-NA
3	B	255	CYC	C1B-CHB-C4A-NA
3	R	255	CYC	C1B-CHB-C4A-NA

There are no ring outliers.

36 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	184	CYC	4	0
3	B	184	CYC	5	0
3	B	255	CYC	4	0
3	C	184	CYC	4	0
3	D	184	CYC	3	0
3	D	255	CYC	3	0
3	E	184	CYC	2	0
3	F	184	CYC	4	0
3	F	255	CYC	4	0
3	G	184	CYC	1	0
3	H	184	CYC	4	0
3	H	255	CYC	4	0
3	I	184	CYC	1	0
3	J	184	CYC	2	0
3	J	255	CYC	3	0
3	K	184	CYC	2	0
3	L	184	CYC	4	0
3	L	255	CYC	5	0
3	M	184	CYC	3	0
3	N	184	CYC	6	0
3	N	255	CYC	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	184	CYC	4	0
3	P	184	CYC	4	0
3	P	255	CYC	4	0
3	Q	184	CYC	3	0
3	R	184	CYC	4	0
3	R	255	CYC	3	0
3	S	184	CYC	5	0
3	T	184	CYC	3	0
3	T	255	CYC	4	0
3	U	184	CYC	5	0
3	V	184	CYC	2	0
3	V	255	CYC	3	0
3	W	184	CYC	3	0
3	X	184	CYC	3	0
3	X	255	CYC	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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