



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:12 PM GMT

PDB ID : 1IZL
Title : Crystal Structure of Photosystem II
Authors : Kamiya, N.; Shen, J.-R.
Deposited on : 2002-10-04
Resolution : 3.70 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

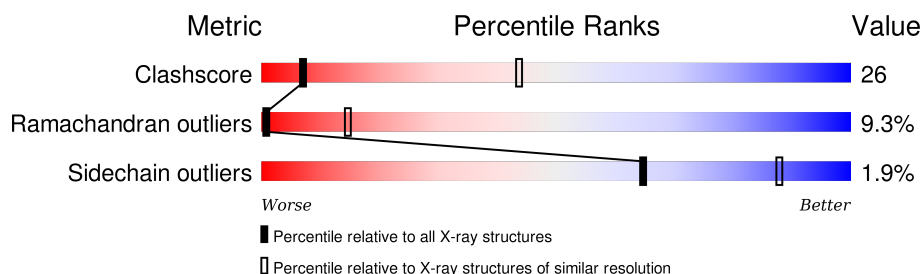
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)






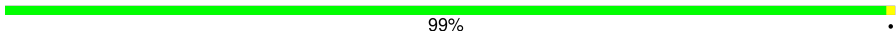
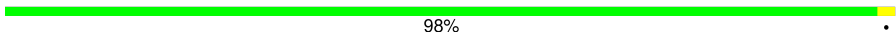
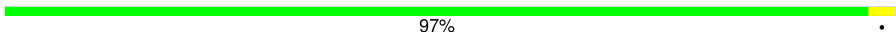







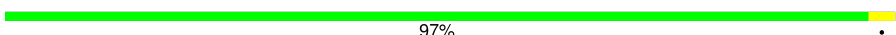
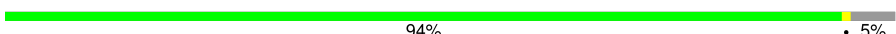




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	J	360	
2	B	472	
2	L	472	
3	C	473	
3	M	473	
4	D	352	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	N	352	
5	E	83	
5	P	83	
6	F	44	
6	Q	44	
7	G	220	
7	R	220	
8	H	33	
8	S	33	
9	I	26	
9	T	26	
10	K	37	
10	W	37	
11	O	205	
11	Y	205	
12	U	97	
12	Z	97	
13	0	137	
13	V	137	
14	1	25	
14	X	25	

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
17	CLA	A	365	X	-	-	-
17	CLA	A	366	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	368	X	-	X	-
17	CLA	A	369	X	-	-	-
17	CLA	B	1107	X	-	-	-
17	CLA	B	1108	X	-	-	-
17	CLA	B	1109	X	-	-	-
17	CLA	B	1110	X	-	-	-
17	CLA	B	1111	X	-	-	-
17	CLA	B	1112	X	-	-	-
17	CLA	B	1113	X	-	-	-
17	CLA	B	1114	X	-	-	-
17	CLA	B	1115	X	-	-	-
17	CLA	B	1116	X	-	-	-
17	CLA	B	1117	X	-	-	-
17	CLA	B	1118	X	-	-	-
17	CLA	B	1119	X	-	-	-
17	CLA	B	1120	X	-	-	-
17	CLA	B	1121	X	-	-	-
17	CLA	B	1122	X	-	-	-
17	CLA	C	1078	X	-	-	-
17	CLA	C	1079	X	-	-	-
17	CLA	C	1080	X	-	-	-
17	CLA	C	1081	X	-	-	-
17	CLA	C	1082	X	-	-	-
17	CLA	C	1083	X	-	-	-
17	CLA	C	1084	X	-	-	-
17	CLA	C	1085	X	-	-	-
17	CLA	C	1086	X	-	-	-
17	CLA	C	1087	X	-	-	-
17	CLA	C	1088	X	-	-	-
17	CLA	C	1089	X	-	X	-
17	CLA	D	354	X	-	-	-
17	CLA	D	355	X	-	-	-
17	CLA	D	357	X	-	-	-
17	CLA	G	221	X	-	-	-
17	CLA	J	365	X	-	-	-
17	CLA	J	367	X	-	X	-
17	CLA	J	368	X	-	-	-
17	CLA	L	1107	X	-	-	-
17	CLA	L	1108	X	-	-	-
17	CLA	L	1109	X	-	-	-
17	CLA	L	1110	X	-	-	-
17	CLA	L	1111	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	L	1112	X	-	-	-
17	CLA	L	1113	X	-	-	-
17	CLA	L	1114	X	-	-	-
17	CLA	L	1115	X	-	-	-
17	CLA	L	1116	X	-	-	-
17	CLA	L	1117	X	-	-	-
17	CLA	L	1118	X	-	-	-
17	CLA	L	1119	X	-	X	-
17	CLA	L	1120	X	-	X	-
17	CLA	L	1121	X	-	-	-
17	CLA	L	1122	X	-	-	-
17	CLA	M	1078	X	-	-	-
17	CLA	M	1079	X	-	-	-
17	CLA	M	1080	X	-	-	-
17	CLA	M	1081	X	-	-	-
17	CLA	M	1082	X	-	-	-
17	CLA	M	1083	X	-	-	-
17	CLA	M	1084	X	-	-	-
17	CLA	M	1085	X	-	-	-
17	CLA	M	1086	X	-	-	-
17	CLA	M	1087	X	-	-	-
17	CLA	M	1088	X	-	-	-
17	CLA	N	354	X	-	-	-
17	CLA	N	355	X	-	-	-
17	CLA	N	356	X	-	-	-
17	CLA	N	358	X	-	-	-
17	CLA	R	221	X	-	-	-
17	CLA	W	64	X	-	-	-
18	PHO	N	357	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 22804 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 Photosystem II: Subunit PsbA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	0	0	0
			1595	975	310	310			
1	J	299	Total	C	N	O	0	0	0
			1602	984	308	310			

- Molecule 2 is a protein called Photosystem II: Subunit PsbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	48
			2004	1238	386	379	1			
2	L	424	Total	C	N	O		0	0	48
			2001	1242	383	376				

- Molecule 3 is a protein called Photosystem II: Subunit PsbC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	349	Total	C	N	O	0	0	0
			1792	1082	358	352			
3	M	347	Total	C	N	O	0	0	0
			1759	1057	354	348			

- Molecule 4 is a protein called Photosystem II: Subunit PsbD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	277	Total	C	N	O	0	0	0
			1460	899	282	279			
4	N	277	Total	C	N	O	0	0	0
			1451	888	284	279			

- Molecule 5 is a protein called Photosystem II: Subunit PsbE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	35	Total	C	N	O	0	0	0
			175	105	35	35			
5	P	17	Total	C	N	O	0	0	0
			83	49	17	17			

- Molecule 6 is a protein called Photosystem II: Subunit PsbF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	30	Total	C	N	O	0	0	0
			166	105	31	30			
6	Q	26	Total	C	N	O	0	0	0
			129	77	26	26			

- Molecule 7 is a protein called Photosystem II: Subunit PsbG.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	G	220	Total	C	0	0	220
			220	220			
7	R	220	Total	C	0	0	220
			220	220			

- Molecule 8 is a protein called Photosystem II: Subunit PsbH.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	33	Total	C	N	O	0	0	0
			165	99	33	33			
8	S	32	Total	C	N	O	0	0	0
			160	96	32	32			

- Molecule 9 is a protein called Photosystem II: Subunit PsbI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	26	Total	C	N	O	0	0	0
			130	78	26	26			
9	T	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 10 is a protein called Photosystem II: Subunit PsbK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	27	Total	C	N	O	0	0	0
			137	83	27	27			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	W	27	Total	C	N	O	0	0	0
			137	83	27	27			

- Molecule 11 is a protein called Photosystem II: Subunit PsbO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	205	Total	C	N	O	0	0	0
			1025	615	205	205			
11	Y	192	Total	C	N	O	0	0	0
			960	576	192	192			

- Molecule 12 is a protein called Photosystem II: Subunit PsbU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	U	97	Total	C	N	O	0	0	0
			485	291	97	97			
12	Z	92	Total	C	N	O	0	0	0
			460	276	92	92			

- Molecule 13 is a protein called Photosystem II: Subunit PsbV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	V	129	Total	C	N	O	0	0	0
			676	410	136	130			
13	0	115	Total	C	N	O	0	0	0
			597	360	121	116			

- Molecule 14 is a protein called Photosystem II: Subunit PsbX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	X	25	Total	C	N	O	0	0	0
			125	75	25	25			
14	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

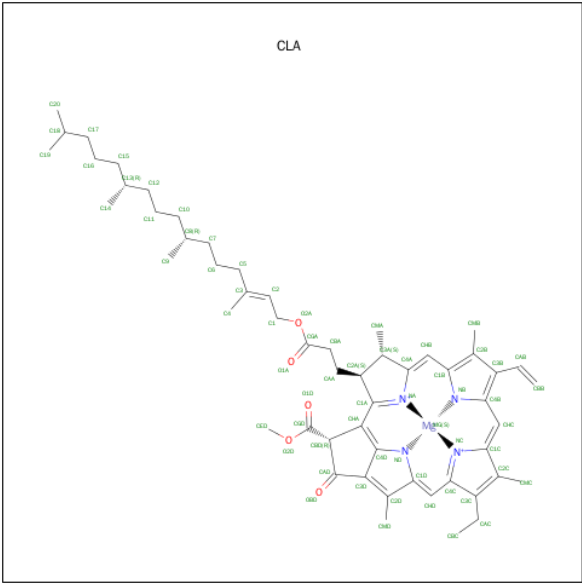
- Molecule 15 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	4	Total	Mn	0	0
			4	4		
15	A	4	Total	Mn	0	0
			4	4		

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total	Fe	0	0
			1	1		
16	N	1	Total	Fe	0	0
			1	1		

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

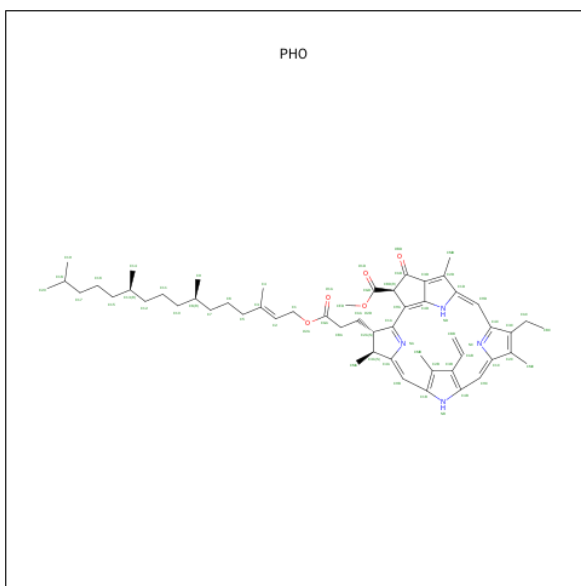
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	G	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	W	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

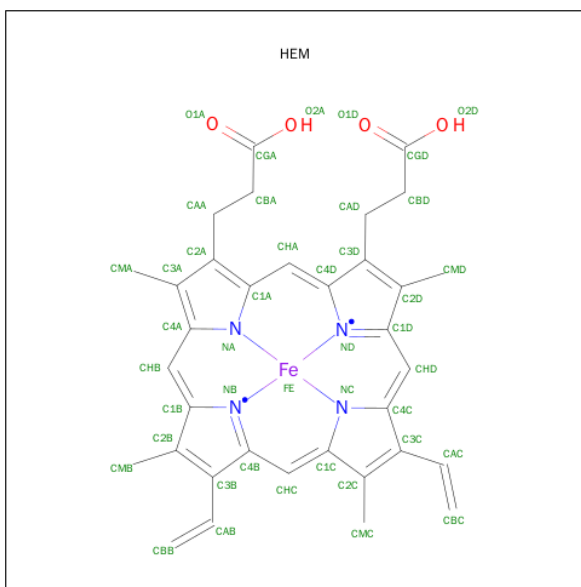
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	R	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

- Molecule 18 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



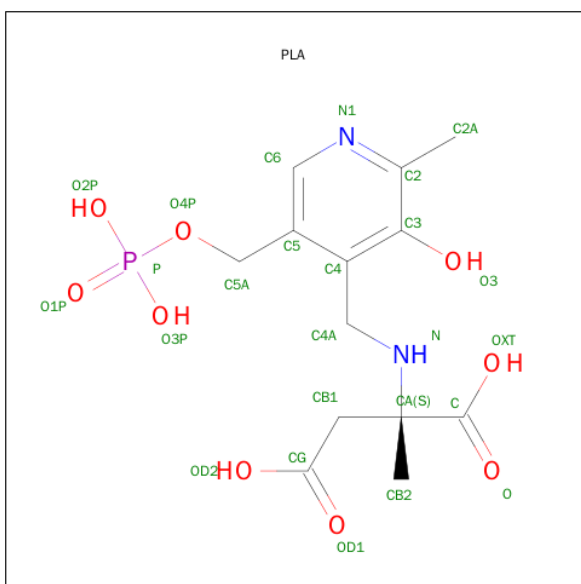
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	N	O	0	0
			34	29	4	1		
18	A	1	Total	C	N	O	0	0
			34	29	4	1		
18	N	1	Total	C	N	O	0	0
			34	29	4	1		
18	J	1	Total	C	N	O	0	0
			34	29	4	1		

- Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



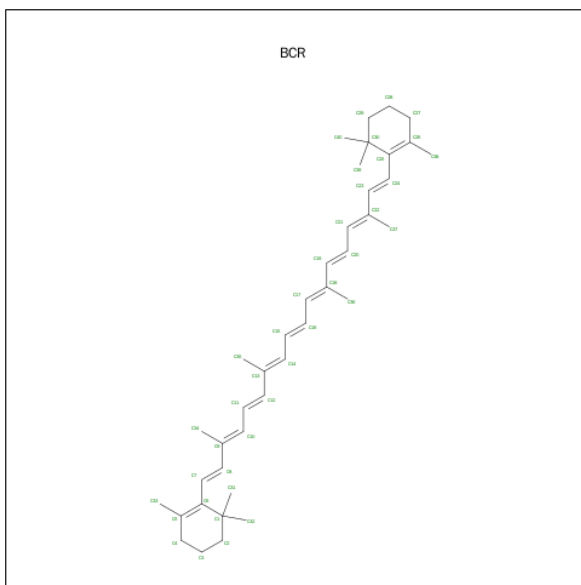
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	E	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	V	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	P	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	0	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 20 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C N 6 5 1	0	0
20	N	1	Total C N 6 5 1	0	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



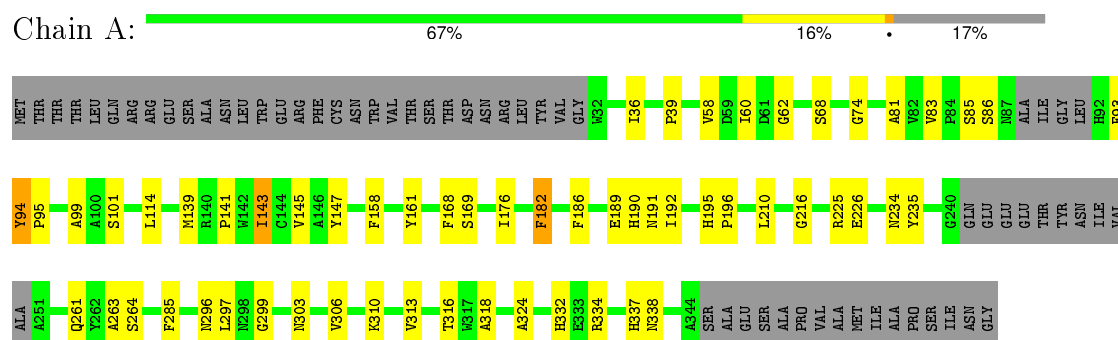
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C 22 22	0	0
21	D	1	Total C 40 40	0	0

3 Residue-property plots

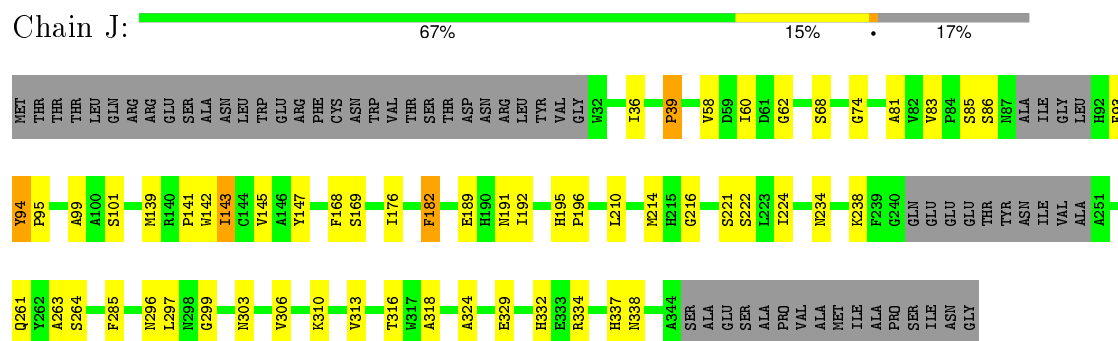
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

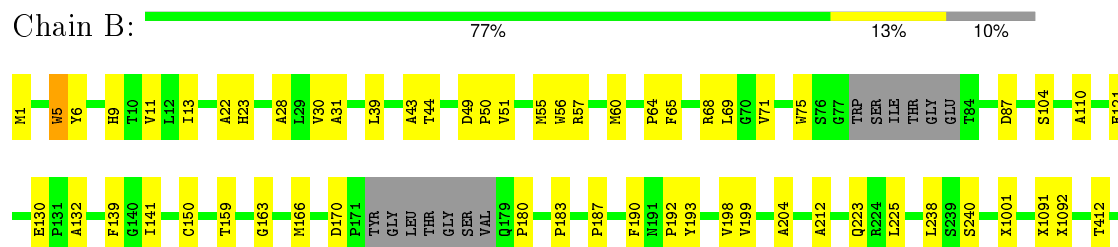
• Molecule 1: Photosystem II: Subunit PsbA

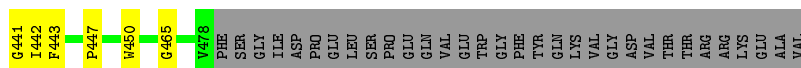


• Molecule 1: Photosystem II: Subunit PsbA



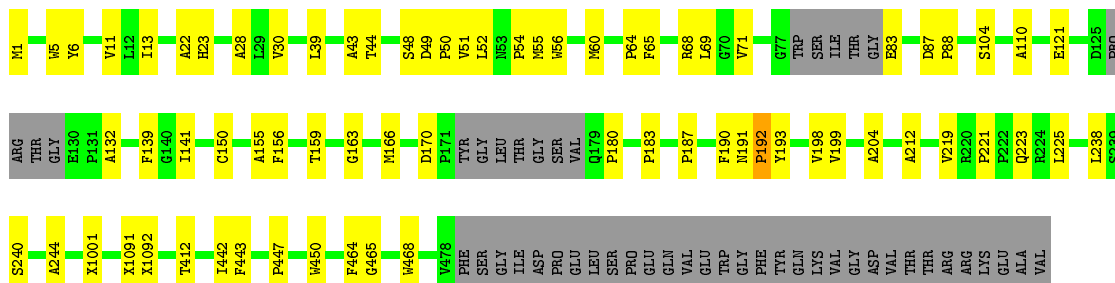
• Molecule 2: Photosystem II: Subunit PsbB





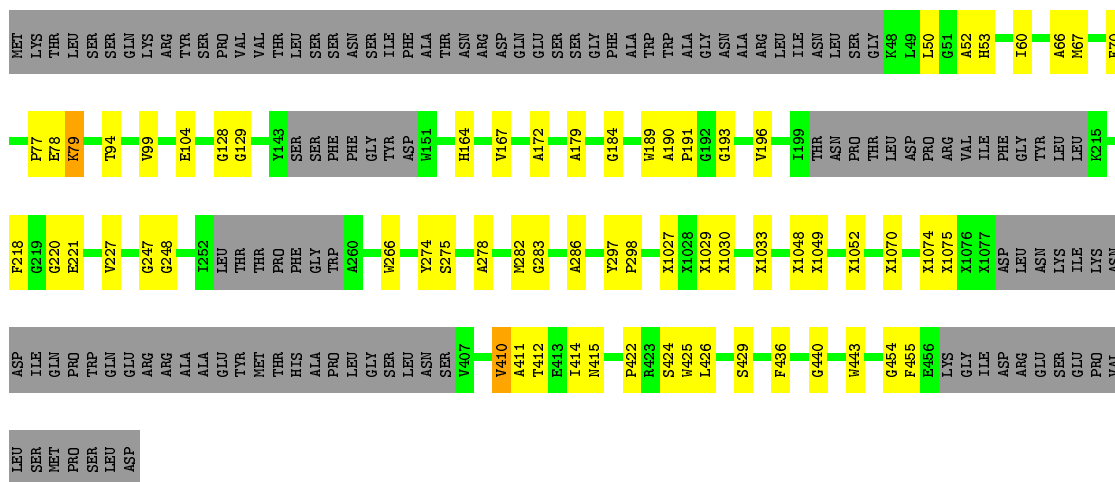
- Molecule 2: Photosystem II: Subunit PsbB

Chain L: 75% 15% 10%



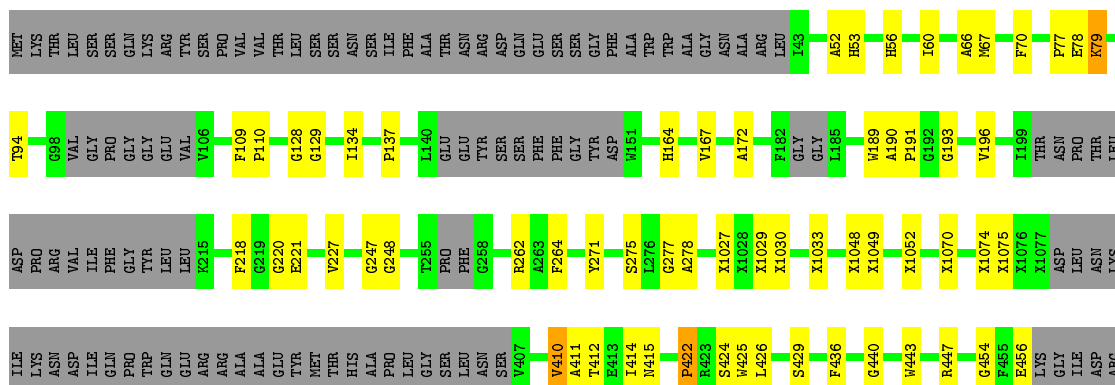
- Molecule 3: Photosystem II: Subunit PsbC

Chain C:  60% 13% 26%



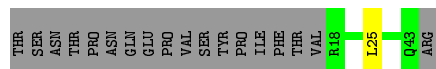
- Molecule 3: Photosystem II: Subunit PsbC

Chain M:  60% 13% 27%



- Molecule 6: Photosystem II: Subunit PsbF

Chain Q:  57% 41%



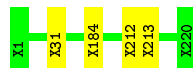
- Molecule 7: Photosystem II: Subunit PsbG

Chain G:  99%



- Molecule 7: Photosystem II: Subunit PsbG

Chain R:  98%



- Molecule 8: Photosystem II: Subunit PsbH

Chain H:  97%




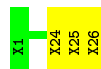
- Molecule 8: Photosystem II: Subunit PsbH

Chain S:  94%




- Molecule 9: Photosystem II: Subunit PsbI

Chain I:  88% 12%



- Molecule 9: Photosystem II: Subunit PsbI

Chain T:  88% 8%



- Molecule 10: Photosystem II: Subunit PsbK

Chain K:  62% 8% 27%



- Molecule 10: Photosystem II: Subunit PsbK

Chain W:  62% 8% 27%




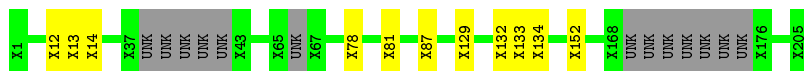
- Molecule 11: Photosystem II: Subunit PsbO

Chain O:  93% 7%



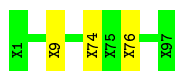
- Molecule 11: Photosystem II: Subunit PsbO

Chain Y:  88% 5% 6%



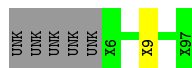
- Molecule 12: Photosystem II: Subunit PsbU

Chain U:  97%




- Molecule 12: Photosystem II: Subunit PsbU

Chain Z:  94% 5%



- Molecule 13: Photosystem II: Subunit PsbV

Chain V:  84% 10% 6%



- Molecule 13: Photosystem II: Subunit PsbV

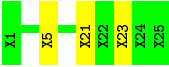
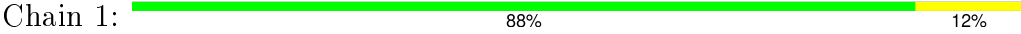
Chain 0:  75% 9% 16%



● Molecule 14: Photosystem II: Subunit PsbX



● Molecule 14: Photosystem II: Subunit PsbX



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.38Å 225.19Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.70	Depositor
% Data completeness (in resolution range)	100.0 (25.00-3.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	0.530 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22804	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: PHO, MN, CLA, FE, PLA, HEM, BCR

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	0.25	0/1613	0.40	0/2229
1	J	0.26	0/1621	0.40	0/2239
2	B	0.24	0/1685	0.41	0/2331
2	L	0.26	0/1682	0.40	0/2323
3	C	0.24	0/1421	0.40	0/1961
3	M	0.25	0/1379	0.40	0/1898
4	D	0.27	0/1475	0.40	0/2037
4	N	0.27	0/1464	0.39	0/2022
5	E	0.24	0/175	0.46	0/243
5	P	0.31	0/82	0.42	0/112
6	F	0.28	0/169	0.47	0/234
6	Q	0.26	0/128	0.40	0/177
10	K	0.25	0/137	0.45	0/191
10	W	0.25	0/137	0.45	0/191
13	O	0.24	0/600	0.37	0/831
13	V	0.23	0/683	0.38	0/949
All	All	0.25	0/14451	0.40	0/19968

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

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	1595	0	834	94	0
1	J	1602	0	843	80	0
2	B	2004	0	968	141	0
2	L	2001	0	961	139	0
3	C	1792	0	842	122	0
3	M	1759	0	793	112	0
4	D	1460	0	761	69	0
4	N	1451	0	746	67	0
5	E	175	0	81	6	0
5	P	83	0	40	2	0
6	F	166	0	95	4	0
6	Q	129	0	66	4	0
7	G	220	0	0	8	0
7	R	220	0	0	10	0
8	H	165	0	36	1	0
8	S	160	0	35	2	0
9	I	130	0	30	2	0
9	T	125	0	29	1	0
10	K	137	0	68	11	0
10	W	137	0	68	11	0
11	O	1025	0	279	37	0
11	Y	960	0	265	34	0
12	U	485	0	112	5	0
12	Z	460	0	106	1	0
13	0	597	0	278	15	0
13	V	676	0	323	16	0
14	1	125	0	28	3	0
14	X	125	0	29	6	0
15	A	4	0	0	0	0
15	J	4	0	0	0	0
16	D	1	0	0	0	0
16	N	1	0	0	0	0
17	A	140	0	68	36	0
17	B	560	0	272	113	0
17	C	420	0	204	95	0
17	D	105	0	48	12	0
17	G	35	0	17	0	0
17	J	105	0	50	23	0
17	L	560	0	272	126	0
17	M	385	0	187	75	0
17	N	140	0	68	10	0
17	R	35	0	17	0	0
17	W	35	0	17	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	34	0	19	20	0
18	D	34	0	19	8	0
18	J	34	0	19	19	0
18	N	34	0	19	28	0
19	O	25	0	4	8	0
19	E	25	0	4	0	0
19	P	25	0	4	0	0
19	V	25	0	4	8	0
20	D	6	0	1	0	0
20	N	6	0	1	0	0
21	D	40	0	56	9	0
21	K	22	0	24	1	0
All	All	22804	0	10110	848	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (848) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:HB3	17:B:1110:CLA:CMB	1.26	1.64
3:M:52:ALA:HB1	17:M:1081:CLA:CAB	1.27	1.62
2:B:465:GLY:CA	17:B:1119:CLA:HMA1	1.22	1.60
2:B:1:MET:HA	7:G:31:UNK:CA	1.20	1.60
1:A:95:PRO:HA	17:A:368:CLA:C3A	1.32	1.59
1:A:235:TYR:CE2	2:B:5:TRP:HA	1.11	1.58
2:L:204:ALA:CB	17:L:1117:CLA:HHC	1.16	1.57
11:O:152:UNK:CB	12:U:9:UNK:CB	1.77	1.57
2:B:204:ALA:CB	17:B:1117:CLA:HHC	1.16	1.56
3:C:52:ALA:HB1	17:C:1082:CLA:CAB	1.28	1.55
2:L:1:MET:HA	7:R:31:UNK:CA	1.21	1.54
2:L:223:GLN:CB	7:R:184:UNK:CA	1.78	1.53
11:Y:152:UNK:CB	12:Z:9:UNK:CB	1.85	1.51
18:A:367:PHO:CMC	4:D:148:ALA:HB1	1.37	1.51
2:L:223:GLN:H	7:R:184:UNK:CA	1.25	1.50
2:B:450:TRP:CB	17:B:1110:CLA:HMB2	1.41	1.50
4:D:212:ALA:HB3	18:D:356:PHO:CAC	1.37	1.49
2:L:450:TRP:HB3	17:L:1110:CLA:CMB	1.40	1.49
3:C:167:VAL:CB	17:C:1086:CLA:HMD2	1.40	1.47
2:L:1:MET:CA	7:R:31:UNK:CA	1.93	1.47
1:A:95:PRO:CA	17:A:368:CLA:H3A	0.99	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:PRO:HA	17:J:367:CLA:C3A	0.98	1.45
2:B:223:GLN:H	7:G:184:UNK:CA	1.28	1.44
2:B:1:MET:CA	7:G:31:UNK:CA	1.93	1.44
17:M:1081:CLA:CMA	17:W:64:CLA:HMD2	1.46	1.43
2:L:450:TRP:CB	17:L:1110:CLA:HMB2	1.47	1.42
1:A:143:ILE:CB	4:D:216:ALA:O	1.64	1.42
1:J:143:ILE:CB	4:N:216:ALA:O	1.64	1.41
1:A:235:TYR:CE2	2:B:5:TRP:CA	2.02	1.39
2:B:223:GLN:CB	7:G:184:UNK:CA	2.01	1.37
3:M:425:TRP:CD2	17:M:1079:CLA:CAB	2.08	1.37
1:A:297:LEU:CA	3:C:1074:UNK:O	1.64	1.36
2:L:223:GLN:N	7:R:184:UNK:CA	1.87	1.36
1:A:310:LYS:CB	13:V:2:GLU:C	1.86	1.36
3:M:129:GLY:CA	17:M:1087:CLA:HMB1	1.44	1.36
5:E:33:GLY:HA2	14:X:5:UNK:CB	1.54	1.35
2:L:23:HIS:CB	17:L:1118:CLA:CMC	2.05	1.35
5:E:8:PRO:HG3	14:X:25:UNK:CB	1.55	1.34
1:A:95:PRO:N	17:A:368:CLA:H3A	1.38	1.34
3:C:425:TRP:CD2	17:C:1079:CLA:CAB	2.08	1.33
5:P:33:GLY:HA2	14:1:5:UNK:CB	1.55	1.33
2:L:22:ALA:CB	17:L:1109:CLA:CAB	2.07	1.32
17:B:1108:CLA:CAC	17:B:1119:CLA:CAD	2.06	1.31
3:M:79:LYS:CB	13:O:102:PRO:CB	2.09	1.31
1:J:210:LEU:CB	18:J:366:PHO:C2C	2.07	1.30
3:C:79:LYS:CB	13:V:102:PRO:CB	2.07	1.30
2:L:465:GLY:HA2	17:L:1119:CLA:CMA	1.61	1.30
2:B:9:HIS:HE1	17:B:1116:CLA:ND	1.28	1.30
2:B:23:HIS:CB	17:B:1118:CLA:CMC	2.09	1.30
2:L:1092:UNK:CA	11:Y:132:UNK:O	1.80	1.29
3:C:53:HIS:CB	17:C:1086:CLA:CAB	2.12	1.28
3:M:53:HIS:CB	17:M:1085:CLA:CAB	2.10	1.28
2:B:465:GLY:HA2	17:B:1119:CLA:CMA	1.53	1.28
11:O:87:UNK:CB	2:L:87:ASP:CB	2.11	1.27
1:J:297:LEU:CA	3:M:1074:UNK:O	1.64	1.27
17:C:1080:CLA:CAB	10:K:21:VAL:CB	2.12	1.27
2:B:223:GLN:N	7:G:184:UNK:CA	1.96	1.27
21:D:359:BCR:C31	21:D:359:BCR:H343	1.63	1.27
2:B:1092:UNK:CA	11:O:132:UNK:O	1.80	1.27
18:A:367:PHO:C2C	4:D:148:ALA:HB1	1.65	1.25
3:M:79:LYS:CB	13:O:102:PRO:O	1.84	1.25
2:L:30:VAL:CB	17:L:1108:CLA:CAA	2.13	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:LYS:CB	13:V:102:PRO:C	2.05	1.25
4:D:200:GLY:O	17:D:354:CLA:HMA1	1.35	1.25
3:M:79:LYS:CB	13:O:102:PRO:C	2.04	1.24
1:J:297:LEU:HA	3:M:1074:UNK:O	1.19	1.24
17:M:1081:CLA:HMA2	17:W:64:CLA:CMD	1.69	1.23
1:A:95:PRO:HA	17:A:368:CLA:C2A	1.68	1.23
2:L:223:GLN:CA	7:R:184:UNK:CA	2.17	1.23
3:C:79:LYS:CB	13:V:102:PRO:O	1.86	1.23
1:A:216:GLY:O	4:D:271:MET:CB	1.88	1.22
3:M:456:GLU:O	4:N:247:VAL:CB	1.86	1.22
10:W:21:VAL:CB	17:W:64:CLA:CAB	2.17	1.21
3:M:52:ALA:CB	17:M:1081:CLA:CAB	2.16	1.21
2:B:87:ASP:CB	11:Y:87:UNK:CB	2.18	1.21
2:B:465:GLY:HA3	17:B:1119:CLA:HMA2	1.21	1.21
3:C:425:TRP:CE3	17:C:1079:CLA:CAB	2.24	1.21
2:L:238:LEU:HA	17:L:1109:CLA:HMD3	1.20	1.20
1:J:216:GLY:O	4:N:271:MET:CB	1.90	1.20
4:N:209:LEU:HA	18:N:357:PHO:C3C	1.72	1.19
2:L:212:ALA:CB	17:L:1107:CLA:HMD3	1.73	1.18
1:J:324:ALA:O	4:N:330:ALA:CB	1.90	1.18
2:B:87:ASP:CB	11:Y:87:UNK:CA	2.22	1.18
3:M:425:TRP:CE3	17:M:1079:CLA:CAB	2.27	1.18
1:A:235:TYR:CZ	2:B:5:TRP:HA	1.79	1.18
1:A:324:ALA:O	4:D:330:ALA:CB	1.91	1.18
2:L:22:ALA:HB1	17:L:1109:CLA:HMB1	1.22	1.17
3:C:275:SER:CA	17:C:1089:CLA:HMA3	1.74	1.17
3:M:1027:UNK:CB	11:Y:78:UNK:CB	2.22	1.17
3:M:129:GLY:CA	17:M:1087:CLA:CMB	2.19	1.16
3:M:129:GLY:C	17:M:1087:CLA:HMB1	1.65	1.16
2:B:23:HIS:CB	17:B:1118:CLA:HMC1	1.70	1.16
1:A:316:THR:CB	4:D:62:GLY:O	1.93	1.16
3:C:1027:UNK:CB	11:O:78:UNK:CB	2.22	1.16
2:B:1:MET:CB	7:G:31:UNK:CA	2.24	1.16
2:L:1:MET:CB	7:R:31:UNK:CA	2.23	1.16
3:M:1052:UNK:CB	11:Y:12:UNK:CB	2.24	1.16
2:B:22:ALA:HB3	17:B:1109:CLA:CAB	1.72	1.15
2:L:22:ALA:O	17:L:1109:CLA:HMB2	1.00	1.15
2:L:22:ALA:HB3	17:L:1109:CLA:CAB	1.74	1.15
1:J:316:THR:CB	4:N:62:GLY:O	1.93	1.15
3:M:167:VAL:CB	17:M:1085:CLA:HMD2	1.76	1.15
4:N:212:ALA:CB	18:N:357:PHO:CAC	2.23	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:425:TRP:CE2	17:M:1079:CLA:CAB	2.29	1.15
2:B:87:ASP:CB	11:Y:87:UNK:HA	1.77	1.15
17:M:1081:CLA:CMA	17:W:64:CLA:CMD	2.24	1.14
17:C:1080:CLA:HMD2	17:C:1082:CLA:CMA	1.77	1.14
2:B:238:LEU:HA	17:B:1109:CLA:HMD3	1.20	1.14
3:C:275:SER:HA	17:C:1089:CLA:HMA3	1.26	1.14
18:J:366:PHO:C2C	4:N:148:ALA:HB1	1.78	1.13
3:C:425:TRP:CE2	17:C:1079:CLA:CAB	2.31	1.13
1:A:297:LEU:HA	3:C:1074:UNK:O	1.19	1.13
17:M:1081:CLA:HMA3	17:W:64:CLA:HMD2	1.19	1.12
3:C:167:VAL:CB	17:C:1086:CLA:CMD	2.27	1.13
2:L:23:HIS:CB	17:L:1118:CLA:HMC1	1.70	1.12
2:L:465:GLY:HA2	17:L:1119:CLA:HMA3	1.26	1.12
7:G:212:UNK:CA	8:H:3:UNK:CB	2.27	1.12
3:C:425:TRP:O	17:C:1079:CLA:HMC2	1.48	1.12
2:L:465:GLY:CA	17:L:1119:CLA:CMA	2.27	1.12
3:M:128:GLY:O	17:M:1087:CLA:HMB3	1.48	1.11
2:B:22:ALA:HB1	17:B:1109:CLA:HMB1	1.23	1.11
2:B:9:HIS:CE1	17:B:1116:CLA:ND	2.17	1.11
3:M:425:TRP:O	17:M:1079:CLA:HMC2	1.49	1.11
2:B:22:ALA:O	17:B:1109:CLA:HMB2	0.95	1.11
18:A:367:PHO:CMC	4:D:148:ALA:CB	2.29	1.10
1:A:296:ASN:HA	3:C:1074:UNK:CB	1.80	1.10
1:J:210:LEU:CB	18:J:366:PHO:C1C	2.28	1.10
17:C:1080:CLA:HMD2	17:C:1082:CLA:HMA3	1.18	1.09
1:J:296:ASN:HA	3:M:1074:UNK:CB	1.81	1.09
1:J:296:ASN:CA	3:M:1074:UNK:CB	2.27	1.09
4:N:212:ALA:HB2	18:N:357:PHO:CAC	1.81	1.09
2:B:212:ALA:CB	17:B:1107:CLA:HMD3	1.81	1.09
1:A:210:LEU:CB	18:A:367:PHO:C2C	2.31	1.09
2:B:22:ALA:HB1	17:B:1109:CLA:CAB	1.82	1.09
2:B:1092:UNK:HA	11:O:132:UNK:O	1.51	1.09
3:C:275:SER:C	17:C:1089:CLA:HMA3	1.73	1.09
17:A:369:CLA:CAB	17:C:1081:CLA:HMC2	1.82	1.08
2:B:204:ALA:HB1	17:B:1117:CLA:CHC	1.78	1.08
7:R:213:UNK:CA	8:S:3:UNK:CB	2.31	1.08
3:C:278:ALA:HB3	17:C:1089:CLA:HMA2	1.31	1.08
1:A:296:ASN:CA	3:C:1074:UNK:CB	2.27	1.07
1:A:95:PRO:HA	17:A:368:CLA:CAA	1.83	1.07
2:L:244:ALA:HB1	17:L:1120:CLA:HMD3	1.18	1.07
17:L:1111:CLA:H3A	17:L:1114:CLA:HMD2	1.11	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:GLY:HA3	17:B:1119:CLA:CMA	1.68	1.07
1:J:210:LEU:CB	18:J:366:PHO:C3C	2.32	1.07
2:L:1092:UNK:HA	11:Y:132:UNK:O	1.51	1.06
2:L:468:TRP:CH2	17:L:1119:CLA:CHC	2.38	1.06
2:L:212:ALA:HB2	17:L:1107:CLA:CMD	1.85	1.06
2:B:212:ALA:HB2	17:B:1107:CLA:CMD	1.85	1.06
18:A:367:PHO:HMC1	4:D:148:ALA:HB1	1.34	1.05
1:A:310:LYS:CB	13:V:2:GLU:O	2.02	1.05
2:B:204:ALA:HB3	17:B:1117:CLA:CHC	1.79	1.05
1:J:94:TYR:C	17:J:367:CLA:HMA1	1.77	1.05
2:L:68:ARG:CB	17:L:1111:CLA:HMA1	1.87	1.05
21:D:359:BCR:C34	21:D:359:BCR:H311	1.88	1.04
3:C:128:GLY:O	17:C:1088:CLA:HMB3	1.57	1.04
2:L:212:ALA:CB	17:L:1107:CLA:CMD	2.35	1.04
2:B:223:GLN:CA	7:G:184:UNK:CA	2.36	1.04
17:B:1111:CLA:H3A	17:B:1114:CLA:HMD2	1.11	1.04
17:B:1108:CLA:CAC	17:B:1119:CLA:CBD	2.35	1.03
3:C:129:GLY:HA2	17:C:1088:CLA:CMB	1.88	1.03
17:L:1111:CLA:C3A	17:L:1114:CLA:HMD2	1.87	1.03
4:N:200:GLY:O	17:N:354:CLA:HMA1	1.59	1.03
2:B:212:ALA:CB	17:B:1107:CLA:CMD	2.36	1.03
2:L:204:ALA:HB3	17:L:1117:CLA:CHC	1.79	1.03
3:M:275:SER:O	17:M:1088:CLA:HMA3	1.58	1.03
2:B:68:ARG:CB	17:B:1111:CLA:HMA1	1.89	1.03
17:B:1111:CLA:C3A	17:B:1114:CLA:HMD2	1.87	1.03
3:C:275:SER:O	17:C:1089:CLA:HMA3	1.57	1.02
3:C:1048:UNK:N	11:O:14:UNK:CB	2.19	1.02
2:L:1092:UNK:C	11:Y:132:UNK:O	2.07	1.02
2:B:1092:UNK:C	11:O:132:UNK:O	2.07	1.02
5:E:33:GLY:CA	14:X:5:UNK:CB	2.36	1.01
17:M:1081:CLA:HMA2	17:W:64:CLA:HMD2	1.23	1.01
17:L:1108:CLA:HHD	17:L:1119:CLA:OBD	1.58	1.01
5:E:8:PRO:CG	14:X:25:UNK:CB	2.38	1.01
2:L:1092:UNK:CB	11:Y:132:UNK:O	2.08	1.01
2:L:139:PHE:HB2	17:L:1120:CLA:CMB	1.91	1.01
17:M:1086:CLA:CAC	17:W:64:CLA:CAC	2.38	1.01
17:C:1080:CLA:CAC	17:C:1087:CLA:CAC	2.38	1.01
1:J:95:PRO:HA	17:J:367:CLA:C2A	1.90	1.01
2:B:1092:UNK:CB	11:O:132:UNK:O	2.08	1.01
3:C:70:PHE:CB	10:K:10:ASP:HA	1.90	1.01
17:C:1086:CLA:HMA3	17:C:1088:CLA:CAC	1.90	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ALA:HB2	17:C:1083:CLA:OBD	1.60	1.01
4:D:113:PHE:CE1	17:D:357:CLA:C1A	2.42	1.00
21:D:359:BCR:C31	21:D:359:BCR:C34	2.38	1.00
2:L:139:PHE:HB2	17:L:1120:CLA:HMB2	1.01	1.00
2:B:69:LEU:N	17:B:1111:CLA:HMA2	1.76	1.00
3:M:70:PHE:CB	10:W:10:ASP:HA	1.90	1.00
3:M:1049:UNK:CB	11:Y:14:UNK:HA	1.85	1.00
1:A:297:LEU:CB	3:C:424:SER:CB	2.40	0.99
2:L:22:ALA:HB1	17:L:1109:CLA:CAB	1.86	0.99
2:L:1092:UNK:HA	11:Y:132:UNK:C	1.92	0.99
1:A:210:LEU:CB	18:A:367:PHO:C1C	2.41	0.99
18:J:366:PHO:CMC	4:N:148:ALA:HB1	1.93	0.99
4:D:212:ALA:HB1	18:D:356:PHO:CAC	1.90	0.99
3:M:172:ALA:HB2	17:M:1082:CLA:OBD	1.63	0.99
21:D:359:BCR:H343	21:D:359:BCR:H311	1.00	0.98
2:B:1092:UNK:HA	11:O:132:UNK:C	1.92	0.98
1:J:85:SER:CB	3:M:221:GLU:O	2.11	0.98
3:M:1048:UNK:N	11:Y:14:UNK:CB	2.17	0.98
3:C:1052:UNK:CB	11:O:12:UNK:CB	2.41	0.98
2:L:204:ALA:HB1	17:L:1117:CLA:CHC	1.77	0.98
4:D:212:ALA:HB2	18:D:356:PHO:CAC	1.92	0.97
3:C:129:GLY:CA	17:C:1088:CLA:HMB1	1.94	0.97
1:A:94:TYR:C	17:A:368:CLA:CMA	2.33	0.97
1:J:324:ALA:O	4:N:330:ALA:HB3	1.64	0.97
17:A:365:CLA:HMB2	17:D:354:CLA:HMB2	1.44	0.97
18:A:367:PHO:CAC	4:D:148:ALA:HB3	1.94	0.96
2:L:204:ALA:HB2	17:L:1117:CLA:HHC	1.46	0.96
1:A:324:ALA:O	4:D:330:ALA:HB3	1.65	0.96
18:A:367:PHO:HMC2	4:D:148:ALA:HB1	1.45	0.96
3:C:50:LEU:HA	17:C:1086:CLA:HMB3	1.45	0.96
1:A:85:SER:CB	3:C:221:GLU:O	2.13	0.95
11:O:44:UNK:O	2:L:83:GLU:CB	2.14	0.95
1:A:296:ASN:CB	3:C:1074:UNK:HA	1.84	0.95
2:L:244:ALA:CB	17:L:1120:CLA:HMD3	1.95	0.95
11:O:87:UNK:CA	2:L:87:ASP:CB	2.44	0.95
4:N:42:TYR:HE1	6:Q:25:LEU:CB	1.79	0.94
4:N:42:TYR:CE1	6:Q:25:LEU:CB	2.49	0.94
2:B:22:ALA:C	17:B:1109:CLA:HMB2	1.88	0.94
1:A:94:TYR:O	17:A:368:CLA:HMA2	1.66	0.94
17:L:1108:CLA:CAC	17:L:1119:CLA:CAD	2.46	0.94
11:O:87:UNK:HA	2:L:87:ASP:CB	1.97	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:ALA:HB1	17:L:1109:CLA:CMB	1.97	0.94
2:L:204:ALA:HB1	17:L:1117:CLA:HHC	0.94	0.94
18:A:367:PHO:C2C	4:D:148:ALA:CB	2.46	0.93
4:N:212:ALA:HB3	18:N:357:PHO:CAC	1.94	0.93
5:P:33:GLY:CA	14:I:5:UNK:CB	2.47	0.93
1:J:297:LEU:CB	3:M:424:SER:CB	2.47	0.93
17:B:1108:CLA:CAC	17:B:1119:CLA:OBD	2.16	0.93
3:C:129:GLY:C	17:C:1088:CLA:HMB1	1.88	0.93
2:B:204:ALA:HB1	17:B:1117:CLA:HHC	0.94	0.93
1:A:139:MET:O	4:D:221:THR:O	1.86	0.93
1:A:95:PRO:N	17:A:368:CLA:C3A	2.19	0.93
1:J:296:ASN:CB	3:M:1074:UNK:HA	1.85	0.92
2:B:204:ALA:HB2	17:B:1117:CLA:HHC	1.47	0.92
3:C:1049:UNK:CB	11:O:14:UNK:HA	1.85	0.92
1:J:214:MET:CB	18:J:366:PHO:HMD3	1.99	0.92
17:C:1080:CLA:CMD	17:C:1082:CLA:CMA	2.47	0.92
2:L:65:PHE:HA	17:L:1114:CLA:CAC	2.00	0.92
1:A:235:TYR:HE2	2:B:5:TRP:CA	1.60	0.92
3:C:129:GLY:HA2	17:C:1088:CLA:HMB1	1.50	0.92
1:J:139:MET:O	4:N:221:THR:O	1.86	0.92
2:B:238:LEU:HA	17:B:1109:CLA:CMD	2.01	0.91
2:B:22:ALA:HB1	17:B:1109:CLA:CMB	1.99	0.91
2:B:64:PRO:CB	17:B:1114:CLA:HMC2	2.00	0.91
2:L:69:LEU:N	17:L:1111:CLA:HMA2	1.84	0.91
3:C:1049:UNK:CB	11:O:13:UNK:O	2.19	0.91
2:L:22:ALA:C	17:L:1109:CLA:HMB2	1.91	0.91
3:C:52:ALA:O	17:C:1082:CLA:HMB2	1.71	0.90
2:L:238:LEU:HA	17:L:1109:CLA:CMD	2.01	0.90
18:J:366:PHO:C3C	4:N:148:ALA:HB1	2.01	0.90
21:D:359:BCR:H21C	21:K:47:BCR:H373	1.53	0.90
3:C:79:LYS:CB	13:V:102:PRO:CA	2.49	0.90
2:L:30:VAL:CB	17:L:1108:CLA:H3A	2.02	0.90
2:B:465:GLY:C	17:B:1119:CLA:CMA	2.40	0.90
1:A:94:TYR:C	17:A:368:CLA:HMA1	1.92	0.90
3:M:79:LYS:CB	13:O:102:PRO:CA	2.50	0.90
1:A:95:PRO:CB	17:A:368:CLA:H3A	2.01	0.90
2:B:204:ALA:HB3	17:B:1117:CLA:HHC	1.31	0.90
1:A:94:TYR:O	17:A:368:CLA:CMA	2.19	0.89
18:A:367:PHO:CAC	4:D:148:ALA:CB	2.50	0.89
2:L:139:PHE:CB	17:L:1120:CLA:HMB2	1.97	0.89
4:D:113:PHE:HE1	17:D:357:CLA:C1A	1.77	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:1108:CLA:CMA	17:B:1112:CLA:CAB	2.50	0.89
17:L:1108:CLA:CMA	17:L:1112:CLA:CAB	2.50	0.89
2:B:450:TRP:CB	17:B:1110:CLA:CMB	2.18	0.89
2:B:465:GLY:C	17:B:1119:CLA:HMA1	1.91	0.89
2:L:240:SER:CB	17:L:1120:CLA:C1C	2.50	0.89
3:M:1049:UNK:CB	11:Y:13:UNK:O	2.19	0.89
2:L:1092:UNK:C	11:Y:132:UNK:C	2.44	0.89
17:M:1081:CLA:HMA2	17:W:64:CLA:C2D	2.03	0.89
2:L:465:GLY:CA	17:L:1119:CLA:HMA2	2.02	0.88
2:L:1092:UNK:HA	11:Y:133:UNK:C	2.03	0.88
2:L:68:ARG:CB	17:L:1111:CLA:CMA	2.52	0.88
2:L:68:ARG:C	17:L:1111:CLA:CMA	2.42	0.88
2:B:68:ARG:C	17:B:1111:CLA:CMA	2.42	0.88
2:B:1092:UNK:C	11:O:132:UNK:C	2.44	0.88
1:A:95:PRO:CA	17:A:368:CLA:CAA	2.50	0.88
3:C:425:TRP:CZ3	17:C:1079:CLA:CAB	2.57	0.88
11:O:152:UNK:CA	12:U:9:UNK:CB	2.52	0.87
2:B:1092:UNK:CA	11:O:132:UNK:C	2.51	0.87
2:L:1092:UNK:CA	11:Y:132:UNK:C	2.51	0.87
3:C:172:ALA:CB	17:C:1083:CLA:CAD	2.52	0.87
3:M:70:PHE:CB	10:W:10:ASP:CA	2.53	0.87
17:L:1111:CLA:H3A	17:L:1114:CLA:CMD	2.04	0.87
2:B:68:ARG:CB	17:B:1111:CLA:CMA	2.52	0.87
2:B:1092:UNK:HA	11:O:133:UNK:C	2.04	0.87
2:B:212:ALA:HB1	17:B:1107:CLA:C2D	2.04	0.86
17:B:1108:CLA:HMA2	17:B:1112:CLA:CAB	2.05	0.86
1:A:235:TYR:CD2	2:B:5:TRP:O	2.29	0.86
17:J:365:CLA:HMB2	17:N:354:CLA:HMB2	1.53	0.86
2:L:60:MET:CB	17:L:1110:CLA:HMA3	2.05	0.86
17:L:1108:CLA:HMA2	17:L:1112:CLA:CAB	2.05	0.86
18:A:367:PHO:C3C	4:D:148:ALA:CB	2.53	0.86
3:C:70:PHE:CB	10:K:10:ASP:CA	2.53	0.86
1:J:94:TYR:O	17:J:367:CLA:HMA2	1.74	0.86
2:L:1092:UNK:O	11:Y:132:UNK:O	1.88	0.86
3:M:66:ALA:C	10:W:13:VAL:CB	2.44	0.86
3:M:172:ALA:CB	17:M:1082:CLA:CAD	2.54	0.86
3:C:66:ALA:C	10:K:13:VAL:CB	2.44	0.86
2:L:23:HIS:CB	17:L:1118:CLA:HMC2	2.06	0.85
2:L:65:PHE:CB	17:L:1114:CLA:CAC	2.54	0.85
1:A:296:ASN:CB	3:C:1074:UNK:CA	2.54	0.85
1:J:94:TYR:C	17:J:367:CLA:CMA	2.43	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:209:LEU:HA	18:N:357:PHO:C4C	2.06	0.85
3:C:425:TRP:O	17:C:1079:CLA:HMC3	1.76	0.85
2:L:240:SER:CB	17:L:1120:CLA:C2C	2.54	0.85
2:L:465:GLY:CA	17:L:1119:CLA:HMA3	2.02	0.85
4:D:48:TRP:HZ3	21:D:359:BCR:H332	1.41	0.85
3:C:278:ALA:HB3	17:C:1089:CLA:CMA	2.06	0.85
3:C:429:SER:CB	17:C:1079:CLA:HMC2	2.06	0.85
2:B:68:ARG:C	17:B:1111:CLA:HMA2	1.95	0.85
1:J:296:ASN:CB	3:M:1074:UNK:CA	2.54	0.85
3:M:129:GLY:C	17:M:1087:CLA:CMB	2.41	0.85
2:B:238:LEU:CA	17:B:1109:CLA:HMD3	2.06	0.84
1:A:337:HIS:CB	4:D:351:ALA:HB2	2.07	0.84
3:M:429:SER:CB	17:M:1079:CLA:HMC2	2.06	0.84
2:L:212:ALA:HB1	17:L:1107:CLA:HMD3	1.59	0.84
3:M:425:TRP:CZ3	17:M:1079:CLA:CAB	2.61	0.83
2:B:1092:UNK:HA	11:O:133:UNK:O	1.78	0.83
2:L:1092:UNK:HA	11:Y:133:UNK:O	1.77	0.83
3:C:266:TRP:HZ2	17:C:1078:CLA:CAC	1.91	0.83
18:A:367:PHO:HMC1	4:D:148:ALA:CB	1.99	0.83
2:L:238:LEU:CA	17:L:1109:CLA:HMD3	2.06	0.83
2:L:65:PHE:CA	17:L:1114:CLA:CAC	2.56	0.83
1:J:337:HIS:CB	4:N:351:ALA:HB2	2.07	0.83
17:C:1078:CLA:HMD1	17:C:1089:CLA:C3D	2.09	0.83
17:B:1111:CLA:H3A	17:B:1114:CLA:CMD	2.04	0.83
17:M:1081:CLA:CMA	17:W:64:CLA:C2D	2.57	0.83
1:J:95:PRO:CB	17:J:367:CLA:C4A	2.56	0.83
1:A:161:TYR:OH	1:A:190:HIS:CB	2.27	0.83
3:C:275:SER:HA	17:C:1089:CLA:CMA	2.07	0.82
3:M:425:TRP:O	17:M:1079:CLA:HMC3	1.77	0.82
1:J:94:TYR:O	17:J:367:CLA:HMA1	1.72	0.82
4:N:209:LEU:CA	18:N:357:PHO:C3C	2.57	0.82
2:L:139:PHE:HD1	17:L:1120:CLA:CHB	1.93	0.82
3:C:429:SER:CB	17:C:1079:CLA:CMC	2.58	0.82
1:A:95:PRO:CB	17:A:368:CLA:C3A	2.58	0.82
2:L:141:ILE:O	17:L:1118:CLA:HMA2	1.80	0.81
2:L:139:PHE:CD1	17:L:1120:CLA:CHB	2.62	0.81
1:J:182:PHE:O	17:J:365:CLA:HMD2	1.80	0.81
1:J:95:PRO:N	17:J:367:CLA:C3A	2.42	0.81
1:A:158:PHE:HZ	17:A:366:CLA:HMC3	1.45	0.81
3:M:278:ALA:HB3	17:M:1088:CLA:H2A	1.63	0.81
1:J:324:ALA:O	4:N:330:ALA:HB1	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:275:SER:O	17:M:1088:CLA:CMA	2.27	0.80
3:C:172:ALA:HB1	17:C:1083:CLA:CAD	2.12	0.80
2:L:68:ARG:C	17:L:1111:CLA:HMA2	2.01	0.80
3:M:429:SER:CB	17:M:1079:CLA:CMC	2.59	0.80
1:J:95:PRO:CA	17:J:367:CLA:C4A	2.58	0.80
3:C:172:ALA:CB	17:C:1083:CLA:OBD	2.30	0.80
17:C:1080:CLA:CMD	17:C:1082:CLA:HMA2	2.09	0.80
13:O:41:HIS:NE2	19:O:138:HEM:NB	2.30	0.80
18:A:367:PHO:C3C	4:D:148:ALA:HB3	2.11	0.80
13:V:41:HIS:CD2	19:V:138:HEM:C4B	2.70	0.80
3:C:128:GLY:O	17:C:1088:CLA:CMB	2.30	0.80
18:J:366:PHO:C3C	4:N:148:ALA:CB	2.60	0.79
1:J:95:PRO:CB	17:J:367:CLA:C3A	2.59	0.79
21:D:359:BCR:C34	21:D:359:BCR:H312	2.10	0.79
2:L:23:HIS:CB	17:L:1118:CLA:HMC3	2.11	0.79
13:O:41:HIS:CD2	19:O:138:HEM:C4B	2.70	0.79
1:A:235:TYR:OH	2:B:5:TRP:N	2.16	0.78
17:B:1111:CLA:CAA	17:B:1114:CLA:HMD3	2.12	0.78
17:C:1080:CLA:C2D	17:C:1082:CLA:HMA2	2.14	0.78
4:N:208:ALA:HB3	18:N:357:PHO:HMC3	1.66	0.78
17:L:1111:CLA:CAA	17:L:1114:CLA:HMD3	2.12	0.78
3:M:1048:UNK:C	11:Y:14:UNK:N	2.44	0.77
1:A:324:ALA:O	4:D:330:ALA:HB1	1.81	0.77
17:B:1111:CLA:CAA	17:B:1114:CLA:CMD	2.62	0.77
2:L:110:ALA:CB	17:L:1121:CLA:HMB2	2.14	0.77
3:M:425:TRP:CZ2	17:M:1079:CLA:CAB	2.68	0.77
2:B:204:ALA:O	17:B:1117:CLA:HMC3	1.85	0.77
17:L:1111:CLA:CAA	17:L:1114:CLA:CMD	2.62	0.77
17:C:1080:CLA:C2D	17:C:1082:CLA:CMA	2.63	0.77
2:L:212:ALA:HB1	17:L:1107:CLA:C2D	2.15	0.77
2:L:212:ALA:HB2	17:L:1107:CLA:HMD1	1.66	0.77
18:A:367:PHO:C3C	4:D:148:ALA:HB1	2.14	0.77
2:B:9:HIS:HE1	17:B:1116:CLA:C4D	1.97	0.77
3:M:278:ALA:HB3	17:M:1088:CLA:HMA2	1.64	0.77
3:M:277:GLY:HA3	17:M:1080:CLA:CAC	2.15	0.77
1:A:297:LEU:C	3:C:1074:UNK:O	2.22	0.76
3:C:275:SER:O	17:C:1089:CLA:HMA1	1.83	0.76
2:L:69:LEU:CB	17:L:1111:CLA:H2A	2.14	0.76
17:B:1108:CLA:HMA3	17:B:1112:CLA:CAB	2.15	0.76
1:A:235:TYR:CZ	2:B:5:TRP:CA	2.53	0.76
2:B:22:ALA:CB	17:B:1109:CLA:HMB1	2.12	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:310:LYS:CB	13:O:2:GLU:O	2.13	0.76
2:L:204:ALA:O	17:L:1117:CLA:HMC3	1.85	0.76
1:J:297:LEU:C	3:M:1074:UNK:O	2.23	0.76
4:N:208:ALA:O	18:N:357:PHO:CAC	2.34	0.76
3:C:266:TRP:CZ2	17:C:1078:CLA:CAC	2.68	0.76
17:L:1115:CLA:HMA2	17:L:1120:CLA:HMC1	1.67	0.76
17:L:1108:CLA:HMA3	17:L:1112:CLA:CAB	2.15	0.76
4:N:209:LEU:CB	18:N:357:PHO:C1C	2.64	0.76
2:B:23:HIS:CB	17:B:1118:CLA:HMC2	2.12	0.76
1:J:210:LEU:CB	18:J:366:PHO:C4C	2.64	0.76
2:L:212:ALA:HB1	17:L:1107:CLA:CMD	2.13	0.76
3:C:1048:UNK:C	11:O:14:UNK:N	2.45	0.76
3:M:172:ALA:HB1	17:M:1082:CLA:CAD	2.15	0.76
2:B:212:ALA:HB2	17:B:1107:CLA:HMD1	1.66	0.75
3:M:172:ALA:CB	17:M:1082:CLA:OBD	2.34	0.75
2:B:23:HIS:CB	17:B:1118:CLA:HMC3	2.15	0.75
4:N:209:LEU:CB	18:N:357:PHO:NC	2.50	0.75
3:C:425:TRP:CZ2	17:C:1079:CLA:CAB	2.69	0.75
2:L:450:TRP:CB	17:L:1110:CLA:CMB	2.29	0.75
3:M:425:TRP:HB3	17:M:1079:CLA:HHC	1.69	0.75
3:C:129:GLY:C	17:C:1088:CLA:CAB	2.54	0.75
2:B:110:ALA:CB	17:B:1121:CLA:HMB2	2.18	0.73
2:B:450:TRP:CG	17:B:1110:CLA:HMB2	2.24	0.73
9:T:24:UNK:O	9:T:25:UNK:CB	2.37	0.73
18:J:366:PHO:CAC	4:N:148:ALA:CB	2.66	0.73
3:C:66:ALA:CB	10:K:13:VAL:CB	2.67	0.73
3:M:66:ALA:CB	10:W:13:VAL:CB	2.67	0.73
17:C:1078:CLA:HMD1	17:C:1089:CLA:CAD	2.19	0.73
1:A:235:TYR:CE2	2:B:5:TRP:C	2.61	0.72
2:L:468:TRP:CZ2	17:L:1119:CLA:CHC	2.72	0.72
3:M:248:GLY:HA2	17:M:1078:CLA:HMA3	1.70	0.72
9:I:24:UNK:O	9:I:25:UNK:CB	2.37	0.72
17:M:1079:CLA:HMD3	17:M:1084:CLA:CAC	2.19	0.72
2:B:212:ALA:CB	17:B:1107:CLA:C2D	2.65	0.72
2:L:150:CYS:HA	17:L:1113:CLA:HMB2	1.72	0.72
3:C:425:TRP:HB3	17:C:1079:CLA:HHC	1.72	0.72
1:A:158:PHE:HZ	17:A:366:CLA:CMC	2.02	0.71
1:A:94:TYR:C	17:A:368:CLA:H3A	2.09	0.71
1:A:95:PRO:HA	17:A:368:CLA:H3A	0.86	0.71
3:M:164:HIS:HB2	17:M:1088:CLA:CAB	2.20	0.71
2:B:64:PRO:CB	17:B:1114:CLA:CMC	2.68	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:41:HIS:NE2	19:V:138:HEM:NB	2.38	0.71
3:M:129:GLY:N	17:M:1087:CLA:HMB1	2.04	0.71
2:L:139:PHE:HD1	17:L:1120:CLA:C4A	2.03	0.71
1:A:95:PRO:CB	17:A:368:CLA:C4A	2.69	0.70
3:M:271:TYR:CB	17:M:1088:CLA:HHD	2.20	0.70
2:B:465:GLY:O	17:B:1119:CLA:CMA	2.39	0.70
2:L:22:ALA:CB	17:L:1109:CLA:HMB1	2.12	0.70
2:B:150:CYS:HA	17:B:1113:CLA:HMB2	1.73	0.70
3:M:128:GLY:O	17:M:1087:CLA:HMB1	1.91	0.70
2:L:141:ILE:O	17:L:1118:CLA:CMA	2.39	0.70
3:M:271:TYR:CB	17:M:1088:CLA:CHD	2.70	0.70
1:J:95:PRO:N	17:J:367:CLA:HHB	2.07	0.70
4:D:113:PHE:CE1	17:D:357:CLA:NA	2.56	0.69
2:B:465:GLY:CA	17:B:1119:CLA:HMA2	1.82	0.69
1:A:296:ASN:CB	3:C:1074:UNK:CB	2.70	0.69
1:J:296:ASN:CB	3:M:1074:UNK:CB	2.70	0.69
1:A:182:PHE:O	17:A:365:CLA:HMD2	1.92	0.69
4:N:212:ALA:HB3	18:N:357:PHO:HHD	1.73	0.69
2:L:465:GLY:HA3	17:L:1119:CLA:HMA2	1.75	0.68
2:B:212:ALA:HB1	17:B:1107:CLA:CMD	2.19	0.68
2:B:39:LEU:HA	2:B:43:ALA:HB3	1.75	0.68
2:L:465:GLY:HA2	17:L:1119:CLA:HMA1	1.69	0.68
3:C:53:HIS:CB	17:C:1086:CLA:C3B	2.71	0.68
1:J:94:TYR:CB	17:J:367:CLA:HMB3	2.23	0.68
1:A:225:ARG:CB	4:D:268:HIS:CB	2.72	0.68
2:L:60:MET:CB	17:L:1110:CLA:CMA	2.71	0.67
3:C:129:GLY:HA2	17:C:1088:CLA:C2B	2.24	0.67
2:L:244:ALA:HB1	17:L:1120:CLA:CMD	2.12	0.67
2:B:65:PHE:HA	17:B:1114:CLA:CAC	2.23	0.67
17:L:1108:CLA:CHD	17:L:1119:CLA:OBD	2.39	0.67
3:C:172:ALA:HB1	17:C:1083:CLA:C3D	2.24	0.67
3:C:425:TRP:CH2	17:C:1079:CLA:CAB	2.78	0.67
17:L:1111:CLA:C3A	17:L:1114:CLA:CMD	2.68	0.67
1:A:337:HIS:CB	4:D:351:ALA:CB	2.73	0.67
1:A:95:PRO:O	17:A:368:CLA:CAA	2.43	0.67
2:L:139:PHE:CD1	17:L:1120:CLA:C4A	2.78	0.67
18:A:367:PHO:HMD2	4:D:145:ALA:HB2	1.77	0.67
17:B:1111:CLA:C3A	17:B:1114:CLA:CMD	2.68	0.67
4:D:209:LEU:HA	18:D:356:PHO:C3C	2.24	0.66
3:C:425:TRP:C	17:C:1079:CLA:HMC3	2.16	0.66
2:B:1092:UNK:O	11:O:132:UNK:O	1.88	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:PRO:CB	17:L:1114:CLA:HMC2	2.24	0.66
2:L:204:ALA:HB1	17:L:1117:CLA:CMC	2.25	0.66
1:A:94:TYR:C	17:A:368:CLA:C3A	2.61	0.66
1:J:210:LEU:CB	18:J:366:PHO:NC	2.58	0.66
3:M:172:ALA:HB2	17:M:1082:CLA:CAD	2.23	0.66
1:J:337:HIS:CB	4:N:351:ALA:CB	2.73	0.66
17:L:1108:CLA:CAC	17:L:1119:CLA:CBD	2.74	0.66
1:A:235:TYR:CZ	2:B:5:TRP:N	2.64	0.66
4:N:209:LEU:HA	18:N:357:PHO:CAC	2.26	0.66
2:B:465:GLY:HA2	17:B:1119:CLA:HMA1	0.67	0.66
3:M:425:TRP:CH2	17:M:1079:CLA:CAB	2.79	0.66
2:B:204:ALA:HB1	17:B:1117:CLA:CMC	2.26	0.66
2:B:60:MET:CB	17:B:1110:CLA:HMA1	2.26	0.66
3:M:425:TRP:C	17:M:1079:CLA:HMC3	2.15	0.66
1:A:235:TYR:CE2	2:B:5:TRP:O	2.49	0.65
21:D:359:BCR:H312	21:D:359:BCR:H342	1.77	0.65
1:J:147:TYR:CB	18:N:357:PHO:CMD	2.74	0.65
2:B:139:PHE:CB	17:B:1120:CLA:HMB2	2.26	0.65
17:L:1108:CLA:CAC	17:L:1119:CLA:C3D	2.75	0.65
13:O:41:HIS:NE2	19:O:138:HEM:C4B	2.64	0.65
4:D:42:TYR:CE1	6:F:25:LEU:CB	2.80	0.65
3:M:278:ALA:CB	17:M:1088:CLA:H2A	2.26	0.65
1:A:316:THR:CA	4:D:62:GLY:O	2.45	0.65
3:C:172:ALA:HB2	17:C:1083:CLA:CAD	2.23	0.65
3:C:52:ALA:HB3	17:C:1082:CLA:CAB	2.22	0.64
2:B:9:HIS:HE1	17:B:1116:CLA:C1D	2.08	0.64
2:L:30:VAL:CB	17:L:1108:CLA:C3A	2.75	0.64
1:J:316:THR:CA	4:N:62:GLY:O	2.45	0.64
2:B:65:PHE:CA	17:B:1114:CLA:CAC	2.75	0.64
13:V:41:HIS:CD2	19:V:138:HEM:CHC	2.80	0.64
2:L:110:ALA:HB2	17:L:1121:CLA:HMB2	1.78	0.64
3:C:129:GLY:CA	17:C:1088:CLA:CAB	2.76	0.64
2:L:212:ALA:HB2	17:L:1107:CLA:HMD3	1.52	0.64
3:C:129:GLY:O	17:C:1088:CLA:HMB1	1.97	0.64
1:J:210:LEU:CA	18:J:366:PHO:C3C	2.77	0.64
2:L:1092:UNK:CA	11:Y:133:UNK:O	2.38	0.64
4:D:42:TYR:HE1	6:F:25:LEU:CB	2.11	0.63
2:B:60:MET:H	17:B:1110:CLA:HMA3	1.63	0.63
1:J:95:PRO:CB	17:J:367:CLA:CHB	2.76	0.63
13:O:41:HIS:CD2	19:O:138:HEM:CHC	2.82	0.63
2:L:22:ALA:CB	17:L:1109:CLA:CMB	2.76	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ILE:O	17:B:1118:CLA:HMA2	1.98	0.62
1:A:158:PHE:CZ	17:A:366:CLA:HMC3	2.31	0.62
17:C:1080:CLA:CMD	17:C:1082:CLA:HMA3	2.09	0.62
1:J:95:PRO:HA	17:J:367:CLA:CMA	2.15	0.62
2:L:465:GLY:HA3	17:L:1119:CLA:CMA	2.27	0.62
3:M:172:ALA:HB1	17:M:1082:CLA:C3D	2.28	0.62
17:L:1108:CLA:HHD	17:L:1119:CLA:CAD	2.30	0.62
4:D:48:TRP:CZ3	21:D:359:BCR:H332	2.29	0.62
3:C:52:ALA:O	17:C:1082:CLA:CMB	2.45	0.62
3:M:128:GLY:C	17:M:1087:CLA:HMB1	2.20	0.62
1:A:145:VAL:CB	3:C:443:TRP:CB	2.77	0.62
17:N:355:CLA:HMB2	18:N:357:PHO:CMB	2.30	0.61
1:J:337:HIS:O	4:N:350:ASN:O	2.19	0.61
3:M:248:GLY:HA2	17:M:1078:CLA:CMA	2.31	0.61
1:J:147:TYR:CB	18:N:357:PHO:HMD1	2.31	0.61
1:A:337:HIS:O	4:D:350:ASN:O	2.19	0.61
3:M:53:HIS:CB	17:M:1085:CLA:C3B	2.79	0.61
2:L:68:ARG:O	17:L:1111:CLA:HMA3	2.01	0.61
5:E:8:PRO:CD	14:X:25:UNK:CB	2.79	0.60
3:C:1049:UNK:CB	11:O:13:UNK:C	2.79	0.60
2:B:240:SER:CB	17:B:1120:CLA:C1C	2.79	0.60
2:L:68:ARG:C	17:L:1111:CLA:HMA3	2.22	0.60
3:M:66:ALA:HB3	10:W:13:VAL:CB	2.32	0.60
4:N:208:ALA:HB3	18:N:357:PHO:CMC	2.30	0.60
2:L:139:PHE:CD1	17:L:1120:CLA:C1B	2.85	0.60
4:N:42:TYR:CD1	6:Q:25:LEU:CB	2.84	0.60
2:B:60:MET:CB	17:B:1110:CLA:CMA	2.80	0.60
2:L:468:TRP:CH2	17:L:1119:CLA:HHC	2.32	0.60
1:J:221:SER:CB	4:N:138:VAL:CB	2.80	0.60
2:B:204:ALA:C	17:B:1117:CLA:HMC3	2.22	0.60
1:J:210:LEU:HA	18:J:366:PHO:CAC	2.31	0.60
2:B:190:PHE:CB	2:B:1001:UNK:CA	2.80	0.60
1:J:95:PRO:O	17:J:367:CLA:CAA	2.50	0.60
2:B:9:HIS:CE1	17:B:1116:CLA:C1D	2.83	0.60
3:M:275:SER:C	17:M:1088:CLA:HMA3	2.21	0.60
4:D:200:GLY:C	17:D:354:CLA:HMA1	2.21	0.59
1:A:216:GLY:C	4:D:271:MET:CB	2.69	0.59
2:L:212:ALA:CB	17:L:1107:CLA:C2D	2.78	0.59
3:C:274:TYR:HD1	17:C:1081:CLA:HHD	1.67	0.59
2:B:204:ALA:HB3	17:B:1117:CLA:C4B	2.32	0.59
2:B:22:ALA:CB	17:B:1109:CLA:CMB	2.76	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:204:ALA:C	17:L:1117:CLA:HMC3	2.22	0.59
3:C:66:ALA:HB3	10:K:13:VAL:CB	2.32	0.59
2:B:87:ASP:CB	11:Y:87:UNK:C	2.81	0.59
1:J:145:VAL:CB	3:M:443:TRP:CB	2.81	0.59
1:A:216:GLY:O	4:D:271:MET:CA	2.51	0.59
3:C:274:TYR:O	17:C:1089:CLA:H2A	2.02	0.59
2:L:150:CYS:CB	17:L:1113:CLA:CAB	2.81	0.59
1:A:86:SER:CB	3:C:218:PHE:CB	2.81	0.59
2:B:212:ALA:HB2	17:B:1107:CLA:HMD3	1.60	0.59
2:L:190:PHE:CB	2:L:1001:UNK:CA	2.81	0.59
2:L:240:SER:CB	17:L:1120:CLA:CHC	2.81	0.58
3:M:1049:UNK:CB	11:Y:13:UNK:C	2.80	0.58
1:J:86:SER:CB	3:M:218:PHE:CB	2.81	0.58
1:J:39:PRO:CB	17:J:367:CLA:CAC	2.80	0.58
2:B:110:ALA:HB2	17:B:1121:CLA:HMB2	1.85	0.58
2:B:150:CYS:CB	17:B:1113:CLA:CAB	2.82	0.58
3:M:52:ALA:O	17:M:1081:CLA:HMB2	2.03	0.58
2:L:204:ALA:HB3	17:L:1117:CLA:C4B	2.32	0.58
3:M:70:PHE:CB	10:W:10:ASP:CB	2.82	0.58
3:C:60:ILE:CB	17:C:1080:CLA:CAA	2.81	0.58
3:C:1049:UNK:CB	11:O:14:UNK:CA	2.72	0.58
2:L:39:LEU:HA	2:L:43:ALA:HB3	1.83	0.58
2:L:468:TRP:CH2	17:L:1119:CLA:C1C	2.87	0.58
3:M:60:ILE:CB	17:W:64:CLA:CAA	2.82	0.57
4:N:200:GLY:C	17:N:354:CLA:HMA1	2.23	0.57
2:L:110:ALA:HB1	17:L:1121:CLA:HMB2	1.86	0.57
18:J:366:PHO:HMB2	17:N:356:CLA:CAB	2.34	0.57
4:D:113:PHE:CZ	17:D:357:CLA:C1A	2.87	0.57
4:N:209:LEU:CA	18:N:357:PHO:C4C	2.79	0.57
13:V:41:HIS:HD2	19:V:138:HEM:CHC	2.16	0.57
1:J:95:PRO:HA	17:J:367:CLA:CAA	2.35	0.57
2:L:150:CYS:HA	17:L:1113:CLA:CMB	2.34	0.57
1:J:216:GLY:C	4:N:271:MET:CB	2.69	0.57
1:A:235:TYR:HE2	2:B:5:TRP:HA	0.77	0.57
3:C:70:PHE:CB	10:K:10:ASP:CB	2.82	0.56
2:L:468:TRP:CZ2	17:L:1119:CLA:HHC	2.40	0.56
4:D:200:GLY:C	17:D:354:CLA:CMA	2.73	0.56
2:B:150:CYS:HA	17:B:1113:CLA:CMB	2.36	0.56
13:V:41:HIS:NE2	19:V:138:HEM:C4B	2.72	0.56
1:J:147:TYR:CB	18:N:357:PHO:HMD2	2.36	0.56
2:B:68:ARG:C	17:B:1111:CLA:HMA3	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:SER:C	17:C:1089:CLA:CMA	2.52	0.55
3:M:1049:UNK:CB	11:Y:14:UNK:CA	2.73	0.55
4:N:209:LEU:CB	18:N:357:PHO:C4C	2.84	0.55
3:C:278:ALA:HB3	17:C:1089:CLA:C3A	2.35	0.55
2:B:69:LEU:HA	17:B:1111:CLA:H2A	1.88	0.55
2:B:65:PHE:CB	17:B:1114:CLA:CAC	2.73	0.55
2:B:450:TRP:CB	17:B:1110:CLA:HMB3	2.27	0.55
3:C:129:GLY:CA	17:C:1088:CLA:CMB	2.62	0.55
2:B:110:ALA:HB1	17:B:1121:CLA:HMB2	1.88	0.55
3:C:282:MET:O	17:C:1085:CLA:CAA	2.54	0.54
2:B:68:ARG:O	17:B:1111:CLA:HMA3	2.07	0.54
3:M:67:MET:N	10:W:13:VAL:CB	2.69	0.54
3:M:275:SER:CA	17:M:1088:CLA:HMA3	2.38	0.54
17:N:355:CLA:CMB	18:N:357:PHO:HMB2	2.38	0.54
1:A:216:GLY:O	4:D:271:MET:C	2.45	0.54
3:C:67:MET:N	10:K:13:VAL:CB	2.70	0.54
2:L:28:ALA:HB1	2:L:104:SER:HA	1.89	0.54
4:D:160:TYR:HE2	4:D:171:PRO:O	1.91	0.54
3:M:167:VAL:CB	17:M:1085:CLA:CMD	2.68	0.53
7:R:212:UNK:CA	8:S:3:UNK:CB	2.86	0.53
1:A:297:LEU:O	3:C:1075:UNK:CB	2.57	0.53
1:J:324:ALA:O	4:N:330:ALA:HB2	2.02	0.53
3:C:248:GLY:HA2	17:C:1078:CLA:HMA3	1.90	0.53
2:B:465:GLY:O	17:B:1119:CLA:HMA3	2.09	0.53
2:B:465:GLY:HA2	17:B:1119:CLA:C3A	2.32	0.53
11:O:153:UNK:H	12:U:9:UNK:CB	2.21	0.53
3:M:275:SER:HA	17:M:1088:CLA:HMA3	1.91	0.53
1:A:210:LEU:CB	18:A:367:PHO:CMC	2.87	0.52
1:J:297:LEU:O	3:M:1075:UNK:CB	2.57	0.52
2:B:212:ALA:HB1	17:B:1107:CLA:HMD3	1.75	0.52
3:M:278:ALA:HB3	17:M:1088:CLA:C2A	2.37	0.52
13:O:41:HIS:HD2	19:O:138:HEM:CHC	2.22	0.52
4:N:209:LEU:CA	18:N:357:PHO:C2C	2.87	0.52
1:A:158:PHE:CZ	17:A:366:CLA:CMC	2.89	0.52
3:M:164:HIS:CB	17:M:1088:CLA:CAB	2.88	0.52
13:V:40:CYS:CB	19:V:138:HEM:C2B	2.93	0.52
2:L:468:TRP:CZ2	17:L:1119:CLA:C4B	2.92	0.52
17:A:369:CLA:CAB	17:C:1081:CLA:CMC	2.74	0.52
3:C:286:ALA:HB3	17:C:1085:CLA:CAA	2.40	0.52
4:N:208:ALA:CB	18:N:357:PHO:CMC	2.88	0.51
17:A:365:CLA:CMB	17:D:354:CLA:HMB2	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1029:UNK:O	11:Y:129:UNK:CB	2.59	0.51
2:L:240:SER:CB	17:L:1120:CLA:HMC3	2.41	0.51
3:C:1029:UNK:O	11:O:129:UNK:CB	2.58	0.51
2:B:69:LEU:CB	17:B:1111:CLA:H2A	2.41	0.51
3:M:275:SER:HA	17:M:1088:CLA:C1A	2.40	0.51
3:C:66:ALA:O	10:K:13:VAL:CB	2.57	0.51
3:C:297:TYR:N	3:C:298:PRO:HD2	2.25	0.51
17:C:1078:CLA:CMD	17:C:1089:CLA:CAD	2.88	0.51
1:A:85:SER:O	3:C:220:GLY:HA3	2.10	0.51
4:N:42:TYR:HE1	6:Q:25:LEU:CA	2.24	0.51
1:A:210:LEU:CB	18:A:367:PHO:C3C	2.89	0.51
3:C:66:ALA:HB1	10:K:13:VAL:CB	2.41	0.51
17:B:1107:CLA:CMC	17:B:1120:CLA:C4C	2.88	0.51
2:B:65:PHE:CZ	17:B:1114:CLA:CMC	2.90	0.51
4:D:113:PHE:HE1	17:D:357:CLA:NA	1.66	0.51
2:B:240:SER:CB	17:B:1120:CLA:C2C	2.88	0.51
3:M:278:ALA:HB3	17:M:1088:CLA:CMA	2.36	0.51
17:M:1086:CLA:C3C	17:W:64:CLA:CAC	2.89	0.51
17:C:1080:CLA:CAC	17:C:1087:CLA:C3C	2.89	0.51
1:A:147:TYR:CB	18:D:356:PHO:HMD2	2.41	0.50
1:J:95:PRO:CA	17:J:367:CLA:CMA	2.81	0.50
17:C:1086:CLA:CMA	17:C:1088:CLA:CAC	2.79	0.50
3:C:266:TRP:HZ3	17:C:1089:CLA:HMD1	1.77	0.50
1:A:316:THR:HA	4:D:62:GLY:O	2.12	0.50
3:M:66:ALA:HB1	10:W:13:VAL:CB	2.41	0.50
1:A:186:PHE:CB	17:A:365:CLA:HMD3	2.42	0.50
4:N:184:PHE:O	17:N:354:CLA:C3C	2.56	0.50
3:C:278:ALA:CB	17:C:1089:CLA:HMA2	2.21	0.50
3:M:66:ALA:O	10:W:13:VAL:CB	2.59	0.50
18:A:367:PHO:HMC2	4:D:148:ALA:CB	2.24	0.49
2:L:464:PHE:CE2	17:L:1119:CLA:HMB3	2.47	0.49
1:J:324:ALA:C	4:N:330:ALA:HB1	2.33	0.49
1:J:85:SER:O	3:M:220:GLY:HA3	2.12	0.49
1:A:94:TYR:CA	17:A:368:CLA:HMA1	2.43	0.49
4:N:117:HIS:CE1	17:N:358:CLA:NC	2.80	0.49
13:O:92:HIS:NE2	19:O:138:HEM:NB	2.60	0.49
1:J:142:TRP:NE1	3:M:447:ARG:CB	2.75	0.49
2:B:30:VAL:HA	17:B:1108:CLA:H3A	1.94	0.49
1:A:216:GLY:O	4:D:271:MET:O	2.30	0.49
3:M:440:GLY:HA3	17:M:1086:CLA:CAD	2.42	0.49
3:C:440:GLY:HA3	17:C:1087:CLA:CAD	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:THR:HA	4:D:111:TRP:HB2	1.93	0.49
1:J:316:THR:HA	4:N:62:GLY:O	2.12	0.49
4:D:160:TYR:CD2	4:D:172:SER:HA	2.48	0.49
2:L:240:SER:O	17:L:1120:CLA:C4C	2.61	0.48
13:V:92:HIS:NE2	19:V:138:HEM:NB	2.60	0.48
3:C:1030:UNK:HA	11:O:129:UNK:CB	2.43	0.48
13:O:41:HIS:HD2	19:O:138:HEM:C4B	2.30	0.48
1:J:216:GLY:O	4:N:271:MET:C	2.51	0.48
3:C:266:TRP:HZ3	17:C:1089:CLA:CMD	2.26	0.48
11:O:66:UNK:O	11:O:103:UNK:HA	2.14	0.48
2:L:204:ALA:HB1	17:L:1117:CLA:C1C	2.40	0.48
3:C:164:HIS:CE1	17:C:1086:CLA:C1D	2.80	0.48
2:L:244:ALA:HB2	17:L:1120:CLA:HHD	1.96	0.48
4:D:77:ALA:HB3	4:D:171:PRO:HA	1.96	0.48
1:A:39:PRO:CB	17:A:368:CLA:CAC	2.92	0.48
17:A:366:CLA:CAB	18:D:356:PHO:HMB2	2.44	0.48
2:B:69:LEU:CA	17:B:1111:CLA:H2A	2.44	0.48
3:M:1030:UNK:HA	11:Y:129:UNK:CB	2.44	0.48
3:M:129:GLY:O	17:M:1087:CLA:CMB	2.60	0.48
2:L:204:ALA:CB	17:L:1117:CLA:C4B	2.85	0.47
1:J:95:PRO:N	17:J:367:CLA:CHB	2.77	0.47
3:M:52:ALA:O	17:M:1081:CLA:CMB	2.63	0.47
11:O:152:UNK:HA	12:U:9:UNK:CB	2.40	0.47
1:A:143:ILE:HA	4:D:216:ALA:HB1	1.97	0.47
2:B:22:ALA:C	17:B:1109:CLA:CMB	2.65	0.47
1:A:235:TYR:HE2	2:B:5:TRP:CB	2.24	0.47
1:J:210:LEU:HA	18:J:366:PHO:C3C	2.45	0.47
2:L:468:TRP:CH2	17:L:1119:CLA:C4B	2.95	0.47
1:J:324:ALA:HB1	4:N:330:ALA:HB1	1.97	0.47
2:L:240:SER:CB	17:L:1120:CLA:CMC	2.92	0.47
3:C:66:ALA:HB3	10:K:13:VAL:HA	1.97	0.47
1:A:141:PRO:O	4:D:220:ASN:CB	2.63	0.47
1:A:95:PRO:C	17:A:368:CLA:CAA	2.83	0.47
2:B:204:ALA:HB1	17:B:1117:CLA:C1C	2.41	0.47
2:L:30:VAL:CB	17:L:1108:CLA:C2A	2.91	0.47
1:A:324:ALA:O	4:D:330:ALA:HB2	2.03	0.47
4:N:213:ILE:HA	18:N:357:PHO:HMD3	1.97	0.46
2:L:221:PRO:O	7:R:184:UNK:CA	2.64	0.46
1:J:216:GLY:CA	4:N:271:MET:CB	2.92	0.46
4:N:208:ALA:CB	18:N:357:PHO:HMC1	2.44	0.46
1:A:324:ALA:C	4:D:330:ALA:HB1	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:ALA:HB3	17:C:1089:CLA:C2A	2.45	0.46
1:J:141:PRO:O	4:N:220:ASN:CB	2.63	0.46
17:M:1084:CLA:HMC3	17:W:64:CLA:H2A	1.96	0.46
1:J:95:PRO:N	17:J:367:CLA:CMA	2.77	0.46
18:J:366:PHO:C3C	4:N:148:ALA:HB3	2.43	0.46
18:J:366:PHO:HMC2	4:N:148:ALA:HB1	1.92	0.46
2:B:87:ASP:CB	11:Y:87:UNK:O	2.63	0.46
2:B:141:ILE:O	17:B:1118:CLA:CMA	2.61	0.46
2:L:1092:UNK:CA	11:Y:133:UNK:C	2.84	0.46
17:L:1115:CLA:HMA2	17:L:1120:CLA:CMC	2.42	0.46
4:N:75:THR:HA	4:N:111:TRP:HB2	1.98	0.46
4:N:208:ALA:HB1	18:N:357:PHO:HMC1	1.98	0.46
3:M:1048:UNK:HA	11:Y:14:UNK:N	2.30	0.46
13:O:40:CYS:CB	19:O:138:HEM:C2B	2.99	0.46
13:O:34:GLN:HA	13:O:38:ALA:HB2	1.97	0.46
1:J:143:ILE:HA	4:N:216:ALA:HB1	1.97	0.46
3:C:274:TYR:CD1	17:C:1081:CLA:HHD	2.49	0.46
3:M:1033:UNK:CB	11:Y:81:UNK:CB	2.94	0.46
17:C:1078:CLA:HMD1	17:C:1089:CLA:C2D	2.45	0.46
2:L:68:ARG:CB	17:L:1111:CLA:HMA2	2.43	0.46
1:J:189:GLU:HB3	3:M:412:THR:CB	2.46	0.45
1:A:332:HIS:NE2	4:D:349:GLY:N	2.64	0.45
1:A:189:GLU:HB3	3:C:412:THR:CB	2.47	0.45
4:D:258:GLY:HA2	4:D:262:SER:O	2.16	0.45
2:L:464:PHE:CZ	17:L:1119:CLA:HMB3	2.51	0.45
3:C:1052:UNK:CB	11:O:12:UNK:CA	2.95	0.45
3:M:66:ALA:HB3	10:W:13:VAL:HA	1.97	0.45
18:J:366:PHO:CAC	4:N:148:ALA:HB3	2.45	0.45
2:B:1092:UNK:CA	11:O:133:UNK:C	2.84	0.45
1:A:216:GLY:CA	4:D:271:MET:CB	2.95	0.45
3:C:1033:UNK:CB	11:O:81:UNK:CB	2.94	0.45
1:J:216:GLY:O	4:N:271:MET:CA	2.58	0.45
4:D:79:SER:HA	4:D:170:ALA:CB	2.47	0.45
1:J:332:HIS:NE2	4:N:349:GLY:N	2.64	0.45
4:N:258:GLY:HA2	4:N:262:SER:O	2.16	0.45
1:A:114:LEU:CB	17:A:368:CLA:HMA3	2.47	0.45
2:B:204:ALA:CB	17:B:1117:CLA:C4B	2.85	0.45
3:M:128:GLY:C	17:M:1087:CLA:CMB	2.75	0.45
1:A:324:ALA:HB1	4:D:330:ALA:HB1	1.97	0.45
3:C:1048:UNK:HA	11:O:14:UNK:N	2.32	0.45
2:L:1091:UNK:C	11:Y:134:UNK:HA	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:329:GLU:C	4:N:326:ARG:CB	2.55	0.44
17:M:1081:CLA:HMA1	17:W:64:CLA:C1D	2.47	0.44
17:N:355:CLA:CMB	18:N:357:PHO:CMB	2.94	0.44
2:B:60:MET:CB	17:B:1110:CLA:CHB	2.95	0.44
3:M:1052:UNK:CB	11:Y:12:UNK:CA	2.93	0.44
2:B:68:ARG:CB	17:B:1111:CLA:HMA2	2.42	0.44
1:J:142:TRP:HE1	3:M:447:ARG:CB	2.30	0.44
3:C:410:VAL:HA	3:C:415:ASN:HA	2.00	0.44
4:D:200:GLY:O	17:D:354:CLA:HMA2	2.08	0.44
2:B:1091:UNK:C	11:O:134:UNK:HA	2.47	0.44
4:N:212:ALA:CB	18:N:357:PHO:HHD	2.46	0.44
3:M:247:GLY:O	17:M:1078:CLA:HMA1	2.17	0.44
2:B:30:VAL:CB	17:B:1108:CLA:H3A	2.48	0.44
5:E:8:PRO:HD3	14:X:25:UNK:CB	2.48	0.44
2:B:1092:UNK:CA	11:O:133:UNK:O	2.38	0.44
17:C:1078:CLA:HMD3	17:C:1089:CLA:CMD	2.48	0.44
3:C:247:GLY:C	17:C:1078:CLA:CMA	2.86	0.44
13:V:34:GLN:HA	13:V:38:ALA:HB2	1.99	0.44
6:F:40:GLN:HA	9:I:26:UNK:CB	2.47	0.44
17:N:355:CLA:HMB2	18:N:357:PHO:HMB2	1.97	0.44
3:M:1070:UNK:CB	13:O:39:SER:O	2.65	0.44
1:J:143:ILE:CA	4:N:216:ALA:HB1	2.48	0.43
3:C:275:SER:HA	17:C:1089:CLA:C2A	2.48	0.43
13:V:41:HIS:HD2	19:V:138:HEM:C4B	2.25	0.43
3:C:283:GLY:HA2	17:C:1085:CLA:CAA	2.48	0.43
1:A:143:ILE:CA	4:D:216:ALA:HB1	2.49	0.43
2:L:22:ALA:C	17:L:1109:CLA:CMB	2.68	0.43
2:B:69:LEU:CA	17:B:1111:CLA:HMA2	2.48	0.43
3:C:179:ALA:HB1	3:C:184:GLY:HA2	2.01	0.43
3:M:410:VAL:HA	3:M:415:ASN:HA	1.99	0.43
2:B:450:TRP:HB3	17:B:1110:CLA:HMB2	0.47	0.43
3:M:425:TRP:CG	17:M:1079:CLA:CAB	2.92	0.43
17:M:1084:CLA:CMC	17:W:64:CLA:H2A	2.49	0.43
3:M:429:SER:CB	17:M:1079:CLA:HMC1	2.48	0.43
2:B:22:ALA:HB1	17:B:1109:CLA:C2B	2.48	0.43
2:L:1092:UNK:HA	11:Y:133:UNK:CA	2.48	0.43
2:L:204:ALA:HB1	17:L:1117:CLA:HMC3	1.99	0.43
2:L:450:TRP:O	17:L:1110:CLA:HMB1	2.19	0.42
3:C:275:SER:HA	17:C:1089:CLA:C3A	2.49	0.42
17:L:1111:CLA:C4A	17:L:1114:CLA:HMD2	2.47	0.42
1:A:285:PHE:CD1	3:C:436:PHE:HD1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:429:SER:CB	17:C:1079:CLA:HMC1	2.47	0.42
2:B:9:HIS:CE1	17:B:1116:CLA:C4D	2.85	0.42
4:D:79:SER:HA	4:D:170:ALA:HB2	2.01	0.42
2:B:9:HIS:NE2	17:B:1116:CLA:NC	2.67	0.42
2:B:1092:UNK:HA	11:O:133:UNK:CA	2.48	0.42
4:D:184:PHE:O	17:D:354:CLA:CAC	2.68	0.42
1:J:216:GLY:O	4:N:271:MET:O	2.37	0.42
17:B:1107:CLA:CMC	17:B:1120:CLA:C3C	2.98	0.42
3:M:129:GLY:HA2	17:M:1087:CLA:CMB	1.56	0.42
3:C:426:LEU:HA	17:C:1079:CLA:CMC	2.50	0.42
3:C:1070:UNK:CB	13:V:39:SER:O	2.68	0.42
18:A:367:PHO:HMC1	4:D:148:ALA:HB2	1.94	0.42
18:J:366:PHO:CMC	4:N:148:ALA:CB	2.83	0.42
1:J:285:PHE:CD1	3:M:436:PHE:HD1	2.37	0.42
3:C:129:GLY:HA2	17:C:1088:CLA:C3B	2.49	0.41
2:L:139:PHE:CE1	17:L:1120:CLA:NA	2.88	0.41
2:L:155:ALA:O	2:L:156:PHE:HB3	2.19	0.41
4:D:209:LEU:HA	18:D:356:PHO:C2C	2.49	0.41
1:A:186:PHE:CB	17:A:365:CLA:CMD	2.99	0.41
2:L:240:SER:O	17:L:1120:CLA:C3C	2.68	0.41
2:L:191:ASN:HA	2:L:192:PRO:HD3	1.84	0.41
4:D:308:ASP:N	4:D:309:PRO:HD3	2.35	0.41
1:J:85:SER:CB	3:M:221:GLU:C	2.86	0.41
1:A:210:LEU:CB	18:A:367:PHO:HMC3	2.50	0.41
2:B:31:ALA:HB2	17:B:1114:CLA:CHB	2.51	0.41
1:A:235:TYR:OH	2:B:5:TRP:CA	2.64	0.41
1:J:95:PRO:CA	17:J:367:CLA:CAA	2.98	0.41
3:C:274:TYR:CD1	17:C:1081:CLA:HMD3	2.56	0.41
17:M:1081:CLA:HMA1	17:W:64:CLA:C2D	2.46	0.41
1:A:95:PRO:CB	17:A:368:CLA:CAA	2.99	0.41
3:M:56:HIS:CB	17:M:1081:CLA:HMB2	2.51	0.41
3:C:275:SER:HA	17:C:1089:CLA:C1A	2.51	0.41
2:B:28:ALA:HB1	2:B:104:SER:HA	2.03	0.41
12:U:74:UNK:C	12:U:76:UNK:H	2.33	0.41
4:D:209:LEU:CB	18:D:356:PHO:C1C	2.99	0.41
3:M:1048:UNK:CA	11:Y:14:UNK:N	2.82	0.41
4:D:42:TYR:CD1	6:F:25:LEU:CB	3.04	0.41
17:C:1078:CLA:HMD2	17:C:1089:CLA:OBD	2.21	0.41
2:L:150:CYS:CA	17:L:1113:CLA:CMB	2.99	0.41
3:C:164:HIS:ND1	17:C:1086:CLA:C1D	2.84	0.40
3:C:266:TRP:HH2	17:C:1078:CLA:HHD	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:426:LEU:HA	17:M:1079:CLA:CMC	2.51	0.40
1:A:94:TYR:CB	17:A:368:CLA:HHB	2.51	0.40
2:L:64:PRO:CB	17:L:1114:CLA:CMC	2.97	0.40
14:1:21:UNK:C	14:1:23:UNK:H	2.33	0.40
2:B:1092:UNK:HA	11:O:133:UNK:N	2.32	0.40
3:C:425:TRP:CG	17:C:1079:CLA:CAB	2.94	0.40
17:B:1111:CLA:C4A	17:B:1114:CLA:HMD2	2.47	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	293/360 (81%)	195 (67%)	66 (22%)	32 (11%)	0	10
1	J	293/360 (81%)	199 (68%)	59 (20%)	35 (12%)	0	8
2	B	314/472 (66%)	219 (70%)	62 (20%)	33 (10%)	1	11
2	L	309/472 (66%)	215 (70%)	60 (19%)	34 (11%)	0	10
3	C	263/473 (56%)	198 (75%)	47 (18%)	18 (7%)	1	23
3	M	257/473 (54%)	189 (74%)	47 (18%)	21 (8%)	1	17
4	D	269/352 (76%)	187 (70%)	56 (21%)	26 (10%)	1	13
4	N	269/352 (76%)	184 (68%)	59 (22%)	26 (10%)	1	13
5	E	33/83 (40%)	23 (70%)	5 (15%)	5 (15%)	0	5
5	P	15/83 (18%)	11 (73%)	4 (27%)	0	100	100
6	F	28/44 (64%)	22 (79%)	3 (11%)	3 (11%)	0	10
6	Q	24/44 (54%)	22 (92%)	2 (8%)	0	100	100
10	K	25/37 (68%)	14 (56%)	9 (36%)	2 (8%)	1	18
10	W	25/37 (68%)	15 (60%)	8 (32%)	2 (8%)	1	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	0	111/137 (81%)	90 (81%)	17 (15%)	4 (4%)	4	41
13	V	127/137 (93%)	102 (80%)	19 (15%)	6 (5%)	3	33
All	All	2655/3916 (68%)	1885 (71%)	523 (20%)	247 (9%)	1	15

All (247) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	101	SER
1	A	168	PHE
1	A	191	ASN
1	A	192	ILE
1	A	195	HIS
1	A	196	PRO
1	A	306	VAL
1	A	313	VAL
2	B	49	ASP
2	B	130	GLU
2	B	170	ASP
2	B	183	PRO
2	B	447	PRO
3	C	190	ALA
3	C	191	PRO
3	C	196	VAL
3	C	410	VAL
3	C	422	PRO
4	D	56	THR
4	D	57	SER
4	D	122	LEU
4	D	139	ARG
4	D	149	PRO
4	D	330	ALA
6	F	17	VAL
10	K	17	PRO
1	J	94	TYR
1	J	101	SER
1	J	168	PHE
1	J	191	ASN
1	J	192	ILE
1	J	195	HIS
1	J	196	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	222	SER
1	J	306	VAL
1	J	313	VAL
2	L	56	TRP
2	L	170	ASP
2	L	183	PRO
2	L	442	ILE
2	L	447	PRO
3	M	79	LYS
3	M	110	PRO
3	M	190	ALA
3	M	191	PRO
3	M	196	VAL
3	M	410	VAL
4	N	56	THR
4	N	57	SER
4	N	139	ARG
4	N	149	PRO
4	N	308	ASP
4	N	330	ALA
10	W	17	PRO
13	0	45	ILE
1	A	36	ILE
1	A	58	VAL
1	A	143	ILE
1	A	169	SER
1	A	226	GLU
1	A	234	ASN
1	A	261	GLN
1	A	264	SER
1	A	334	ARG
2	B	50	PRO
2	B	159	THR
2	B	180	PRO
2	B	198	VAL
3	C	78	GLU
3	C	79	LYS
3	C	99	VAL
3	C	189	TRP
3	C	227	VAL
4	D	76	VAL
4	D	249	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	341	PHE
4	D	342	PRO
5	E	8	PRO
5	E	20	VAL
1	J	36	ILE
1	J	58	VAL
1	J	143	ILE
1	J	169	SER
1	J	261	GLN
1	J	264	SER
1	J	334	ARG
2	L	6	TYR
2	L	49	ASP
2	L	50	PRO
2	L	51	VAL
2	L	159	THR
2	L	180	PRO
2	L	187	PRO
2	L	198	VAL
3	M	78	GLU
3	M	189	TRP
3	M	227	VAL
3	M	262	ARG
3	M	422	PRO
3	M	454	GLY
4	N	76	VAL
4	N	249	ALA
4	N	341	PHE
4	N	342	PRO
1	A	68	SER
1	A	263	ALA
1	A	318	ALA
2	B	6	TYR
2	B	13	ILE
2	B	75	TRP
2	B	121	GLU
2	B	163	GLY
2	B	187	PRO
2	B	193	TYR
2	B	441	GLY
3	C	94	THR
3	C	411	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	454	GLY
4	D	53	THR
4	D	147	SER
5	E	13	ILE
6	F	18	ARG
13	V	82	TYR
1	J	68	SER
1	J	263	ALA
1	J	318	ALA
2	L	13	ILE
2	L	44	THR
2	L	48	SER
2	L	54	PRO
2	L	55	MET
2	L	132	ALA
3	M	94	THR
3	M	137	PRO
3	M	411	ALA
4	N	53	THR
4	N	123	ILE
4	N	147	SER
4	N	195	PRO
13	0	82	TYR
1	A	93	PHE
1	A	303	ASN
1	A	338	ASN
2	B	132	ALA
2	B	199	VAL
2	B	412	THR
2	B	442	ILE
3	C	77	PRO
3	C	104	GLU
4	D	123	ILE
4	D	313	THR
4	D	345	VAL
5	E	14	THR
6	F	14	ILE
1	J	93	PHE
1	J	303	ASN
1	J	338	ASN
2	L	52	LEU
2	L	88	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	121	GLU
2	L	163	GLY
2	L	193	TYR
2	L	199	VAL
2	L	412	THR
3	M	77	PRO
4	N	313	THR
4	N	345	VAL
1	A	74	GLY
1	A	81	ALA
1	A	99	ALA
1	A	176	ILE
2	B	5	TRP
2	B	11	VAL
2	B	55	MET
2	B	56	TRP
2	B	57	ARG
2	B	166	MET
2	B	192	PRO
2	B	225	LEU
2	B	443	PHE
3	C	455	PHE
4	D	55	VAL
4	D	140	PRO
4	D	170	ALA
4	D	298	PHE
4	D	339	PHE
4	D	348	ARG
13	V	16	GLY
13	V	78	ASN
1	J	74	GLY
1	J	81	ALA
1	J	99	ALA
1	J	176	ILE
1	J	234	ASN
1	J	238	LYS
2	L	5	TRP
2	L	11	VAL
2	L	166	MET
2	L	225	LEU
2	L	443	PHE
3	M	264	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	55	VAL
4	N	170	ALA
4	N	176	ALA
4	N	310	GLU
4	N	339	PHE
4	N	348	ARG
13	0	78	ASN
1	A	62	GLY
1	A	83	VAL
1	A	299	GLY
2	B	44	THR
3	C	193	GLY
3	C	414	ILE
4	D	75	THR
1	J	62	GLY
1	J	83	VAL
1	J	299	GLY
2	L	192	PRO
3	M	109	PHE
3	M	414	ILE
4	N	124	GLY
4	N	140	PRO
2	B	51	VAL
4	D	138	VAL
4	D	346	LEU
13	V	19	ILE
2	L	219	VAL
3	M	193	GLY
4	N	138	VAL
4	N	346	LEU
10	W	21	VAL
10	K	21	VAL
1	J	224	ILE
3	M	134	ILE
2	B	71	VAL
4	D	99	GLY
4	D	124	GLY
5	E	40	GLY
1	A	60	ILE
13	V	45	ILE
13	V	101	PHE
1	J	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	0	101	PHE
1	J	39	PRO
2	L	71	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	21/290 (7%)	20 (95%)	1 (5%)	31	72
1	J	22/290 (8%)	21 (96%)	1 (4%)	34	74
2	B	21/290 (7%)	21 (100%)	0	100	100
2	L	21/290 (7%)	21 (100%)	0	100	100
3	C	16/315 (5%)	16 (100%)	0	100	100
3	M	10/315 (3%)	9 (90%)	1 (10%)	9	44
4	D	16/283 (6%)	16 (100%)	0	100	100
4	N	14/283 (5%)	14 (100%)	0	100	100
5	E	1/72 (1%)	1 (100%)	0	100	100
6	F	3/38 (8%)	3 (100%)	0	100	100
10	K	1/30 (3%)	1 (100%)	0	100	100
10	W	1/30 (3%)	1 (100%)	0	100	100
13	0	5/117 (4%)	5 (100%)	0	100	100
13	V	7/117 (6%)	7 (100%)	0	100	100
All	All	159/2760 (6%)	156 (98%)	3 (2%)	65	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	J	182	PHE
3	M	422	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
2	B	9	HIS
3	C	164	HIS
1	J	332	HIS
3	M	164	HIS
4	N	117	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 94 ligands modelled in this entry, 10 are monoatomic - leaving 84 for Mogul analysis.

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$
19	HEM	0	138	13	25,32,50	3.98	11 (44%)	22,54,82	2.96	10 (45%)
17	CLA	A	365	-	25,43,73	1.61	4 (16%)	28,76,113	2.55	10 (35%)
17	CLA	A	366	-	25,43,73	1.10	3 (12%)	28,76,113	2.15	10 (35%)
18	PHO	A	367	-	37,39,69	1.19	4 (10%)	52,62,99	1.67	5 (9%)
17	CLA	A	368	1	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	369	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1107	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1108	2	25,43,73	1.30	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1109	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1110	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1111	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1112	-	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1113	2	25,43,73	1.31	3 (12%)	28,76,113	2.07	9 (32%)
17	CLA	B	1114	2	25,43,73	1.33	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1115	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	B	1116	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1117	2	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1118	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1119	2	25,43,73	1.33	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1120	-	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1121	-	25,43,73	1.31	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1122	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1078	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1079	3	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	C	1080	3	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	C	1081	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	C	1082	3	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	C	1083	-	25,43,73	1.32	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	C	1084	-	25,43,73	1.33	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	C	1085	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1086	3	25,43,73	1.34	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	C	1087	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1088	3	25,43,73	1.33	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	C	1089	3	25,43,73	1.32	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	D	354	4	25,43,73	1.27	3 (12%)	28,76,113	2.03	8 (28%)
17	CLA	D	355	-	25,43,73	1.09	1 (4%)	28,76,113	2.06	10 (35%)
18	PHO	D	356	4	37,39,69	1.17	4 (10%)	52,62,99	1.69	5 (9%)
17	CLA	D	357	4	25,43,73	1.35	4 (16%)	28,76,113	2.07	9 (32%)
20	PLA	D	358	-	6,6,25	2.91	5 (83%)	6,6,37	0.88	0
21	BCR	D	359	-	41,41,41	1.25	5 (12%)	56,56,56	1.77	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	HEM	E	84	-	25,32,50	3.98	11 (44%)	22,54,82	2.95	10 (45%)
17	CLA	G	221	-	25,43,73	1.34	4 (16%)	28,76,113	1.92	8 (28%)
17	CLA	J	365	-	25,43,73	1.59	3 (12%)	28,76,113	2.66	10 (35%)
18	PHO	J	366	-	37,39,69	1.19	4 (10%)	52,62,99	1.69	5 (9%)
17	CLA	J	367	1	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	J	368	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
21	BCR	K	47	-	19,21,41	0.83	0	20,24,56	1.21	2 (10%)
17	CLA	L	1107	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	L	1108	-	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	L	1109	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	L	1110	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1111	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1112	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	L	1113	2	25,43,73	1.30	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1114	-	25,43,73	1.34	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	L	1115	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1116	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1117	2	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1118	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1119	-	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	L	1120	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	L	1121	2	25,43,73	1.31	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1122	-	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	M	1078	-	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	M	1079	3	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	M	1080	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	M	1081	-	25,43,73	1.32	3 (12%)	28,76,113	2.03	9 (32%)
17	CLA	M	1082	-	25,43,73	1.32	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	M	1083	-	25,43,73	1.31	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	M	1084	-	25,43,73	1.31	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	M	1085	3	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	M	1086	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	M	1087	3	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	M	1088	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	N	354	4	25,43,73	1.27	2 (8%)	28,76,113	2.03	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	N	355	-	25,43,73	1.11	3 (12%)	28,76,113	2.15	10 (35%)
17	CLA	N	356	-	25,43,73	1.08	1 (4%)	28,76,113	2.06	10 (35%)
18	PHO	N	357	-	37,39,69	1.16	4 (10%)	52,62,99	1.70	5 (9%)
17	CLA	N	358	4	25,43,73	1.32	4 (16%)	28,76,113	2.07	9 (32%)
20	PLA	N	359	-	6,6,25	2.91	5 (83%)	6,6,37	0.88	0
19	HEM	P	92	-	25,32,50	3.98	11 (44%)	22,54,82	2.97	10 (45%)
17	CLA	R	221	-	25,43,73	1.34	4 (16%)	28,76,113	1.92	8 (28%)
19	HEM	V	138	13	25,32,50	3.98	11 (44%)	22,54,82	2.95	10 (45%)
17	CLA	W	64	-	25,43,73	1.33	4 (16%)	28,76,113	2.05	9 (32%)

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
19	HEM	0	138	13	-	0/0/40/54	0/0/8/8
17	CLA	A	365	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	A	366	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	A	367	-	-	0/15/60/103	0/1/6/6
17	CLA	A	368	1	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	A	369	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1107	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1108	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1109	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1110	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1111	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1112	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1113	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1114	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1115	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1116	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1117	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1118	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1119	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1120	-	3/3/13/25	0/0/92/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1121	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1122	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1078	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1079	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1080	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1081	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1082	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1083	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1084	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1085	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1086	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1087	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1088	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1089	3	4/4/13/25	0/0/92/135	0/0/9/9
17	CLA	D	354	4	1/1/13/25	0/0/92/135	0/0/9/9
17	CLA	D	355	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	D	356	4	-	0/15/60/103	0/1/6/6
17	CLA	D	357	4	3/3/13/25	0/0/92/135	0/0/9/9
20	PLA	D	358	-	-	0/0/0/23	0/1/1/1
21	BCR	D	359	-	-	0/29/63/63	0/2/2/2
19	HEM	E	84	-	-	0/0/40/54	0/0/8/8
17	CLA	G	221	-	2/2/13/25	0/0/92/135	0/0/9/9
17	CLA	J	365	-	3/3/13/25	0/0/92/135	0/0/9/9
18	PHO	J	366	-	-	0/15/60/103	0/1/6/6
17	CLA	J	367	1	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	J	368	-	3/3/13/25	0/0/92/135	0/0/9/9
21	BCR	K	47	-	-	0/21/23/63	0/0/0/2
17	CLA	L	1107	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1108	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1109	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1110	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1111	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1112	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1113	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1114	-	3/3/13/25	0/0/92/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	L	1115	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1116	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1117	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1118	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1119	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1120	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1121	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1122	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1078	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1079	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1080	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1081	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1082	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1083	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1084	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1085	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1086	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1087	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1088	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	N	354	4	1/1/13/25	0/0/92/135	0/0/9/9
17	CLA	N	355	-	2/2/13/25	0/0/92/135	0/0/9/9
17	CLA	N	356	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	N	357	-	-	0/15/60/103	0/1/6/6
17	CLA	N	358	4	3/3/13/25	0/0/92/135	0/0/9/9
20	PLA	N	359	-	-	0/0/0/23	0/1/1/1
19	HEM	P	92	-	-	0/0/40/54	0/0/8/8
17	CLA	R	221	-	2/2/13/25	0/0/92/135	0/0/9/9
19	HEM	V	138	13	-	0/0/40/54	0/0/8/8
17	CLA	W	64	-	3/3/13/25	0/0/92/135	0/0/9/9

All (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	92	HEM	C2D-C1D	-8.41	1.38	1.50
19	O	138	HEM	C2D-C1D	-8.38	1.38	1.50
19	V	138	HEM	C2D-C1D	-8.34	1.38	1.50
19	E	84	HEM	C2D-C1D	-8.28	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	V	138	HEM	C2B-C1B	-7.32	1.39	1.50
19	O	138	HEM	C2B-C1B	-7.31	1.39	1.50
19	E	84	HEM	C2B-C1B	-7.30	1.39	1.50
19	P	92	HEM	C2B-C1B	-7.26	1.39	1.50
19	E	84	HEM	C3D-C4D	-6.65	1.40	1.50
19	P	92	HEM	C3D-C4D	-6.64	1.40	1.50
19	V	138	HEM	C3D-C4D	-6.64	1.40	1.50
19	O	138	HEM	C3D-C4D	-6.62	1.40	1.50
19	V	138	HEM	C3B-C4B	-6.38	1.41	1.50
19	E	84	HEM	C3B-C4B	-6.37	1.41	1.50
19	O	138	HEM	C3B-C4B	-6.34	1.41	1.50
19	P	92	HEM	C3B-C4B	-6.33	1.41	1.50
17	A	365	CLA	CBD-CAD	-4.31	1.42	1.51
19	P	92	HEM	C3D-C2D	-4.22	1.41	1.52
19	E	84	HEM	C3D-C2D	-4.18	1.41	1.52
19	O	138	HEM	C3D-C2D	-4.17	1.41	1.52
19	V	138	HEM	C3D-C2D	-4.17	1.41	1.52
19	O	138	HEM	C3B-C2B	-4.07	1.42	1.52
19	V	138	HEM	C3B-C2B	-4.03	1.42	1.52
19	E	84	HEM	C3B-C2B	-4.02	1.42	1.52
19	P	92	HEM	C3B-C2B	-4.00	1.42	1.52
17	A	365	CLA	CBD-CHA	-3.53	1.45	1.50
17	A	365	CLA	CAB-C3B	-2.94	1.45	1.51
17	J	365	CLA	CAB-C3B	-2.94	1.45	1.51
19	O	138	HEM	C4D-ND	-2.56	1.34	1.38
19	P	92	HEM	C4D-ND	-2.51	1.35	1.38
19	V	138	HEM	C4D-ND	-2.51	1.35	1.38
19	E	84	HEM	C4D-ND	-2.50	1.35	1.38
17	G	221	CLA	C1B-CHB	-2.47	1.33	1.39
17	R	221	CLA	C1B-CHB	-2.46	1.33	1.39
21	D	359	BCR	C23-C22	-2.29	1.40	1.45
17	N	354	CLA	C1B-CHB	-2.27	1.33	1.39
17	D	354	CLA	C1B-CHB	-2.27	1.33	1.39
18	D	356	PHO	C4D-CHA	-2.12	1.39	1.45
18	N	357	PHO	C4D-CHA	-2.09	1.39	1.45
18	J	366	PHO	C4D-CHA	-2.07	1.39	1.45
18	A	367	PHO	C4D-CHA	-2.06	1.39	1.45
17	N	355	CLA	C1B-CHB	-2.04	1.34	1.39
17	A	366	CLA	C1B-CHB	-2.03	1.34	1.39
17	M	1082	CLA	CMD-C2D	2.00	1.56	1.51
17	L	1107	CLA	CBD-CHA	2.00	1.53	1.50
17	C	1089	CLA	CBD-CHA	2.01	1.53	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	367	CLA	CBD-CHA	2.01	1.53	1.50
17	C	1083	CLA	CMD-C2D	2.01	1.56	1.51
17	D	354	CLA	CHC-C1C	2.01	1.41	1.35
17	C	1088	CLA	CBD-CHA	2.02	1.53	1.50
17	L	1122	CLA	CBD-CHA	2.02	1.53	1.50
17	B	1107	CLA	CBD-CHA	2.04	1.53	1.50
17	W	64	CLA	CBD-CHA	2.04	1.53	1.50
17	C	1079	CLA	CBD-CHA	2.04	1.53	1.50
17	B	1112	CLA	CBD-CHA	2.04	1.53	1.50
17	M	1083	CLA	CBD-CHA	2.05	1.53	1.50
17	C	1084	CLA	CBD-CHA	2.05	1.53	1.50
17	L	1120	CLA	CBD-CHA	2.05	1.53	1.50
17	B	1110	CLA	CBD-CHA	2.05	1.53	1.50
17	M	1085	CLA	CBD-CHA	2.06	1.53	1.50
17	B	1114	CLA	CBD-CHA	2.06	1.53	1.50
17	L	1112	CLA	CBD-CHA	2.07	1.53	1.50
17	L	1114	CLA	CBD-CHA	2.07	1.53	1.50
17	M	1087	CLA	CBD-CHA	2.07	1.53	1.50
17	M	1079	CLA	CBD-CHA	2.08	1.53	1.50
17	L	1119	CLA	CBD-CHA	2.09	1.53	1.50
17	C	1086	CLA	CBD-CHA	2.09	1.53	1.50
17	N	358	CLA	CBD-CHA	2.10	1.53	1.50
17	B	1120	CLA	CBD-CHA	2.11	1.53	1.50
17	A	369	CLA	CBD-CHA	2.12	1.53	1.50
17	D	357	CLA	CBD-CHA	2.18	1.53	1.50
21	D	359	BCR	C26-C25	2.18	1.37	1.34
17	B	1112	CLA	OBD-CAD	2.22	1.26	1.22
17	L	1112	CLA	OBD-CAD	2.24	1.26	1.22
18	N	357	PHO	CMD-C2D	2.27	1.55	1.50
17	B	1114	CLA	OBD-CAD	2.28	1.26	1.22
17	L	1121	CLA	OBD-CAD	2.28	1.26	1.22
17	N	358	CLA	OBD-CAD	2.29	1.26	1.22
17	W	64	CLA	OBD-CAD	2.31	1.26	1.22
17	L	1113	CLA	OBD-CAD	2.32	1.26	1.22
17	B	1121	CLA	OBD-CAD	2.32	1.26	1.22
17	L	1107	CLA	OBD-CAD	2.33	1.26	1.22
17	B	1110	CLA	OBD-CAD	2.33	1.26	1.22
17	A	369	CLA	OBD-CAD	2.34	1.26	1.22
17	B	1107	CLA	OBD-CAD	2.34	1.26	1.22
17	C	1084	CLA	OBD-CAD	2.34	1.26	1.22
17	M	1083	CLA	OBD-CAD	2.35	1.26	1.22
17	L	1120	CLA	OBD-CAD	2.35	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1113	CLA	OBD-CAD	2.35	1.26	1.22
18	D	356	PHO	CMD-C2D	2.35	1.55	1.50
18	J	366	PHO	CMD-C2D	2.36	1.55	1.50
17	M	1084	CLA	OBD-CAD	2.36	1.26	1.22
17	L	1114	CLA	OBD-CAD	2.36	1.26	1.22
17	B	1115	CLA	OBD-CAD	2.36	1.26	1.22
17	N	355	CLA	CBD-CAD	2.36	1.56	1.51
17	M	1085	CLA	OBD-CAD	2.36	1.26	1.22
17	A	365	CLA	CHC-C1C	2.37	1.42	1.35
17	L	1115	CLA	OBD-CAD	2.37	1.26	1.22
17	A	366	CLA	CBD-CAD	2.38	1.56	1.51
17	L	1116	CLA	OBD-CAD	2.38	1.26	1.22
17	C	1086	CLA	OBD-CAD	2.38	1.26	1.22
17	J	367	CLA	OBD-CAD	2.38	1.26	1.22
17	C	1082	CLA	OBD-CAD	2.38	1.26	1.22
17	C	1089	CLA	OBD-CAD	2.38	1.26	1.22
17	J	365	CLA	CHC-C1C	2.38	1.42	1.35
17	C	1080	CLA	OBD-CAD	2.38	1.26	1.22
17	M	1087	CLA	OBD-CAD	2.39	1.26	1.22
17	L	1111	CLA	OBD-CAD	2.39	1.26	1.22
17	B	1118	CLA	OBD-CAD	2.39	1.26	1.22
17	C	1079	CLA	OBD-CAD	2.40	1.26	1.22
17	R	221	CLA	CHC-C1C	2.40	1.42	1.35
17	M	1078	CLA	OBD-CAD	2.40	1.26	1.22
17	M	1088	CLA	OBD-CAD	2.40	1.26	1.22
17	B	1108	CLA	OBD-CAD	2.40	1.26	1.22
17	B	1122	CLA	OBD-CAD	2.40	1.26	1.22
17	B	1117	CLA	OBD-CAD	2.40	1.26	1.22
20	N	359	PLA	C4-C3	2.40	1.44	1.38
17	M	1079	CLA	OBD-CAD	2.41	1.26	1.22
17	L	1118	CLA	OBD-CAD	2.41	1.26	1.22
17	C	1088	CLA	OBD-CAD	2.41	1.26	1.22
17	A	368	CLA	OBD-CAD	2.41	1.26	1.22
17	L	1117	CLA	OBD-CAD	2.41	1.26	1.22
17	C	1087	CLA	OBD-CAD	2.41	1.26	1.22
17	G	221	CLA	CHC-C1C	2.41	1.42	1.35
17	C	1078	CLA	OBD-CAD	2.41	1.26	1.22
17	B	1111	CLA	OBD-CAD	2.42	1.26	1.22
17	L	1110	CLA	OBD-CAD	2.42	1.26	1.22
17	B	1116	CLA	OBD-CAD	2.42	1.26	1.22
17	C	1085	CLA	OBD-CAD	2.42	1.26	1.22
17	L	1122	CLA	OBD-CAD	2.42	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1119	CLA	OBD-CAD	2.42	1.26	1.22
17	M	1080	CLA	OBD-CAD	2.42	1.26	1.22
17	M	1081	CLA	OBD-CAD	2.43	1.26	1.22
20	D	358	PLA	C4-C3	2.43	1.44	1.38
17	D	357	CLA	OBD-CAD	2.43	1.26	1.22
17	L	1119	CLA	OBD-CAD	2.43	1.26	1.22
17	C	1083	CLA	OBD-CAD	2.44	1.26	1.22
17	L	1108	CLA	OBD-CAD	2.44	1.26	1.22
17	L	1109	CLA	OBD-CAD	2.44	1.26	1.22
17	B	1109	CLA	OBD-CAD	2.44	1.26	1.22
17	M	1086	CLA	OBD-CAD	2.44	1.26	1.22
17	C	1081	CLA	OBD-CAD	2.44	1.26	1.22
17	G	221	CLA	CAA-C2A	2.45	1.58	1.53
17	J	368	CLA	OBD-CAD	2.45	1.26	1.22
17	B	1120	CLA	OBD-CAD	2.46	1.26	1.22
17	R	221	CLA	CAA-C2A	2.46	1.58	1.53
17	M	1082	CLA	OBD-CAD	2.48	1.26	1.22
18	A	367	PHO	CMD-C2D	2.48	1.56	1.50
17	A	366	CLA	CHC-C1C	2.54	1.43	1.35
17	N	355	CLA	CHC-C1C	2.57	1.43	1.35
17	L	1108	CLA	CAA-C2A	2.58	1.59	1.53
17	B	1108	CLA	CAA-C2A	2.60	1.59	1.53
17	M	1082	CLA	CAA-C2A	2.62	1.59	1.53
17	C	1083	CLA	CAA-C2A	2.65	1.59	1.53
17	C	1082	CLA	CAA-C2A	2.65	1.59	1.53
17	L	1107	CLA	CAA-C2A	2.66	1.59	1.53
17	M	1084	CLA	CAA-C2A	2.66	1.59	1.53
17	M	1079	CLA	CAA-C2A	2.67	1.59	1.53
17	M	1081	CLA	CAA-C2A	2.67	1.59	1.53
18	D	356	PHO	CAA-C2A	2.67	1.59	1.53
17	B	1113	CLA	CAA-C2A	2.67	1.59	1.53
17	L	1115	CLA	CAA-C2A	2.67	1.59	1.53
17	L	1111	CLA	CAA-C2A	2.68	1.59	1.53
17	M	1083	CLA	CAA-C2A	2.68	1.59	1.53
17	B	1116	CLA	CAA-C2A	2.68	1.59	1.53
17	B	1110	CLA	CAA-C2A	2.68	1.59	1.53
17	B	1107	CLA	CAA-C2A	2.68	1.59	1.53
17	J	368	CLA	CAA-C2A	2.68	1.59	1.53
17	L	1112	CLA	CAA-C2A	2.68	1.59	1.53
17	N	356	CLA	CHC-C1C	2.68	1.43	1.35
17	N	358	CLA	CAA-C2A	2.69	1.59	1.53
17	C	1089	CLA	CAA-C2A	2.69	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1121	CLA	CAA-C2A	2.69	1.59	1.53
17	L	1119	CLA	CAA-C2A	2.69	1.59	1.53
17	N	354	CLA	CBD-CAD	2.69	1.57	1.51
17	L	1121	CLA	CAA-C2A	2.70	1.59	1.53
17	L	1120	CLA	CAA-C2A	2.70	1.59	1.53
17	J	367	CLA	CAA-C2A	2.70	1.59	1.53
17	C	1088	CLA	CAA-C2A	2.70	1.59	1.53
17	C	1081	CLA	CAA-C2A	2.70	1.59	1.53
17	B	1114	CLA	CAA-C2A	2.70	1.59	1.53
17	L	1110	CLA	CAA-C2A	2.70	1.59	1.53
17	B	1112	CLA	CAA-C2A	2.70	1.59	1.53
17	B	1117	CLA	CAA-C2A	2.71	1.59	1.53
17	B	1115	CLA	CAA-C2A	2.71	1.59	1.53
17	B	1122	CLA	CAA-C2A	2.71	1.59	1.53
17	B	1109	CLA	CAA-C2A	2.71	1.59	1.53
17	C	1084	CLA	CAA-C2A	2.72	1.59	1.53
17	B	1111	CLA	CAA-C2A	2.72	1.59	1.53
17	B	1120	CLA	CAA-C2A	2.72	1.59	1.53
17	M	1086	CLA	CAA-C2A	2.72	1.59	1.53
17	B	1119	CLA	CAA-C2A	2.72	1.59	1.53
17	D	354	CLA	CBD-CAD	2.72	1.57	1.51
17	M	1080	CLA	CAA-C2A	2.72	1.59	1.53
17	C	1085	CLA	CAA-C2A	2.72	1.59	1.53
18	N	357	PHO	CAA-C2A	2.72	1.59	1.53
17	B	1118	CLA	CAA-C2A	2.72	1.59	1.53
17	L	1116	CLA	CAA-C2A	2.72	1.59	1.53
17	L	1122	CLA	CAA-C2A	2.73	1.59	1.53
17	A	369	CLA	CAA-C2A	2.73	1.59	1.53
17	C	1087	CLA	CAA-C2A	2.73	1.59	1.53
17	D	357	CLA	CAA-C2A	2.73	1.59	1.53
17	L	1113	CLA	CAA-C2A	2.73	1.59	1.53
17	A	368	CLA	CAA-C2A	2.73	1.59	1.53
17	L	1117	CLA	CAA-C2A	2.73	1.59	1.53
17	M	1088	CLA	CAA-C2A	2.73	1.59	1.53
17	M	1087	CLA	CAA-C2A	2.73	1.59	1.53
17	C	1080	CLA	CAA-C2A	2.74	1.59	1.53
17	C	1079	CLA	CAA-C2A	2.74	1.59	1.53
18	J	366	PHO	CAA-C2A	2.74	1.59	1.53
18	A	367	PHO	CAA-C2A	2.74	1.59	1.53
17	L	1109	CLA	CAA-C2A	2.74	1.59	1.53
17	C	1086	CLA	CAA-C2A	2.74	1.59	1.53
17	M	1085	CLA	CAA-C2A	2.75	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	1078	CLA	CAA-C2A	2.75	1.59	1.53
17	D	355	CLA	CHC-C1C	2.76	1.43	1.35
21	D	359	BCR	C29-C30	2.76	1.60	1.54
20	N	359	PLA	C5-C4	2.76	1.45	1.38
17	L	1114	CLA	CAA-C2A	2.77	1.59	1.53
17	W	64	CLA	CAA-C2A	2.77	1.59	1.53
17	C	1078	CLA	CAA-C2A	2.77	1.59	1.53
17	L	1118	CLA	CAA-C2A	2.77	1.59	1.53
21	D	359	BCR	C30-C25	2.78	1.57	1.53
20	D	358	PLA	C5-C4	2.78	1.45	1.38
17	B	1121	CLA	CHC-C1C	2.86	1.44	1.35
17	M	1083	CLA	CHC-C1C	2.88	1.44	1.35
18	D	356	PHO	CHC-C1C	2.89	1.44	1.38
20	N	359	PLA	C5-C6	2.89	1.46	1.37
20	D	358	PLA	C5-C6	2.89	1.46	1.37
17	B	1118	CLA	CHC-C1C	2.89	1.44	1.35
18	N	357	PHO	CHC-C1C	2.90	1.44	1.38
17	M	1085	CLA	CHC-C1C	2.90	1.44	1.35
17	L	1109	CLA	CHC-C1C	2.90	1.44	1.35
17	J	367	CLA	CHC-C1C	2.91	1.44	1.35
17	L	1118	CLA	CHC-C1C	2.91	1.44	1.35
17	L	1121	CLA	CHC-C1C	2.91	1.44	1.35
17	C	1084	CLA	CHC-C1C	2.91	1.44	1.35
17	B	1116	CLA	CHC-C1C	2.91	1.44	1.35
17	A	368	CLA	CHC-C1C	2.92	1.44	1.35
17	C	1082	CLA	CHC-C1C	2.92	1.44	1.35
17	L	1119	CLA	CHC-C1C	2.92	1.44	1.35
17	B	1115	CLA	CHC-C1C	2.92	1.44	1.35
17	B	1111	CLA	CHC-C1C	2.92	1.44	1.35
17	M	1081	CLA	CHC-C1C	2.92	1.44	1.35
17	L	1122	CLA	CHC-C1C	2.92	1.44	1.35
17	M	1082	CLA	CHC-C1C	2.92	1.44	1.35
17	C	1079	CLA	CHC-C1C	2.92	1.44	1.35
17	C	1078	CLA	CHC-C1C	2.92	1.44	1.35
17	B	1107	CLA	CHC-C1C	2.93	1.44	1.35
18	A	367	PHO	CHC-C1C	2.93	1.44	1.38
17	L	1111	CLA	CHC-C1C	2.93	1.44	1.35
17	M	1088	CLA	CHC-C1C	2.93	1.44	1.35
17	B	1109	CLA	CHC-C1C	2.93	1.44	1.35
17	D	357	CLA	CHC-C1C	2.93	1.44	1.35
17	M	1079	CLA	CHC-C1C	2.93	1.44	1.35
17	C	1086	CLA	CHC-C1C	2.93	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1108	CLA	CHC-C1C	2.93	1.44	1.35
18	J	366	PHO	CHC-C1C	2.93	1.44	1.38
17	C	1083	CLA	CHC-C1C	2.93	1.44	1.35
17	L	1115	CLA	CHC-C1C	2.93	1.44	1.35
17	C	1088	CLA	CHC-C1C	2.94	1.44	1.35
17	B	1119	CLA	CHC-C1C	2.94	1.44	1.35
17	L	1120	CLA	CHC-C1C	2.94	1.44	1.35
17	B	1110	CLA	CHC-C1C	2.94	1.44	1.35
17	N	358	CLA	CHC-C1C	2.94	1.44	1.35
17	L	1107	CLA	CHC-C1C	2.94	1.44	1.35
17	B	1122	CLA	CHC-C1C	2.95	1.44	1.35
17	L	1113	CLA	CHC-C1C	2.95	1.44	1.35
17	C	1085	CLA	CHC-C1C	2.95	1.44	1.35
17	B	1117	CLA	CHC-C1C	2.95	1.44	1.35
17	L	1108	CLA	CHC-C1C	2.95	1.44	1.35
17	L	1117	CLA	CHC-C1C	2.95	1.44	1.35
17	M	1086	CLA	CHC-C1C	2.95	1.44	1.35
17	M	1087	CLA	CHC-C1C	2.95	1.44	1.35
17	L	1116	CLA	CHC-C1C	2.95	1.44	1.35
17	C	1087	CLA	CHC-C1C	2.95	1.44	1.35
17	L	1110	CLA	CHC-C1C	2.96	1.44	1.35
17	M	1078	CLA	CHC-C1C	2.96	1.44	1.35
17	B	1113	CLA	CHC-C1C	2.96	1.44	1.35
17	B	1120	CLA	CHC-C1C	2.96	1.44	1.35
17	L	1112	CLA	CHC-C1C	2.96	1.44	1.35
17	C	1080	CLA	CHC-C1C	2.97	1.44	1.35
17	B	1112	CLA	CHC-C1C	2.97	1.44	1.35
17	M	1084	CLA	CHC-C1C	2.97	1.44	1.35
17	J	368	CLA	CHC-C1C	2.97	1.44	1.35
17	C	1081	CLA	CHC-C1C	2.98	1.44	1.35
17	C	1089	CLA	CHC-C1C	2.98	1.44	1.35
17	W	64	CLA	CHC-C1C	2.98	1.44	1.35
17	B	1114	CLA	CHC-C1C	2.98	1.44	1.35
17	A	369	CLA	CHC-C1C	2.99	1.44	1.35
19	E	84	HEM	FE-NB	2.99	2.13	1.97
19	P	92	HEM	FE-NB	2.99	2.13	1.97
19	V	138	HEM	FE-NB	2.99	2.13	1.97
19	0	138	HEM	FE-NB	2.99	2.13	1.97
21	D	359	BCR	C2-C1	3.00	1.61	1.54
17	L	1114	CLA	CHC-C1C	3.00	1.44	1.35
17	M	1080	CLA	CHC-C1C	3.02	1.44	1.35
17	G	221	CLA	CBD-CAD	3.41	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	359	PLA	C2-N1	3.45	1.44	1.33
20	D	358	PLA	C2-N1	3.46	1.44	1.33
17	R	221	CLA	CBD-CAD	3.48	1.59	1.51
20	D	358	PLA	C6-N1	3.60	1.44	1.33
20	N	359	PLA	C6-N1	3.63	1.44	1.33
19	V	138	HEM	FE-NC	4.39	2.13	1.95
19	P	92	HEM	FE-NC	4.40	2.13	1.95
19	E	84	HEM	FE-NC	4.40	2.13	1.95
19	O	138	HEM	FE-NC	4.42	2.13	1.95
17	J	365	CLA	CBD-CHA	5.37	1.58	1.50
19	O	138	HEM	C3A-C4A	6.77	1.51	1.40
19	E	84	HEM	C3A-C4A	6.79	1.51	1.40
19	P	92	HEM	C3A-C4A	6.79	1.51	1.40
19	V	138	HEM	C3A-C4A	6.80	1.51	1.40
19	P	92	HEM	C2A-C1A	7.31	1.52	1.40
19	V	138	HEM	C2A-C1A	7.33	1.52	1.40
19	O	138	HEM	C2A-C1A	7.37	1.52	1.40
19	E	84	HEM	C2A-C1A	7.41	1.52	1.40

All (729) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	365	CLA	OBD-CAD-CBD	-7.98	109.14	125.98
19	O	138	HEM	C3D-C4D-CHA	-7.10	116.89	124.06
19	P	92	HEM	C3D-C4D-CHA	-7.06	116.93	124.06
19	V	138	HEM	C3D-C4D-CHA	-7.01	116.98	124.06
19	E	84	HEM	C3D-C4D-CHA	-6.98	117.01	124.06
18	J	366	PHO	CAB-C3B-C2B	-5.63	115.25	126.81
18	N	357	PHO	CAB-C3B-C2B	-5.61	115.27	126.81
18	D	356	PHO	CAB-C3B-C2B	-5.60	115.30	126.81
18	A	367	PHO	CAB-C3B-C2B	-5.56	115.38	126.81
19	P	92	HEM	C2D-C3D-C4D	-5.09	98.80	103.90
19	O	138	HEM	C2D-C3D-C4D	-5.08	98.81	103.90
19	E	84	HEM	C2D-C3D-C4D	-5.04	98.86	103.90
19	V	138	HEM	C2D-C3D-C4D	-5.03	98.87	103.90
17	N	355	CLA	CAB-C3B-C2B	-4.96	114.99	125.14
17	A	366	CLA	CAB-C3B-C2B	-4.96	115.00	125.14
17	A	365	CLA	OBD-CAD-CBD	-4.93	115.58	125.98
17	A	369	CLA	CAB-C3B-C2B	-4.85	115.22	125.14
17	J	368	CLA	CAB-C3B-C2B	-4.84	115.25	125.14
17	B	1113	CLA	CAB-C3B-C2B	-4.82	115.28	125.14
17	N	358	CLA	CAB-C3B-C2B	-4.82	115.28	125.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	1120	CLA	CAB-C3B-C2B	-4.82	115.28	125.14
17	C	1089	CLA	CAB-C3B-C2B	-4.82	115.28	125.14
17	M	1087	CLA	CAB-C3B-C2B	-4.81	115.29	125.14
17	B	1107	CLA	CAB-C3B-C2B	-4.81	115.30	125.14
17	M	1083	CLA	CAB-C3B-C2B	-4.81	115.30	125.14
17	C	1086	CLA	CAB-C3B-C2B	-4.81	115.30	125.14
17	M	1085	CLA	CAB-C3B-C2B	-4.81	115.31	125.14
17	J	367	CLA	CAB-C3B-C2B	-4.81	115.31	125.14
17	L	1113	CLA	CAB-C3B-C2B	-4.81	115.31	125.14
17	C	1079	CLA	CAB-C3B-C2B	-4.80	115.31	125.14
17	C	1084	CLA	CAB-C3B-C2B	-4.80	115.31	125.14
17	C	1082	CLA	CAB-C3B-C2B	-4.80	115.32	125.14
17	C	1080	CLA	CAB-C3B-C2B	-4.80	115.33	125.14
17	A	368	CLA	CAB-C3B-C2B	-4.80	115.33	125.14
17	L	1121	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	M	1079	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	L	1107	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	B	1115	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	B	1120	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	W	64	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	B	1108	CLA	CAB-C3B-C2B	-4.79	115.34	125.14
17	C	1088	CLA	CAB-C3B-C2B	-4.79	115.35	125.14
17	M	1088	CLA	CAB-C3B-C2B	-4.79	115.35	125.14
17	M	1080	CLA	CAB-C3B-C2B	-4.79	115.35	125.14
17	B	1114	CLA	CAB-C3B-C2B	-4.79	115.35	125.14
17	L	1110	CLA	CAB-C3B-C2B	-4.79	115.35	125.14
17	L	1112	CLA	CAB-C3B-C2B	-4.78	115.36	125.14
17	D	357	CLA	CAB-C3B-C2B	-4.78	115.36	125.14
17	M	1084	CLA	CAB-C3B-C2B	-4.78	115.37	125.14
17	L	1114	CLA	CAB-C3B-C2B	-4.78	115.37	125.14
17	C	1078	CLA	CAB-C3B-C2B	-4.77	115.38	125.14
17	M	1078	CLA	CAB-C3B-C2B	-4.77	115.39	125.14
17	B	1119	CLA	CAB-C3B-C2B	-4.77	115.39	125.14
17	C	1081	CLA	CAB-C3B-C2B	-4.77	115.39	125.14
17	M	1082	CLA	CAB-C3B-C2B	-4.76	115.40	125.14
17	B	1121	CLA	CAB-C3B-C2B	-4.76	115.40	125.14
17	B	1117	CLA	CAB-C3B-C2B	-4.76	115.41	125.14
17	B	1110	CLA	CAB-C3B-C2B	-4.76	115.41	125.14
17	M	1086	CLA	CAB-C3B-C2B	-4.75	115.42	125.14
17	L	1116	CLA	CAB-C3B-C2B	-4.75	115.42	125.14
17	L	1119	CLA	CAB-C3B-C2B	-4.75	115.42	125.14
17	L	1108	CLA	CAB-C3B-C2B	-4.75	115.42	125.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1085	CLA	CAB-C3B-C2B	-4.75	115.42	125.14
17	L	1117	CLA	CAB-C3B-C2B	-4.75	115.43	125.14
17	L	1115	CLA	CAB-C3B-C2B	-4.75	115.43	125.14
17	B	1122	CLA	CAB-C3B-C2B	-4.75	115.43	125.14
17	B	1111	CLA	CAB-C3B-C2B	-4.75	115.43	125.14
17	B	1109	CLA	CAB-C3B-C2B	-4.75	115.43	125.14
17	L	1118	CLA	CAB-C3B-C2B	-4.74	115.44	125.14
17	L	1111	CLA	CAB-C3B-C2B	-4.74	115.44	125.14
17	B	1116	CLA	CAB-C3B-C2B	-4.74	115.45	125.14
17	M	1081	CLA	CAB-C3B-C2B	-4.74	115.45	125.14
17	B	1112	CLA	CAB-C3B-C2B	-4.73	115.46	125.14
17	C	1087	CLA	CAB-C3B-C2B	-4.73	115.46	125.14
17	L	1109	CLA	CAB-C3B-C2B	-4.73	115.47	125.14
17	B	1118	CLA	CAB-C3B-C2B	-4.73	115.47	125.14
17	L	1122	CLA	CAB-C3B-C2B	-4.72	115.48	125.14
17	C	1083	CLA	CAB-C3B-C2B	-4.72	115.48	125.14
17	J	365	CLA	CMA-C3A-C2A	-4.35	105.79	116.20
17	A	365	CLA	CMA-C3A-C2A	-4.34	105.80	116.20
17	R	221	CLA	CMA-C3A-C2A	-4.27	105.98	116.20
17	G	221	CLA	CMA-C3A-C2A	-4.25	106.02	116.20
17	N	354	CLA	CMA-C3A-C2A	-4.21	106.11	116.20
17	D	354	CLA	CMA-C3A-C2A	-4.19	106.17	116.20
17	D	355	CLA	CAB-C3B-C2B	-4.17	116.61	125.14
17	N	356	CLA	CAB-C3B-C2B	-4.16	116.64	125.14
17	N	354	CLA	CAA-C2A-C3A	-4.15	106.27	116.20
17	D	354	CLA	CAA-C2A-C3A	-4.13	106.31	116.20
17	R	221	CLA	CAA-C2A-C3A	-4.06	106.48	116.20
17	G	221	CLA	CAA-C2A-C3A	-4.02	106.56	116.20
17	J	365	CLA	CAA-C2A-C3A	-4.01	106.59	116.20
17	A	365	CLA	CAA-C2A-C3A	-3.99	106.65	116.20
17	J	365	CLA	CAD-CBD-CHA	-3.70	100.87	105.18
17	N	355	CLA	CAA-C2A-C3A	-3.51	107.80	116.20
17	D	354	CLA	CAB-C3B-C2B	-3.51	117.97	125.14
17	N	354	CLA	CAB-C3B-C2B	-3.49	118.00	125.14
17	A	366	CLA	CAA-C2A-C3A	-3.49	107.84	116.20
17	A	365	CLA	CAB-C3B-C2B	-3.40	118.18	125.14
17	J	365	CLA	CAB-C3B-C2B	-3.37	118.25	125.14
17	N	356	CLA	CAA-C2A-C3A	-3.35	108.18	116.20
17	D	355	CLA	CAA-C2A-C3A	-3.33	108.22	116.20
17	M	1080	CLA	CMA-C3A-C2A	-3.18	108.59	116.20
17	L	1119	CLA	CMA-C3A-C2A	-3.14	108.67	116.20
17	M	1078	CLA	CMA-C3A-C2A	-3.14	108.68	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	356	PHO	CMA-C3A-C2A	-3.14	108.69	116.20
17	B	1119	CLA	CMA-C3A-C2A	-3.14	108.69	116.20
17	B	1116	CLA	CMA-C3A-C2A	-3.13	108.70	116.20
17	B	1110	CLA	CMA-C3A-C2A	-3.13	108.70	116.20
17	C	1081	CLA	CMA-C3A-C2A	-3.13	108.70	116.20
17	C	1078	CLA	CMA-C3A-C2A	-3.13	108.70	116.20
17	L	1122	CLA	CMA-C3A-C2A	-3.13	108.70	116.20
17	L	1116	CLA	CMA-C3A-C2A	-3.13	108.71	116.20
17	J	367	CLA	CMA-C3A-C2A	-3.13	108.71	116.20
17	L	1115	CLA	CMA-C3A-C2A	-3.13	108.71	116.20
17	L	1114	CLA	CMA-C3A-C2A	-3.13	108.71	116.20
17	C	1085	CLA	CMA-C3A-C2A	-3.13	108.72	116.20
18	J	366	PHO	CMA-C3A-C2A	-3.13	108.72	116.20
17	C	1079	CLA	CMA-C3A-C2A	-3.12	108.72	116.20
17	L	1110	CLA	CMA-C3A-C2A	-3.12	108.72	116.20
17	C	1086	CLA	CMA-C3A-C2A	-3.12	108.72	116.20
18	N	357	PHO	CMA-C3A-C2A	-3.12	108.73	116.20
17	L	1108	CLA	CMA-C3A-C2A	-3.12	108.73	116.20
17	M	1082	CLA	CMA-C3A-C2A	-3.12	108.73	116.20
17	B	1115	CLA	CMA-C3A-C2A	-3.12	108.73	116.20
17	B	1108	CLA	CMA-C3A-C2A	-3.12	108.74	116.20
17	L	1111	CLA	CMA-C3A-C2A	-3.11	108.74	116.20
17	C	1087	CLA	CMA-C3A-C2A	-3.11	108.75	116.20
17	M	1084	CLA	CMA-C3A-C2A	-3.11	108.75	116.20
18	A	367	PHO	CMA-C3A-C2A	-3.11	108.76	116.20
17	L	1109	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	B	1114	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	M	1086	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	B	1109	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	M	1085	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	L	1121	CLA	CMA-C3A-C2A	-3.11	108.76	116.20
17	M	1079	CLA	CMA-C3A-C2A	-3.10	108.77	116.20
17	B	1111	CLA	CMA-C3A-C2A	-3.10	108.77	116.20
17	B	1122	CLA	CMA-C3A-C2A	-3.10	108.77	116.20
17	C	1088	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	A	368	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	C	1082	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	C	1080	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	C	1089	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	M	1087	CLA	CMA-C3A-C2A	-3.10	108.78	116.20
17	B	1107	CLA	CMA-C3A-C2A	-3.09	108.80	116.20
17	M	1081	CLA	CMA-C3A-C2A	-3.09	108.80	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1083	CLA	CMA-C3A-C2A	-3.09	108.80	116.20
17	B	1118	CLA	CMA-C3A-C2A	-3.09	108.80	116.20
17	A	369	CLA	CMA-C3A-C2A	-3.09	108.80	116.20
17	C	1084	CLA	CMA-C3A-C2A	-3.09	108.80	116.20
17	L	1112	CLA	CMA-C3A-C2A	-3.09	108.81	116.20
17	B	1117	CLA	CMA-C3A-C2A	-3.09	108.81	116.20
17	M	1088	CLA	CMA-C3A-C2A	-3.09	108.81	116.20
17	L	1118	CLA	CMA-C3A-C2A	-3.09	108.81	116.20
17	L	1107	CLA	CMA-C3A-C2A	-3.08	108.82	116.20
17	W	64	CLA	CMA-C3A-C2A	-3.08	108.82	116.20
17	B	1121	CLA	CMA-C3A-C2A	-3.08	108.82	116.20
17	B	1112	CLA	CMA-C3A-C2A	-3.08	108.82	116.20
17	L	1117	CLA	CMA-C3A-C2A	-3.08	108.83	116.20
17	J	368	CLA	CMA-C3A-C2A	-3.08	108.83	116.20
17	B	1120	CLA	CMA-C3A-C2A	-3.08	108.84	116.20
17	M	1083	CLA	CMA-C3A-C2A	-3.07	108.84	116.20
17	B	1113	CLA	CMA-C3A-C2A	-3.07	108.84	116.20
17	D	357	CLA	CMA-C3A-C2A	-3.07	108.84	116.20
17	L	1113	CLA	CMA-C3A-C2A	-3.07	108.85	116.20
17	L	1120	CLA	CMA-C3A-C2A	-3.07	108.86	116.20
17	N	358	CLA	CMA-C3A-C2A	-3.06	108.86	116.20
21	D	359	BCR	C38-C26-C27	-2.98	107.79	113.43
17	G	221	CLA	CMB-C2B-C1B	-2.90	123.56	128.36
21	D	359	BCR	C33-C5-C4	-2.86	108.00	113.43
17	R	221	CLA	CMB-C2B-C1B	-2.83	123.68	128.36
17	D	355	CLA	CMA-C3A-C2A	-2.82	109.45	116.20
17	N	356	CLA	CMA-C3A-C2A	-2.81	109.47	116.20
17	M	1088	CLA	CMB-C2B-C1B	-2.80	123.72	128.36
17	N	358	CLA	CMB-C2B-C1B	-2.80	123.74	128.36
17	M	1083	CLA	CMB-C2B-C1B	-2.79	123.74	128.36
17	L	1107	CLA	CMB-C2B-C1B	-2.79	123.75	128.36
17	L	1120	CLA	CMB-C2B-C1B	-2.79	123.75	128.36
17	D	357	CLA	CMB-C2B-C1B	-2.79	123.75	128.36
17	L	1117	CLA	CMB-C2B-C1B	-2.78	123.76	128.36
17	L	1112	CLA	CMB-C2B-C1B	-2.78	123.77	128.36
17	B	1112	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
17	B	1117	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
17	C	1080	CLA	CMB-C2B-C1B	-2.77	123.79	128.36
17	W	64	CLA	CMB-C2B-C1B	-2.76	123.79	128.36
17	B	1113	CLA	CMB-C2B-C1B	-2.76	123.80	128.36
17	L	1110	CLA	CMB-C2B-C1B	-2.75	123.81	128.36
17	B	1120	CLA	CMB-C2B-C1B	-2.75	123.81	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1086	CLA	CMB-C2B-C1B	-2.75	123.82	128.36
17	C	1084	CLA	CMB-C2B-C1B	-2.74	123.82	128.36
17	B	1107	CLA	CMB-C2B-C1B	-2.74	123.82	128.36
17	C	1081	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
17	C	1082	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
17	L	1111	CLA	CMB-C2B-C1B	-2.73	123.85	128.36
17	L	1113	CLA	CMB-C2B-C1B	-2.73	123.85	128.36
17	L	1121	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	M	1086	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	B	1118	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	L	1109	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	M	1084	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	M	1085	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	C	1088	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
17	M	1080	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	B	1110	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	B	1121	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	L	1114	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	B	1109	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	B	1114	CLA	CMB-C2B-C1B	-2.72	123.87	128.36
17	C	1089	CLA	CMB-C2B-C1B	-2.71	123.87	128.36
17	A	369	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
17	B	1111	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
17	L	1108	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
17	C	1079	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
17	M	1079	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
17	L	1118	CLA	CMB-C2B-C1B	-2.70	123.90	128.36
17	C	1087	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	C	1085	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	L	1116	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	J	368	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	B	1119	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	L	1115	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
17	B	1108	CLA	CMB-C2B-C1B	-2.69	123.92	128.36
17	J	367	CLA	CMB-C2B-C1B	-2.68	123.92	128.36
17	B	1115	CLA	CMB-C2B-C1B	-2.68	123.92	128.36
17	M	1087	CLA	CMB-C2B-C1B	-2.68	123.92	128.36
17	M	1078	CLA	CMB-C2B-C1B	-2.68	123.93	128.36
17	C	1083	CLA	CMB-C2B-C1B	-2.68	123.93	128.36
17	L	1119	CLA	CMB-C2B-C1B	-2.68	123.94	128.36
17	B	1122	CLA	CMB-C2B-C1B	-2.67	123.94	128.36
17	B	1116	CLA	CMB-C2B-C1B	-2.67	123.95	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1078	CLA	CMB-C2B-C1B	-2.67	123.95	128.36
17	A	368	CLA	CMB-C2B-C1B	-2.66	123.96	128.36
17	M	1081	CLA	CMB-C2B-C1B	-2.65	123.98	128.36
17	D	355	CLA	OBD-CAD-CBD	-2.64	120.40	125.98
17	N	356	CLA	CMB-C2B-C1B	-2.64	123.99	128.36
17	D	355	CLA	CMB-C2B-C1B	-2.64	124.00	128.36
17	M	1082	CLA	CMB-C2B-C1B	-2.64	124.00	128.36
17	L	1122	CLA	CMB-C2B-C1B	-2.63	124.01	128.36
17	N	356	CLA	OBD-CAD-CBD	-2.63	120.43	125.98
17	A	366	CLA	CMB-C2B-C1B	-2.59	124.09	128.36
17	N	355	CLA	CMB-C2B-C1B	-2.58	124.09	128.36
17	A	366	CLA	OBD-CAD-CBD	-2.55	120.59	125.98
21	D	359	BCR	C8-C9-C10	-2.54	114.89	118.98
17	N	355	CLA	OBD-CAD-CBD	-2.54	120.62	125.98
17	N	355	CLA	CMA-C3A-C2A	-2.54	110.12	116.20
17	A	366	CLA	CMA-C3A-C2A	-2.53	110.15	116.20
19	E	84	HEM	CHB-C1B-NB	-2.51	122.00	124.52
17	M	1083	CLA	C2C-C1C-NC	-2.49	108.39	110.24
19	O	138	HEM	CHB-C1B-NB	-2.48	122.04	124.52
17	A	365	CLA	CMB-C2B-C1B	-2.47	124.28	128.36
19	V	138	HEM	CHB-C1B-NB	-2.47	122.05	124.52
17	J	365	CLA	CMB-C2B-C1B	-2.46	124.29	128.36
19	P	92	HEM	CHB-C1B-NB	-2.45	122.06	124.52
17	A	366	CLA	C2C-C1C-NC	-2.41	108.45	110.24
17	C	1084	CLA	C2C-C1C-NC	-2.37	108.48	110.24
17	N	355	CLA	C2C-C1C-NC	-2.33	108.51	110.24
17	M	1088	CLA	C2C-C1C-NC	-2.33	108.51	110.24
17	B	1107	CLA	C2C-C1C-NC	-2.32	108.52	110.24
17	L	1111	CLA	C2C-C1C-NC	-2.32	108.52	110.24
17	L	1122	CLA	C2C-C1C-NC	-2.31	108.53	110.24
17	D	357	CLA	C2C-C1C-NC	-2.30	108.53	110.24
17	L	1107	CLA	C2C-C1C-NC	-2.29	108.54	110.24
17	L	1120	CLA	C2C-C1C-NC	-2.29	108.54	110.24
17	M	1078	CLA	C2C-C1C-NC	-2.29	108.54	110.24
17	M	1085	CLA	C2C-C1C-NC	-2.29	108.54	110.24
17	B	1113	CLA	C2C-C1C-NC	-2.29	108.54	110.24
17	B	1118	CLA	C2C-C1C-NC	-2.28	108.54	110.24
17	C	1086	CLA	OBD-CAD-CBD	-2.28	121.16	125.98
17	L	1118	CLA	C2C-C1C-NC	-2.28	108.54	110.24
17	L	1114	CLA	OBD-CAD-CBD	-2.28	121.18	125.98
17	L	1109	CLA	C2C-C1C-NC	-2.27	108.55	110.24
17	B	1117	CLA	C2C-C1C-NC	-2.27	108.55	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1081	CLA	C2C-C1C-NC	-2.27	108.55	110.24
17	C	1089	CLA	C2C-C1C-NC	-2.27	108.56	110.24
17	C	1086	CLA	C2C-C1C-NC	-2.26	108.56	110.24
17	L	1117	CLA	OBD-CAD-CBD	-2.26	121.20	125.98
17	M	1085	CLA	OBD-CAD-CBD	-2.26	121.21	125.98
17	C	1080	CLA	C2C-C1C-NC	-2.26	108.56	110.24
17	M	1088	CLA	OBD-CAD-CBD	-2.26	121.21	125.98
17	J	368	CLA	OBD-CAD-CBD	-2.26	121.21	125.98
17	B	1121	CLA	C2C-C1C-NC	-2.26	108.56	110.24
17	B	1120	CLA	C2C-C1C-NC	-2.25	108.56	110.24
17	L	1121	CLA	C2C-C1C-NC	-2.25	108.56	110.24
17	L	1110	CLA	C2C-C1C-NC	-2.25	108.57	110.24
17	B	1113	CLA	OBD-CAD-CBD	-2.25	121.23	125.98
19	O	138	HEM	C3A-C2A-C1A	-2.25	104.32	106.29
17	B	1111	CLA	C2C-C1C-NC	-2.25	108.57	110.24
17	L	1110	CLA	OBD-CAD-CBD	-2.25	121.24	125.98
17	M	1082	CLA	OBD-CAD-CBD	-2.24	121.25	125.98
19	E	84	HEM	C3A-C2A-C1A	-2.24	104.33	106.29
18	J	366	PHO	OBD-CAD-CBD	-2.24	121.10	125.95
17	C	1081	CLA	OBD-CAD-CBD	-2.24	121.26	125.98
17	M	1083	CLA	OBD-CAD-CBD	-2.23	121.27	125.98
17	B	1120	CLA	OBD-CAD-CBD	-2.23	121.27	125.98
17	B	1117	CLA	OBD-CAD-CBD	-2.23	121.27	125.98
17	L	1112	CLA	OBD-CAD-CBD	-2.23	121.27	125.98
17	L	1108	CLA	C2C-C1C-NC	-2.23	108.58	110.24
17	B	1110	CLA	OBD-CAD-CBD	-2.23	121.28	125.98
17	L	1121	CLA	OBD-CAD-CBD	-2.23	121.28	125.98
17	D	357	CLA	OBD-CAD-CBD	-2.23	121.28	125.98
17	M	1082	CLA	C2C-C1C-NC	-2.23	108.58	110.24
17	W	64	CLA	OBD-CAD-CBD	-2.23	121.28	125.98
17	C	1088	CLA	C2C-C1C-NC	-2.23	108.59	110.24
17	C	1083	CLA	C2C-C1C-NC	-2.22	108.59	110.24
17	M	1081	CLA	C2C-C1C-NC	-2.22	108.59	110.24
17	M	1080	CLA	OBD-CAD-CBD	-2.22	121.29	125.98
17	L	1115	CLA	C2C-C1C-NC	-2.22	108.59	110.24
17	M	1086	CLA	C2C-C1C-NC	-2.22	108.59	110.24
17	L	1113	CLA	C2C-C1C-NC	-2.22	108.59	110.24
17	B	1112	CLA	OBD-CAD-CBD	-2.22	121.30	125.98
17	L	1120	CLA	OBD-CAD-CBD	-2.22	121.30	125.98
17	C	1084	CLA	OBD-CAD-CBD	-2.22	121.30	125.98
17	B	1114	CLA	OBD-CAD-CBD	-2.22	121.30	125.98
17	L	1107	CLA	OBD-CAD-CBD	-2.22	121.30	125.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	1119	CLA	OBD-CAD-CBD	-2.22	121.30	125.98
17	B	1107	CLA	OBD-CAD-CBD	-2.22	121.31	125.98
19	P	92	HEM	C3A-C2A-C1A	-2.21	104.35	106.29
17	L	1116	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	C	1078	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	C	1082	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	A	369	CLA	OBD-CAD-CBD	-2.21	121.32	125.98
17	B	1116	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	B	1114	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	N	358	CLA	C2C-C1C-NC	-2.21	108.60	110.24
17	L	1116	CLA	OBD-CAD-CBD	-2.21	121.33	125.98
17	C	1083	CLA	OBD-CAD-CBD	-2.20	121.33	125.98
17	L	1115	CLA	OBD-CAD-CBD	-2.20	121.33	125.98
17	L	1114	CLA	C2C-C1C-NC	-2.20	108.60	110.24
17	L	1112	CLA	C2C-C1C-NC	-2.20	108.60	110.24
19	V	138	HEM	C3A-C2A-C1A	-2.20	104.36	106.29
17	M	1080	CLA	C2C-C1C-NC	-2.20	108.61	110.24
17	M	1087	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	C	1080	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	C	1085	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	L	1113	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	B	1110	CLA	C2C-C1C-NC	-2.20	108.61	110.24
21	D	359	BCR	C30-C25-C26	-2.20	119.43	122.66
17	M	1079	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	C	1089	CLA	OBD-CAD-CBD	-2.20	121.34	125.98
17	W	64	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	N	358	CLA	OBD-CAD-CBD	-2.19	121.35	125.98
17	M	1087	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	C	1079	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	B	1108	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	B	1109	CLA	OBD-CAD-CBD	-2.19	121.36	125.98
17	B	1121	CLA	OBD-CAD-CBD	-2.19	121.36	125.98
17	C	1085	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	L	1117	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	B	1112	CLA	C2C-C1C-NC	-2.19	108.61	110.24
17	A	368	CLA	C2C-C1C-NC	-2.19	108.62	110.24
17	C	1088	CLA	OBD-CAD-CBD	-2.18	121.37	125.98
17	J	367	CLA	OBD-CAD-CBD	-2.18	121.37	125.98
17	B	1118	CLA	OBD-CAD-CBD	-2.18	121.38	125.98
17	C	1079	CLA	OBD-CAD-CBD	-2.18	121.38	125.98
17	A	368	CLA	OBD-CAD-CBD	-2.18	121.38	125.98
17	M	1084	CLA	OBD-CAD-CBD	-2.18	121.38	125.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	1082	CLA	OBD-CAD-CBD	-2.18	121.38	125.98
17	L	1109	CLA	OBD-CAD-CBD	-2.18	121.39	125.98
17	J	367	CLA	C2C-C1C-NC	-2.18	108.62	110.24
17	B	1109	CLA	C2C-C1C-NC	-2.18	108.62	110.24
17	B	1115	CLA	OBD-CAD-CBD	-2.18	121.39	125.98
17	B	1122	CLA	OBD-CAD-CBD	-2.18	121.39	125.98
17	B	1111	CLA	OBD-CAD-CBD	-2.17	121.39	125.98
17	M	1078	CLA	OBD-CAD-CBD	-2.17	121.40	125.98
17	C	1087	CLA	OBD-CAD-CBD	-2.17	121.40	125.98
17	B	1122	CLA	C2C-C1C-NC	-2.17	108.63	110.24
17	B	1116	CLA	OBD-CAD-CBD	-2.17	121.41	125.98
17	L	1122	CLA	OBD-CAD-CBD	-2.16	121.41	125.98
17	L	1111	CLA	OBD-CAD-CBD	-2.16	121.42	125.98
21	D	359	BCR	C23-C22-C21	-2.16	115.50	118.98
17	B	1119	CLA	OBD-CAD-CBD	-2.16	121.42	125.98
17	M	1086	CLA	OBD-CAD-CBD	-2.16	121.42	125.98
17	B	1115	CLA	C2C-C1C-NC	-2.16	108.64	110.24
17	L	1118	CLA	OBD-CAD-CBD	-2.16	121.43	125.98
17	C	1078	CLA	OBD-CAD-CBD	-2.16	121.43	125.98
17	C	1087	CLA	C2C-C1C-NC	-2.16	108.64	110.24
17	J	368	CLA	C2C-C1C-NC	-2.15	108.64	110.24
17	L	1108	CLA	OBD-CAD-CBD	-2.15	121.45	125.98
17	B	1119	CLA	C2C-C1C-NC	-2.14	108.65	110.24
17	M	1084	CLA	C2C-C1C-NC	-2.14	108.65	110.24
18	N	357	PHO	OBD-CAD-CBD	-2.13	121.33	125.95
17	M	1081	CLA	OBD-CAD-CBD	-2.13	121.48	125.98
18	D	356	PHO	OBD-CAD-CBD	-2.13	121.34	125.95
18	A	367	PHO	OBD-CAD-CBD	-2.13	121.34	125.95
17	M	1079	CLA	C2C-C1C-NC	-2.12	108.66	110.24
17	B	1108	CLA	OBD-CAD-CBD	-2.12	121.50	125.98
17	A	369	CLA	C2C-C1C-NC	-2.12	108.67	110.24
17	L	1119	CLA	C2C-C1C-NC	-2.12	108.67	110.24
17	G	221	CLA	CAB-C3B-C2B	-2.11	120.81	125.14
21	D	359	BCR	C1-C6-C5	-2.10	119.57	122.66
17	R	221	CLA	CAB-C3B-C2B	-2.10	120.85	125.14
17	N	354	CLA	OBD-CAD-CBD	-2.02	121.72	125.98
17	D	354	CLA	OBD-CAD-CBD	-2.01	121.75	125.98
21	D	359	BCR	C30-C25-C24	2.05	121.56	115.82
21	D	359	BCR	C23-C24-C25	2.07	133.52	127.32
21	D	359	BCR	C11-C10-C9	2.16	130.32	127.20
17	R	221	CLA	CMB-C2B-C3B	2.20	129.64	125.14
17	A	366	CLA	C1D-CHD-C4C	2.21	125.94	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	355	CLA	C1D-CHD-C4C	2.21	125.95	122.60
17	G	221	CLA	CMB-C2B-C3B	2.22	129.67	125.14
21	K	47	BCR	C15-C14-C13	2.22	130.41	127.20
21	K	47	BCR	C11-C10-C9	2.25	130.44	127.20
21	D	359	BCR	C15-C14-C13	2.26	130.46	127.20
17	A	366	CLA	OBD-CAD-C3D	2.27	131.07	127.55
17	N	355	CLA	OBD-CAD-C3D	2.28	131.08	127.55
21	D	359	BCR	C24-C23-C22	2.29	129.71	126.22
21	D	359	BCR	C34-C9-C8	2.34	121.99	118.10
19	E	84	HEM	CHA-C4D-ND	2.34	126.86	124.52
17	D	355	CLA	C2A-C1A-CHA	2.36	128.22	123.89
19	P	92	HEM	CHA-C4D-ND	2.37	126.89	124.52
19	V	138	HEM	CHA-C4D-ND	2.37	126.89	124.52
17	W	64	CLA	C1D-CHD-C4C	2.41	126.25	122.60
19	0	138	HEM	CHA-C4D-ND	2.42	126.94	124.52
17	N	356	CLA	C2A-C1A-CHA	2.43	128.35	123.89
17	R	221	CLA	C1D-CHD-C4C	2.49	126.36	122.60
17	B	1121	CLA	C1D-CHD-C4C	2.49	126.37	122.60
17	G	221	CLA	C1D-CHD-C4C	2.50	126.39	122.60
17	M	1085	CLA	C1D-CHD-C4C	2.51	126.39	122.60
17	L	1110	CLA	C1D-CHD-C4C	2.52	126.41	122.60
17	D	354	CLA	C1D-CHD-C4C	2.52	126.42	122.60
19	P	92	HEM	C2B-C1B-CHB	2.52	126.60	124.06
17	N	354	CLA	OBD-CAD-C3D	2.52	131.47	127.55
17	B	1110	CLA	C1D-CHD-C4C	2.53	126.42	122.60
17	C	1088	CLA	C1D-CHD-C4C	2.53	126.43	122.60
17	C	1080	CLA	C1D-CHD-C4C	2.53	126.43	122.60
17	M	1087	CLA	C1D-CHD-C4C	2.54	126.44	122.60
17	M	1083	CLA	C1D-CHD-C4C	2.54	126.44	122.60
17	D	354	CLA	OBD-CAD-C3D	2.54	131.49	127.55
17	L	1121	CLA	C1D-CHD-C4C	2.54	126.44	122.60
17	C	1086	CLA	C1D-CHD-C4C	2.54	126.45	122.60
17	L	1114	CLA	C1D-CHD-C4C	2.54	126.45	122.60
17	N	354	CLA	C1D-CHD-C4C	2.55	126.45	122.60
17	B	1114	CLA	C1D-CHD-C4C	2.55	126.46	122.60
17	C	1084	CLA	C1D-CHD-C4C	2.55	126.46	122.60
17	C	1079	CLA	C1D-CHD-C4C	2.55	126.47	122.60
17	B	1117	CLA	C1D-CHD-C4C	2.56	126.47	122.60
17	D	355	CLA	C1D-CHD-C4C	2.57	126.48	122.60
17	C	1085	CLA	C1D-CHD-C4C	2.57	126.48	122.60
17	L	1107	CLA	C1D-CHD-C4C	2.57	126.49	122.60
17	A	365	CLA	C1D-CHD-C4C	2.57	126.49	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	1117	CLA	C1D-CHD-C4C	2.57	126.49	122.60
17	L	1112	CLA	C1D-CHD-C4C	2.57	126.49	122.60
17	M	1079	CLA	C1D-CHD-C4C	2.57	126.49	122.60
17	A	369	CLA	C1D-CHD-C4C	2.57	126.49	122.60
19	V	138	HEM	C2B-C1B-CHB	2.58	126.65	124.06
17	C	1087	CLA	C1D-CHD-C4C	2.58	126.50	122.60
17	M	1086	CLA	C1D-CHD-C4C	2.58	126.50	122.60
17	C	1081	CLA	C1D-CHD-C4C	2.58	126.50	122.60
17	M	1088	CLA	C1D-CHD-C4C	2.58	126.50	122.60
19	O	138	HEM	C2B-C1B-CHB	2.58	126.66	124.06
17	M	1082	CLA	C1D-CHD-C4C	2.58	126.51	122.60
17	B	1112	CLA	C1D-CHD-C4C	2.58	126.51	122.60
17	B	1122	CLA	C1D-CHD-C4C	2.58	126.51	122.60
17	B	1118	CLA	C1D-CHD-C4C	2.59	126.53	122.60
17	L	1113	CLA	C1D-CHD-C4C	2.59	126.53	122.60
17	B	1109	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	B	1111	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	B	1120	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	J	368	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	M	1081	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	C	1082	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	C	1083	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	L	1111	CLA	C1D-CHD-C4C	2.60	126.53	122.60
17	N	356	CLA	C1D-CHD-C4C	2.60	126.54	122.60
17	L	1120	CLA	C1D-CHD-C4C	2.60	126.54	122.60
17	L	1119	CLA	C1D-CHD-C4C	2.60	126.54	122.60
19	E	84	HEM	C2B-C1B-CHB	2.61	126.68	124.06
17	L	1109	CLA	C1D-CHD-C4C	2.61	126.54	122.60
17	C	1089	CLA	C1D-CHD-C4C	2.61	126.55	122.60
17	B	1113	CLA	C1D-CHD-C4C	2.61	126.55	122.60
17	C	1078	CLA	C1D-CHD-C4C	2.61	126.55	122.60
17	M	1084	CLA	C1D-CHD-C4C	2.61	126.56	122.60
17	B	1108	CLA	C1D-CHD-C4C	2.61	126.56	122.60
17	M	1080	CLA	C1D-CHD-C4C	2.61	126.56	122.60
17	B	1107	CLA	C1D-CHD-C4C	2.61	126.56	122.60
17	L	1122	CLA	C1D-CHD-C4C	2.62	126.57	122.60
17	B	1116	CLA	C1D-CHD-C4C	2.63	126.57	122.60
17	L	1118	CLA	C1D-CHD-C4C	2.63	126.57	122.60
17	D	355	CLA	OBD-CAD-C3D	2.63	131.62	127.55
17	J	365	CLA	C1D-CHD-C4C	2.63	126.58	122.60
17	N	358	CLA	C1D-CHD-C4C	2.65	126.60	122.60
17	A	368	CLA	C1D-CHD-C4C	2.65	126.61	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	1108	CLA	C1D-CHD-C4C	2.65	126.61	122.60
17	J	367	CLA	C1D-CHD-C4C	2.66	126.62	122.60
17	M	1078	CLA	C1D-CHD-C4C	2.66	126.62	122.60
17	D	357	CLA	C1D-CHD-C4C	2.66	126.63	122.60
17	L	1115	CLA	C1D-CHD-C4C	2.67	126.63	122.60
17	B	1119	CLA	C1D-CHD-C4C	2.67	126.64	122.60
17	N	356	CLA	OBD-CAD-C3D	2.67	131.69	127.55
17	L	1116	CLA	C1D-CHD-C4C	2.67	126.64	122.60
17	B	1115	CLA	C1D-CHD-C4C	2.68	126.66	122.60
17	B	1108	CLA	OBD-CAD-C3D	2.76	131.82	127.55
17	M	1081	CLA	OBD-CAD-C3D	2.76	131.83	127.55
17	L	1108	CLA	OBD-CAD-C3D	2.77	131.85	127.55
17	M	1086	CLA	OBD-CAD-C3D	2.78	131.87	127.55
17	C	1087	CLA	OBD-CAD-C3D	2.78	131.87	127.55
17	C	1078	CLA	OBD-CAD-C3D	2.79	131.88	127.55
17	M	1078	CLA	OBD-CAD-C3D	2.81	131.91	127.55
17	L	1122	CLA	OBD-CAD-C3D	2.81	131.91	127.55
17	L	1118	CLA	OBD-CAD-C3D	2.82	131.92	127.55
17	C	1083	CLA	OBD-CAD-C3D	2.82	131.92	127.55
17	A	368	CLA	OBD-CAD-C3D	2.82	131.93	127.55
17	M	1084	CLA	OBD-CAD-C3D	2.82	131.93	127.55
17	J	367	CLA	OBD-CAD-C3D	2.83	131.93	127.55
17	B	1116	CLA	OBD-CAD-C3D	2.83	131.94	127.55
17	C	1082	CLA	OBD-CAD-C3D	2.83	131.94	127.55
17	B	1119	CLA	OBD-CAD-C3D	2.83	131.94	127.55
17	B	1118	CLA	OBD-CAD-C3D	2.84	131.96	127.55
17	B	1122	CLA	OBD-CAD-C3D	2.85	131.97	127.55
17	B	1109	CLA	OBD-CAD-C3D	2.85	131.97	127.55
17	C	1085	CLA	OBD-CAD-C3D	2.85	131.97	127.55
17	B	1115	CLA	OBD-CAD-C3D	2.86	131.98	127.55
17	C	1088	CLA	OBD-CAD-C3D	2.86	131.99	127.55
17	B	1111	CLA	OBD-CAD-C3D	2.86	131.99	127.55
19	O	138	HEM	C3B-C2B-C1B	2.86	106.77	103.90
19	V	138	HEM	C3B-C2B-C1B	2.87	106.78	103.90
17	L	1109	CLA	OBD-CAD-C3D	2.87	132.00	127.55
17	M	1087	CLA	OBD-CAD-C3D	2.87	132.01	127.55
19	E	84	HEM	C3B-C2B-C1B	2.87	106.78	103.90
17	L	1116	CLA	OBD-CAD-C3D	2.88	132.01	127.55
17	C	1079	CLA	OBD-CAD-C3D	2.88	132.01	127.55
17	M	1082	CLA	OBD-CAD-C3D	2.88	132.02	127.55
19	P	92	HEM	C3B-C2B-C1B	2.88	106.79	103.90
17	L	1111	CLA	OBD-CAD-C3D	2.88	132.02	127.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	1107	CLA	OBD-CAD-C3D	2.89	132.03	127.55
17	M	1080	CLA	OBD-CAD-C3D	2.89	132.03	127.55
17	L	1107	CLA	OBD-CAD-C3D	2.89	132.04	127.55
17	M	1079	CLA	OBD-CAD-C3D	2.89	132.04	127.55
17	L	1119	CLA	OBD-CAD-C3D	2.89	132.04	127.55
17	C	1081	CLA	OBD-CAD-C3D	2.90	132.04	127.55
17	L	1113	CLA	OBD-CAD-C3D	2.90	132.04	127.55
17	D	357	CLA	OBD-CAD-C3D	2.90	132.05	127.55
17	C	1089	CLA	OBD-CAD-C3D	2.91	132.06	127.55
17	N	358	CLA	OBD-CAD-C3D	2.91	132.07	127.55
17	L	1115	CLA	OBD-CAD-C3D	2.92	132.07	127.55
19	E	84	HEM	C3D-C4D-ND	2.92	116.12	110.17
19	V	138	HEM	C3D-C4D-ND	2.92	116.12	110.17
17	C	1080	CLA	OBD-CAD-C3D	2.92	132.09	127.55
17	B	1112	CLA	OBD-CAD-C3D	2.93	132.10	127.55
17	A	369	CLA	OBD-CAD-C3D	2.93	132.10	127.55
21	D	359	BCR	C29-C30-C25	2.93	115.01	110.36
17	B	1117	CLA	OBD-CAD-C3D	2.94	132.11	127.55
17	B	1120	CLA	OBD-CAD-C3D	2.94	132.11	127.55
19	0	138	HEM	C3D-C4D-ND	2.94	116.17	110.17
17	B	1121	CLA	OBD-CAD-C3D	2.95	132.12	127.55
19	P	92	HEM	C3D-C4D-ND	2.95	116.18	110.17
17	J	368	CLA	OBD-CAD-C3D	2.95	132.12	127.55
17	B	1114	CLA	OBD-CAD-C3D	2.95	132.13	127.55
17	L	1117	CLA	OBD-CAD-C3D	2.95	132.13	127.55
17	M	1083	CLA	OBD-CAD-C3D	2.95	132.13	127.55
17	B	1113	CLA	OBD-CAD-C3D	2.96	132.14	127.55
17	W	64	CLA	OBD-CAD-C3D	2.96	132.14	127.55
17	B	1110	CLA	OBD-CAD-C3D	2.96	132.15	127.55
17	L	1120	CLA	OBD-CAD-C3D	2.96	132.15	127.55
17	L	1112	CLA	OBD-CAD-C3D	2.97	132.15	127.55
17	M	1085	CLA	OBD-CAD-C3D	2.97	132.15	127.55
17	C	1084	CLA	OBD-CAD-C3D	2.97	132.16	127.55
17	L	1110	CLA	OBD-CAD-C3D	2.98	132.18	127.55
17	R	221	CLA	CAB-C3B-C4B	2.98	133.30	128.36
21	D	359	BCR	C7-C8-C9	2.99	130.77	126.22
17	G	221	CLA	CAB-C3B-C4B	3.00	133.32	128.36
17	L	1121	CLA	OBD-CAD-C3D	3.00	132.20	127.55
17	M	1088	CLA	OBD-CAD-C3D	3.02	132.24	127.55
17	L	1114	CLA	OBD-CAD-C3D	3.02	132.24	127.55
17	C	1086	CLA	OBD-CAD-C3D	3.03	132.25	127.55
19	0	138	HEM	C3B-C4B-CHC	3.16	128.17	122.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	138	HEM	C3B-C4B-CHC	3.16	128.18	122.58
19	P	92	HEM	C3B-C4B-CHC	3.17	128.19	122.58
19	E	84	HEM	C3B-C4B-CHC	3.18	128.21	122.58
21	D	359	BCR	C2-C1-C6	3.21	115.45	110.36
18	A	367	PHO	C4A-NA-C1A	3.22	111.09	108.21
18	J	366	PHO	C4A-NA-C1A	3.26	111.12	108.21
17	J	365	CLA	C4A-NA-C1A	3.33	110.67	106.36
17	A	365	CLA	C4A-NA-C1A	3.36	110.70	106.36
17	A	366	CLA	C4A-NA-C1A	3.41	110.76	106.36
18	D	356	PHO	C4A-NA-C1A	3.43	111.27	108.21
17	N	355	CLA	C4A-NA-C1A	3.50	110.88	106.36
17	D	355	CLA	C4A-NA-C1A	3.54	110.93	106.36
18	N	357	PHO	C4A-NA-C1A	3.54	111.37	108.21
17	N	356	CLA	C4A-NA-C1A	3.58	110.98	106.36
17	G	221	CLA	C4A-NA-C1A	3.58	110.98	106.36
17	R	221	CLA	C4A-NA-C1A	3.65	111.07	106.36
17	L	1120	CLA	C4A-NA-C1A	3.65	111.08	106.36
17	B	1120	CLA	C4A-NA-C1A	3.67	111.10	106.36
17	B	1107	CLA	C4A-NA-C1A	3.70	111.14	106.36
17	L	1116	CLA	C4A-NA-C1A	3.70	111.14	106.36
17	L	1117	CLA	C4A-NA-C1A	3.70	111.14	106.36
17	L	1108	CLA	C4A-NA-C1A	3.71	111.15	106.36
17	B	1117	CLA	C4A-NA-C1A	3.71	111.16	106.36
17	W	64	CLA	C4A-NA-C1A	3.72	111.16	106.36
17	L	1109	CLA	C4A-NA-C1A	3.72	111.17	106.36
17	J	365	CLA	CAB-C3B-C4B	3.72	134.52	128.36
17	A	368	CLA	C4A-NA-C1A	3.72	111.17	106.36
17	B	1108	CLA	C4A-NA-C1A	3.72	111.17	106.36
17	C	1084	CLA	C4A-NA-C1A	3.72	111.17	106.36
17	L	1111	CLA	C4A-NA-C1A	3.73	111.18	106.36
17	J	367	CLA	C4A-NA-C1A	3.73	111.18	106.36
17	L	1107	CLA	C4A-NA-C1A	3.73	111.18	106.36
17	C	1088	CLA	C4A-NA-C1A	3.73	111.19	106.36
17	C	1085	CLA	C4A-NA-C1A	3.74	111.20	106.36
17	A	365	CLA	CAB-C3B-C4B	3.74	134.56	128.36
17	B	1109	CLA	C4A-NA-C1A	3.75	111.20	106.36
17	B	1121	CLA	C4A-NA-C1A	3.75	111.21	106.36
17	L	1113	CLA	C4A-NA-C1A	3.75	111.21	106.36
17	M	1087	CLA	C4A-NA-C1A	3.75	111.21	106.36
17	B	1112	CLA	C4A-NA-C1A	3.76	111.22	106.36
17	C	1080	CLA	C4A-NA-C1A	3.76	111.22	106.36
17	M	1083	CLA	C4A-NA-C1A	3.76	111.22	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	1122	CLA	C4A-NA-C1A	3.77	111.23	106.36
17	C	1086	CLA	C4A-NA-C1A	3.77	111.23	106.36
17	B	1116	CLA	C4A-NA-C1A	3.77	111.24	106.36
17	M	1078	CLA	C4A-NA-C1A	3.77	111.24	106.36
17	C	1083	CLA	C4A-NA-C1A	3.78	111.24	106.36
17	B	1111	CLA	C4A-NA-C1A	3.78	111.25	106.36
17	L	1121	CLA	C4A-NA-C1A	3.78	111.25	106.36
17	B	1113	CLA	C4A-NA-C1A	3.78	111.25	106.36
17	M	1082	CLA	C4A-NA-C1A	3.78	111.25	106.36
17	L	1115	CLA	C4A-NA-C1A	3.78	111.25	106.36
17	L	1112	CLA	C4A-NA-C1A	3.79	111.25	106.36
17	M	1086	CLA	C4A-NA-C1A	3.79	111.26	106.36
17	B	1119	CLA	C4A-NA-C1A	3.79	111.27	106.36
17	B	1118	CLA	C4A-NA-C1A	3.79	111.27	106.36
17	C	1081	CLA	C4A-NA-C1A	3.80	111.27	106.36
17	B	1114	CLA	C4A-NA-C1A	3.80	111.27	106.36
17	M	1088	CLA	C4A-NA-C1A	3.80	111.27	106.36
17	C	1079	CLA	C4A-NA-C1A	3.80	111.27	106.36
17	M	1084	CLA	C4A-NA-C1A	3.80	111.28	106.36
17	C	1078	CLA	C4A-NA-C1A	3.80	111.28	106.36
17	L	1122	CLA	C4A-NA-C1A	3.80	111.28	106.36
17	C	1082	CLA	C4A-NA-C1A	3.81	111.28	106.36
17	M	1085	CLA	C4A-NA-C1A	3.81	111.28	106.36
17	J	368	CLA	C4A-NA-C1A	3.81	111.28	106.36
17	L	1110	CLA	C4A-NA-C1A	3.81	111.29	106.36
17	L	1118	CLA	C4A-NA-C1A	3.81	111.29	106.36
17	M	1079	CLA	C4A-NA-C1A	3.81	111.29	106.36
17	A	369	CLA	C4A-NA-C1A	3.82	111.29	106.36
17	M	1080	CLA	C4A-NA-C1A	3.82	111.30	106.36
17	B	1110	CLA	C4A-NA-C1A	3.82	111.30	106.36
17	L	1114	CLA	C4A-NA-C1A	3.82	111.30	106.36
17	C	1087	CLA	C4A-NA-C1A	3.82	111.31	106.36
17	B	1115	CLA	C4A-NA-C1A	3.83	111.31	106.36
17	M	1081	CLA	C4A-NA-C1A	3.83	111.31	106.36
17	L	1119	CLA	C4A-NA-C1A	3.83	111.31	106.36
17	N	358	CLA	C4A-NA-C1A	3.85	111.34	106.36
17	D	357	CLA	C4A-NA-C1A	3.87	111.37	106.36
17	C	1089	CLA	C4A-NA-C1A	3.89	111.39	106.36
17	D	354	CLA	C4A-NA-C1A	3.93	111.44	106.36
17	N	354	CLA	C4A-NA-C1A	3.93	111.44	106.36
17	N	354	CLA	CAB-C3B-C4B	3.98	134.95	128.36
17	D	354	CLA	CAB-C3B-C4B	3.99	134.97	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	356	CLA	CAB-C3B-C4B	4.25	135.40	128.36
17	D	355	CLA	CAB-C3B-C4B	4.30	135.48	128.36
21	D	359	BCR	C33-C5-C6	4.38	128.90	124.61
21	D	359	BCR	C38-C26-C25	4.46	128.98	124.61
17	A	365	CLA	OBD-CAD-C3D	4.61	134.71	127.55
17	J	365	CLA	OBD-CAD-C3D	4.65	134.77	127.55
17	M	1088	CLA	CAB-C3B-C4B	4.66	136.07	128.36
17	L	1111	CLA	CAB-C3B-C4B	4.69	136.13	128.36
17	C	1088	CLA	CAB-C3B-C4B	4.70	136.14	128.36
17	L	1120	CLA	CAB-C3B-C4B	4.70	136.14	128.36
17	M	1083	CLA	CAB-C3B-C4B	4.70	136.15	128.36
17	D	357	CLA	CAB-C3B-C4B	4.71	136.16	128.36
17	L	1109	CLA	CAB-C3B-C4B	4.71	136.16	128.36
17	B	1110	CLA	CAB-C3B-C4B	4.71	136.16	128.36
17	B	1114	CLA	CAB-C3B-C4B	4.71	136.16	128.36
17	B	1112	CLA	CAB-C3B-C4B	4.72	136.17	128.36
17	L	1121	CLA	CAB-C3B-C4B	4.72	136.17	128.36
17	B	1111	CLA	CAB-C3B-C4B	4.72	136.18	128.36
17	M	1081	CLA	CAB-C3B-C4B	4.72	136.18	128.36
17	W	64	CLA	CAB-C3B-C4B	4.73	136.18	128.36
17	C	1081	CLA	CAB-C3B-C4B	4.73	136.18	128.36
17	M	1087	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	L	1117	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	M	1085	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	B	1120	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	B	1117	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	M	1080	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	L	1107	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	B	1107	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	C	1082	CLA	CAB-C3B-C4B	4.73	136.19	128.36
17	B	1119	CLA	CAB-C3B-C4B	4.73	136.20	128.36
17	C	1085	CLA	CAB-C3B-C4B	4.73	136.20	128.36
17	L	1122	CLA	CAB-C3B-C4B	4.73	136.20	128.36
17	C	1089	CLA	CAB-C3B-C4B	4.74	136.20	128.36
17	L	1119	CLA	CAB-C3B-C4B	4.74	136.20	128.36
17	C	1080	CLA	CAB-C3B-C4B	4.74	136.20	128.36
17	B	1121	CLA	CAB-C3B-C4B	4.74	136.20	128.36
17	C	1078	CLA	CAB-C3B-C4B	4.74	136.21	128.36
17	L	1112	CLA	CAB-C3B-C4B	4.74	136.21	128.36
17	B	1109	CLA	CAB-C3B-C4B	4.75	136.22	128.36
17	L	1114	CLA	CAB-C3B-C4B	4.75	136.22	128.36
17	L	1118	CLA	CAB-C3B-C4B	4.75	136.22	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	368	CLA	CAB-C3B-C4B	4.75	136.22	128.36
17	C	1087	CLA	CAB-C3B-C4B	4.75	136.23	128.36
17	L	1110	CLA	CAB-C3B-C4B	4.75	136.23	128.36
17	B	1116	CLA	CAB-C3B-C4B	4.76	136.24	128.36
17	L	1108	CLA	CAB-C3B-C4B	4.76	136.24	128.36
17	B	1122	CLA	CAB-C3B-C4B	4.76	136.24	128.36
17	C	1083	CLA	CAB-C3B-C4B	4.76	136.24	128.36
17	M	1084	CLA	CAB-C3B-C4B	4.76	136.25	128.36
17	C	1086	CLA	CAB-C3B-C4B	4.76	136.25	128.36
17	B	1118	CLA	CAB-C3B-C4B	4.77	136.25	128.36
17	B	1113	CLA	CAB-C3B-C4B	4.77	136.25	128.36
17	L	1116	CLA	CAB-C3B-C4B	4.77	136.25	128.36
17	C	1084	CLA	CAB-C3B-C4B	4.77	136.26	128.36
17	M	1078	CLA	CAB-C3B-C4B	4.77	136.26	128.36
17	L	1113	CLA	CAB-C3B-C4B	4.77	136.26	128.36
17	M	1086	CLA	CAB-C3B-C4B	4.78	136.27	128.36
17	M	1082	CLA	CAB-C3B-C4B	4.78	136.27	128.36
17	A	369	CLA	CAB-C3B-C4B	4.78	136.27	128.36
17	J	367	CLA	CAB-C3B-C4B	4.78	136.27	128.36
17	B	1108	CLA	CAB-C3B-C4B	4.79	136.28	128.36
17	N	358	CLA	CAB-C3B-C4B	4.79	136.29	128.36
17	J	368	CLA	CAB-C3B-C4B	4.80	136.31	128.36
17	C	1079	CLA	CAB-C3B-C4B	4.80	136.31	128.36
17	L	1115	CLA	CAB-C3B-C4B	4.81	136.33	128.36
17	A	366	CLA	CAB-C3B-C4B	4.83	136.35	128.36
17	B	1115	CLA	CAB-C3B-C4B	4.83	136.35	128.36
17	N	355	CLA	CAB-C3B-C4B	4.85	136.39	128.36
17	M	1079	CLA	CAB-C3B-C4B	4.88	136.43	128.36
17	A	365	CLA	CAD-CBD-CHA	6.14	112.34	105.18
18	A	367	PHO	CAB-C3B-C4B	6.84	136.19	125.06
18	D	356	PHO	CAB-C3B-C4B	6.89	136.27	125.06
18	N	357	PHO	CAB-C3B-C4B	6.92	136.33	125.06
18	J	366	PHO	CAB-C3B-C4B	6.95	136.38	125.06
19	O	138	HEM	C3D-C2D-C1D	7.38	111.30	103.90
19	V	138	HEM	C3D-C2D-C1D	7.39	111.30	103.90
19	E	84	HEM	C3D-C2D-C1D	7.41	111.32	103.90
19	P	92	HEM	C3D-C2D-C1D	7.47	111.38	103.90

All (207) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	L	1111	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	L	1111	CLA	ND
17	L	1111	CLA	NA
17	J	367	CLA	NC
17	J	367	CLA	ND
17	J	367	CLA	NA
17	M	1084	CLA	NC
17	M	1084	CLA	ND
17	M	1084	CLA	NA
17	N	355	CLA	ND
17	N	355	CLA	NA
17	B	1110	CLA	NC
17	B	1110	CLA	ND
17	B	1110	CLA	NA
17	B	1120	CLA	NC
17	B	1120	CLA	ND
17	B	1120	CLA	NA
17	N	358	CLA	NC
17	N	358	CLA	ND
17	N	358	CLA	NA
17	M	1078	CLA	NC
17	M	1078	CLA	ND
17	M	1078	CLA	NA
17	C	1080	CLA	NC
17	C	1080	CLA	ND
17	C	1080	CLA	NA
17	B	1109	CLA	NC
17	B	1109	CLA	ND
17	B	1109	CLA	NA
17	C	1087	CLA	NC
17	C	1087	CLA	ND
17	C	1087	CLA	NA
17	L	1109	CLA	NC
17	L	1109	CLA	ND
17	L	1109	CLA	NA
17	B	1115	CLA	NC
17	B	1115	CLA	ND
17	B	1115	CLA	NA
17	N	354	CLA	ND
17	L	1115	CLA	NC
17	L	1115	CLA	ND
17	L	1115	CLA	NA
17	L	1121	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	L	1121	CLA	ND
17	L	1121	CLA	NA
17	A	366	CLA	ND
17	A	366	CLA	NA
17	R	221	CLA	ND
17	R	221	CLA	NA
17	M	1086	CLA	NC
17	M	1086	CLA	ND
17	M	1086	CLA	NA
17	M	1080	CLA	NC
17	M	1080	CLA	ND
17	M	1080	CLA	NA
17	C	1088	CLA	NC
17	C	1088	CLA	ND
17	C	1088	CLA	NA
17	L	1107	CLA	NC
17	L	1107	CLA	ND
17	L	1107	CLA	NA
17	B	1122	CLA	NC
17	B	1122	CLA	ND
17	B	1122	CLA	NA
17	M	1085	CLA	NC
17	M	1085	CLA	ND
17	M	1085	CLA	NA
17	B	1118	CLA	NC
17	B	1118	CLA	ND
17	B	1118	CLA	NA
17	C	1079	CLA	NC
17	C	1079	CLA	ND
17	C	1079	CLA	NA
17	M	1079	CLA	NC
17	M	1079	CLA	ND
17	M	1079	CLA	NA
17	D	355	CLA	ND
17	D	355	CLA	NA
17	J	368	CLA	NC
17	J	368	CLA	ND
17	J	368	CLA	NA
17	M	1083	CLA	NC
17	M	1083	CLA	ND
17	M	1083	CLA	NA
17	C	1085	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	C	1085	CLA	ND
17	C	1085	CLA	NA
17	B	1117	CLA	NC
17	B	1117	CLA	ND
17	B	1117	CLA	NA
17	L	1110	CLA	NC
17	L	1110	CLA	ND
17	L	1110	CLA	NA
17	B	1112	CLA	NC
17	B	1112	CLA	ND
17	B	1112	CLA	NA
17	B	1107	CLA	NC
17	B	1107	CLA	ND
17	B	1107	CLA	NA
17	M	1087	CLA	NC
17	M	1087	CLA	ND
17	M	1087	CLA	NA
17	B	1113	CLA	NC
17	B	1113	CLA	ND
17	B	1113	CLA	NA
17	C	1081	CLA	NC
17	C	1081	CLA	ND
17	C	1081	CLA	NA
17	L	1116	CLA	NC
17	L	1116	CLA	ND
17	L	1116	CLA	NA
17	A	369	CLA	NC
17	A	369	CLA	ND
17	A	369	CLA	NA
17	B	1111	CLA	NC
17	B	1111	CLA	ND
17	B	1111	CLA	NA
17	D	357	CLA	NC
17	D	357	CLA	ND
17	D	357	CLA	NA
17	M	1088	CLA	NC
17	M	1088	CLA	ND
17	M	1088	CLA	NA
17	C	1086	CLA	NC
17	C	1086	CLA	ND
17	C	1086	CLA	NA
17	C	1089	CLA	CBD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	C	1089	CLA	NC
17	C	1089	CLA	ND
17	C	1089	CLA	NA
17	C	1083	CLA	NC
17	C	1083	CLA	ND
17	C	1083	CLA	NA
17	J	365	CLA	NC
17	J	365	CLA	ND
17	J	365	CLA	NA
17	N	356	CLA	ND
17	N	356	CLA	NA
17	L	1119	CLA	NC
17	L	1119	CLA	ND
17	L	1119	CLA	NA
17	W	64	CLA	NC
17	W	64	CLA	ND
17	W	64	CLA	NA
17	L	1108	CLA	NC
17	L	1108	CLA	ND
17	L	1108	CLA	NA
17	C	1078	CLA	NC
17	C	1078	CLA	ND
17	C	1078	CLA	NA
17	B	1119	CLA	NC
17	B	1119	CLA	ND
17	B	1119	CLA	NA
17	L	1113	CLA	NC
17	L	1113	CLA	ND
17	L	1113	CLA	NA
17	B	1116	CLA	NC
17	B	1116	CLA	ND
17	B	1116	CLA	NA
17	L	1114	CLA	NC
17	L	1114	CLA	ND
17	L	1114	CLA	NA
17	M	1081	CLA	NC
17	M	1081	CLA	ND
17	M	1081	CLA	NA
17	L	1122	CLA	NC
17	L	1122	CLA	ND
17	L	1122	CLA	NA
17	B	1108	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	B	1108	CLA	ND
17	B	1108	CLA	NA
17	A	368	CLA	NC
17	A	368	CLA	ND
17	A	368	CLA	NA
17	C	1084	CLA	NC
17	C	1084	CLA	ND
17	C	1084	CLA	NA
17	D	354	CLA	ND
17	C	1082	CLA	NC
17	C	1082	CLA	ND
17	C	1082	CLA	NA
17	A	365	CLA	NC
17	A	365	CLA	ND
17	A	365	CLA	NA
17	G	221	CLA	ND
17	G	221	CLA	NA
17	B	1121	CLA	NC
17	B	1121	CLA	ND
17	B	1121	CLA	NA
17	B	1114	CLA	NC
17	B	1114	CLA	ND
17	B	1114	CLA	NA
17	L	1117	CLA	NC
17	L	1117	CLA	ND
17	L	1117	CLA	NA
17	L	1118	CLA	NC
17	L	1118	CLA	ND
17	L	1118	CLA	NA
17	M	1082	CLA	NC
17	M	1082	CLA	ND
17	M	1082	CLA	NA
17	L	1112	CLA	NC
17	L	1112	CLA	ND
17	L	1112	CLA	NA
17	L	1120	CLA	NC
17	L	1120	CLA	ND
17	L	1120	CLA	NA

There are no torsion outliers.

There are no ring outliers.

70 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	0	138	HEM	8	0
17	A	365	CLA	5	0
17	A	366	CLA	5	0
18	A	367	PHO	20	0
17	A	368	CLA	24	0
17	A	369	CLA	2	0
17	B	1107	CLA	11	0
17	B	1108	CLA	8	0
17	B	1109	CLA	13	0
17	B	1110	CLA	10	0
17	B	1111	CLA	19	0
17	B	1112	CLA	3	0
17	B	1113	CLA	3	0
17	B	1114	CLA	14	0
17	B	1116	CLA	7	0
17	B	1117	CLA	12	0
17	B	1118	CLA	6	0
17	B	1119	CLA	14	0
17	B	1120	CLA	5	0
17	B	1121	CLA	3	0
17	C	1078	CLA	11	0
17	C	1079	CLA	15	0
17	C	1080	CLA	11	0
17	C	1081	CLA	5	0
17	C	1082	CLA	11	0
17	C	1083	CLA	6	0
17	C	1085	CLA	3	0
17	C	1086	CLA	9	0
17	C	1087	CLA	3	0
17	C	1088	CLA	14	0
17	C	1089	CLA	24	0
17	D	354	CLA	7	0
18	D	356	PHO	8	0
17	D	357	CLA	5	0
21	D	359	BCR	9	0
17	J	365	CLA	2	0
18	J	366	PHO	19	0
17	J	367	CLA	21	0
21	K	47	BCR	1	0
17	L	1107	CLA	9	0
17	L	1108	CLA	13	0
17	L	1109	CLA	13	0
17	L	1110	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	1111	CLA	16	0
17	L	1112	CLA	3	0
17	L	1113	CLA	4	0
17	L	1114	CLA	12	0
17	L	1115	CLA	2	0
17	L	1117	CLA	12	0
17	L	1118	CLA	6	0
17	L	1119	CLA	23	0
17	L	1120	CLA	22	0
17	L	1121	CLA	3	0
17	M	1078	CLA	3	0
17	M	1079	CLA	16	0
17	M	1080	CLA	1	0
17	M	1081	CLA	14	0
17	M	1082	CLA	6	0
17	M	1084	CLA	3	0
17	M	1085	CLA	4	0
17	M	1086	CLA	3	0
17	M	1087	CLA	11	0
17	M	1088	CLA	15	0
17	N	354	CLA	4	0
17	N	355	CLA	4	0
17	N	356	CLA	1	0
18	N	357	PHO	28	0
17	N	358	CLA	1	0
19	V	138	HEM	8	0
17	W	64	CLA	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.