



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:41 am GMT

PDB ID : 3KZI
Title : Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors : Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on : 2009-12-08
Resolution : 3.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

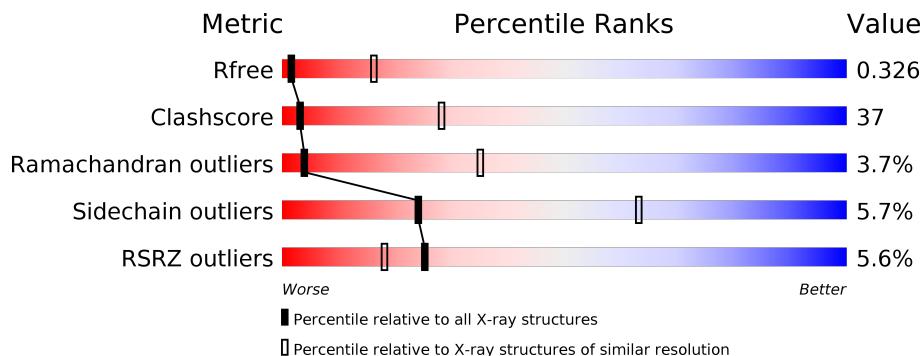
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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




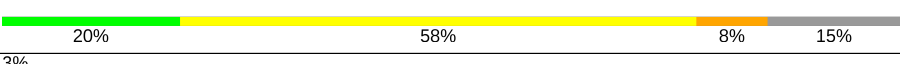
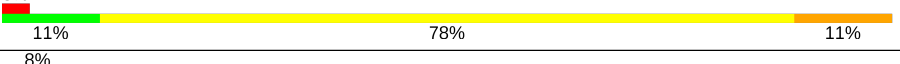
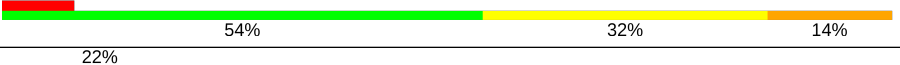

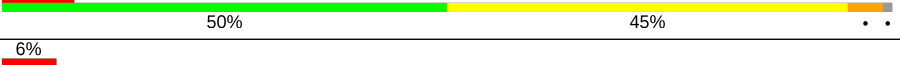


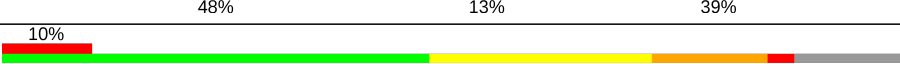
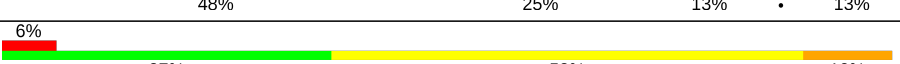
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>6%</div> <div> <div>47%</div> <div>46%</div> <div>5%</div> </div> </div>
2	B	510	<div> <div>3%</div> <div> <div>53%</div> <div>38%</div> <div>5%</div> </div> </div>
3	C	461	<div> <div>4%</div> <div> <div>41%</div> <div>50%</div> <div>6%</div> </div> </div>
4	D	352	<div> <div>7%</div> <div> <div>51%</div> <div>39%</div> <div>7%</div> </div> </div>
5	E	83	<div> <div>2%</div> <div> <div>28%</div> <div>57%</div> <div>7%</div> </div> </div>
6	F	44	<div> <div>14%</div> <div> <div>25%</div> <div>50%</div> <div>11%</div> <div>14%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	H	65	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	36	
13	O	246	
14	T	32	
15	U	104	
16	V	137	
17	y	46	
18	X	40	
19	Z	62	

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
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	X
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	X
21	CLA	B	511	X	-	-	X
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	X
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	X
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	X
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	X
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
25	BCR	A	369	-	-	-	X
25	BCR	B	527	-	-	-	X
25	BCR	B	529	-	-	-	X
25	BCR	B	530	-	-	-	X
25	BCR	C	490	-	-	-	X
25	BCR	J	115	-	-	-	X
25	BCR	X	107	-	-	-	X
25	BCR	Z	116	-	-	-	X
26	DGD	B	528	-	-	X	-
26	DGD	C	474	-	-	-	X
26	DGD	C	492	X	-	-	-
26	DGD	C	493	X	-	X	-
26	DGD	D	362	-	-	-	X
28	SQD	C	475	-	-	-	X
28	SQD	F	224	-	-	-	X
28	SQD	L	213	-	-	-	X
29	LMG	A	373	-	-	X	X
29	LMG	C	494	-	-	-	X
29	LMG	D	360	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LMG	J	492	-	-	-	X
29	LMG	M	217	-	-	-	X
30	LMT	A	376	-	-	-	X
30	LMT	D	363	-	-	-	X
30	LMT	I	274	-	-	-	X
32	PL9	D	357	-	-	X	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 24678 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	0	0
			3812	2505	635	659	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3455	2262	580	600	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			635	417	103	115			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	38	Total	C	N	O	S	0	0	0
			307	207	50	49	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			774	491	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	35	Total	C	N	O		0	0	0
			254	172	38	44				

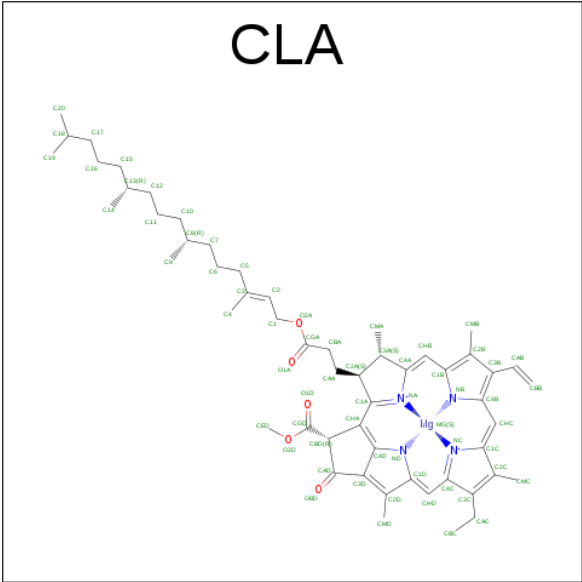
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



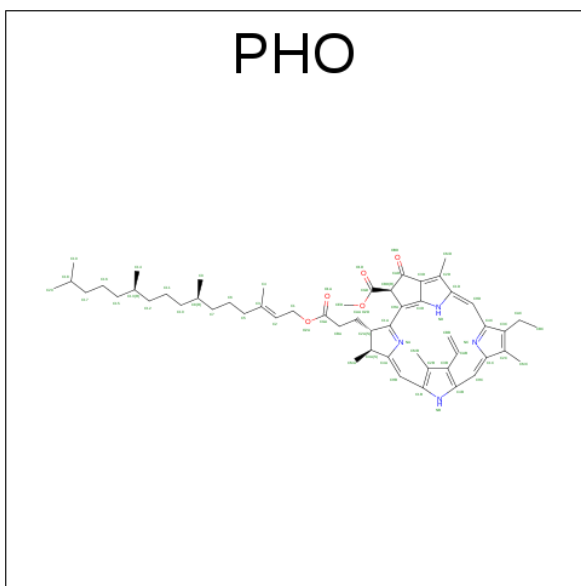
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

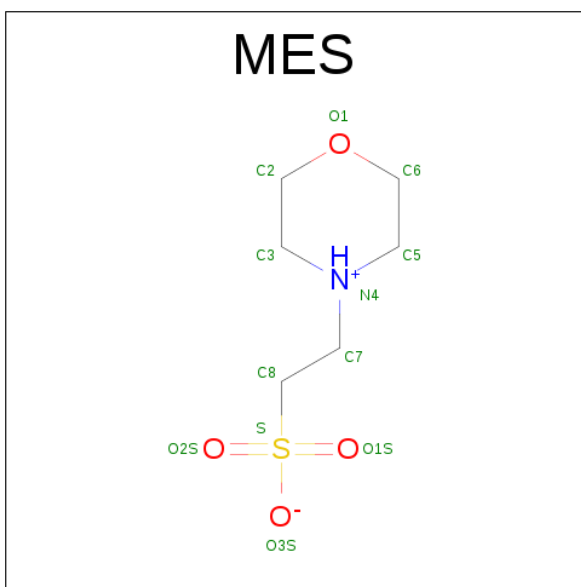
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



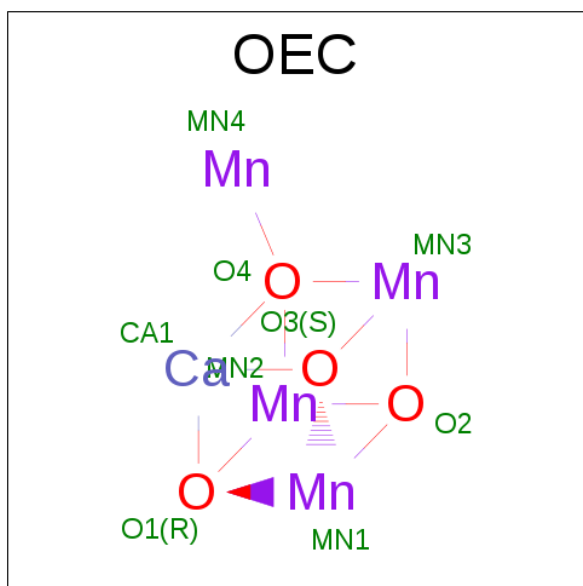
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



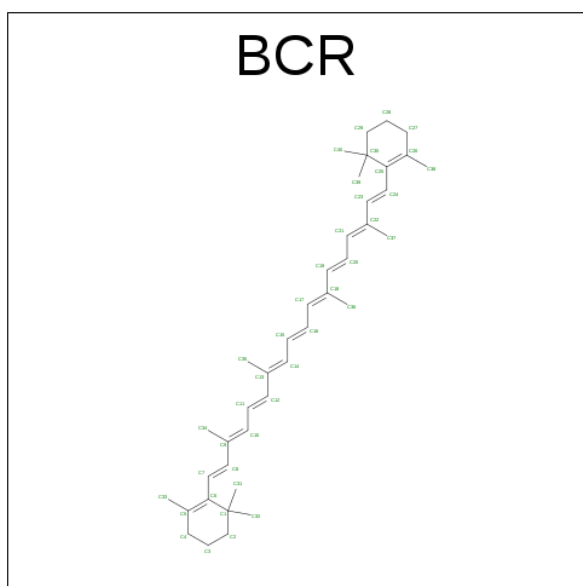
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 24 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



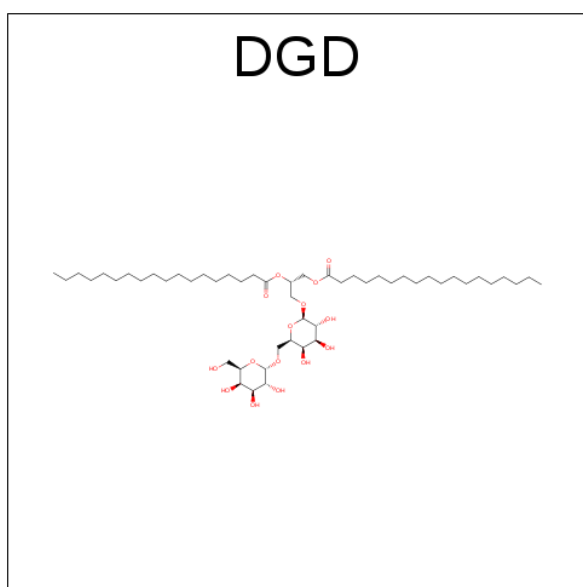
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



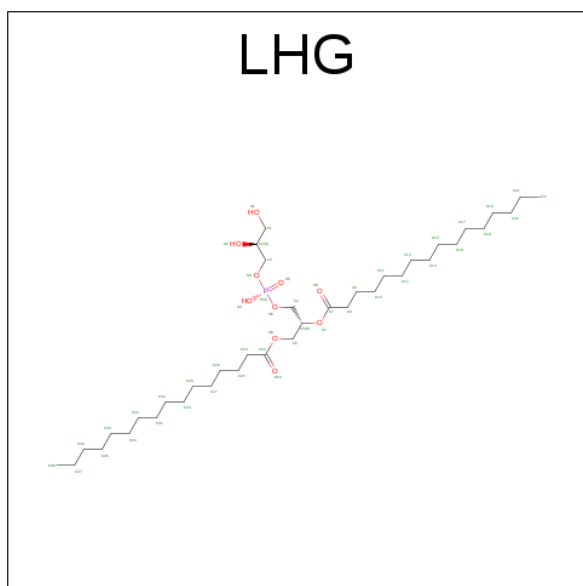
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	X	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	Z	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



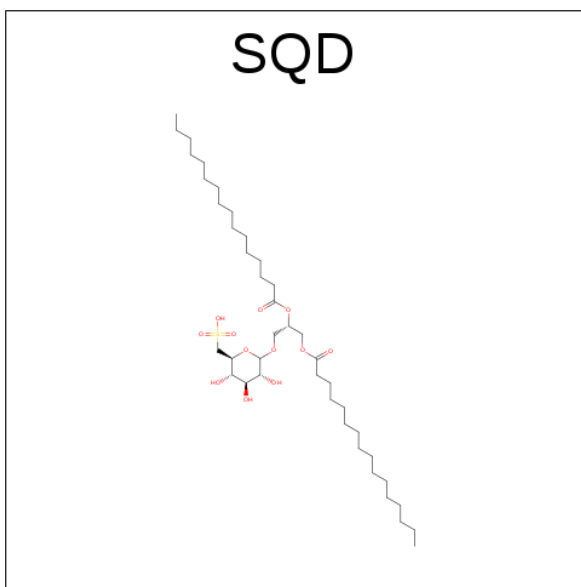
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			56	41	15		
26	A	1	Total	C	O	0	0
			52	37	15		
26	B	1	Total	C	O	0	0
			66	51	15		
26	C	1	Total	C	O	0	0
			53	38	15		
26	C	1	Total	C	O	0	0
			62	47	15		
26	C	1	Total	C	O	0	0
			66	51	15		
26	D	1	Total	C	O	0	0
			63	48	15		
26	B	1	Total	C	O	0	0
			58	43	15		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



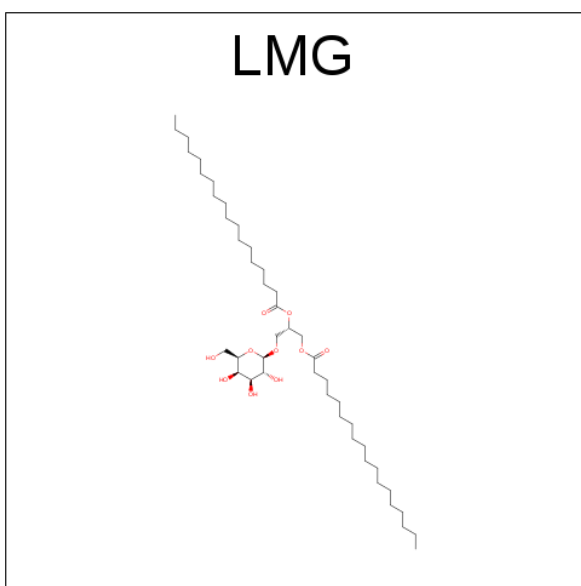
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



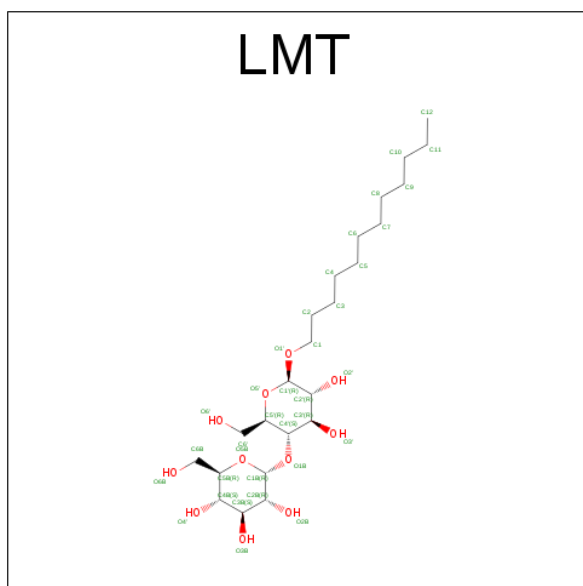
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total	C	O	S	0	0
			51	38	12	1		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	F	1	Total	C	O	S	0	0
			45	32	12	1		
28	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			49	39	10		
29	J	1	Total	C	O	0	0
			48	38	10		
29	C	1	Total	C	O	0	0
			45	35	10		
29	D	1	Total	C	O	0	0
			46	36	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	I	1	Total	C	O	0	0
			43	33	10		
29	M	1	Total	C	O	0	0
			42	32	10		

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



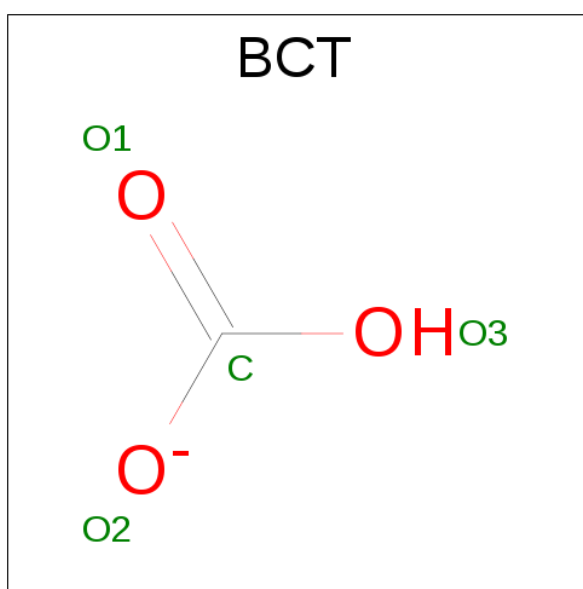
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	D	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

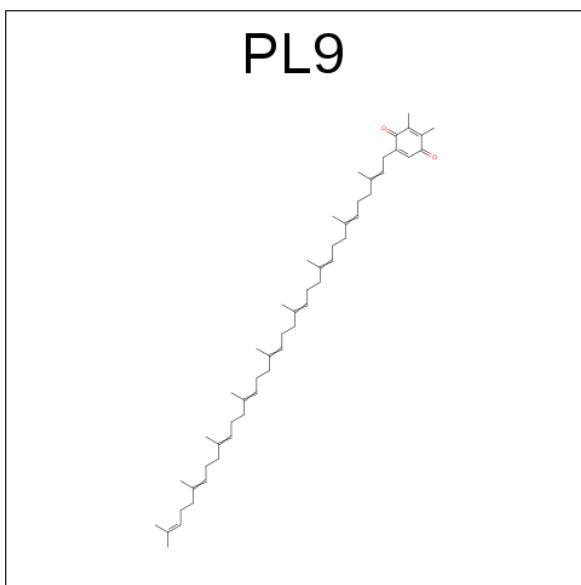
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total	C	O	0	0
			31	20	11		
30	T	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	O	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



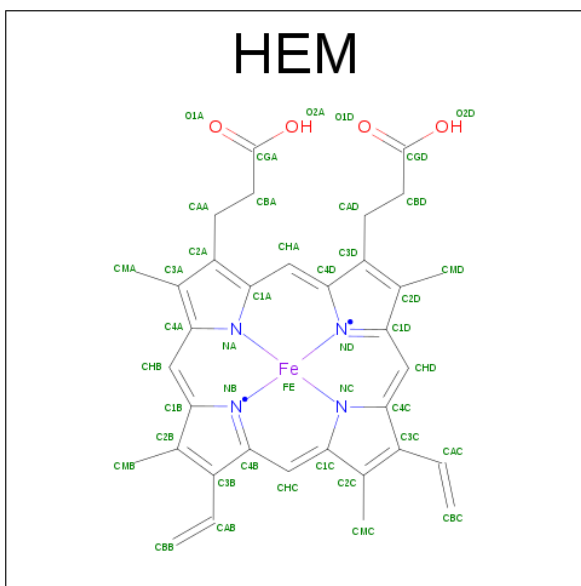
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			55	53	2		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

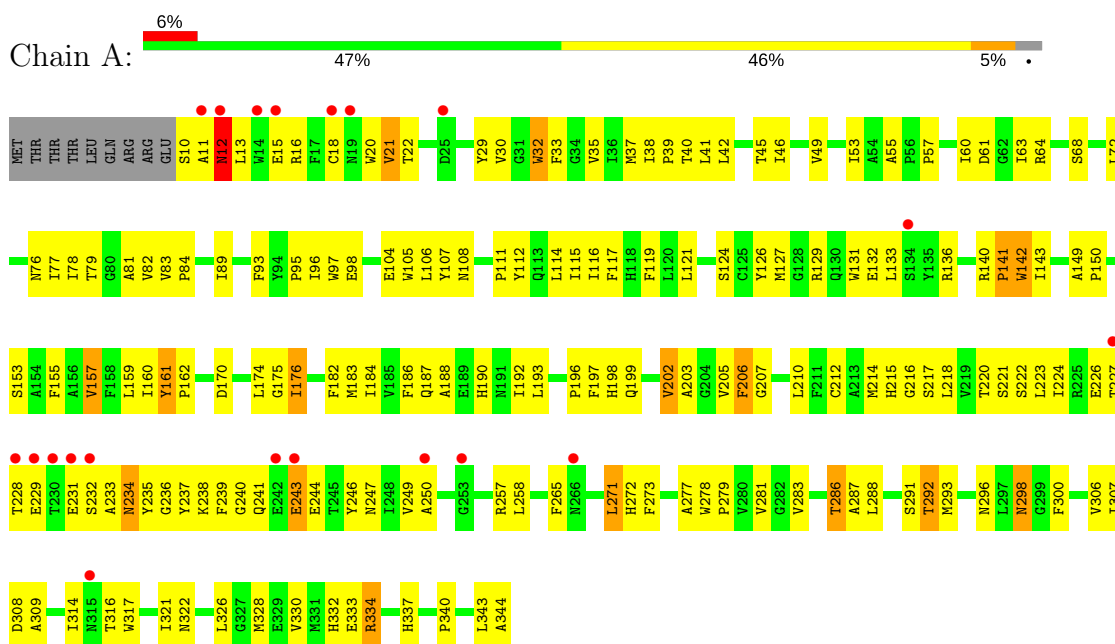
- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	O	1	Total 1	Ca 1	0	0
34	K	1	Total 1	Ca 1	0	0
34	F	1	Total 1	Ca 1	0	0

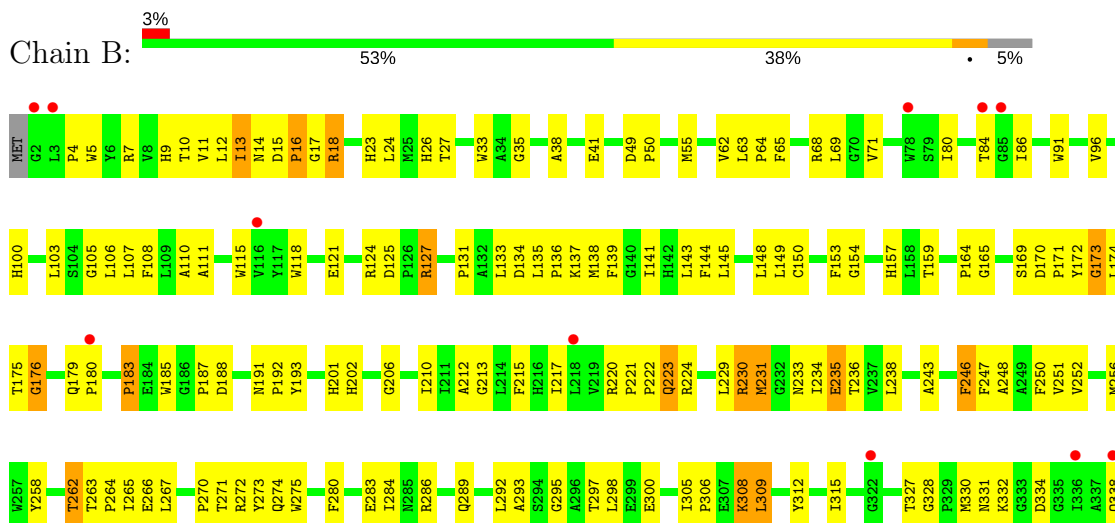
3 Residue-property plots

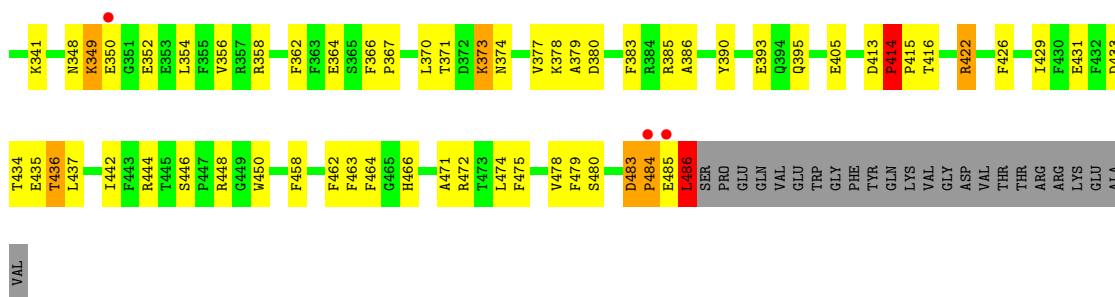
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Photosystem Q(B) protein 1



• Molecule 2: Photosystem II core light harvesting protein



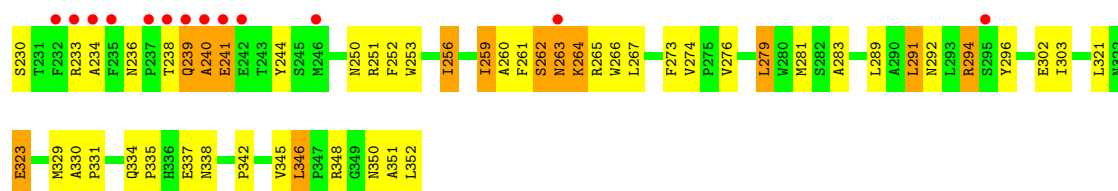


• Molecule 3: Photosystem II CP43 protein

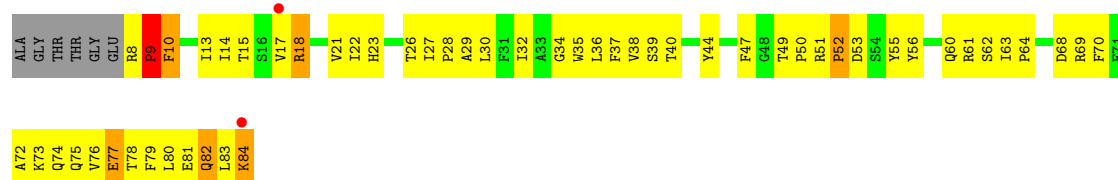


• Molecule 4: Photosystem II D2 protein

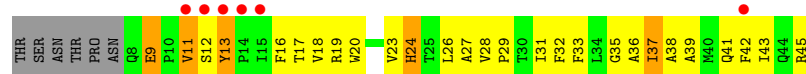




• Molecule 5: Cytochrome b559 subunit alpha



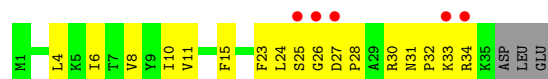
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein I

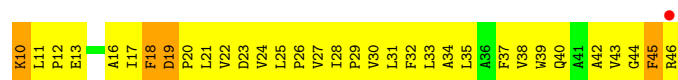


• Molecule 9: Photosystem II reaction center protein J

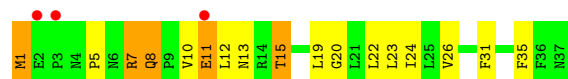


• Molecule 10: Photosystem II reaction center protein K





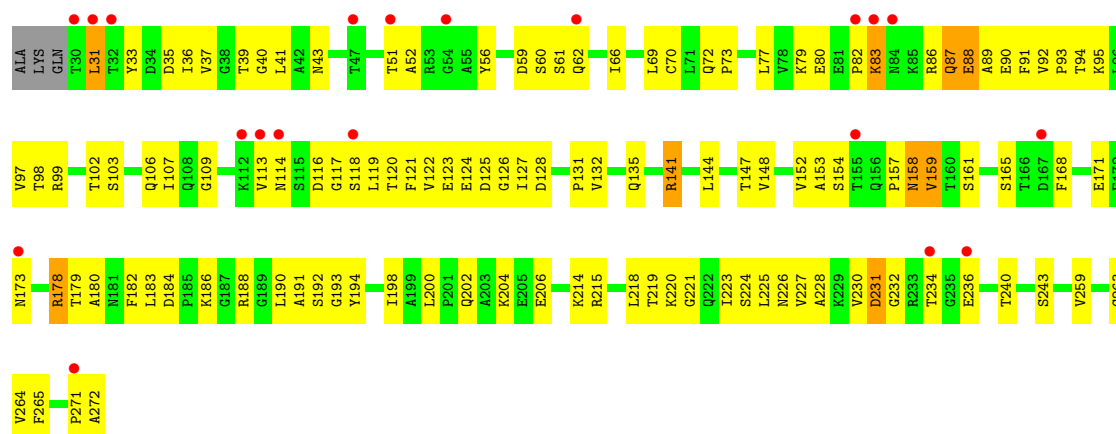
- Molecule 11: Photosystem II reaction center protein L



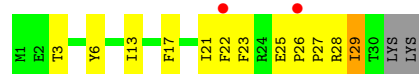
- Molecule 12: Photosystem II reaction center protein M



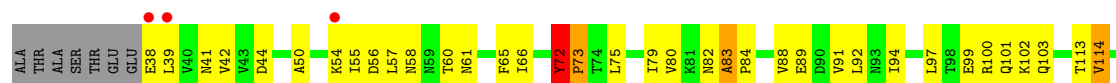
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

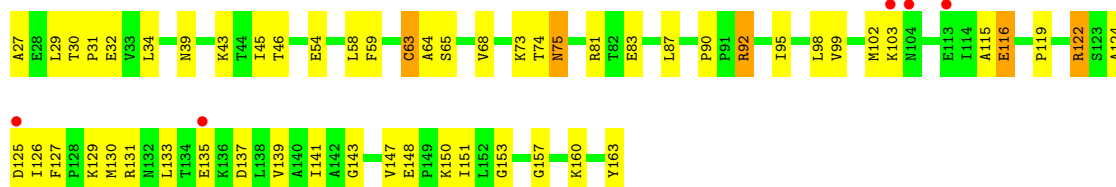


- Molecule 15: Photosystem II 12 kDa extrinsic protein

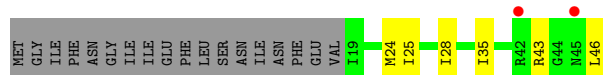




• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.3 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.303 , 0.326	Depositor DCC
R_{free} test set	1054 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CA, LMT, CLA, PL9, BCT, FE2, MES, OEC, HEM, LMG, BCR, SQD

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	0.44	0/2713	0.66	0/3700
2	B	0.43	0/3947	0.66	1/5379 (0.0%)
3	C	0.41	0/3567	0.64	1/4856 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.43	0/654	0.69	0/891
6	F	0.62	0/317	0.71	0/433
7	H	0.38	0/520	0.67	0/709
8	I	0.51	0/293	0.68	0/395
9	J	0.41	0/255	0.68	0/346
10	K	0.41	0/303	0.62	0/416
11	L	0.37	0/311	0.65	0/422
12	M	0.44	0/270	0.70	0/367
13	O	0.44	0/1876	0.70	0/2548
14	T	0.49	0/265	0.63	0/359
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.39	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.42	0/257	0.59	0/348
19	Z	0.45	0/490	0.69	0/669
All	All	0.43	0/20907	0.66	3/28460 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	6.98	131.36	115.30
3	C	32	GLY	N-CA-C	-5.55	99.23	113.10
15	U	72	TYR	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	244	0
2	B	3812	0	3683	272	0
3	C	3455	0	3378	373	0
4	D	2706	0	2608	238	0
5	E	635	0	625	82	0
6	F	307	0	312	49	0
7	H	507	0	521	67	0
8	I	286	0	308	18	0
9	J	249	0	262	50	0
10	K	293	0	305	56	0
11	L	304	0	316	28	0
12	M	267	0	289	34	0
13	O	1845	0	1801	119	0
14	T	256	0	262	24	0
15	U	774	0	773	47	0
16	V	1060	0	1068	49	0
17	y	201	0	226	0	0
18	X	254	0	282	28	0
19	Z	479	0	516	64	0
20	A	1	0	0	0	0
21	A	260	0	288	49	0
21	B	1040	0	1152	151	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	780	0	864	143	0
21	D	130	0	144	20	0
21	K	65	0	72	15	0
22	A	64	0	74	8	0
22	D	64	0	74	12	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	8	0
25	B	120	0	168	7	0
25	C	80	0	112	26	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	6	0
25	Z	40	0	56	4	0
26	A	52	0	62	1	0
26	B	124	0	170	42	0
26	C	237	0	311	76	0
26	D	63	0	87	0	0
27	A	39	0	51	7	0
27	C	37	0	44	5	0
28	C	51	0	68	5	0
28	D	43	0	49	9	0
28	F	45	0	53	0	0
28	L	47	0	60	2	0
29	A	51	0	72	40	0
29	B	49	0	68	6	0
29	C	45	0	60	6	0
29	D	94	0	127	36	0
29	I	43	0	56	0	0
29	J	48	0	66	4	0
29	M	42	0	54	3	0
30	A	35	0	46	0	0
30	B	35	0	46	2	0
30	D	66	0	81	3	0
30	I	35	0	46	2	0
30	O	35	0	46	1	0
30	T	35	0	46	1	0
31	D	4	0	0	0	0
32	D	55	0	80	31	0
33	F	43	0	30	6	0
33	V	43	0	30	5	0
34	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1799	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 37.

All (1799) 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)
28:C:475:SQD:C4	28:C:475:SQD:C3	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
29:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17
26:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.25	1.13
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.18	1.13
2:B:327:THR:HA	21:B:517:CLA:O1A	1.49	1.12
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.23	1.11
1:A:271:LEU:CD1	23:A:367:MES:H82	1.80	1.11
3:C:174:LEU:HD22	21:C:478:CLA:H161	1.21	1.10
10:K:10:LYS:HG2	10:K:10:LYS:O	1.44	1.10
3:C:293:ASN:HA	26:C:491:DGD:O2E	1.53	1.09
29:A:373:LMG:H332	12:M:22:LEU:HD21	1.27	1.08
3:C:174:LEU:CD2	21:C:478:CLA:H161	1.84	1.07
21:B:518:CLA:H42	4:D:127:LEU:HD11	1.07	1.05
5:E:15:THR:HG22	9:J:7:ARG:CG	1.85	1.05
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.31	1.05
26:B:528:DGD:O1B	26:B:528:DGD:HG12	1.57	1.04
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.20	1.04
5:E:15:THR:CG2	9:J:7:ARG:HG2	1.86	1.04
3:C:254:THR:HG22	3:C:255:THR:H	1.18	1.04
4:D:23:LYS:HZ1	28:D:361:SQD:H462	1.22	1.04
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.18	1.04
26:B:528:DGD:O2D	4:D:87:HIS:HB2	1.58	1.03
29:D:360:LMG:O6	11:L:15:THR:HG21	1.62	1.00
2:B:250:PHE:HD1	26:B:528:DGD:HB92	1.22	1.00
29:A:373:LMG:H112	4:D:266:TRP:HH2	0.85	1.00
2:B:149:LEU:HG	21:B:513:CLA:HBC1	1.41	1.00
29:A:373:LMG:H372	12:M:18:PRO:CB	1.91	0.98
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.00	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:373:LMG:C37	12:M:18:PRO:HB3	1.93	0.96
29:A:373:LMG:H372	12:M:18:PRO:HB3	0.97	0.96
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.49	0.95
13:O:230:VAL:HG12	13:O:231:ASP:H	1.30	0.94
14:T:29:ILE:HD12	14:T:29:ILE:H	1.33	0.94
15:U:83:ALA:HB1	15:U:84:PRO:CD	1.98	0.93
25:C:489:BCR:H312	19:Z:9:LEU:HD11	1.51	0.93
1:A:11:ALA:O	1:A:12:ASN:HB2	1.67	0.93
2:B:332:LYS:HE3	26:B:533:DGD:O4D	1.68	0.92
29:A:373:LMG:C11	4:D:266:TRP:HH2	1.80	0.92
11:L:1:MET:HG2	11:L:1:MET:O	1.70	0.92
3:C:407:VAL:HA	26:C:493:DGD:O2E	1.70	0.91
21:B:517:CLA:H202	4:D:281:MET:SD	2.11	0.91
4:D:186:GLN:HB2	21:D:354:CLA:HBC1	1.52	0.91
21:C:477:CLA:HMB3	25:C:490:BCR:H403	1.51	0.90
3:C:225:VAL:HG21	26:C:491:DGD:HG11	1.52	0.90
3:C:52:ALA:HA	21:C:486:CLA:HMB3	1.53	0.90
1:A:286:THR:HG23	21:A:362:CLA:HED3	1.50	0.90
29:D:360:LMG:O7	11:L:19:LEU:HD21	1.71	0.89
29:D:360:LMG:H212	14:T:17:PHE:HZ	1.36	0.89
21:B:524:CLA:H18	26:B:533:DGD:HAS1	1.53	0.89
5:E:15:THR:CG2	9:J:7:ARG:CG	2.48	0.89
3:C:224:ILE:O	3:C:227:VAL:HG23	1.73	0.89
26:B:528:DGD:HO2D	4:D:87:HIS:CG	1.90	0.89
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.55	0.88
21:B:514:CLA:H11	21:B:522:CLA:H152	1.54	0.88
2:B:434:THR:HG23	13:O:204:LYS:HE3	1.54	0.88
26:C:493:DGD:HE62	9:J:40:LEU:HD21	1.54	0.88
2:B:271:THR:HG22	2:B:273:TYR:H	1.39	0.88
5:E:15:THR:HG21	9:J:7:ARG:HG2	1.56	0.87
3:C:305:THR:HG22	3:C:308:GLU:H	1.40	0.87
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.57	0.87
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.56	0.87
13:O:69:LEU:HD12	13:O:70:CYS:H	1.39	0.87
29:A:373:LMG:H231	29:D:360:LMG:H202	1.54	0.87
3:C:155:ASN:HD21	3:C:255:THR:HB	1.40	0.87
26:B:528:DGD:HBE1	4:D:159:ILE:HG23	1.57	0.87
3:C:447:ARG:HH11	3:C:447:ARG:HG2	1.40	0.86
2:B:250:PHE:HD1	26:B:528:DGD:C9B	1.88	0.86
16:V:30:THR:HB	16:V:31:PRO:HD2	1.54	0.86
4:D:259:ILE:HG12	29:D:360:LMG:H301	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.40	0.86
25:C:489:BCR:H353	25:J:112:BCR:H321	1.56	0.85
13:O:178:ARG:CG	13:O:178:ARG:HH11	1.88	0.85
1:A:121:LEU:HD21	21:A:366:CLA:HMB3	1.58	0.85
4:D:129:GLN:NE2	4:D:143:ALA:HA	1.92	0.85
21:B:513:CLA:HBB1	21:B:515:CLA:H171	1.59	0.85
7:H:12:ARG:HD3	7:H:12:ARG:O	1.76	0.85
11:L:8:GLN:HE21	11:L:8:GLN:N	1.75	0.85
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.60	0.84
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.57	0.84
2:B:250:PHE:CD1	26:B:528:DGD:HB92	2.12	0.84
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.60	0.83
1:A:39:PRO:HG3	25:A:369:BCR:HC8	1.58	0.83
3:C:437:PHE:CZ	21:K:483:CLA:HMB3	2.14	0.83
26:B:533:DGD:HG31	12:M:6:LEU:HD12	1.59	0.83
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.39	0.83
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.43	0.83
29:D:360:LMG:H221	14:T:13:ILE:HG21	1.60	0.83
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.61	0.83
21:C:478:CLA:H12	21:C:479:CLA:H42	1.61	0.82
26:B:528:DGD:O2D	4:D:87:HIS:CB	2.27	0.82
1:A:214:MET:HB3	23:A:367:MES:H61	1.59	0.82
4:D:135:LEU:HD23	28:D:361:SQD:O2	1.78	0.82
3:C:407:VAL:HA	26:C:493:DGD:HO2E	1.45	0.82
21:B:518:CLA:CBB	4:D:123:ILE:HG12	2.10	0.81
21:C:487:CLA:HMA2	21:C:487:CLA:H172	1.61	0.81
3:C:407:VAL:HG22	26:C:493:DGD:O2E	1.81	0.81
3:C:28:GLN:OE1	3:C:28:GLN:HA	1.78	0.81
29:D:360:LMG:H341	14:T:21:ILE:HD11	1.62	0.81
2:B:247:PHE:HE1	21:B:512:CLA:H8	1.46	0.81
3:C:254:THR:HG22	3:C:255:THR:N	1.96	0.81
4:D:23:LYS:NZ	28:D:361:SQD:H462	1.97	0.80
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.63	0.80
4:D:323:GLU:HG2	13:O:194:TYR:OH	1.81	0.80
1:A:192:ILE:HA	1:A:293:MET:HE3	1.64	0.80
5:E:84:LYS:NZ	5:E:84:LYS:HB2	1.97	0.80
29:A:373:LMG:C20	32:D:357:PL9:H212	2.13	0.79
25:C:489:BCR:HC22	10:K:18:PHE:HD1	1.46	0.79
3:C:473:ASP:HB2	14:T:26:PRO:CB	2.11	0.79
28:C:475:SQD:C3	28:C:475:SQD:C5	2.60	0.79
26:B:533:DGD:HAH1	12:M:17:VAL:CG2	2.08	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:10:LYS:O	10:K:10:LYS:CG	2.30	0.78
2:B:238:LEU:HB2	21:B:522:CLA:HMD3	1.65	0.78
13:O:230:VAL:HG12	13:O:231:ASP:N	1.98	0.78
21:C:484:CLA:H141	21:K:483:CLA:H162	1.64	0.78
2:B:434:THR:CG2	13:O:204:LYS:HE3	2.12	0.78
19:Z:36:SER:HA	19:Z:39:LEU:HG	1.64	0.78
1:A:215:HIS:HA	23:A:367:MES:H51	1.63	0.78
2:B:383:PHE:O	13:O:192:SER:HA	1.84	0.78
3:C:110:PRO:HG3	29:C:494:LMG:H141	1.65	0.78
21:C:480:CLA:H143	21:C:484:CLA:H152	1.66	0.77
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.65	0.77
1:A:218:LEU:HD22	23:A:367:MES:H52	1.66	0.77
3:C:233:VAL:HA	25:C:490:BCR:H281	1.65	0.77
4:D:152:VAL:HG11	21:D:354:CLA:H11	1.67	0.77
7:H:35:MET:HE2	25:X:107:BCR:HC21	1.65	0.77
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.67	0.77
1:A:271:LEU:HD21	23:A:367:MES:HN4	1.50	0.77
29:D:360:LMG:H201	11:L:22:LEU:HD11	1.66	0.77
29:A:373:LMG:H332	12:M:22:LEU:CD2	2.12	0.77
3:C:284:PHE:HB3	26:C:491:DGD:HA52	1.66	0.77
3:C:135:ARG:HE	19:Z:33:TRP:HE1	1.30	0.76
2:B:134:ASP:OD2	2:B:137:LYS:HE3	1.86	0.76
1:A:131:TRP:CH2	21:C:481:CLA:HBA2	2.20	0.76
4:D:192:THR:HG23	21:D:354:CLA:HBC2	1.68	0.76
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.20	0.76
2:B:271:THR:HG22	2:B:273:TYR:N	1.98	0.76
3:C:209:ILE:HG23	25:C:490:BCR:H382	1.65	0.76
19:Z:49:ALA:O	19:Z:53:VAL:HG23	1.86	0.76
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.00	0.75
1:A:93:PHE:CZ	21:A:366:CLA:HBA1	2.20	0.75
1:A:46:ILE:HD13	26:A:375:DGD:HBE2	1.68	0.75
28:C:475:SQD:H251	27:C:476:LHG:H102	1.66	0.75
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.14	0.75
18:X:12:ILE:O	18:X:12:ILE:HG23	1.85	0.75
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.07	0.75
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.66	0.75
3:C:391:ARG:HB2	3:C:391:ARG:NH1	2.02	0.75
3:C:437:PHE:HZ	21:K:483:CLA:HMB3	1.50	0.75
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.67	0.75
8:I:4:LEU:HD22	30:I:274:LMT:H52	1.69	0.75
4:D:279:LEU:HG	22:D:355:PHO:HBC3	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.68	0.75
21:B:523:CLA:H2	21:B:523:CLA:HED3	1.68	0.74
16:V:63:CYS:SG	33:V:164:HEM:CAB	2.61	0.74
21:B:518:CLA:H42	4:D:127:LEU:CD1	2.03	0.74
1:A:214:MET:CB	23:A:367:MES:H61	2.16	0.74
29:A:373:LMG:H192	32:D:357:PL9:H221	1.69	0.74
3:C:135:ARG:NE	19:Z:33:TRP:HE1	1.85	0.74
3:C:223:TRP:CZ2	26:C:474:DGD:HA62	2.23	0.74
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.17	0.74
19:Z:32:ASP:HB2	19:Z:35:ARG:HG2	1.67	0.74
4:D:244:TYR:OH	4:D:264:LYS:HE3	1.88	0.74
5:E:18:ARG:HH11	5:E:18:ARG:HB3	1.52	0.74
29:A:373:LMG:C33	12:M:22:LEU:HD21	2.14	0.74
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.68	0.74
3:C:418:ASN:HB2	26:C:493:DGD:O4E	1.88	0.73
2:B:234:ILE:HD11	21:B:520:CLA:H191	1.70	0.73
3:C:155:ASN:HA	3:C:158:THR:HG22	1.69	0.73
4:D:41:ALA:HB2	22:D:355:PHO:H43	1.70	0.73
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.03	0.73
3:C:135:ARG:HB2	19:Z:27:TYR:HB3	1.69	0.73
19:Z:32:ASP:CG	19:Z:33:TRP:H	1.90	0.73
4:D:262:SER:HG	29:D:360:LMG:HO3	1.33	0.73
21:B:518:CLA:H142	21:B:518:CLA:H102	1.69	0.73
1:A:214:MET:HA	1:A:214:MET:CE	2.17	0.73
1:A:41:LEU:O	1:A:45:THR:HG22	1.89	0.73
5:E:15:THR:HG22	9:J:7:ARG:HG3	1.71	0.73
28:C:475:SQD:C4	28:C:475:SQD:C2	2.66	0.73
18:X:34:PHE:O	18:X:38:ILE:HG12	1.88	0.73
1:A:42:LEU:HD12	25:A:369:BCR:C11	2.18	0.73
3:C:241:GLY:O	3:C:245:ILE:HG13	1.88	0.73
3:C:85:GLY:O	21:C:480:CLA:HED1	1.89	0.73
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.23	0.73
5:E:17:VAL:O	5:E:21:VAL:HG23	1.88	0.73
29:A:373:LMG:H202	32:D:357:PL9:H212	1.70	0.72
3:C:225:VAL:CG2	26:C:491:DGD:HG11	2.20	0.72
1:A:35:VAL:HA	25:A:369:BCR:H333	1.70	0.72
3:C:168:LEU:HD13	21:C:483:CLA:H43	1.71	0.72
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.70	0.72
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.72	0.72
4:D:261:PHE:HB2	32:D:357:PL9:H522	1.71	0.72
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.55	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:CG2	3:C:308:GLU:H	2.02	0.72
2:B:450:TRP:HB3	21:B:517:CLA:HMB2	1.71	0.72
3:C:240:ILE:O	3:C:244:CYS:HB2	1.88	0.72
3:C:254:THR:CG2	3:C:255:THR:H	2.00	0.72
3:C:415:ASN:O	3:C:416:SER:HB3	1.89	0.72
25:C:489:BCR:H11C	25:J:112:BCR:H322	1.69	0.71
3:C:91:HIS:CD2	21:C:478:CLA:HBA1	2.25	0.71
3:C:404:LEU:HG	26:C:493:DGD:O1A	1.90	0.71
29:D:360:LMG:H192	11:L:22:LEU:HD21	1.71	0.71
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.04	0.71
2:B:327:THR:CA	21:B:517:CLA:O1A	2.36	0.71
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.73	0.71
21:B:513:CLA:H161	7:H:38:PHE:HE2	1.54	0.71
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.19	0.71
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.56	0.71
1:A:93:PHE:HZ	21:A:366:CLA:HBA1	1.54	0.71
2:B:250:PHE:CD1	26:B:528:DGD:C9B	2.72	0.71
4:D:129:GLN:HE22	4:D:143:ALA:HA	1.55	0.71
4:D:44:ALA:HB3	22:D:355:PHO:H92	1.72	0.71
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.72	0.71
3:C:348:GLU:OE2	13:O:37:VAL:HA	1.91	0.70
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.74	0.70
2:B:135:LEU:HA	2:B:138:MET:HE3	1.72	0.70
3:C:116:VAL:HG12	25:C:489:BCR:H332	1.72	0.70
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.02	0.70
2:B:224:ARG:HG2	7:H:24:GLY:O	1.91	0.70
13:O:33:TYR:O	13:O:37:VAL:HG23	1.92	0.70
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.74	0.70
13:O:69:LEU:HD12	13:O:70:CYS:N	2.05	0.70
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.26	0.70
2:B:222:PRO:HG3	7:H:27:THR:H	1.57	0.70
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.27	0.70
13:O:35:ASP:C	13:O:36:ILE:HD12	2.12	0.70
16:V:115:ALA:CB	16:V:122:ARG:HD2	2.22	0.70
3:C:219:GLY:HA2	26:C:491:DGD:O3D	1.92	0.70
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.74	0.70
26:B:533:DGD:CDA	12:M:17:VAL:HG21	2.12	0.69
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.06	0.69
3:C:54:VAL:HG13	21:C:487:CLA:HED1	1.74	0.69
4:D:259:ILE:HG12	29:D:360:LMG:C30	2.21	0.69
15:U:38:GLU:HG2	15:U:39:LEU:N	2.05	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:O	21:B:515:CLA:HBA1	1.92	0.69
21:B:521:CLA:H193	21:B:523:CLA:H92	1.74	0.69
2:B:284:ILE:HG12	2:B:309:LEU:CD1	2.22	0.69
4:D:39:PRO:O	4:D:43:LEU:HD22	1.93	0.69
2:B:137:LYS:HD2	7:H:14:LEU:O	1.93	0.69
3:C:404:LEU:HD21	26:C:493:DGD:HA31	1.73	0.69
21:B:513:CLA:H161	7:H:38:PHE:CE2	2.28	0.69
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.27	0.69
1:A:119:PHE:HZ	21:A:362:CLA:H101	1.58	0.69
21:C:478:CLA:O1A	21:C:479:CLA:H11	1.92	0.69
4:D:41:ALA:CB	22:D:355:PHO:H43	2.23	0.69
9:J:22:ILE:HG21	29:J:492:LMG:H202	1.75	0.69
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.74	0.69
3:C:284:PHE:CB	26:C:491:DGD:HA52	2.23	0.69
19:Z:30:PRO:HG3	19:Z:33:TRP:HZ3	1.58	0.69
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.74	0.69
3:C:158:THR:O	3:C:251:HIS:HB3	1.92	0.69
3:C:60:ILE:HG21	21:C:479:CLA:H191	1.75	0.69
29:J:492:LMG:O8	29:J:492:LMG:O9	2.11	0.69
19:Z:28:ALA:O	19:Z:30:PRO:HD3	1.93	0.69
3:C:68:THR:OG1	21:C:479:CLA:HED1	1.92	0.69
5:E:81:GLU:C	5:E:83:LEU:H	1.96	0.69
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.75	0.68
21:B:524:CLA:OBD	11:L:10:VAL:HG21	1.93	0.68
5:E:81:GLU:O	5:E:83:LEU:N	2.24	0.68
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.76	0.68
3:C:130:VAL:HG13	21:C:486:CLA:H92	1.74	0.68
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.68
19:Z:32:ASP:HB3	19:Z:35:ARG:NH1	2.07	0.68
21:B:521:CLA:H52	21:B:524:CLA:HBC3	1.74	0.68
29:A:373:LMG:HC92	2:B:5:TRP:HE1	1.59	0.68
26:C:493:DGD:HD3	9:J:32:ALA:O	1.93	0.68
25:D:358:BCR:H403	9:J:25:VAL:HG21	1.75	0.68
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.76	0.68
16:V:29:LEU:HD13	16:V:151:ILE:HD11	1.75	0.68
3:C:166:ILE:O	3:C:170:ILE:HG13	1.94	0.68
10:K:19:ASP:N	10:K:20:PRO:HD2	2.09	0.68
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.59	0.68
3:C:405:ASN:HA	26:C:493:DGD:HG12	1.75	0.68
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.29	0.68
1:A:271:LEU:HD11	23:A:367:MES:H82	0.83	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HB3	2:B:138:MET:CE	2.24	0.68
1:A:307:ILE:HG13	6:F:45:ARG:HD2	1.76	0.68
2:B:464:PHE:HD2	21:B:521:CLA:HAC2	1.58	0.67
2:B:328:GLY:O	21:B:517:CLA:HBA1	1.94	0.67
2:B:332:LYS:HE3	26:B:533:DGD:C4D	2.24	0.67
4:D:152:VAL:CG1	21:D:354:CLA:H11	2.24	0.67
6:F:18:VAL:HG13	6:F:19:ARG:H	1.59	0.67
3:C:30:SER:HB2	10:K:46:ARG:O	1.94	0.67
3:C:472:LEU:HD12	3:C:473:ASP:H	1.59	0.67
3:C:113:VAL:HG12	29:C:494:LMG:H192	1.76	0.67
5:E:78:THR:O	5:E:81:GLU:HB2	1.94	0.67
4:D:27:PHE:CD2	6:F:19:ARG:HD3	2.29	0.67
1:A:39:PRO:HB2	21:A:366:CLA:HBB1	1.75	0.67
7:H:63:LYS:C	7:H:65:LEU:H	1.98	0.67
1:A:183:MET:HG2	21:A:363:CLA:HBC1	1.77	0.67
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.59	0.67
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.77	0.67
26:B:533:DGD:HA81	12:M:14:PHE:HA	1.75	0.67
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.58	0.67
4:D:180:ARG:CG	4:D:180:ARG:HH11	2.08	0.67
2:B:135:LEU:HD23	2:B:138:MET:CE	2.25	0.67
21:C:479:CLA:H171	21:K:483:CLA:HBB2	1.77	0.67
26:C:492:DGD:O3D	25:J:115:BCR:H382	1.94	0.67
1:A:45:THR:HB	22:A:365:PHO:H8	1.77	0.67
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.78	0.67
1:A:278:TRP:HA	26:C:493:DGD:HAG1	1.76	0.67
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.66
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.26	0.66
25:C:489:BCR:HC22	10:K:18:PHE:CD1	2.31	0.66
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.78	0.66
2:B:483:ASP:OD2	2:B:484:PRO:HD2	1.94	0.66
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.77	0.66
3:C:155:ASN:HD21	3:C:255:THR:CB	2.07	0.66
3:C:377:LEU:O	3:C:381:LYS:HB2	1.95	0.66
26:C:493:DGD:HBF1	29:D:359:LMG:H211	1.77	0.66
2:B:62:VAL:CG1	21:B:515:CLA:HED3	2.26	0.66
3:C:305:THR:HG22	3:C:308:GLU:CB	2.26	0.66
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.48	0.66
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.77	0.66
2:B:271:THR:CG2	2:B:273:TYR:H	2.08	0.66
29:A:373:LMG:C11	4:D:266:TRP:CH2	2.66	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:THR:HG22	9:J:7:ARG:CB	2.25	0.66
19:Z:33:TRP:O	19:Z:37:LYS:HB2	1.95	0.66
1:A:119:PHE:CZ	21:A:362:CLA:H101	2.30	0.66
26:C:492:DGD:HB52	25:J:115:BCR:H352	1.78	0.66
2:B:385:ARG:HD3	13:O:191:ALA:O	1.96	0.65
4:D:192:THR:CG2	21:D:354:CLA:HBC2	2.26	0.65
13:O:206:GLU:CD	13:O:206:GLU:H	1.97	0.65
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.62	0.65
2:B:271:THR:HB	2:B:274:GLN:HG3	1.78	0.65
29:D:360:LMG:O9	29:D:360:LMG:C7	2.43	0.65
3:C:437:PHE:HA	21:C:484:CLA:CMC	2.26	0.65
21:C:486:CLA:H151	19:Z:24:PRO:HG3	1.79	0.65
1:A:121:LEU:CD2	21:A:366:CLA:HMB3	2.25	0.65
21:B:517:CLA:H141	21:B:517:CLA:H172	1.79	0.65
3:C:453:ALA:O	8:I:34:ARG:HB2	1.97	0.65
3:C:220:GLY:N	26:C:491:DGD:O3D	2.29	0.65
3:C:165:LEU:HD21	21:C:482:CLA:HHC	1.78	0.65
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.78	0.65
15:U:83:ALA:CB	15:U:84:PRO:HD2	2.14	0.65
2:B:86:ILE:O	2:B:86:ILE:HD12	1.97	0.65
3:C:89:ILE:N	3:C:90:PRO:HD2	2.11	0.65
1:A:64:ARG:NH1	13:O:98:THR:HG21	2.12	0.65
21:B:513:CLA:O2A	21:B:513:CLA:H3A	1.97	0.64
16:V:143:GLY:O	16:V:147:VAL:HG23	1.97	0.64
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.79	0.64
32:D:357:PL9:H262	32:D:357:PL9:C30	2.27	0.64
2:B:442:ILE:HD11	13:O:200:LEU:HD23	1.76	0.64
21:D:356:CLA:H42	18:X:26:GLY:HA3	1.79	0.64
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.32	0.64
2:B:7:ARG:HA	21:B:521:CLA:HBA1	1.78	0.64
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.78	0.64
2:B:250:PHE:HB3	26:B:528:DGD:HB82	1.78	0.64
11:L:7:ARG:HD2	11:L:7:ARG:O	1.97	0.64
2:B:331:ASN:HB3	2:B:437:LEU:HD12	1.79	0.64
21:C:483:CLA:OBD	21:C:485:CLA:H152	1.96	0.64
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.63	0.64
3:C:281:MET:HE2	26:C:474:DGD:HAE1	1.79	0.64
13:O:120:THR:HG22	13:O:154:SER:OG	1.96	0.64
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.78	0.64
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.77	0.64
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:LEU:O	5:E:40:THR:HG23	1.98	0.64
2:B:284:ILE:HG23	2:B:305:ILE:HD12	1.80	0.63
19:Z:55:GLY:HA2	25:Z:116:BCR:H312	1.80	0.63
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.32	0.63
1:A:57:PRO:HG3	1:A:68:SER:CB	2.28	0.63
14:T:29:ILE:CD1	14:T:29:ILE:H	1.95	0.63
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.80	0.63
2:B:297:THR:OG1	2:B:300:GLU:HG3	1.98	0.63
2:B:486:LEU:O	2:B:486:LEU:HD13	1.98	0.63
3:C:310:SER:OG	3:C:355:THR:HG23	1.98	0.63
32:D:357:PL9:H262	32:D:357:PL9:H302	1.80	0.63
2:B:187:PRO:HB3	21:B:511:CLA:HMB2	1.81	0.63
6:F:19:ARG:NH2	33:F:85:HEM:O2D	2.32	0.63
5:E:26:THR:O	5:E:29:ALA:HB3	1.98	0.63
2:B:247:PHE:HB2	21:B:518:CLA:HBC1	1.80	0.63
21:B:513:CLA:CGA	21:B:513:CLA:H3A	2.29	0.62
21:B:517:CLA:H11	26:B:533:DGD:HB32	1.79	0.62
1:A:300:PHE:CZ	3:C:404:LEU:HD23	2.33	0.62
3:C:407:VAL:CA	26:C:493:DGD:O2E	2.45	0.62
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.32	0.62
29:A:373:LMG:H201	32:D:357:PL9:H212	1.80	0.62
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.82	0.62
3:C:293:ASN:CA	26:C:491:DGD:O2E	2.40	0.62
1:A:22:THR:HG21	8:I:30:ARG:CD	2.29	0.62
3:C:135:ARG:NE	19:Z:33:TRP:NE1	2.47	0.62
1:A:18:CYS:O	1:A:22:THR:HG22	2.00	0.62
3:C:44:ASN:C	3:C:45:LEU:HD12	2.20	0.62
13:O:117:GLY:O	13:O:159:VAL:HG12	1.98	0.62
5:E:23:HIS:HA	5:E:26:THR:OG1	2.00	0.62
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.34	0.62
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.80	0.62
1:A:343:LEU:O	1:A:344:ALA:HB2	2.00	0.62
3:C:107:ASP:OD2	3:C:110:PRO:HD3	1.99	0.62
13:O:234:THR:OG1	13:O:236:GLU:HG2	2.00	0.62
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.82	0.62
21:C:486:CLA:H141	19:Z:20:VAL:O	2.00	0.62
1:A:228:THR:HG22	1:A:229:GLU:H	1.65	0.62
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.80	0.62
26:B:528:DGD:HE5	26:B:528:DGD:HD61	1.82	0.62
3:C:418:ASN:HA	26:C:493:DGD:HE2	1.81	0.62
10:K:18:PHE:HD2	10:K:18:PHE:N	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD12	25:A:369:BCR:H11C	1.81	0.62
2:B:371:THR:HG22	2:B:377:VAL:HA	1.81	0.62
3:C:286:ALA:HB2	21:C:478:CLA:CMD	2.30	0.62
5:E:10:PHE:CE2	6:F:19:ARG:NH1	2.67	0.62
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.81	0.61
3:C:119:LEU:HG	25:C:489:BCR:H10C	1.82	0.61
3:C:44:ASN:O	3:C:45:LEU:HD12	1.99	0.61
5:E:18:ARG:O	5:E:22:ILE:HG13	2.00	0.61
2:B:69:LEU:HD11	21:B:513:CLA:OBD	2.00	0.61
27:C:476:LHG:H171	26:C:492:DGD:HBG2	1.82	0.61
3:C:41:ARG:NH1	21:C:486:CLA:HMD1	2.14	0.61
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.30	0.61
5:E:64:PRO:HB3	5:E:84:LYS:HE2	1.82	0.61
19:Z:32:ASP:CB	19:Z:35:ARG:HG2	2.30	0.61
1:A:218:LEU:CD2	23:A:367:MES:H52	2.30	0.61
2:B:69:LEU:HD12	21:B:515:CLA:HBA2	1.82	0.61
2:B:462:PHE:CE1	21:B:523:CLA:HMB3	2.36	0.61
3:C:41:ARG:NH1	21:C:486:CLA:OBD	2.33	0.61
26:C:492:DGD:HB42	26:C:493:DGD:HA21	1.81	0.61
4:D:267:LEU:HD23	4:D:267:LEU:C	2.20	0.61
15:U:66:ILE:HG22	15:U:66:ILE:O	1.98	0.61
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.81	0.61
3:C:113:VAL:HG11	29:C:494:LMG:H172	1.81	0.61
3:C:461:ARG:HG3	3:C:461:ARG:HH11	1.65	0.61
4:D:342:PRO:O	4:D:345:VAL:HG12	2.01	0.61
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.31	0.61
3:C:224:ILE:HD11	21:C:477:CLA:H93	1.81	0.61
3:C:248:GLY:O	3:C:252:ILE:HG12	2.00	0.61
29:B:531:LMG:HC2	4:D:141:TYR:OH	2.00	0.61
6:F:31:ILE:HD12	6:F:31:ILE:N	2.16	0.61
14:T:29:ILE:HD12	14:T:29:ILE:N	2.10	0.61
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.15	0.61
15:U:94:ILE:O	15:U:97:LEU:HG	2.00	0.61
21:B:517:CLA:HBC3	25:B:529:BCR:H10C	1.83	0.61
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.82	0.61
3:C:405:ASN:HB2	26:C:493:DGD:HG32	1.82	0.61
1:A:53:ILE:HD11	32:D:357:PL9:H501	1.82	0.61
3:C:114:VAL:HG22	29:C:494:LMG:H211	1.83	0.61
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.61
5:E:79:PHE:O	5:E:84:LYS:HB3	2.01	0.61
7:H:19:GLY:O	7:H:21:VAL:HG13	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:THR:CG2	9:J:8:ILE:H	2.13	0.61
13:O:39:THR:OG1	13:O:41:LEU:HB2	2.01	0.61
4:D:209:LEU:HD23	4:D:209:LEU:C	2.22	0.61
10:K:18:PHE:CD2	10:K:18:PHE:N	2.68	0.61
29:A:373:LMG:H331	11:L:24:ILE:HD11	1.81	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
3:C:88:LEU:HB3	21:C:479:CLA:HED3	1.83	0.61
9:J:18:GLY:HA3	25:J:112:BCR:H371	1.82	0.61
3:C:143:TYR:O	3:C:144:SER:HB2	2.00	0.60
21:C:480:CLA:H93	26:C:492:DGD:HAT2	1.83	0.60
21:B:518:CLA:HBB2	4:D:123:ILE:HG12	1.82	0.60
16:V:90:PRO:O	16:V:92:ARG:HD3	2.01	0.60
21:A:362:CLA:H111	22:A:365:PHO:H3A	1.83	0.60
29:A:373:LMG:H192	32:D:357:PL9:C22	2.31	0.60
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.36	0.60
1:A:322:ASN:OD1	3:C:412:THR:HA	2.01	0.60
6:F:38:ALA:O	6:F:41:GLN:HG2	2.01	0.60
13:O:86:ARG:HG3	13:O:86:ARG:HH11	1.66	0.60
15:U:97:LEU:O	15:U:102:LYS:HE2	2.01	0.60
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.82	0.60
10:K:17:ILE:HD12	10:K:17:ILE:N	2.17	0.60
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.13	0.60
3:C:204:LEU:HD21	3:C:238:ILE:HG21	1.84	0.60
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.36	0.60
13:O:230:VAL:CG1	13:O:231:ASP:H	2.10	0.60
1:A:153:SER:HB2	21:A:362:CLA:H43	1.83	0.60
7:H:58:VAL:HG13	7:H:58:VAL:O	2.00	0.60
4:D:47:GLY:HA2	25:D:358:BCR:H332	1.83	0.60
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.83	0.60
18:X:12:ILE:HG12	18:X:16:LEU:CD1	2.30	0.60
19:Z:33:TRP:O	19:Z:33:TRP:HD1	1.84	0.60
1:A:107:TYR:CD1	13:O:141:ARG:NH1	2.69	0.60
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.02	0.60
3:C:264:PHE:HE2	21:C:482:CLA:O1A	1.85	0.60
29:A:373:LMG:H311	11:L:20:GLY:HA2	1.82	0.60
3:C:178:LYS:HB2	21:C:478:CLA:H162	1.83	0.60
1:A:306:VAL:HG13	1:A:314:ILE:O	2.01	0.60
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.60
2:B:143:LEU:HA	21:B:520:CLA:HED1	1.83	0.60
2:B:238:LEU:HD13	21:B:522:CLA:C1D	2.32	0.60
5:E:18:ARG:NH1	5:E:18:ARG:HB3	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:217:ILE:HG13	2.02	0.60
2:B:462:PHE:HA	21:B:521:CLA:HMC1	1.84	0.60
3:C:141:GLU:H	3:C:141:GLU:CD	2.05	0.59
3:C:39:ASN:OD1	21:C:485:CLA:HBB2	2.02	0.59
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.82	0.59
13:O:87:GLN:O	13:O:88:GLU:HB3	2.02	0.59
15:U:113:THR:O	15:U:114:VAL:HG23	2.02	0.59
1:A:22:THR:HG21	8:I:30:ARG:NE	2.16	0.59
21:B:517:CLA:H142	29:B:531:LMG:H382	1.84	0.59
21:C:477:CLA:H151	21:C:483:CLA:HMB3	1.84	0.59
5:E:15:THR:HG23	9:J:8:ILE:O	2.01	0.59
1:A:257:ARG:HH11	1:A:257:ARG:HG3	1.66	0.59
29:B:531:LMG:H291	29:B:531:LMG:H201	1.83	0.59
3:C:292:PHE:O	26:C:491:DGD:O2E	2.20	0.59
13:O:31:LEU:N	13:O:31:LEU:HD12	2.17	0.59
1:A:309:ALA:HB3	16:V:27:ALA:O	2.03	0.59
21:B:520:CLA:HBB1	21:B:520:CLA:HHC	1.83	0.59
3:C:233:VAL:HA	25:C:490:BCR:C28	2.32	0.59
16:V:102:MET:HE3	16:V:141:ILE:HG21	1.83	0.59
1:A:214:MET:HA	1:A:214:MET:HE3	1.85	0.59
2:B:172:TYR:O	2:B:174:LEU:HG	2.02	0.59
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.37	0.59
6:F:16:PHE:HE2	33:F:85:HEM:HMA2	1.66	0.59
21:A:363:CLA:H42	22:A:365:PHO:HMB3	1.85	0.59
2:B:149:LEU:CG	21:B:513:CLA:HBC1	2.26	0.59
10:K:33:LEU:HD23	21:K:483:CLA:OBD	2.03	0.59
21:B:512:CLA:C4	7:H:45:ILE:HD11	2.33	0.59
6:F:27:ALA:HB1	33:F:85:HEM:HBC2	1.82	0.59
1:A:22:THR:HG21	8:I:30:ARG:HE	1.67	0.59
5:E:56:TYR:O	16:V:27:ALA:HB2	2.02	0.59
21:B:511:CLA:HHC	21:B:511:CLA:HBB1	1.84	0.59
3:C:418:ASN:CB	26:C:493:DGD:HE2	2.32	0.59
21:C:480:CLA:H42	26:C:493:DGD:HA32	1.84	0.59
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.01	0.59
2:B:458:PHE:HB3	21:B:514:CLA:HBC2	1.84	0.59
3:C:318:LEU:C	3:C:318:LEU:HD23	2.24	0.59
3:C:37:ALA:C	21:C:484:CLA:HBA1	2.23	0.59
21:C:480:CLA:H43	26:C:492:DGD:HA91	1.85	0.59
6:F:23:VAL:O	6:F:27:ALA:HB2	2.03	0.59
3:C:112:PHE:O	3:C:116:VAL:HG13	2.03	0.58
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:437:PHE:HA	21:C:484:CLA:HMC3	1.86	0.58
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.68	0.58
3:C:369:LEU:HD21	3:C:384:ILE:HD13	1.85	0.58
21:C:481:CLA:H12	8:I:23:PHE:CD2	2.38	0.58
4:D:55:VAL:HG21	4:D:110:LEU:CD1	2.33	0.58
9:J:22:ILE:HG13	25:J:115:BCR:H10C	1.85	0.58
13:O:80:GLU:O	13:O:89:ALA:HB1	2.03	0.58
1:A:238:LYS:O	1:A:241:GLN:HG3	2.03	0.58
3:C:380:ILE:HA	3:C:384:ILE:HD11	1.85	0.58
3:C:418:ASN:CA	26:C:493:DGD:HE2	2.34	0.58
3:C:95:LEU:HD11	21:C:479:CLA:HBA2	1.83	0.58
29:D:360:LMG:O9	29:D:360:LMG:HC72	2.03	0.58
5:E:8:ARG:N	6:F:13:TYR:CE1	2.71	0.58
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.86	0.58
3:C:28:GLN:HB2	21:C:486:CLA:HED2	1.86	0.58
4:D:32:TRP:CG	28:D:361:SQD:H251	2.38	0.58
10:K:17:ILE:HD12	10:K:17:ILE:H	1.69	0.58
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.04	0.58
5:E:76:VAL:O	5:E:80:LEU:HD22	2.03	0.58
5:E:15:THR:HG23	9:J:8:ILE:H	1.68	0.58
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.86	0.58
2:B:262:THR:HG21	21:B:513:CLA:HBA2	1.86	0.58
21:B:516:CLA:H161	21:B:526:CLA:H161	1.84	0.58
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.67	0.58
2:B:150:CYS:HA	21:B:513:CLA:HBC2	1.85	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD13	21:D:354:CLA:HBA2	1.86	0.58
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.03	0.58
1:A:205:VAL:HG21	21:A:362:CLA:HMA1	1.86	0.58
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.58
3:C:52:ALA:HA	21:C:486:CLA:CMB	2.31	0.58
13:O:123:GLU:HG2	13:O:124:GLU:N	2.18	0.58
15:U:38:GLU:HG2	15:U:39:LEU:H	1.68	0.58
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.34	0.58
19:Z:14:ILE:O	19:Z:18:VAL:HG23	2.04	0.58
2:B:462:PHE:HA	21:B:521:CLA:CMC	2.33	0.58
3:C:122:SER:OG	25:C:489:BCR:H14C	2.04	0.58
3:C:305:THR:HG23	3:C:307:PRO:CD	2.32	0.58
4:D:239:GLN:O	4:D:240:ALA:HB3	2.03	0.58
1:A:203:ALA:HB1	26:C:493:DGD:HBV2	1.86	0.57
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:7:ARG:C	11:L:8:GLN:HE21	2.06	0.57
3:C:80:PRO:HD2	16:V:129:LYS:HZ1	1.69	0.57
3:C:60:ILE:HG21	21:C:479:CLA:C19	2.34	0.57
32:D:357:PL9:H43	29:D:360:LMG:C25	2.34	0.57
9:J:14:ALA:HB1	25:J:112:BCR:C38	2.34	0.57
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.87	0.57
3:C:289:PHE:CD1	21:C:477:CLA:H12	2.38	0.57
3:C:447:ARG:CG	3:C:447:ARG:HH11	2.14	0.57
32:D:357:PL9:H303	32:D:357:PL9:H23	1.87	0.57
5:E:15:THR:O	9:J:8:ILE:HD12	2.03	0.57
3:C:272:LEU:HA	21:C:485:CLA:HMD3	1.86	0.57
3:C:362:ARG:HG2	26:C:491:DGD:HE61	1.86	0.57
26:C:493:DGD:O3D	9:J:37:GLY:O	2.22	0.57
2:B:393:GLU:HG2	15:U:44:ASP:O	2.03	0.57
19:Z:55:GLY:CA	25:Z:116:BCR:H312	2.34	0.57
2:B:224:ARG:NE	7:H:25:TRP:NE1	2.52	0.57
2:B:150:CYS:CA	21:B:513:CLA:HBC2	2.35	0.57
4:D:252:PHE:O	4:D:256:ILE:HG22	2.05	0.57
4:D:279:LEU:CD1	21:D:354:CLA:HBA2	2.35	0.57
6:F:20:TRP:O	6:F:24:HIS:HB2	2.04	0.57
1:A:234:ASN:HB2	29:A:373:LMG:HC3	1.87	0.57
3:C:39:ASN:HB2	21:C:484:CLA:HBA2	1.85	0.57
4:D:122:LEU:HD21	22:D:355:PHO:H62	1.86	0.57
4:D:188:PHE:HE2	4:D:329:MET:CE	2.17	0.57
7:H:63:LYS:O	7:H:65:LEU:N	2.37	0.57
16:V:74:THR:O	16:V:75:ASN:HB2	2.04	0.57
21:B:511:CLA:HMD2	21:B:511:CLA:H152	1.87	0.57
21:B:521:CLA:OBD	29:B:531:LMG:HC8	2.05	0.57
1:A:214:MET:HB3	23:A:367:MES:C6	2.33	0.57
1:A:233:ALA:HB3	29:B:531:LMG:HC4	1.86	0.57
29:D:360:LMG:C20	11:L:22:LEU:HD11	2.34	0.57
12:M:29:THR:O	12:M:32:GLN:HG3	2.05	0.57
1:A:244:GLU:HG3	1:A:246:TYR:H	1.70	0.57
1:A:38:ILE:O	1:A:42:LEU:HG	2.05	0.57
2:B:230:ARG:O	2:B:233:ASN:HB3	2.05	0.57
2:B:262:THR:HG21	21:B:513:CLA:CBA	2.35	0.57
3:C:343:ARG:NH1	3:C:347:GLY:O	2.38	0.57
5:E:84:LYS:HB2	5:E:84:LYS:HZ3	1.70	0.57
10:K:31:LEU:O	10:K:34:ALA:HB3	2.04	0.57
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.34	0.57
18:X:45:LYS:HD3	18:X:45:LYS:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD11	26:C:491:DGD:HA91	1.86	0.56
2:B:256:MET:HA	2:B:263:THR:HG21	1.87	0.56
2:B:110:ALA:CB	21:B:526:CLA:HMB2	2.34	0.56
26:B:528:DGD:HO2D	4:D:87:HIS:CB	2.09	0.56
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.88	0.56
4:D:152:VAL:HG21	4:D:279:LEU:CD1	2.35	0.56
4:D:113:PHE:CE2	25:D:358:BCR:HC41	2.40	0.56
10:K:26:PRO:O	10:K:29:PRO:HD2	2.05	0.56
1:A:13:LEU:HD12	1:A:13:LEU:H	1.69	0.56
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.87	0.56
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.88	0.56
3:C:305:THR:HG22	3:C:308:GLU:N	2.16	0.56
3:C:374:GLY:O	3:C:375:LEU:C	2.44	0.56
21:C:477:CLA:H141	21:C:483:CLA:HMA1	1.87	0.56
29:A:373:LMG:H202	32:D:357:PL9:H201	1.86	0.56
4:D:36:LEU:O	4:D:39:PRO:HD2	2.05	0.56
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.70	0.56
18:X:12:ILE:CG1	18:X:16:LEU:HD12	2.33	0.56
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.35	0.56
7:H:12:ARG:HD3	7:H:12:ARG:C	2.24	0.56
1:A:193:LEU:HD21	21:A:362:CLA:C2C	2.36	0.56
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.41	0.56
29:A:373:LMG:C25	29:D:360:LMG:C22	2.83	0.56
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.40	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
19:Z:16:SER:O	19:Z:20:VAL:HG23	2.04	0.56
4:D:18:LEU:O	4:D:22:LEU:HG	2.05	0.56
13:O:178:ARG:NH1	13:O:178:ARG:CG	2.55	0.56
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.88	0.56
7:H:58:VAL:O	7:H:58:VAL:CG1	2.53	0.56
11:L:11:GLU:HG2	11:L:12:LEU:N	2.19	0.56
4:D:18:LEU:HD22	18:X:38:ILE:HD13	1.86	0.56
3:C:113:VAL:CG1	29:C:494:LMG:H192	2.36	0.56
2:B:224:ARG:HG3	7:H:25:TRP:CD1	2.41	0.56
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.41	0.56
10:K:10:LYS:O	10:K:11:LEU:C	2.43	0.56
13:O:31:LEU:HD12	13:O:31:LEU:H	1.71	0.56
4:D:267:LEU:HD23	4:D:267:LEU:O	2.06	0.56
4:D:85:MET:CE	5:E:69:ARG:HA	2.36	0.56
13:O:88:GLU:OE2	13:O:90:GLU:HG2	2.06	0.56
1:A:292:THR:OG1	26:C:492:DGD:CEA	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:PHE:CZ	25:D:358:BCR:HC41	2.41	0.56
6:F:18:VAL:HG13	6:F:19:ARG:N	2.21	0.56
15:U:89:GLU:CD	15:U:89:GLU:H	2.09	0.56
16:V:87:LEU:HD12	16:V:87:LEU:N	2.20	0.56
1:A:187:GLN:HB2	21:A:362:CLA:HAC2	1.88	0.55
19:Z:26:ALA:CB	19:Z:40:ILE:HD11	2.36	0.55
21:A:362:CLA:H202	21:A:363:CLA:H112	1.88	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CE2	2.41	0.55
3:C:167:VAL:CG1	21:C:487:CLA:H11	2.36	0.55
19:Z:21:ILE:O	19:Z:25:VAL:HG22	2.07	0.55
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.08	0.55
3:C:107:ASP:OD2	3:C:109:PHE:HB3	2.06	0.55
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.88	0.55
1:A:37:MET:HG2	1:A:41:LEU:HD12	1.89	0.55
21:B:512:CLA:H203	26:B:528:DGD:HB91	1.88	0.55
25:J:112:BCR:HC31	10:K:21:LEU:HD21	1.89	0.55
1:A:217:SER:HA	1:A:220:THR:HG22	1.88	0.55
3:C:199:ILE:N	3:C:199:ILE:HD12	2.22	0.55
4:D:48:TRP:CE2	22:D:355:PHO:H161	2.42	0.55
5:E:30:LEU:HD12	33:F:85:HEM:HMC1	1.88	0.55
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.42	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.87	0.55
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.41	0.55
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.88	0.55
3:C:239:TRP:CE3	3:C:243:ILE:HD11	2.42	0.55
3:C:337:LEU:HD12	13:O:131:PRO:HG3	1.88	0.55
3:C:286:ALA:HB2	21:C:478:CLA:HMD1	1.88	0.55
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.42	0.55
2:B:191:ASN:HD21	7:H:60:VAL:HA	1.72	0.55
16:V:59:PHE:HA	16:V:63:CYS:SG	2.47	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CZ2	2.42	0.55
21:C:478:CLA:H122	21:C:479:CLA:HMB2	1.89	0.55
8:I:11:VAL:O	8:I:15:PHE:HD2	1.89	0.55
13:O:227:VAL:HG12	13:O:228:ALA:N	2.22	0.55
18:X:32:LEU:N	18:X:32:LEU:HD23	2.22	0.55
19:Z:29:SER:HB2	19:Z:31:GLN:HG3	1.88	0.55
2:B:100:HIS:CE1	21:B:516:CLA:H11	2.42	0.55
21:C:477:CLA:HMB3	25:C:490:BCR:C40	2.30	0.55
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.22	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.89	0.55
19:Z:23:VAL:O	19:Z:26:ALA:HB3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:371:LHG:HC2	4:D:229:ALA:HB1	1.87	0.55
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.70	0.55
19:Z:36:SER:OG	19:Z:39:LEU:HD12	2.07	0.55
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.36	0.54
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.22	0.54
4:D:85:MET:HE2	5:E:69:ARG:HA	1.89	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.75	0.54
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.07	0.54
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.88	0.54
21:B:520:CLA:H111	21:B:525:CLA:HAA1	1.88	0.54
3:C:127:PHE:HE1	19:Z:23:VAL:HG21	1.72	0.54
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.90	0.54
3:C:55:ALA:HB1	25:C:489:BCR:H373	1.89	0.54
5:E:55:TYR:O	5:E:84:LYS:HE3	2.07	0.54
13:O:141:ARG:HH11	13:O:141:ARG:HG2	1.71	0.54
13:O:154:SER:O	13:O:168:PHE:HA	2.07	0.54
29:A:373:LMG:C25	29:D:360:LMG:H222	2.37	0.54
3:C:54:VAL:CG1	21:C:488:CLA:HMC3	2.36	0.54
2:B:238:LEU:CB	21:B:522:CLA:HMD3	2.37	0.54
3:C:155:ASN:O	3:C:158:THR:HG22	2.07	0.54
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.89	0.54
4:D:152:VAL:HG11	21:D:354:CLA:C1	2.34	0.54
4:D:152:VAL:HG11	21:D:354:CLA:HBA1	1.88	0.54
2:B:169:SER:O	7:H:65:LEU:HD13	2.06	0.54
28:L:213:SQD:H261	29:M:217:LMG:H191	1.90	0.54
15:U:66:ILE:CG2	15:U:66:ILE:O	2.56	0.54
1:A:197:PHE:CE2	26:C:492:DGD:CEA	2.90	0.54
21:C:477:CLA:H3A	21:C:477:CLA:O2A	2.08	0.54
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.07	0.54
19:Z:36:SER:HA	19:Z:39:LEU:CG	2.35	0.54
2:B:247:PHE:CE1	21:B:512:CLA:H8	2.33	0.54
21:B:518:CLA:H111	4:D:120:PHE:CE1	2.42	0.54
4:D:180:ARG:HG3	4:D:180:ARG:NH1	2.23	0.54
5:E:84:LYS:HZ2	5:E:84:LYS:HB2	1.68	0.54
1:A:45:THR:OG1	21:A:363:CLA:H141	2.08	0.54
21:C:477:CLA:C3D	21:C:479:CLA:H2	2.38	0.54
15:U:100:ARG:O	15:U:103:GLN:HB3	2.07	0.54
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.89	0.54
3:C:53:HIS:CB	21:C:487:CLA:HMD1	2.38	0.54
21:B:519:CLA:HAC2	7:H:34:PHE:CE2	2.43	0.54
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:135:GLU:O	16:V:139:VAL:HG23	2.08	0.54
4:D:303:ILE:HD13	12:M:2:GLU:HG2	1.88	0.54
6:F:43:ILE:HG22	9:J:36:LEU:HD21	1.90	0.54
13:O:218:LEU:HD22	15:U:119:THR:CG2	2.35	0.54
1:A:183:MET:HE1	21:A:363:CLA:HMD3	1.90	0.54
21:B:511:CLA:HBB2	7:H:44:ILE:HG21	1.90	0.54
2:B:474:LEU:O	4:D:134:ARG:NH1	2.41	0.54
21:A:364:CLA:H203	29:D:359:LMG:H402	1.89	0.54
19:Z:35:ARG:O	19:Z:38:GLN:HB3	2.07	0.54
3:C:125:LEU:HD22	21:C:487:CLA:CED	2.37	0.53
7:H:12:ARG:N	7:H:13:PRO:HD2	2.23	0.53
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.90	0.53
4:D:239:GLN:O	4:D:240:ALA:CB	2.55	0.53
4:D:86:GLY:O	4:D:166:SER:HB2	2.08	0.53
5:E:15:THR:O	9:J:8:ILE:CD1	2.56	0.53
3:C:418:ASN:HB2	26:C:493:DGD:HE2	1.89	0.53
3:C:165:LEU:HD21	21:C:482:CLA:HBB1	1.89	0.53
26:C:492:DGD:HG11	29:J:492:LMG:H301	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.90	0.53
32:D:357:PL9:H352	11:L:26:VAL:HB	1.90	0.53
2:B:235:GLU:O	2:B:235:GLU:HG2	2.08	0.53
21:B:521:CLA:H52	21:B:524:CLA:CB	2.38	0.53
25:B:530:BCR:HC31	30:B:535:LMT:H72	1.90	0.53
3:C:223:TRP:CH2	26:C:474:DGD:HA62	2.44	0.53
3:C:174:LEU:HD12	21:C:487:CLA:H51	1.89	0.53
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.91	0.53
10:K:43:VAL:O	10:K:43:VAL:HG13	2.09	0.53
2:B:10:THR:C	2:B:12:LEU:H	2.12	0.53
2:B:150:CYS:N	21:B:513:CLA:HBC2	2.23	0.53
2:B:471:ALA:HB2	4:D:130:PHE:CE2	2.44	0.53
9:J:15:THR:O	9:J:19:MET:HG3	2.08	0.53
3:C:416:SER:H	26:C:493:DGD:C3E	2.22	0.53
3:C:425:TRP:CZ2	21:C:480:CLA:HBA2	2.44	0.53
1:A:160:ILE:HD11	26:C:491:DGD:HA81	1.90	0.53
3:C:407:VAL:CG2	26:C:493:DGD:O2E	2.55	0.53
21:B:512:CLA:H201	4:D:159:ILE:HG12	1.89	0.53
12:M:25:LEU:O	12:M:28:GLN:HG3	2.08	0.53
13:O:82:PRO:HB3	13:O:87:GLN:HG3	1.89	0.53
16:V:116:GLU:O	16:V:116:GLU:HG3	2.08	0.53
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.37	0.53
2:B:106:LEU:HD22	21:B:516:CLA:H193	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:404:LEU:CD2	26:C:493:DGD:HA31	2.37	0.53
3:C:54:VAL:HA	21:C:487:CLA:CED	2.39	0.53
1:A:193:LEU:HD11	21:A:362:CLA:HMC3	1.91	0.53
21:A:363:CLA:H101	29:D:360:LMG:C25	2.39	0.53
3:C:406:SER:O	26:C:493:DGD:O2E	2.23	0.53
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.91	0.53
7:H:55:LEU:O	7:H:58:VAL:HG12	2.09	0.53
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.09	0.53
3:C:53:HIS:HB3	21:C:487:CLA:OBD	2.09	0.53
25:C:489:BCR:C11	25:J:112:BCR:H322	2.38	0.53
32:D:357:PL9:C35	11:L:26:VAL:HB	2.38	0.53
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.90	0.53
33:V:164:HEM:HMA2	33:V:164:HEM:HBA1	1.90	0.53
4:D:18:LEU:HD22	18:X:38:ILE:CD1	2.38	0.53
21:B:515:CLA:H92	21:B:522:CLA:H18	1.91	0.53
4:D:238:THR:O	4:D:239:GLN:O	2.27	0.53
4:D:261:PHE:CB	32:D:357:PL9:H522	2.39	0.53
1:A:107:TYR:HD1	13:O:141:ARG:NH1	2.05	0.53
19:Z:30:PRO:C	19:Z:32:ASP:H	2.12	0.53
21:B:520:CLA:O1D	21:B:520:CLA:H121	2.09	0.52
3:C:449:ARG:HG2	21:C:481:CLA:HED3	1.91	0.52
26:C:493:DGD:O2D	9:J:32:ALA:HB1	2.10	0.52
25:D:358:BCR:H391	9:J:21:VAL:HG11	1.91	0.52
10:K:24:VAL:O	10:K:27:VAL:HG12	2.10	0.52
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.07	0.52
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.90	0.52
3:C:239:TRP:HE3	3:C:243:ILE:HD11	1.74	0.52
3:C:391:ARG:CB	3:C:391:ARG:HH11	2.19	0.52
21:C:484:CLA:H43	21:C:486:CLA:HAC1	1.90	0.52
1:A:278:TRP:HA	26:C:493:DGD:CIA	2.38	0.52
4:D:44:ALA:CB	22:D:355:PHO:H92	2.39	0.52
15:U:100:ARG:HH11	15:U:103:GLN:HG2	1.73	0.52
13:O:190:LEU:HD12	15:U:41:ASN:ND2	2.24	0.52
19:Z:3:ILE:O	19:Z:7:LEU:HG	2.09	0.52
3:C:216:SER:HB2	26:C:474:DGD:HG31	1.91	0.52
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.91	0.52
27:C:476:LHG:H142	25:J:115:BCR:HC21	1.89	0.52
2:B:143:LEU:CA	21:B:520:CLA:HED1	2.39	0.52
2:B:464:PHE:CD2	21:B:521:CLA:HAC2	2.44	0.52
26:B:528:DGD:HE5	26:B:528:DGD:C6D	2.39	0.52
2:B:7:ARG:HE	21:B:521:CLA:HED1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.73	0.52
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.40	0.52
4:D:76:VAL:O	4:D:77:ALA:HB2	2.10	0.52
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.92	0.52
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.38	0.52
19:Z:55:GLY:N	25:Z:116:BCR:H312	2.23	0.52
1:A:218:LEU:HD23	23:A:367:MES:H72	1.90	0.52
21:C:480:CLA:H193	26:C:492:DGD:HBV1	1.91	0.52
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.45	0.52
1:A:334:ARG:HD2	13:O:183:LEU:HB2	1.92	0.52
26:B:533:DGD:HAE1	12:M:17:VAL:HG21	1.92	0.52
3:C:452:ALA:O	3:C:454:GLY:N	2.42	0.52
3:C:405:ASN:CB	26:C:493:DGD:HG32	2.40	0.52
29:D:360:LMG:H212	14:T:17:PHE:CZ	2.28	0.52
2:B:191:ASN:ND2	7:H:60:VAL:HA	2.24	0.52
1:A:334:ARG:NH1	13:O:183:LEU:O	2.42	0.52
13:O:240:THR:HA	13:O:264:VAL:HA	1.92	0.52
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.34	0.52
21:C:486:CLA:HMB2	25:C:489:BCR:H382	1.92	0.52
9:J:11:TRP:CG	10:K:42:ALA:HA	2.45	0.52
15:U:83:ALA:CB	15:U:84:PRO:CD	2.77	0.52
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.75	0.52
2:B:341:LYS:HD2	2:B:429:ILE:HG22	1.90	0.52
3:C:193:GLY:O	3:C:194:GLY:C	2.48	0.52
3:C:393:ALA:HB1	33:V:164:HEM:HBC1	1.91	0.52
3:C:447:ARG:NH1	3:C:447:ARG:HG2	2.16	0.52
3:C:47:GLY:O	3:C:50:LEU:HB3	2.10	0.52
4:D:221:THR:HG23	4:D:221:THR:O	2.10	0.52
13:O:141:ARG:HG2	13:O:141:ARG:NH1	2.24	0.52
15:U:66:ILE:HG13	15:U:72:TYR:CD1	2.44	0.52
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.74	0.52
19:Z:31:GLN:O	19:Z:32:ASP:HB3	2.10	0.52
1:A:49:VAL:O	1:A:53:ILE:HG13	2.10	0.52
3:C:281:MET:CE	21:C:481:CLA:HAC2	2.40	0.52
3:C:271:TYR:CE1	21:C:483:CLA:HAC1	2.44	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
11:L:1:MET:CG	11:L:1:MET:O	2.48	0.52
2:B:12:LEU:CD2	2:B:18:ARG:HB2	2.40	0.52
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.52
19:Z:32:ASP:C	19:Z:34:ASP:N	2.60	0.52
1:A:228:THR:HG22	1:A:229:GLU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:334:GLN:N	4:D:335:PRO:HD3	2.25	0.51
5:E:61:ARG:NH2	16:V:153:GLY:HA3	2.25	0.51
4:D:136:VAL:O	4:D:136:VAL:HG12	2.10	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.45	0.51
4:D:346:LEU:O	4:D:348:ARG:HG3	2.10	0.51
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.75	0.51
2:B:222:PRO:CG	7:H:27:THR:H	2.21	0.51
25:D:358:BCR:H391	25:J:115:BCR:H332	1.91	0.51
10:K:30:VAL:HA	21:K:483:CLA:H191	1.93	0.51
19:Z:32:ASP:OD1	19:Z:36:SER:HB2	2.11	0.51
1:A:202:VAL:HG11	21:A:364:CLA:OBD	2.09	0.51
3:C:346:THR:O	13:O:40:GLY:HA2	2.10	0.51
16:V:147:VAL:O	16:V:150:LYS:HB2	2.10	0.51
7:H:38:PHE:HB2	25:X:107:BCR:H10C	1.92	0.51
18:X:12:ILE:CG2	18:X:12:ILE:O	2.58	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.45	0.51
3:C:227:VAL:HG11	25:C:490:BCR:H282	1.93	0.51
3:C:95:LEU:CD1	21:C:479:CLA:HBA2	2.40	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
1:A:334:ARG:NH1	13:O:184:ASP:C	2.64	0.51
2:B:334:ASP:HB3	13:O:202:GLN:HG3	1.92	0.51
2:B:149:LEU:HD22	21:B:514:CLA:H161	1.92	0.51
21:B:518:CLA:H143	21:D:356:CLA:HMB2	1.93	0.51
1:A:78:ILE:O	1:A:176:ILE:HB	2.10	0.51
1:A:183:MET:HB3	21:A:362:CLA:HBC2	1.92	0.51
1:A:150:PRO:O	21:A:362:CLA:H43	2.11	0.51
21:A:363:CLA:HED2	4:D:198:MET:SD	2.50	0.51
3:C:128:GLY:HA3	21:C:488:CLA:C3C	2.40	0.51
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.10	0.51
3:C:60:ILE:HG23	21:K:483:CLA:HMC2	1.92	0.51
5:E:15:THR:CG2	9:J:7:ARG:CB	2.85	0.51
25:J:112:BCR:C15	10:K:31:LEU:HB3	2.41	0.51
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.35	0.51
2:B:327:THR:HG22	21:B:517:CLA:H12	1.92	0.51
3:C:415:ASN:O	3:C:416:SER:CB	2.57	0.51
5:E:81:GLU:C	5:E:83:LEU:N	2.64	0.51
13:O:118:SER:HB3	13:O:157:PRO:HA	1.93	0.51
19:Z:47:TRP:O	19:Z:50:LEU:HB2	2.11	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.92	0.51
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.11	0.51
10:K:17:ILE:H	10:K:17:ILE:CD1	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.41	0.51
2:B:229:LEU:O	2:B:231:MET:N	2.43	0.51
3:C:158:THR:HG21	3:C:254:THR:O	2.10	0.51
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.91	0.51
13:O:59:ASP:C	13:O:61:SER:H	2.14	0.51
18:X:17:LYS:O	18:X:21:ILE:HG13	2.10	0.51
2:B:293:ALA:C	2:B:295:GLY:H	2.14	0.51
2:B:91:TRP:HE1	30:B:535:LMT:H41	1.75	0.51
10:K:25:LEU:HB2	10:K:26:PRO:HD3	1.93	0.51
29:A:373:LMG:O4	11:L:13:ASN:ND2	2.44	0.51
15:U:72:TYR:O	15:U:73:PRO:C	2.48	0.51
16:V:30:THR:HB	16:V:31:PRO:CD	2.35	0.51
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.46	0.50
19:Z:17:PHE:CE2	19:Z:21:ILE:HD11	2.45	0.50
1:A:227:THR:HA	1:A:231:GLU:OE2	2.10	0.50
21:B:518:CLA:HBA1	28:D:361:SQD:H101	1.93	0.50
2:B:55:MET:CE	2:B:80:ILE:HD12	2.42	0.50
21:B:518:CLA:HMB2	4:D:127:LEU:HG	1.93	0.50
21:A:364:CLA:HBB1	4:D:157:PHE:CE2	2.45	0.50
4:D:86:GLY:HA2	4:D:166:SER:HB3	1.93	0.50
19:Z:5:PHE:HA	19:Z:57:LEU:CD2	2.40	0.50
2:B:125:ASP:OD2	2:B:127:ARG:HB3	2.11	0.50
3:C:137:PRO:HB2	3:C:139:THR:O	2.12	0.50
3:C:250:TRP:CD1	3:C:250:TRP:C	2.84	0.50
21:C:481:CLA:O1A	8:I:23:PHE:CZ	2.64	0.50
21:A:364:CLA:HED1	26:C:493:DGD:HBW2	1.93	0.50
3:C:81:MET:CE	3:C:89:ILE:HG22	2.41	0.50
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.40	0.50
4:D:99:GLY:HA3	30:D:363:LMT:H2'	1.94	0.50
8:I:27:ASP:N	8:I:28:PRO:CD	2.74	0.50
13:O:271:PRO:HG2	13:O:272:ALA:H	1.76	0.50
1:A:20:TRP:O	1:A:21:VAL:C	2.50	0.50
29:A:373:LMG:C25	29:D:360:LMG:H231	2.41	0.50
2:B:137:LYS:O	2:B:141:ILE:HG13	2.11	0.50
26:C:493:DGD:HG31	9:J:33:TYR:CZ	2.47	0.50
26:C:493:DGD:HB51	29:D:359:LMG:H121	1.94	0.50
18:X:16:LEU:HD13	18:X:16:LEU:C	2.31	0.50
1:A:283:VAL:O	1:A:286:THR:HG22	2.11	0.50
29:A:373:LMG:HC61	11:L:11:GLU:OE2	2.11	0.50
2:B:250:PHE:O	26:B:528:DGD:HB82	2.11	0.50
4:D:53:THR:HG22	4:D:67:TYR:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.92	0.50
7:H:62:TRP:O	7:H:63:LYS:O	2.30	0.50
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.93	0.50
3:C:155:ASN:CA	3:C:158:THR:HG22	2.39	0.50
3:C:159:THR:HG23	3:C:252:ILE:HD13	1.93	0.50
32:D:357:PL9:H301	32:D:357:PL9:H33	1.93	0.50
13:O:94:THR:HB	13:O:135:GLN:O	2.12	0.50
30:D:363:LMT:O2'	18:X:21:ILE:HD12	2.11	0.50
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.93	0.50
21:B:512:CLA:H43	21:B:512:CLA:HBD	1.92	0.50
21:C:481:CLA:HAA2	21:C:481:CLA:HBD	1.92	0.50
21:C:486:CLA:H13	19:Z:20:VAL:HG13	1.93	0.50
4:D:180:ARG:CG	4:D:180:ARG:NH1	2.70	0.50
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.93	0.50
1:A:126:TYR:OH	22:A:365:PHO:O1D	2.23	0.50
3:C:116:VAL:CG1	25:C:489:BCR:H332	2.40	0.50
3:C:405:ASN:HA	26:C:493:DGD:C1G	2.40	0.50
3:C:72:LEU:HD11	3:C:108:THR:HB	1.93	0.50
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.34	0.50
13:O:43:ASN:OD1	13:O:103:SER:HB2	2.12	0.50
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.92	0.50
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.40	0.50
3:C:224:ILE:CD1	21:C:477:CLA:H93	2.42	0.50
19:Z:5:PHE:CE1	19:Z:54:VAL:HG13	2.46	0.50
1:A:106:LEU:HD11	25:A:369:BCR:H402	1.94	0.49
1:A:239:PHE:O	14:T:29:ILE:HA	2.12	0.49
2:B:23:HIS:C	21:B:525:CLA:HED1	2.33	0.49
26:B:533:DGD:HAW2	12:M:13:LEU:HD13	1.93	0.49
3:C:155:ASN:HA	3:C:158:THR:CG2	2.38	0.49
7:H:63:LYS:C	7:H:65:LEU:N	2.65	0.49
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.47	0.49
21:B:511:CLA:HMC1	21:B:511:CLA:HBC3	1.92	0.49
3:C:126:GLY:O	3:C:130:VAL:HG23	2.12	0.49
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.47	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
18:X:43:ILE:O	18:X:43:ILE:HG22	2.12	0.49
1:A:215:HIS:N	23:A:367:MES:H61	2.27	0.49
29:A:373:LMG:H202	32:D:357:PL9:C21	2.40	0.49
3:C:264:PHE:CE1	21:C:483:CLA:HBB1	2.48	0.49
3:C:405:ASN:CA	26:C:493:DGD:HG12	2.42	0.49
3:C:449:ARG:HG2	21:C:481:CLA:CED	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:484:CLA:C4	21:C:486:CLA:HAC1	2.42	0.49
3:C:33:PHE:CE1	4:D:229:ALA:CB	2.96	0.49
29:D:360:LMG:H192	11:L:22:LEU:CD2	2.42	0.49
2:B:256:MET:O	2:B:448:ARG:NH1	2.42	0.49
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.01	0.49
19:Z:12:LEU:HB2	19:Z:50:LEU:HD22	1.93	0.49
3:C:165:LEU:HD21	21:C:482:CLA:CHC	2.43	0.49
4:D:192:THR:HG23	21:D:354:CLA:CBC	2.39	0.49
2:B:134:ASP:OD2	2:B:137:LYS:HB2	2.12	0.49
2:B:183:PRO:HB2	2:B:185:TRP:CH2	2.46	0.49
2:B:286:ARG:NH1	2:B:286:ARG:HG2	2.26	0.49
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.95	0.49
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.49
5:E:30:LEU:CD1	6:F:28:VAL:HG13	2.41	0.49
7:H:53:LEU:HD12	18:X:19:PHE:CD1	2.47	0.49
13:O:159:VAL:O	13:O:159:VAL:HG13	2.13	0.49
13:O:59:ASP:HB3	13:O:62:GLN:HB3	1.93	0.49
19:Z:5:PHE:HA	19:Z:57:LEU:HD21	1.95	0.49
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.12	0.49
21:B:526:CLA:HMD1	7:H:5:THR:OG1	2.12	0.49
3:C:281:MET:HE1	21:C:481:CLA:HAC2	1.94	0.49
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.46	0.49
2:B:26:HIS:HB2	21:B:522:CLA:HMB2	1.93	0.49
21:B:518:CLA:H161	21:B:519:CLA:H203	1.95	0.49
4:D:283:ALA:HA	21:D:354:CLA:CED	2.43	0.49
9:J:34:ALA:O	9:J:35:GLY:O	2.31	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.13	0.49
3:C:89:ILE:N	3:C:90:PRO:CD	2.75	0.49
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.94	0.49
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.95	0.49
21:C:478:CLA:CGA	21:C:479:CLA:H11	2.43	0.49
21:C:481:CLA:CB	21:C:481:CLA:HAA2	2.41	0.49
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.73	0.49
4:D:126:MET:CE	4:D:150:ILE:HG13	2.43	0.49
29:A:373:LMG:H192	32:D:357:PL9:C23	2.43	0.49
6:F:9:GLU:C	6:F:11:VAL:H	2.15	0.49
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.93	0.49
11:L:12:LEU:HD22	12:M:25:LEU:HD12	1.93	0.49
26:B:533:DGD:C3G	12:M:6:LEU:HD12	2.38	0.49
13:O:126:GLY:O	13:O:128:ASP:N	2.45	0.49
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:486:CLA:H111	10:K:32:PHE:HE1	1.77	0.48
10:K:30:VAL:HA	21:K:483:CLA:H201	1.94	0.48
16:V:95:ILE:O	16:V:99:VAL:HG23	2.12	0.48
1:A:13:LEU:CD1	1:A:13:LEU:H	2.27	0.48
1:A:235:TYR:C	1:A:237:TYR:H	2.16	0.48
21:B:520:CLA:H11	21:B:522:CLA:H201	1.95	0.48
3:C:116:VAL:HG23	3:C:117:VAL:N	2.28	0.48
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.94	0.48
5:E:28:PRO:O	5:E:32:ILE:HG13	2.13	0.48
9:J:14:ALA:HB1	25:J:112:BCR:H382	1.94	0.48
13:O:226:ASN:HD22	13:O:226:ASN:N	2.11	0.48
18:X:42:GLN:O	18:X:43:ILE:HG13	2.12	0.48
1:A:224:ILE:O	1:A:226:GLU:OE2	2.30	0.48
3:C:167:VAL:HG13	21:C:487:CLA:H11	1.96	0.48
3:C:315:MET:O	3:C:319:ILE:HG13	2.12	0.48
3:C:390:ARG:NH2	16:V:126:ILE:HD13	2.29	0.48
4:D:210:LEU:HD21	32:D:357:PL9:H13	1.95	0.48
6:F:31:ILE:CD1	6:F:31:ILE:N	2.76	0.48
13:O:223:ILE:HG12	13:O:224:SER:N	2.27	0.48
33:V:164:HEM:CMA	33:V:164:HEM:HBA1	2.42	0.48
18:X:32:LEU:O	18:X:36:VAL:HG23	2.13	0.48
21:C:486:CLA:H161	19:Z:20:VAL:HG13	1.94	0.48
1:A:193:LEU:HD21	21:A:362:CLA:HMC3	1.94	0.48
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.48	0.48
2:B:35:GLY:O	2:B:38:ALA:HB3	2.13	0.48
4:D:60:THR:HG23	4:D:61:HIS:HD2	1.75	0.48
13:O:86:ARG:HG3	13:O:86:ARG:NH1	2.26	0.48
2:B:154:GLY:O	2:B:159:THR:HG23	2.13	0.48
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.49	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.14	0.48
21:B:519:CLA:HMD1	7:H:27:THR:HB	1.95	0.48
29:D:360:LMG:C22	14:T:13:ILE:HG21	2.36	0.48
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.48
1:A:193:LEU:HD11	21:A:362:CLA:CMC	2.43	0.48
1:A:199:GLN:NE2	21:A:364:CLA:HED2	2.29	0.48
3:C:315:MET:CE	3:C:366:LEU:HD13	2.44	0.48
21:A:366:CLA:C1	26:C:474:DGD:HB22	2.44	0.48
3:C:91:HIS:NE2	21:C:478:CLA:HBA1	2.28	0.48
4:D:274:VAL:HA	32:D:357:PL9:H253	1.95	0.48
26:B:528:DGD:HD3	4:D:87:HIS:ND1	2.29	0.48
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:483:CLA:H192	21:K:483:CLA:HMD3	1.96	0.48
4:D:303:ILE:CD1	12:M:2:GLU:HG2	2.44	0.48
21:B:516:CLA:H62	25:B:530:BCR:H342	1.95	0.48
29:A:373:LMG:H312	12:M:22:LEU:HD11	1.95	0.48
2:B:458:PHE:CG	21:B:514:CLA:HMC3	2.49	0.48
3:C:135:ARG:HB2	19:Z:27:TYR:CB	2.42	0.48
21:C:480:CLA:C4	26:C:493:DGD:HA32	2.43	0.48
21:C:486:CLA:C4D	10:K:39:TRP:HH2	2.26	0.48
3:C:71:GLU:OE1	3:C:89:ILE:HG13	2.13	0.48
4:D:180:ARG:HG3	4:D:180:ARG:HH11	1.79	0.48
21:B:513:CLA:H52	21:B:513:CLA:HMB2	1.94	0.48
21:B:523:CLA:H161	25:B:529:BCR:H312	1.96	0.48
3:C:154:LYS:HE2	3:C:261:ARG:HD2	1.94	0.48
3:C:413:GLU:HG3	3:C:414:ILE:H	1.78	0.48
4:D:201:VAL:O	4:D:205:LEU:HB2	2.13	0.48
4:D:26:ARG:HD3	6:F:18:VAL:HG21	1.95	0.48
10:K:11:LEU:HD12	10:K:19:ASP:HA	1.96	0.48
2:B:328:GLY:C	21:B:517:CLA:HBA1	2.34	0.48
21:B:512:CLA:H42	7:H:45:ILE:CD1	2.44	0.48
2:B:9:HIS:HB2	21:B:521:CLA:O1A	2.13	0.48
21:B:523:CLA:H61	21:B:523:CLA:H41	1.59	0.48
3:C:413:GLU:HG3	3:C:414:ILE:N	2.28	0.48
4:D:146:PHE:O	4:D:150:ILE:HG12	2.14	0.48
10:K:20:PRO:O	10:K:23:ASP:HB2	2.13	0.48
13:O:36:ILE:N	13:O:36:ILE:HD12	2.29	0.48
19:Z:32:ASP:C	19:Z:34:ASP:H	2.17	0.48
1:A:10:SER:C	1:A:12:ASN:H	2.16	0.47
1:A:114:LEU:HD23	1:A:114:LEU:C	2.34	0.47
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.95	0.47
2:B:175:THR:O	2:B:176:GLY:O	2.31	0.47
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.48	0.47
2:B:221:PRO:HA	21:B:519:CLA:HED3	1.95	0.47
3:C:457:LYS:HE3	4:D:228:GLY:O	2.13	0.47
28:C:475:SQD:O8	4:D:233:ARG:HG3	2.14	0.47
4:D:337:GLU:O	4:D:338:ASN:C	2.51	0.47
7:H:30:LEU:HD11	7:H:34:PHE:HE1	1.78	0.47
8:I:24:LEU:O	8:I:26:GLY:N	2.41	0.47
12:M:8:LEU:HD21	30:T:226:LMT:H81	1.95	0.47
1:A:111:PRO:O	1:A:115:ILE:HG13	2.14	0.47
1:A:287:ALA:HA	21:A:362:CLA:HED2	1.96	0.47
1:A:330:VAL:HG11	4:D:348:ARG:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:CD2	21:B:516:CLA:H193	2.44	0.47
2:B:135:LEU:HD23	2:B:138:MET:HE1	1.95	0.47
3:C:30:SER:OG	4:D:233:ARG:NH2	2.47	0.47
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.95	0.47
21:C:487:CLA:H121	21:C:488:CLA:H202	1.96	0.47
4:D:135:LEU:HD23	28:D:361:SQD:HO2	1.78	0.47
4:D:93:TRP:HA	4:D:99:GLY:H	1.80	0.47
5:E:22:ILE:O	5:E:26:THR:HG23	2.14	0.47
13:O:79:LYS:HE2	13:O:89:ALA:HB3	1.95	0.47
1:A:190:HIS:HB3	1:A:293:MET:CE	2.43	0.47
1:A:281:VAL:HB	26:C:493:DGD:HAG3	1.96	0.47
21:B:517:CLA:H61	21:B:517:CLA:H41	1.67	0.47
3:C:94:THR:HG22	3:C:298:PRO:HD2	1.96	0.47
3:C:437:PHE:CE1	21:K:483:CLA:HMB3	2.48	0.47
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.26	0.47
2:B:124:ARG:HD3	2:B:131:PRO:N	2.30	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.47	0.47
3:C:272:LEU:CA	21:C:485:CLA:HMD3	2.43	0.47
21:C:487:CLA:H172	21:C:487:CLA:CMA	2.37	0.47
32:D:357:PL9:C33	32:D:357:PL9:H301	2.45	0.47
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.95	0.47
16:V:45:ILE:HG12	16:V:46:THR:N	2.28	0.47
1:A:287:ALA:HA	21:A:362:CLA:CED	2.44	0.47
27:A:371:LHG:H341	21:C:480:CLA:H203	1.96	0.47
2:B:265:ILE:HG13	2:B:266:GLU:N	2.30	0.47
2:B:373:LYS:HD2	2:B:373:LYS:HA	1.55	0.47
2:B:250:PHE:CB	26:B:528:DGD:HB82	2.45	0.47
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.49	0.47
4:D:23:LYS:HZ1	28:D:361:SQD:C46	2.10	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.42	0.47
1:A:124:SER:O	1:A:127:MET:HB3	2.15	0.47
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.96	0.47
1:A:243:GLU:HA	4:D:241:GLU:HA	1.97	0.47
1:A:183:MET:CE	21:A:363:CLA:HMD3	2.44	0.47
2:B:258:TYR:CE2	26:B:528:DGD:O1B	2.67	0.47
3:C:29:GLU:HA	10:K:46:ARG:HH12	1.79	0.47
29:D:360:LMG:H361	14:T:21:ILE:HD11	1.97	0.47
4:D:32:TRP:CZ3	28:D:361:SQD:H282	2.49	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.83	0.47
2:B:274:GLN:NE2	7:H:62:TRP:NE1	2.63	0.47
10:K:35:LEU:HA	10:K:38:VAL:HG23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.96	0.47
19:Z:32:ASP:CG	19:Z:33:TRP:N	2.60	0.47
2:B:24:LEU:HD21	21:B:526:CLA:CAB	2.44	0.47
3:C:288:CYS:SG	26:C:491:DGD:HA21	2.55	0.47
7:H:25:TRP:O	7:H:26:GLY:C	2.53	0.47
1:A:22:THR:CG2	8:I:30:ARG:HD3	2.42	0.47
19:Z:29:SER:C	19:Z:31:GLN:H	2.17	0.47
2:B:248:ALA:HA	21:B:513:CLA:H42	1.97	0.47
2:B:68:ARG:HH22	21:B:514:CLA:HED3	1.80	0.47
3:C:447:ARG:CG	3:C:447:ARG:NH1	2.74	0.47
4:D:122:LEU:CD2	22:D:355:PHO:H62	2.44	0.47
4:D:259:ILE:HG12	29:D:360:LMG:C29	2.44	0.47
8:I:30:ARG:O	8:I:31:ASN:HB3	2.14	0.47
11:L:24:ILE:HD12	11:L:24:ILE:N	2.29	0.47
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.49	0.47
1:A:214:MET:HE2	1:A:214:MET:HA	1.95	0.47
3:C:135:ARG:HB2	19:Z:27:TYR:CG	2.50	0.47
4:D:134:ARG:HA	4:D:134:ARG:HE	1.78	0.47
1:A:176:ILE:HG23	21:A:363:CLA:O1D	2.14	0.47
2:B:110:ALA:HB2	21:B:526:CLA:HMB2	1.97	0.47
21:B:517:CLA:HBC3	25:B:529:BCR:HC8	1.97	0.47
21:C:477:CLA:H171	21:C:483:CLA:HMB3	1.97	0.47
13:O:225:LEU:C	13:O:226:ASN:HD22	2.17	0.47
21:B:522:CLA:H12	21:B:525:CLA:HAA2	1.96	0.47
3:C:365:TRP:CB	3:C:391:ARG:HG2	2.45	0.47
4:D:261:PHE:HB2	32:D:357:PL9:C52	2.43	0.47
4:D:202:ALA:HB3	32:D:357:PL9:C30	2.44	0.47
13:O:135:GLN:HG2	13:O:141:ARG:HG3	1.97	0.47
27:A:371:LHG:O4	4:D:230:SER:HA	2.14	0.46
5:E:8:ARG:HA	6:F:13:TYR:CE2	2.50	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	0.46
1:A:10:SER:C	1:A:12:ASN:N	2.69	0.46
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.43	0.46
21:B:519:CLA:OBD	7:H:27:THR:HB	2.15	0.46
3:C:127:PHE:HA	21:C:486:CLA:H192	1.96	0.46
3:C:436:PHE:O	21:C:484:CLA:HAC1	2.14	0.46
3:C:52:ALA:CA	21:C:486:CLA:HMB3	2.37	0.46
30:D:536:LMT:H5'	28:D:361:SQD:H5	1.97	0.46
5:E:9:PRO:O	5:E:10:PHE:C	2.53	0.46
13:O:113:VAL:HA	13:O:119:LEU:HD23	1.97	0.46
16:V:68:VAL:O	16:V:68:VAL:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.97	0.46
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.81	0.46
1:A:105:TRP:CZ3	25:A:369:BCR:H371	2.49	0.46
26:B:528:DGD:O2D	4:D:87:HIS:CG	2.54	0.46
3:C:193:GLY:O	3:C:194:GLY:O	2.33	0.46
4:D:261:PHE:O	4:D:262:SER:HB3	2.14	0.46
14:T:25:GLU:O	14:T:26:PRO:C	2.54	0.46
16:V:148:GLU:OE1	16:V:148:GLU:HA	2.14	0.46
1:A:215:HIS:O	1:A:216:GLY:C	2.53	0.46
26:B:533:DGD:HA81	12:M:14:PHE:CA	2.42	0.46
4:D:27:PHE:CD2	6:F:19:ARG:CD	2.97	0.46
1:A:12:ASN:O	1:A:16:ARG:HG3	2.15	0.46
21:A:363:CLA:H43	22:A:365:PHO:HMA1	1.98	0.46
2:B:138:MET:SD	21:B:525:CLA:HAC1	2.55	0.46
2:B:246:PHE:CD1	2:B:246:PHE:C	2.88	0.46
2:B:252:VAL:HG13	21:B:513:CLA:H12	1.97	0.46
2:B:462:PHE:CZ	21:B:523:CLA:HMB3	2.51	0.46
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
3:C:265:ILE:HG13	21:C:481:CLA:HED1	1.97	0.46
4:D:274:VAL:HG13	32:D:357:PL9:H253	1.97	0.46
13:O:82:PRO:O	13:O:83:LYS:CB	2.64	0.46
1:A:216:GLY:O	1:A:220:THR:HG22	2.16	0.46
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.46	0.46
1:A:157:VAL:HG21	21:A:363:CLA:CMC	2.45	0.46
2:B:172:TYR:O	2:B:173:GLY:C	2.52	0.46
3:C:213:LEU:HD21	25:C:490:BCR:C20	2.46	0.46
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.45	0.46
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.51	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
2:B:238:LEU:CA	21:B:522:CLA:HMD3	2.45	0.46
3:C:390:ARG:CZ	16:V:126:ILE:HD13	2.46	0.46
1:A:221:SER:HB2	4:D:139:ARG:O	2.16	0.46
7:H:35:MET:HE2	25:X:107:BCR:H322	1.97	0.46
9:J:15:THR:HA	25:J:112:BCR:C37	2.46	0.46
3:C:396:MET:HE1	16:V:73:LYS:O	2.16	0.46
19:Z:36:SER:C	19:Z:38:GLN:N	2.69	0.46
19:Z:5:PHE:HE1	19:Z:54:VAL:HG13	1.80	0.46
1:A:45:THR:HG23	1:A:46:ILE:N	2.31	0.46
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.96	0.46
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.44	0.46
3:C:472:LEU:HD12	3:C:473:ASP:N	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:HD21	21:C:484:CLA:CBB	2.46	0.46
3:C:42:LEU:CD2	21:C:486:CLA:HED3	2.44	0.46
4:D:217:THR:O	4:D:221:THR:HB	2.15	0.46
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.97	0.46
12:M:18:PRO:O	12:M:21:PHE:HB3	2.16	0.46
3:C:370:ARG:HD3	13:O:33:TYR:CE2	2.51	0.46
16:V:54:GLU:HA	16:V:54:GLU:OE1	2.16	0.46
7:H:35:MET:HG3	25:X:107:BCR:H323	1.98	0.46
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.75	0.46
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.51	0.46
1:A:121:LEU:HD11	21:C:481:CLA:H171	1.98	0.46
3:C:125:LEU:HA	21:C:488:CLA:HMC1	1.98	0.46
26:C:492:DGD:HBE2	26:C:493:DGD:HA92	1.97	0.46
1:A:306:VAL:HG11	1:A:316:THR:HG23	1.97	0.46
3:C:143:TYR:O	3:C:144:SER:CB	2.64	0.46
3:C:39:ASN:HD21	21:C:486:CLA:C1C	2.29	0.46
3:C:452:ALA:C	3:C:454:GLY:N	2.68	0.46
3:C:49:LEU:O	3:C:53:HIS:ND1	2.43	0.46
3:C:56:HIS:C	3:C:58:GLY:N	2.68	0.46
4:D:201:VAL:HA	21:D:354:CLA:HMB3	1.97	0.46
21:D:354:CLA:H101	22:D:355:PHO:H2	1.98	0.46
5:E:51:ARG:O	5:E:53:ASP:N	2.49	0.46
1:A:64:ARG:O	13:O:178:ARG:NH2	2.49	0.46
1:A:214:MET:O	1:A:215:HIS:C	2.54	0.45
1:A:326:LEU:HD21	3:C:412:THR:HB	1.98	0.45
1:A:32:TRP:HA	1:A:32:TRP:HE3	1.76	0.45
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.98	0.45
3:C:435:PHE:O	3:C:438:LEU:N	2.49	0.45
21:C:486:CLA:H8	25:C:489:BCR:H402	1.97	0.45
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.51	0.45
29:D:359:LMG:O3	9:J:32:ALA:HA	2.16	0.45
4:D:41:ALA:HB2	22:D:355:PHO:C4	2.44	0.45
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.46	0.45
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.45	0.45
2:B:229:LEU:O	2:B:230:ARG:C	2.54	0.45
21:B:519:CLA:C3D	7:H:31:MET:HB2	2.45	0.45
3:C:328:VAL:HG23	3:C:329:GLY:N	2.31	0.45
21:A:366:CLA:H12	26:C:474:DGD:HB22	1.98	0.45
1:A:131:TRP:CZ3	21:C:481:CLA:HBA2	2.51	0.45
5:E:64:PRO:HD3	5:E:84:LYS:HE2	1.98	0.45
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:206:PHE:HB2	2.17	0.45
1:A:39:PRO:HB2	21:A:366:CLA:CBB	2.44	0.45
2:B:15:ASP:O	2:B:17:GLY:N	2.50	0.45
2:B:212:ALA:HB2	21:B:519:CLA:HMC3	1.99	0.45
2:B:68:ARG:HH12	21:B:514:CLA:CED	2.30	0.45
3:C:210:PHE:HZ	3:C:243:ILE:HD11	1.81	0.45
3:C:176:VAL:HG11	3:C:238:ILE:HG12	1.99	0.45
3:C:223:TRP:CH2	26:C:474:DGD:HA82	2.51	0.45
3:C:282:MET:O	21:C:478:CLA:HMD3	2.16	0.45
3:C:54:VAL:HG22	21:C:487:CLA:HED1	1.99	0.45
6:F:12:SER:O	6:F:13:TYR:HB2	2.16	0.45
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.45	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.80	0.45
2:B:68:ARG:HH12	21:B:514:CLA:HED1	1.81	0.45
21:B:518:CLA:C14	21:B:518:CLA:H102	2.41	0.45
26:B:528:DGD:C6D	26:B:528:DGD:C5E	2.94	0.45
3:C:276:LEU:CD1	3:C:444:HIS:HD2	2.30	0.45
6:F:23:VAL:HG22	6:F:23:VAL:O	2.17	0.45
4:D:14:TRP:CE3	18:X:38:ILE:HD12	2.52	0.45
19:Z:35:ARG:HG3	19:Z:36:SER:N	2.30	0.45
1:A:243:GLU:CD	1:A:243:GLU:H	2.16	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.97	0.45
21:B:515:CLA:H61	21:B:515:CLA:H41	1.51	0.45
3:C:245:ILE:O	3:C:249:ILE:HG12	2.16	0.45
3:C:258:GLY:CA	3:C:262:ARG:HH12	2.28	0.45
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.45
4:D:126:MET:HE3	4:D:150:ILE:HG13	1.99	0.45
5:E:10:PHE:CZ	6:F:19:ARG:HD2	2.51	0.45
9:J:14:ALA:HB1	25:J:112:BCR:C26	2.46	0.45
13:O:56:TYR:O	13:O:161:SER:HA	2.17	0.45
13:O:88:GLU:HG2	13:O:89:ALA:N	2.31	0.45
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.99	0.45
16:V:30:THR:O	16:V:34:LEU:HG	2.17	0.45
21:B:516:CLA:HHC	21:B:516:CLA:HBB1	1.99	0.45
21:B:517:CLA:C1	26:B:533:DGD:HB32	2.46	0.45
3:C:168:LEU:HD13	21:C:483:CLA:C4	2.45	0.45
3:C:318:LEU:O	3:C:318:LEU:HD23	2.16	0.45
27:A:371:LHG:HC11	3:C:447:ARG:CZ	2.46	0.45
4:D:36:LEU:C	4:D:39:PRO:HD2	2.37	0.45
15:U:80:VAL:HG22	15:U:127:ARG:HH21	1.82	0.45
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HB	25:A:369:BCR:H331	1.99	0.45
3:C:460:ASP:O	3:C:461:ARG:C	2.55	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CD2	2.52	0.45
7:H:21:VAL:HG23	7:H:22:ALA:O	2.16	0.45
21:A:363:CLA:H2	29:A:373:LMG:H242	1.99	0.45
2:B:145:LEU:CD1	21:B:525:CLA:HMB2	2.46	0.45
2:B:62:VAL:HG11	21:B:515:CLA:HED3	1.99	0.45
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.98	0.45
4:D:213:ILE:HG23	4:D:214:HIS:N	2.30	0.45
4:D:56:THR:HB	5:E:49:THR:HG23	1.97	0.45
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.43	0.45
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.17	0.45
1:A:214:MET:CE	4:D:142:ASN:ND2	2.80	0.45
29:A:373:LMG:O10	29:A:373:LMG:O9	2.34	0.45
2:B:10:THR:O	2:B:13:ILE:HG13	2.16	0.45
2:B:422:ARG:HH11	2:B:422:ARG:HG2	1.82	0.45
3:C:258:GLY:HA3	3:C:262:ARG:HH12	1.81	0.45
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.29	0.45
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.45
13:O:69:LEU:HB3	13:O:107:ILE:CB	2.35	0.45
2:B:247:PHE:CD2	21:B:513:CLA:H111	2.52	0.45
2:B:71:VAL:HG21	2:B:96:VAL:CG2	2.47	0.45
3:C:163:PHE:CD1	3:C:252:ILE:HD11	2.52	0.45
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.99	0.45
21:C:479:CLA:H61	21:C:479:CLA:H41	1.58	0.45
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
15:U:100:ARG:NH1	15:U:103:GLN:HG2	2.31	0.45
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.52	0.45
1:A:39:PRO:HB3	21:A:366:CLA:HMC3	1.99	0.44
2:B:141:ILE:O	2:B:144:PHE:HB3	2.17	0.44
25:B:529:BCR:H361	25:B:529:BCR:H20C	1.80	0.44
3:C:110:PRO:O	3:C:114:VAL:HG23	2.17	0.44
3:C:68:THR:OG1	21:C:479:CLA:CED	2.63	0.44
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.47	0.44
29:A:373:LMG:H171	11:L:23:LEU:HD13	1.99	0.44
3:C:337:LEU:CD1	13:O:131:PRO:HG3	2.47	0.44
13:O:173:ASN:ND2	13:O:220:LYS:HD3	2.32	0.44
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.52	0.44
4:D:122:LEU:CG	22:D:355:PHO:H62	2.47	0.44
1:A:214:MET:HE1	4:D:142:ASN:ND2	2.33	0.44
4:D:19:ASP:O	4:D:20:ASP:C	2.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:GLY:HA2	6:F:32:PHE:CE2	2.53	0.44
7:H:28:THR:O	7:H:31:MET:HB3	2.18	0.44
7:H:9:ASP:O	7:H:12:ARG:HB3	2.17	0.44
8:I:4:LEU:O	8:I:8:VAL:HG23	2.17	0.44
2:B:148:LEU:HG	21:B:514:CLA:H193	1.99	0.44
3:C:436:PHE:HB3	21:K:483:CLA:H93	1.99	0.44
25:D:358:BCR:H331	25:D:358:BCR:C8	2.47	0.44
29:D:360:LMG:H221	14:T:13:ILE:CG2	2.38	0.44
6:F:36:ALA:O	6:F:38:ALA:N	2.50	0.44
3:C:334:PRO:HA	13:O:179:THR:OG1	2.17	0.44
18:X:16:LEU:HD11	18:X:20:PHE:CE2	2.53	0.44
3:C:264:PHE:CE2	21:C:482:CLA:O1A	2.66	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.44
9:J:22:ILE:HG21	29:J:492:LMG:C20	2.45	0.44
10:K:17:ILE:C	10:K:18:PHE:HD2	2.21	0.44
10:K:17:ILE:N	10:K:17:ILE:CD1	2.81	0.44
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.44
21:B:512:CLA:C20	26:B:528:DGD:HB91	2.48	0.44
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.99	0.44
3:C:276:LEU:HD21	21:C:484:CLA:HBB1	1.99	0.44
3:C:28:GLN:CB	21:C:486:CLA:HED2	2.47	0.44
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.44
4:D:253:TRP:HB2	4:D:260:ALA:HB2	2.00	0.44
15:U:72:TYR:CB	15:U:73:PRO:CD	2.92	0.44
16:V:59:PHE:CD1	16:V:63:CYS:SG	3.08	0.44
16:V:81:ARG:HH11	16:V:81:ARG:HG2	1.83	0.44
1:A:60:ILE:HG23	1:A:61:ASP:N	2.32	0.44
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.16	0.44
2:B:435:GLU:O	2:B:436:THR:C	2.56	0.44
2:B:86:ILE:C	2:B:86:ILE:HD12	2.38	0.44
3:C:281:MET:CE	21:C:481:CLA:HMC1	2.47	0.44
5:E:15:THR:CG2	9:J:7:ARG:HB3	2.47	0.44
6:F:36:ALA:O	6:F:39:ALA:N	2.51	0.44
1:A:159:LEU:C	1:A:162:PRO:HD2	2.38	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.44
4:D:209:LEU:O	4:D:213:ILE:HG22	2.18	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
7:H:41:PHE:O	7:H:45:ILE:HG23	2.18	0.44
2:B:444:ARG:HH11	2:B:444:ARG:HG3	1.82	0.44
3:C:394:GLU:OE2	3:C:398:HIS:CD2	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:ALA:HB3	32:D:357:PL9:H302	2.00	0.44
32:D:357:PL9:C43	29:D:360:LMG:C25	2.95	0.44
13:O:120:THR:HG22	13:O:154:SER:CB	2.47	0.44
18:X:44:ASP:O	18:X:45:LYS:HB3	2.17	0.44
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.38	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.18	0.44
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.44
21:B:517:CLA:CBC	25:B:529:BCR:H10C	2.48	0.44
3:C:82:TYR:HA	3:C:422:PRO:HG2	2.00	0.44
3:C:92:ILE:HD11	21:C:479:CLA:HED2	1.99	0.44
3:C:54:VAL:HA	21:C:487:CLA:HED1	2.00	0.44
4:D:154:VAL:O	4:D:158:LEU:HB2	2.18	0.44
4:D:221:THR:CG2	4:D:244:TYR:HB2	2.48	0.44
25:D:358:BCR:C39	9:J:21:VAL:HG11	2.48	0.44
29:D:360:LMG:H111	29:D:360:LMG:H292	1.98	0.44
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.99	0.44
7:H:44:ILE:HG12	18:X:19:PHE:CZ	2.52	0.44
1:A:217:SER:O	1:A:220:THR:HG22	2.18	0.43
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.17	0.43
21:C:487:CLA:HHC	21:C:487:CLA:HBB1	2.00	0.43
21:C:488:CLA:C1	21:C:488:CLA:HAA1	2.47	0.43
4:D:67:TYR:OH	29:D:359:LMG:H291	2.18	0.43
5:E:74:GLN:HG3	5:E:75:GLN:N	2.31	0.43
6:F:45:ARG:NH2	6:F:45:ARG:HB3	2.33	0.43
10:K:17:ILE:HG22	10:K:17:ILE:O	2.17	0.43
27:A:371:LHG:HC32	4:D:229:ALA:O	2.18	0.43
2:B:10:THR:C	2:B:12:LEU:N	2.71	0.43
2:B:206:GLY:O	2:B:210:ILE:HG13	2.18	0.43
2:B:271:THR:CG2	2:B:273:TYR:HB2	2.48	0.43
2:B:484:PRO:O	2:B:485:GLU:HG2	2.18	0.43
21:B:518:CLA:C1	4:D:127:LEU:HD21	2.48	0.43
2:B:238:LEU:N	21:B:522:CLA:HMD3	2.32	0.43
3:C:235:GLY:O	3:C:238:ILE:HB	2.18	0.43
4:D:101:PHE:O	4:D:104:TRP:HB3	2.18	0.43
26:B:533:DGD:HA32	12:M:10:ALA:HB1	2.00	0.43
13:O:116:ASP:OD1	13:O:157:PRO:HB3	2.18	0.43
13:O:225:LEU:HD12	13:O:225:LEU:N	2.33	0.43
16:V:39:ASN:HD21	16:V:43:LYS:HB3	1.82	0.43
21:D:356:CLA:C4	18:X:26:GLY:HA3	2.47	0.43
1:A:29:TYR:OH	1:A:132:GLU:OE2	2.26	0.43
1:A:198:HIS:O	1:A:202:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:HG2	2:B:165:GLY:H	1.82	0.43
2:B:463:PHE:CE1	26:B:528:DGD:CFA	3.01	0.43
3:C:168:LEU:O	21:C:477:CLA:HMC1	2.18	0.43
3:C:416:SER:OG	16:V:68:VAL:HG23	2.17	0.43
5:E:72:ALA:O	5:E:76:VAL:HG23	2.18	0.43
2:B:434:THR:HG21	13:O:204:LYS:HE3	1.97	0.43
3:C:390:ARG:NE	16:V:126:ILE:CG2	2.82	0.43
16:V:63:CYS:O	16:V:64:ALA:C	2.55	0.43
19:Z:17:PHE:HE2	19:Z:21:ILE:HD11	1.84	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
2:B:348:ASN:OD1	2:B:352:GLU:HB2	2.18	0.43
2:B:327:THR:HG22	21:B:517:CLA:C1	2.49	0.43
21:B:514:CLA:H142	21:B:525:CLA:H52	2.01	0.43
26:B:533:DGD:HA32	12:M:10:ALA:CB	2.49	0.43
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.54	0.43
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.54	0.43
3:C:362:ARG:CG	26:C:491:DGD:HE61	2.48	0.43
10:K:18:PHE:CE1	19:Z:9:LEU:HG	2.53	0.43
10:K:30:VAL:N	21:K:483:CLA:H191	2.34	0.43
13:O:72:GLN:O	13:O:263:GLY:HA3	2.17	0.43
15:U:54:LYS:HD2	15:U:113:THR:CG2	2.49	0.43
1:A:309:ALA:HB3	5:E:53:ASP:HA	2.00	0.43
21:B:512:CLA:CAA	7:H:45:ILE:HD12	2.48	0.43
2:B:247:PHE:HD2	21:B:513:CLA:H111	1.83	0.43
21:B:518:CLA:C14	21:D:356:CLA:HMB2	2.48	0.43
3:C:72:LEU:HG	10:K:10:LYS:N	2.33	0.43
5:E:38:VAL:CG2	6:F:36:ALA:HB1	2.47	0.43
21:C:486:CLA:H122	10:K:32:PHE:CE1	2.53	0.43
13:O:70:CYS:O	13:O:265:PHE:HB2	2.18	0.43
16:V:64:ALA:O	16:V:65:SER:C	2.56	0.43
19:Z:36:SER:HA	19:Z:39:LEU:CD1	2.48	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	1.99	0.43
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.53	0.43
3:C:437:PHE:HA	21:C:484:CLA:HMC1	2.00	0.43
5:E:8:ARG:HA	6:F:13:TYR:CZ	2.52	0.43
1:A:187:GLN:HB2	21:A:362:CLA:CAC	2.48	0.43
29:A:373:LMG:H301	12:M:22:LEU:HD22	1.99	0.43
1:A:42:LEU:HA	1:A:45:THR:HG22	2.00	0.43
2:B:284:ILE:HG23	2:B:305:ILE:CD1	2.48	0.43
2:B:450:TRP:HB3	21:B:517:CLA:CMB	2.47	0.43
2:B:252:VAL:HG11	21:B:514:CLA:OBD	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:GLY:N	21:C:488:CLA:HAC2	2.33	0.43
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.01	0.43
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.00	0.43
30:I:274:LMT:H6D	13:O:95:LYS:NZ	2.34	0.43
10:K:46:ARG:HB2	10:K:46:ARG:NH1	2.34	0.43
21:A:363:CLA:HMB3	22:A:365:PHO:H172	2.01	0.43
2:B:289:GLN:OE1	2:B:292:LEU:HD12	2.19	0.43
2:B:263:THR:HB	2:B:448:ARG:HH12	1.82	0.43
3:C:433:LEU:HD13	21:C:478:CLA:CHC	2.49	0.43
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.43
4:D:263:ASN:O	4:D:265:ARG:N	2.52	0.43
4:D:291:LEU:O	4:D:292:ASN:HB2	2.18	0.43
13:O:109:GLY:HA3	13:O:122:VAL:O	2.18	0.43
13:O:171:GLU:HA	13:O:221:GLY:O	2.19	0.43
3:C:473:ASP:HA	14:T:27:PRO:HD2	2.01	0.43
2:B:327:THR:O	2:B:444:ARG:NE	2.46	0.43
3:C:55:ALA:C	25:C:489:BCR:H373	2.39	0.43
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.43
6:F:33:PHE:C	6:F:35:GLY:H	2.22	0.43
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.49	0.43
12:M:33:GLN:HG2	12:M:34:LYS:N	2.33	0.43
18:X:32:LEU:HD23	18:X:32:LEU:H	1.83	0.43
2:B:103:LEU:HD21	21:B:515:CLA:HMC3	2.01	0.43
21:B:517:CLA:HMB1	21:B:517:CLA:HAB	1.85	0.43
3:C:48:LYS:CD	3:C:138:GLU:HG3	2.49	0.43
3:C:55:ALA:HB1	25:C:489:BCR:C37	2.49	0.43
3:C:33:PHE:CE1	4:D:229:ALA:HB3	2.54	0.43
26:C:492:DGD:HB41	9:J:29:PHE:CZ	2.54	0.43
10:K:43:VAL:O	10:K:46:ARG:HG3	2.19	0.43
12:M:1:MET:HG2	12:M:2:GLU:H	1.84	0.43
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.43
1:A:247:ASN:HB3	1:A:250:ALA:HB3	2.00	0.42
1:A:286:THR:CG2	21:A:362:CLA:HED3	2.35	0.42
1:A:45:THR:CB	22:A:365:PHO:H8	2.48	0.42
2:B:222:PRO:HG3	7:H:27:THR:N	2.28	0.42
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.42
2:B:413:ASP:OD1	2:B:416:THR:HB	2.19	0.42
21:C:484:CLA:H41	21:C:484:CLA:H62	1.64	0.42
4:D:125:PHE:O	4:D:128:ARG:HB3	2.19	0.42
5:E:34:GLY:O	5:E:37:PHE:HB3	2.19	0.42
9:J:12:ILE:O	9:J:16:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:91:VAL:HG13	15:U:92:LEU:N	2.33	0.42
1:A:55:ALA:HA	25:A:369:BCR:C27	2.50	0.42
2:B:215:PHE:C	2:B:215:PHE:CD2	2.93	0.42
26:B:528:DGD:HD61	26:B:528:DGD:C5E	2.48	0.42
3:C:318:LEU:HG	3:C:328:VAL:CG1	2.48	0.42
3:C:164:HIS:CB	21:C:483:CLA:HED3	2.49	0.42
3:C:164:HIS:HB2	21:C:483:CLA:HED3	2.00	0.42
5:E:35:TRP:CD1	5:E:35:TRP:C	2.93	0.42
12:M:33:GLN:CG	12:M:34:LYS:N	2.82	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.55	0.42
19:Z:30:PRO:C	19:Z:32:ASP:N	2.72	0.42
1:A:239:PHE:HB3	14:T:28:ARG:O	2.19	0.42
2:B:105:GLY:O	2:B:108:PHE:HB3	2.19	0.42
2:B:33:TRP:HZ3	21:B:515:CLA:HMD1	1.83	0.42
2:B:348:ASN:O	2:B:349:LYS:C	2.57	0.42
2:B:349:LYS:HG2	2:B:395:GLN:O	2.19	0.42
3:C:101:PRO:O	3:C:104:GLU:HB2	2.19	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.42
3:C:363:GLY:O	3:C:364:PRO:C	2.56	0.42
3:C:406:SER:HA	3:C:420:VAL:CG2	2.49	0.42
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.54	0.42
9:J:14:ALA:C	25:J:112:BCR:H382	2.40	0.42
3:C:29:GLU:CB	10:K:46:ARG:NH1	2.80	0.42
29:A:373:LMG:HC92	2:B:5:TRP:NE1	2.32	0.42
2:B:251:VAL:HB	21:B:513:CLA:C4	2.50	0.42
2:B:150:CYS:HB2	21:B:513:CLA:HMC3	2.01	0.42
3:C:202:PRO:HB2	3:C:235:GLY:HA2	2.01	0.42
21:C:483:CLA:H41	21:C:483:CLA:H61	1.92	0.42
3:C:37:ALA:O	21:C:484:CLA:HBA1	2.19	0.42
3:C:436:PHE:O	21:C:484:CLA:HMC1	2.19	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.84	0.42
27:A:371:LHG:H351	21:K:483:CLA:H71	2.01	0.42
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.70	0.42
13:O:59:ASP:O	13:O:61:SER:N	2.53	0.42
16:V:130:MET:SD	16:V:133:LEU:HD12	2.60	0.42
1:A:207:GLY:O	1:A:210:LEU:HB3	2.20	0.42
2:B:234:ILE:C	2:B:236:THR:H	2.23	0.42
2:B:413:ASP:O	2:B:414:PRO:C	2.57	0.42
3:C:162:GLY:O	3:C:166:ILE:HG13	2.18	0.42
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:16:ALA:O	10:K:19:ASP:HB2	2.20	0.42
1:A:160:ILE:HD11	26:C:491:DGD:C9A	2.50	0.42
1:A:222:SER:O	1:A:246:TYR:HB2	2.19	0.42
2:B:330:MET:SD	2:B:446:SER:HB3	2.59	0.42
21:B:524:CLA:H41	21:B:524:CLA:H61	1.85	0.42
21:B:526:CLA:C1D	7:H:7:LEU:HD23	2.50	0.42
3:C:205:ASP:OD1	3:C:207:ARG:HB3	2.19	0.42
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.72	0.42
21:C:477:CLA:C2D	21:C:479:CLA:H2	2.50	0.42
1:A:33:PHE:CE2	21:C:481:CLA:O1A	2.73	0.42
5:E:69:ARG:HG3	5:E:70:PHE:N	2.34	0.42
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.42
3:C:414:ILE:HG22	3:C:415:ASN:N	2.35	0.42
3:C:442:LEU:HD21	21:C:481:CLA:HMB3	2.02	0.42
26:C:493:DGD:HBW1	29:D:359:LMG:H181	2.02	0.42
5:E:35:TRP:CG	6:F:39:ALA:HB2	2.55	0.42
10:K:44:GLY:O	10:K:45:PHE:C	2.57	0.42
16:V:83:GLU:H	16:V:83:GLU:CD	2.23	0.42
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.55	0.42
1:A:273:PHE:CD1	27:A:371:LHG:H242	2.55	0.42
1:A:39:PRO:CB	21:A:366:CLA:HBB1	2.45	0.42
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.02	0.42
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.92	0.42
3:C:365:TRP:HB3	3:C:391:ARG:HG2	2.02	0.42
27:C:476:LHG:H171	26:C:492:DGD:HBN1	2.00	0.42
1:A:328:MET:CE	4:D:183:LEU:HD22	2.49	0.42
4:D:52:THR:HG22	4:D:67:TYR:CE2	2.54	0.42
5:E:78:THR:HA	5:E:81:GLU:HG2	2.02	0.42
2:B:222:PRO:HB3	7:H:26:GLY:N	2.34	0.42
7:H:39:LEU:HD23	7:H:39:LEU:C	2.39	0.42
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.33	0.42
28:L:213:SQD:H82	29:M:217:LMG:H152	2.01	0.42
1:A:129:ARG:C	1:A:131:TRP:H	2.23	0.42
1:A:317:TRP:O	1:A:321:ILE:HG13	2.20	0.42
1:A:234:ASN:CB	29:A:373:LMG:HC3	2.48	0.42
1:A:42:LEU:HA	1:A:45:THR:CG2	2.49	0.42
2:B:448:ARG:HH11	2:B:448:ARG:HG3	1.84	0.42
26:C:492:DGD:HB52	25:J:115:BCR:C35	2.47	0.42
5:E:15:THR:HG23	9:J:8:ILE:N	2.34	0.42
7:H:35:MET:HA	25:X:107:BCR:C32	2.50	0.42
2:B:191:ASN:HB2	7:H:58:VAL:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:O:274:LMT:H1B	30:O:274:LMT:H5'	1.92	0.42
3:C:125:LEU:HG	25:Z:116:BCR:C36	2.49	0.42
29:A:373:LMG:C31	12:M:22:LEU:HD21	2.50	0.42
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.54	0.42
2:B:472:ARG:HG2	2:B:472:ARG:HH11	1.84	0.42
3:C:140:LEU:HB2	3:C:148:GLY:HA2	2.02	0.42
3:C:148:GLY:O	3:C:156:LYS:NZ	2.51	0.42
3:C:461:ARG:NH1	3:C:461:ARG:HG3	2.32	0.42
22:A:365:PHO:HAC2	4:D:212:ALA:HB3	2.01	0.42
4:D:261:PHE:N	32:D:357:PL9:O1	2.51	0.42
7:H:18:TYR:CG	7:H:19:GLY:N	2.85	0.42
10:K:30:VAL:CA	21:K:483:CLA:H191	2.50	0.42
18:X:12:ILE:C	18:X:12:ILE:HD13	2.40	0.42
29:A:373:LMG:C25	29:D:360:LMG:C21	2.97	0.41
29:A:373:LMG:H131	4:D:273:PHE:CE2	2.55	0.41
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.41
2:B:280:PHE:O	2:B:284:ILE:HG13	2.20	0.41
26:B:533:DGD:HG11	12:M:6:LEU:HD12	2.02	0.41
4:D:204:VAL:HG22	4:D:279:LEU:HD21	2.01	0.41
9:J:15:THR:O	25:J:112:BCR:H372	2.19	0.41
6:F:45:ARG:CZ	9:J:40:LEU:OXT	2.68	0.41
21:C:486:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
29:A:373:LMG:C31	11:L:20:GLY:HA2	2.49	0.41
13:O:227:VAL:CG1	13:O:228:ALA:N	2.82	0.41
14:T:22:PHE:C	14:T:23:PHE:CD2	2.93	0.41
15:U:72:TYR:CG	15:U:73:PRO:N	2.87	0.41
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.55	0.41
1:A:131:TRP:CH2	21:C:481:CLA:CBA	2.99	0.41
1:A:228:THR:HB	1:A:231:GLU:HB3	2.01	0.41
3:C:208:VAL:O	3:C:209:ILE:C	2.57	0.41
3:C:405:ASN:HB2	26:C:493:DGD:O6D	2.20	0.41
21:C:478:CLA:O1A	21:C:479:CLA:HBD	2.19	0.41
21:A:362:CLA:HMC3	4:D:182:LEU:HD13	2.02	0.41
4:D:122:LEU:HG	22:D:355:PHO:H62	2.02	0.41
10:K:11:LEU:O	10:K:12:PRO:C	2.57	0.41
1:A:104:GLU:OE2	13:O:99:ARG:HD3	2.20	0.41
1:A:236:GLY:HA3	4:D:265:ARG:NH1	2.35	0.41
2:B:462:PHE:HE1	21:B:523:CLA:HMB3	1.82	0.41
3:C:125:LEU:HD22	21:C:487:CLA:HED3	2.00	0.41
4:D:128:ARG:O	4:D:129:GLN:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:GLU:HA	4:D:302:GLU:OE1	2.20	0.41
1:A:332:HIS:HB3	4:D:321:LEU:HD21	2.01	0.41
15:U:50:ALA:HB1	15:U:113:THR:HG21	2.01	0.41
15:U:75:LEU:O	15:U:79:ILE:HG13	2.20	0.41
15:U:82:ASN:ND2	15:U:94:ILE:HG23	2.34	0.41
1:A:10:SER:OG	1:A:13:LEU:HD12	2.20	0.41
1:A:193:LEU:HD21	21:A:362:CLA:CMC	2.50	0.41
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.02	0.41
21:B:513:CLA:H203	21:B:519:CLA:H92	2.02	0.41
3:C:109:PHE:CD2	29:C:494:LMG:H112	2.55	0.41
3:C:264:PHE:HE2	21:C:482:CLA:CGA	2.33	0.41
3:C:292:PHE:CD2	26:C:491:DGD:HG31	2.55	0.41
3:C:456:GLU:N	3:C:456:GLU:OE1	2.53	0.41
3:C:72:LEU:O	10:K:10:LYS:N	2.52	0.41
4:D:274:VAL:HG13	32:D:357:PL9:H222	2.02	0.41
9:J:36:LEU:C	9:J:38:SER:H	2.23	0.41
15:U:55:ILE:HG21	15:U:65:PHE:CE1	2.56	0.41
19:Z:5:PHE:CD2	19:Z:61:VAL:HG21	2.54	0.41
21:B:511:CLA:CMD	21:B:511:CLA:H152	2.49	0.41
27:C:476:LHG:H242	27:C:476:LHG:H121	2.02	0.41
3:C:272:LEU:N	21:C:485:CLA:HMD3	2.36	0.41
3:C:55:ALA:CB	25:C:489:BCR:H373	2.51	0.41
29:B:531:LMG:C2	4:D:141:TYR:OH	2.67	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.71	0.41
4:D:259:ILE:HG21	29:D:360:LMG:H292	2.01	0.41
6:F:28:VAL:CB	6:F:29:PRO:HD3	2.46	0.41
9:J:11:TRP:CE2	9:J:12:ILE:HG12	2.55	0.41
11:L:22:LEU:O	11:L:26:VAL:HG13	2.21	0.41
13:O:215:ARG:NE	15:U:39:LEU:HD22	2.34	0.41
1:A:307:ILE:HG13	6:F:45:ARG:CD	2.49	0.41
2:B:328:GLY:N	21:B:517:CLA:O1A	2.54	0.41
3:C:189:TRP:O	3:C:190:ALA:C	2.58	0.41
1:A:296:ASN:HB2	3:C:400:PRO:O	2.20	0.41
3:C:45:LEU:O	3:C:46:SER:C	2.58	0.41
3:C:464:GLU:O	3:C:467:LEU:HB2	2.19	0.41
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.48	0.41
4:D:161:PRO:CB	4:D:170:ALA:HB2	2.51	0.41
5:E:14:ILE:O	5:E:14:ILE:HG22	2.20	0.41
10:K:28:ILE:O	10:K:31:LEU:HB2	2.21	0.41
1:A:105:TRP:CZ3	1:A:111:PRO:HG3	2.55	0.41
1:A:155:PHE:CD1	26:C:491:DGD:HAE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:O	1:A:15:GLU:HB3	2.20	0.41
1:A:96:ILE:C	1:A:98:GLU:H	2.23	0.41
2:B:12:LEU:O	2:B:14:ASN:N	2.54	0.41
2:B:222:PRO:O	2:B:223:GLN:C	2.59	0.41
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.21	0.41
2:B:479:PHE:O	2:B:480:SER:CB	2.68	0.41
3:C:187:ASP:HB2	3:C:230:LEU:CD1	2.48	0.41
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.01	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.41
15:U:58:ASN:HD22	15:U:114:VAL:HG13	1.84	0.41
1:A:277:ALA:O	1:A:281:VAL:HG23	2.21	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.85	0.41
2:B:49:ASP:HA	2:B:50:PRO:HD2	1.88	0.41
21:C:480:CLA:HBB1	21:C:480:CLA:HHC	2.03	0.41
6:F:24:HIS:HE1	33:F:85:HEM:ND	2.19	0.41
5:E:44:TYR:OH	6:F:43:ILE:HD13	2.21	0.41
7:H:13:PRO:HG2	7:H:14:LEU:H	1.85	0.41
2:B:220:ARG:NH1	7:H:20:LYS:O	2.51	0.41
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.41
6:F:38:ALA:HB1	9:J:27:LEU:CD2	2.50	0.41
13:O:120:THR:HA	13:O:153:ALA:O	2.21	0.41
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.03	0.41
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.51	0.41
19:Z:36:SER:C	19:Z:38:GLN:H	2.24	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.88	0.41
2:B:354:LEU:HD12	2:B:378:LYS:HB2	2.02	0.41
3:C:142:GLU:C	3:C:144:SER:H	2.24	0.41
3:C:175:LEU:HA	21:C:478:CLA:H141	2.02	0.41
3:C:199:ILE:CD1	3:C:199:ILE:N	2.83	0.41
3:C:451:ALA:HA	3:C:456:GLU:CD	2.41	0.41
21:C:478:CLA:HMB1	21:C:480:CLA:HMC3	2.03	0.41
25:C:489:BCR:H361	25:C:489:BCR:H20C	1.87	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:A:114:LEU:O	1:A:114:LEU:HD23	2.21	0.41
2:B:475:PHE:HB3	2:B:478:VAL:CG2	2.51	0.41
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.01	0.41
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.03	0.41
1:A:18:CYS:O	1:A:22:THR:CG2	2.69	0.41
2:B:191:ASN:OD1	2:B:193:TYR:N	2.52	0.41
2:B:380:ASP:OD1	2:B:380:ASP:C	2.60	0.41
3:C:267:SER:O	3:C:271:TYR:CD2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:CH2	26:C:493:DGD:HBV1	2.56	0.41
21:A:364:CLA:H91	21:D:354:CLA:H203	2.02	0.41
5:E:64:PRO:HB3	5:E:84:LYS:CD	2.51	0.41
6:F:37:ILE:O	6:F:37:ILE:HG22	2.20	0.41
6:F:31:ILE:HG12	33:F:85:HEM:HMC2	2.03	0.41
7:H:10:ILE:HG13	7:H:10:ILE:H	1.70	0.41
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.86	0.41
13:O:73:PRO:HG2	13:O:102:THR:HB	2.03	0.41
13:O:147:THR:OG1	13:O:148:VAL:N	2.54	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.41
1:A:234:ASN:HA	1:A:234:ASN:HD22	1.66	0.40
2:B:414:PRO:CB	2:B:415:PRO:HD3	2.40	0.40
2:B:238:LEU:HD13	21:B:522:CLA:C2D	2.51	0.40
3:C:216:SER:HA	26:C:474:DGD:HG12	2.03	0.40
3:C:271:TYR:CE1	21:C:483:CLA:CAC	3.04	0.40
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.02	0.40
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.56	0.40
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.56	0.40
3:C:327:ASN:HB3	13:O:125:ASP:OD1	2.21	0.40
3:C:369:LEU:CD2	3:C:384:ILE:HD13	2.51	0.40
3:C:64:ALA:HB2	21:C:479:CLA:C2D	2.51	0.40
4:D:274:VAL:HG22	32:D:357:PL9:H253	2.03	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.55	0.40
21:A:363:CLA:H92	32:D:357:PL9:H422	2.02	0.40
12:M:10:ALA:O	12:M:14:PHE:HB2	2.21	0.40
12:M:31:SER:HA	29:M:217:LMG:HC72	2.03	0.40
13:O:190:LEU:HD12	15:U:41:ASN:CG	2.41	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:288:LEU:O	1:A:292:THR:HB	2.21	0.40
2:B:224:ARG:NE	7:H:25:TRP:HE1	2.19	0.40
2:B:472:ARG:HE	21:B:521:CLA:HED2	1.86	0.40
21:B:518:CLA:H11	4:D:127:LEU:HD21	2.04	0.40
21:B:525:CLA:H41	21:B:525:CLA:H62	1.72	0.40
3:C:116:VAL:CG2	3:C:117:VAL:N	2.84	0.40
3:C:188:THR:CG2	3:C:298:PRO:HB3	2.50	0.40
4:D:90:LEU:O	21:D:356:CLA:HED1	2.21	0.40
6:F:45:ARG:CB	6:F:45:ARG:HH21	2.35	0.40
25:J:115:BCR:H20C	25:J:115:BCR:H361	1.96	0.40
5:E:15:THR:HG22	9:J:8:ILE:H	1.83	0.40
13:O:226:ASN:ND2	13:O:226:ASN:N	2.68	0.40
1:A:217:SER:HA	1:A:220:THR:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:373:LMG:C20	32:D:357:PL9:C21	2.92	0.40
21:B:513:CLA:CBB	21:B:515:CLA:H171	2.42	0.40
21:B:517:CLA:C2	26:B:533:DGD:HB52	2.52	0.40
2:B:327:THR:HG1	26:B:533:DGD:HO2D	1.70	0.40
3:C:350:ILE:CG2	3:C:359:TRP:HB2	2.51	0.40
3:C:54:VAL:HG11	21:C:488:CLA:HMC3	2.02	0.40
3:C:59:LEU:HD11	25:C:489:BCR:H372	2.03	0.40
1:A:309:ALA:HB2	5:E:52:PRO:C	2.42	0.40
7:H:53:LEU:HD21	7:H:55:LEU:HD21	2.03	0.40
9:J:24:ILE:HG23	9:J:25:VAL:N	2.37	0.40
10:K:18:PHE:O	10:K:19:ASP:C	2.60	0.40
10:K:34:ALA:O	10:K:37:PHE:HB2	2.20	0.40
13:O:157:PRO:O	13:O:158:ASN:O	2.38	0.40
18:X:11:THR:OG1	25:X:107:BCR:H282	2.21	0.40
2:B:150:CYS:HA	21:B:513:CLA:CBC	2.52	0.40
2:B:272:ARG:HG3	2:B:273:TYR:N	2.36	0.40
21:B:522:CLA:H102	21:B:522:CLA:H13	1.86	0.40
3:C:258:GLY:C	3:C:262:ARG:NH1	2.74	0.40
21:C:483:CLA:H121	25:C:490:BCR:H362	2.04	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
4:D:185:PHE:HE2	4:D:289:LEU:HD12	1.87	0.40
4:D:239:GLN:HB3	4:D:240:ALA:H	1.33	0.40
29:D:360:LMG:H361	14:T:21:ILE:CD1	2.51	0.40
4:D:84:SER:HB3	5:E:68:ASP:HA	2.04	0.40
5:E:30:LEU:CD2	6:F:28:VAL:HG13	2.51	0.40
6:F:33:PHE:C	6:F:35:GLY:N	2.74	0.40
21:K:483:CLA:HBB1	21:K:483:CLA:HHC	2.03	0.40
3:C:127:PHE:CE1	19:Z:23:VAL:HG21	2.54	0.40
21:C:486:CLA:C14	19:Z:24:PRO:HG2	2.51	0.40
1:A:116:ILE:HG13	1:A:117:PHE:N	2.37	0.40
1:A:238:LYS:HD3	1:A:238:LYS:HA	1.86	0.40
1:A:214:MET:HB2	23:A:367:MES:H61	1.99	0.40
2:B:153:PHE:O	2:B:157:HIS:HB3	2.22	0.40
2:B:262:THR:HG21	21:B:513:CLA:HBA1	2.03	0.40
2:B:26:HIS:CE1	21:B:522:CLA:HMA1	2.57	0.40
2:B:463:PHE:CD2	2:B:463:PHE:C	2.94	0.40
2:B:483:ASP:CB	2:B:484:PRO:CD	2.97	0.40
3:C:141:GLU:HA	3:C:148:GLY:HA3	2.04	0.40
21:C:481:CLA:O1A	8:I:23:PHE:CE1	2.74	0.40
4:D:17:ILE:HG21	18:X:42:GLN:HG3	2.03	0.40
4:D:279:LEU:CD1	21:D:354:CLA:CBA	3.00	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:PHE:CD1	6:F:42:PHE:N	2.90	0.40
7:H:11:LEU:C	7:H:13:PRO:HD2	2.41	0.40
7:H:7:LEU:HG	7:H:11:LEU:CD1	2.52	0.40
13:O:215:ARG:HD2	15:U:39:LEU:HD22	2.04	0.40
1:A:72:LEU:HD23	14:T:3:THR:HG21	2.03	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	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	8	48
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	6	42
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	4	36
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	6	42
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	2	25
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0	5
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0	5
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	22
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1	21
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	2	23
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	3	29
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100	100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	31
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	25	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	4
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	1	12
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	26
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	4	35

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	141	PRO
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
3	C	452	ALA
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
5	E	82	GLN
7	H	18	TYR
7	H	63	LYS
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
15	U	72	TYR
15	U	83	ALA
16	V	75	ASN
17	y	43	ARG
19	Z	32	ASP
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	209	ILE
3	C	456	GLU
4	D	234	ALA
4	D	264	LYS
6	F	37	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	H	26	GLY
9	J	38	SER
13	O	83	LYS
13	O	231	ASP
15	U	73	PRO
17	y	25	ILE
18	X	43	ILE
2	B	13	ILE
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	375	LEU
3	C	453	ALA
4	D	263	ASN
5	E	9	PRO
6	F	17	THR
7	H	16	SER
7	H	64	ALA
10	K	13	GLU
10	K	45	PHE
13	O	60	SER
13	O	158	ASN
13	O	165	SER
19	Z	24	PRO
19	Z	28	ALA
2	B	173	GLY
2	B	231	MET
2	B	235	GLU
3	C	154	LYS
4	D	73	PHE
5	E	10	PHE
13	O	51	THR
17	y	24	MET
18	X	44	ASP
1	A	97	TRP
3	C	462	GLU
6	F	13	TYR
7	H	6	TRP
7	H	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	U	42	VAL
18	X	12	ILE
1	A	334	ARG
4	D	351	ALA
7	H	14	LEU
1	A	21	VAL
2	B	16	PRO
13	O	159	VAL
3	C	201	ASN
6	F	9	GLU
6	F	11	VAL
17	y	35	ILE
5	E	52	PRO
7	H	60	VAL
8	I	32	PRO
13	O	232	GLY
1	A	176	ILE
4	D	160	TYR
13	O	127	ILE
13	O	152	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	271/280 (97%)	257 (95%)	14 (5%)	27	65
2	B	385/407 (95%)	369 (96%)	16 (4%)	34	71
3	C	348/362 (96%)	327 (94%)	21 (6%)	22	62
4	D	275/283 (97%)	256 (93%)	19 (7%)	18	56
5	E	69/72 (96%)	64 (93%)	5 (7%)	17	55
6	F	32/38 (84%)	31 (97%)	1 (3%)	45	79
7	H	53/54 (98%)	49 (92%)	4 (8%)	16	53
8	I	32/35 (91%)	31 (97%)	1 (3%)	45	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	23 (96%)	1 (4%)	34	71
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	41
11	L	35/35 (100%)	30 (86%)	5 (14%)	4	26
12	M	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	193 (96%)	9 (4%)	32	70
14	T	27/29 (93%)	26 (96%)	1 (4%)	39	74
15	U	84/89 (94%)	80 (95%)	4 (5%)	30	68
16	V	116/117 (99%)	111 (96%)	5 (4%)	33	71
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	41
18	X	28/33 (85%)	24 (86%)	4 (14%)	4	26
19	Z	52/52 (100%)	47 (90%)	5 (10%)	10	43
All	All	2114/2222 (95%)	1994 (94%)	120 (6%)	24	63

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	170	ASP
1	A	202	VAL
1	A	206	PHE
1	A	234	ASN
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	298	ASN
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	223	GLN
2	B	246	PHE
2	B	262	THR
2	B	308	LYS
2	B	309	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	362	PHE
2	B	373	LYS
2	B	374	ASN
2	B	414	PRO
2	B	422	ARG
2	B	433	ASP
2	B	483	ASP
2	B	486	LEU
3	C	26	ARG
3	C	27	ASP
3	C	28	GLN
3	C	29	GLU
3	C	78	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	201	ASN
3	C	207	ARG
3	C	232	ASP
3	C	244	CYS
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	401	LEU
3	C	447	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	60	THR
4	D	84	SER
4	D	91	LEU
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	221	THR
4	D	236	ASN
4	D	241	GLU
4	D	256	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
6	F	24	HIS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
10	K	10	LYS
10	K	18	PHE
10	K	19	ASP
11	L	1	MET
11	L	7	ARG
11	L	8	GLN
11	L	11	GLU
11	L	15	THR
13	O	31	LEU
13	O	87	GLN
13	O	88	GLU
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	141	ARG
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	32	GLU
16	V	63	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	V	92	ARG
16	V	116	GLU
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	42	GLN
18	X	45	LYS
19	Z	14	ILE
19	Z	25	VAL
19	Z	33	TRP
19	Z	58	ASN
19	Z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	241	GLN
1	A	261	GLN
2	B	201	HIS
2	B	216	HIS
2	B	374	ASN
3	C	155	ASN
3	C	251	HIS
3	C	398	HIS
3	C	418	ASN
3	C	444	HIS
4	D	98	GLN
4	D	117	HIS
4	D	129	GLN
4	D	142	ASN
4	D	239	GLN
4	D	250	ASN
5	E	74	GLN
6	F	44	GLN
7	H	59	ASN
11	L	6	ASN
11	L	8	GLN
12	M	33	GLN
13	O	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	O	135	GLN
13	O	150	ASN
13	O	173	ASN
13	O	222	GLN
13	O	226	ASN
15	U	82	ASN
18	X	42	GLN
19	Z	6	GLN

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 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\# Z > 2$
21	CLA	A	362	-	56,73,73	2.31	14 (25%)	65,113,113	1.62	14 (21%)
21	CLA	A	363	-	56,73,73	2.39	15 (26%)	65,113,113	1.83	16 (24%)
21	CLA	A	364	-	56,73,73	2.48	14 (25%)	65,113,113	1.67	15 (23%)
22	PHO	A	365	-	67,69,69	2.26	14 (20%)	87,99,99	1.45	14 (16%)
21	CLA	A	366	-	56,73,73	2.56	13 (23%)	65,113,113	1.49	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	MES	A	367	-	12,12,12	1.46	1 (8%)	14,16,16	1.56	3 (21%)
24	OEC	A	368	1,3	0,0,13	0.00	-	0,0,27	0.00	-
25	BCR	A	369	-	41,41,41	1.90	6 (14%)	56,56,56	2.09	19 (33%)
27	LHG	A	371	-	38,38,48	2.13	6 (15%)	39,44,54	1.45	4 (10%)
29	LMG	A	373	-	51,51,55	0.54	1 (1%)	59,59,63	1.14	6 (10%)
26	DGD	A	375	-	53,53,67	2.06	13 (24%)	67,67,81	2.52	22 (32%)
30	LMT	A	376	-	36,36,36	2.02	11 (30%)	47,47,47	1.51	8 (17%)
21	CLA	B	511	-	56,73,73	3.36	19 (33%)	65,113,113	1.59	15 (23%)
21	CLA	B	512	-	56,73,73	2.34	13 (23%)	65,113,113	1.49	11 (16%)
21	CLA	B	513	-	56,73,73	2.39	14 (25%)	65,113,113	1.71	16 (24%)
21	CLA	B	514	-	56,73,73	2.58	13 (23%)	65,113,113	1.50	15 (23%)
21	CLA	B	515	-	56,73,73	2.60	15 (26%)	65,113,113	1.65	12 (18%)
21	CLA	B	516	-	56,73,73	2.75	15 (26%)	65,113,113	1.80	19 (29%)
21	CLA	B	517	-	56,73,73	2.68	16 (28%)	65,113,113	2.12	23 (35%)
21	CLA	B	518	-	56,73,73	2.81	18 (32%)	65,113,113	1.97	21 (32%)
21	CLA	B	519	-	56,73,73	2.61	13 (23%)	65,113,113	1.65	15 (23%)
21	CLA	B	520	-	56,73,73	2.55	13 (23%)	65,113,113	1.52	12 (18%)
21	CLA	B	521	-	56,73,73	2.59	14 (25%)	65,113,113	1.79	16 (24%)
21	CLA	B	522	-	56,73,73	2.37	14 (25%)	65,113,113	1.54	14 (21%)
21	CLA	B	523	-	56,73,73	2.34	14 (25%)	65,113,113	1.45	13 (20%)
21	CLA	B	524	-	56,73,73	2.79	16 (28%)	65,113,113	1.76	15 (23%)
21	CLA	B	525	-	56,73,73	2.72	17 (30%)	65,113,113	1.56	13 (20%)
21	CLA	B	526	-	56,73,73	2.87	14 (25%)	65,113,113	1.60	13 (20%)
25	BCR	B	527	-	41,41,41	1.78	7 (17%)	56,56,56	2.34	20 (35%)
26	DGD	B	528	-	59,59,67	0.59	2 (3%)	73,73,81	1.10	8 (10%)
25	BCR	B	529	-	41,41,41	2.16	9 (21%)	56,56,56	2.17	19 (33%)
25	BCR	B	530	-	41,41,41	2.49	11 (26%)	56,56,56	2.23	23 (41%)
29	LMG	B	531	-	49,49,55	1.63	6 (12%)	57,57,63	2.81	18 (31%)
26	DGD	B	533	-	67,67,67	1.48	14 (20%)	81,81,81	1.86	20 (24%)
30	LMT	B	535	-	36,36,36	1.89	10 (27%)	47,47,47	1.18	2 (4%)
26	DGD	C	474	-	57,57,67	2.08	15 (26%)	71,71,81	3.74	25 (35%)
28	SQD	C	475	-	50,51,54	2.58	27 (54%)	60,62,65	3.11	20 (33%)
27	LHG	C	476	-	36,36,48	2.30	7 (19%)	37,42,54	1.54	4 (10%)
21	CLA	C	477	-	56,73,73	2.60	13 (23%)	65,113,113	1.70	14 (21%)
21	CLA	C	478	-	56,73,73	2.49	14 (25%)	65,113,113	1.57	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	C	479	-	56,73,73	2.73	16 (28%)	65,113,113	1.72	16 (24%)
21	CLA	C	480	-	56,73,73	2.67	16 (28%)	65,113,113	1.89	14 (21%)
21	CLA	C	481	-	56,73,73	2.82	14 (25%)	65,113,113	2.18	16 (24%)
21	CLA	C	482	-	56,73,73	3.13	19 (33%)	65,113,113	1.58	16 (24%)
21	CLA	C	483	-	56,73,73	2.77	17 (30%)	65,113,113	1.55	13 (20%)
21	CLA	C	484	-	56,73,73	2.68	14 (25%)	65,113,113	1.70	17 (26%)
21	CLA	C	485	-	56,73,73	2.57	13 (23%)	65,113,113	1.48	12 (18%)
21	CLA	C	486	3	56,73,73	2.84	17 (30%)	65,113,113	1.88	17 (26%)
21	CLA	C	487	-	56,73,73	3.13	18 (32%)	65,113,113	1.59	11 (16%)
21	CLA	C	488	-	56,73,73	2.69	15 (26%)	65,113,113	1.84	16 (24%)
25	BCR	C	489	-	41,41,41	1.89	9 (21%)	56,56,56	2.09	16 (28%)
25	BCR	C	490	-	41,41,41	1.97	8 (19%)	56,56,56	2.22	21 (37%)
26	DGD	C	491	-	54,54,67	1.63	9 (16%)	68,68,81	3.07	23 (33%)
26	DGD	C	492	-	63,63,67	1.36	10 (15%)	77,77,81	2.79	21 (27%)
26	DGD	C	493	-	67,67,67	1.45	16 (23%)	81,81,81	3.10	29 (35%)
29	LMG	C	494	-	45,45,55	1.89	8 (17%)	53,53,63	2.27	16 (30%)
31	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	D	354	-	56,73,73	2.51	14 (25%)	65,113,113	1.72	15 (23%)
22	PHO	D	355	-	67,69,69	2.19	14 (20%)	87,99,99	1.38	15 (17%)
21	CLA	D	356	-	56,73,73	2.61	16 (28%)	65,113,113	1.64	15 (23%)
32	PL9	D	357	-	55,55,55	3.00	21 (38%)	69,69,69	2.83	26 (37%)
25	BCR	D	358	-	41,41,41	1.70	7 (17%)	56,56,56	2.29	19 (33%)
29	LMG	D	359	-	46,46,55	1.69	6 (13%)	54,54,63	2.61	16 (29%)
29	LMG	D	360	-	48,48,55	0.55	1 (2%)	56,56,63	1.15	6 (10%)
28	SQD	D	361	-	42,43,54	2.57	19 (45%)	52,54,65	3.45	18 (34%)
26	DGD	D	362	-	64,64,67	2.09	22 (34%)	78,78,81	2.58	21 (26%)
30	LMT	D	363	-	32,32,36	1.83	7 (21%)	43,43,47	1.49	6 (13%)
30	LMT	D	536	-	36,36,36	1.71	10 (27%)	47,47,47	1.60	8 (17%)
28	SQD	F	224	-	44,45,54	2.65	21 (47%)	54,56,65	3.36	19 (35%)
33	HEM	F	85	5	28,50,50	2.62	10 (35%)	17,82,82	4.02	7 (41%)
29	LMG	I	220	-	43,43,55	2.00	12 (27%)	51,51,63	2.21	14 (27%)
30	LMT	I	274	-	36,36,36	1.88	12 (33%)	47,47,47	1.35	7 (14%)
25	BCR	J	112	-	41,41,41	1.88	8 (19%)	56,56,56	2.41	25 (44%)
25	BCR	J	115	-	41,41,41	2.23	11 (26%)	56,56,56	3.21	18 (32%)
29	LMG	J	492	-	48,48,55	1.92	9 (18%)	56,56,63	1.91	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	K	483	-	56,73,73	2.42	13 (23%)	65,113,113	1.51	12 (18%)
28	SQD	L	213	-	46,47,54	2.60	23 (50%)	56,58,65	3.37	21 (37%)
29	LMG	M	217	-	42,42,55	1.91	8 (19%)	50,50,63	1.55	7 (14%)
30	LMT	O	274	-	36,36,36	2.03	12 (33%)	47,47,47	1.41	7 (14%)
30	LMT	T	226	-	36,36,36	1.80	9 (25%)	47,47,47	1.01	2 (4%)
33	HEM	V	164	16	28,50,50	2.13	7 (25%)	17,82,82	3.84	6 (35%)
25	BCR	X	107	-	41,41,41	1.53	6 (14%)	56,56,56	2.40	20 (35%)
25	BCR	Z	116	-	41,41,41	1.93	8 (19%)	56,56,56	2.08	20 (35%)

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
21	CLA	A	362	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	A	363	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	A	364	-	4/4/20/25	0/37/135/135	0/0/9/9
22	PHO	A	365	-	1/1/17/22	0/53/103/103	0/1/6/6
21	CLA	A	366	-	4/4/20/25	0/37/135/135	0/0/9/9
23	MES	A	367	-	-	0/6/14/14	0/1/1/1
24	OEC	A	368	1,3	-	0/0/0/54	0/0/0/5
25	BCR	A	369	-	-	0/29/63/63	0/2/2/2
27	LHG	A	371	-	-	0/43/43/53	0/0/0/0
29	LMG	A	373	-	-	0/46/66/70	0/1/1/1
26	DGD	A	375	-	-	0/41/81/95	0/2/2/2
30	LMT	A	376	-	-	0/21/61/61	0/2/2/2
21	CLA	B	511	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	512	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	513	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	514	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	515	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	516	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	517	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	518	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	519	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	520	-	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	521	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	522	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	523	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	524	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	525	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	526	-	4/4/20/25	0/37/135/135	0/0/9/9
25	BCR	B	527	-	-	0/29/63/63	0/2/2/2
26	DGD	B	528	-	-	0/47/87/95	0/2/2/2
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
25	BCR	B	530	-	-	0/29/63/63	0/2/2/2
29	LMG	B	531	-	-	0/44/64/70	0/1/1/1
26	DGD	B	533	-	-	0/55/95/95	0/2/2/2
30	LMT	B	535	-	-	0/21/61/61	0/2/2/2
26	DGD	C	474	-	-	0/45/85/95	0/2/2/2
28	SQD	C	475	-	-	0/46/66/69	0/1/1/1
27	LHG	C	476	-	-	0/41/41/53	0/0/0/0
21	CLA	C	477	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	478	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	479	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	480	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	481	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	482	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	483	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	484	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	485	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	486	3	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	487	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	488	-	4/4/20/25	0/37/135/135	0/0/9/9
25	BCR	C	489	-	-	0/29/63/63	0/2/2/2
25	BCR	C	490	-	-	0/29/63/63	0/2/2/2
26	DGD	C	491	-	-	0/42/82/95	0/2/2/2
26	DGD	C	492	-	1/1/13/13	0/51/91/95	0/2/2/2
26	DGD	C	493	-	1/1/13/13	0/55/95/95	0/2/2/2
29	LMG	C	494	-	-	0/40/60/70	0/1/1/1
31	BCT	D	353	20	-	0/0/0/0	0/0/0/0
21	CLA	D	354	-	4/4/20/25	0/37/135/135	0/0/9/9
22	PHO	D	355	-	1/1/17/22	0/53/103/103	0/1/6/6
21	CLA	D	356	-	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PL9	D	357	-	-	2/53/73/73	0/1/1/1
25	BCR	D	358	-	-	0/29/63/63	0/2/2/2
29	LMG	D	359	-	-	0/41/61/70	0/1/1/1
29	LMG	D	360	-	-	0/43/63/70	0/1/1/1
28	SQD	D	361	-	-	2/38/58/69	0/1/1/1
26	DGD	D	362	-	-	0/52/92/95	0/2/2/2
30	LMT	D	363	-	-	0/17/57/61	0/2/2/2
30	LMT	D	536	-	-	0/21/61/61	0/2/2/2
28	SQD	F	224	-	-	0/40/60/69	0/1/1/1
33	HEM	F	85	5	-	0/6/54/54	0/0/8/8
29	LMG	I	220	-	-	0/38/58/70	0/1/1/1
30	LMT	I	274	-	-	0/21/61/61	0/2/2/2
25	BCR	J	112	-	-	0/29/63/63	0/2/2/2
25	BCR	J	115	-	-	0/29/63/63	0/2/2/2
29	LMG	J	492	-	-	0/43/63/70	0/1/1/1
21	CLA	K	483	-	4/4/20/25	0/37/135/135	0/0/9/9
28	SQD	L	213	-	-	0/42/62/69	0/1/1/1
29	LMG	M	217	-	-	0/37/57/70	0/1/1/1
30	LMT	O	274	-	-	0/21/61/61	0/2/2/2
30	LMT	T	226	-	-	0/21/61/61	0/2/2/2
33	HEM	V	164	16	-	0/6/54/54	0/0/8/8
25	BCR	X	107	-	-	0/29/63/63	0/2/2/2
25	BCR	Z	116	-	-	0/29/63/63	0/2/2/2

All (1006) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	531	LMG	O1-C1	-9.46	1.23	1.40
29	M	217	LMG	O1-C1	-9.43	1.23	1.40
29	I	220	LMG	O1-C1	-9.39	1.23	1.40
29	C	494	LMG	O1-C1	-9.36	1.23	1.40
29	J	492	LMG	O1-C1	-9.35	1.23	1.40
29	D	359	LMG	O1-C1	-9.34	1.23	1.40
32	D	357	PL9	C3-C4	-5.83	1.39	1.49
21	B	516	CLA	C3A-C2A	-5.34	1.39	1.54
21	B	517	CLA	C3A-C2A	-5.33	1.39	1.54
21	C	477	CLA	C3A-C2A	-5.32	1.39	1.54
21	B	513	CLA	C3A-C2A	-5.32	1.39	1.54
21	B	523	CLA	C3A-C2A	-5.32	1.39	1.54
21	D	356	CLA	C3A-C2A	-5.32	1.39	1.54
21	B	521	CLA	C3A-C2A	-5.32	1.39	1.54
21	B	512	CLA	C3A-C2A	-5.31	1.39	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	366	CLA	C3A-C2A	-5.31	1.39	1.54
21	C	478	CLA	C3A-C2A	-5.31	1.39	1.54
21	C	485	CLA	C3A-C2A	-5.31	1.39	1.54
21	C	484	CLA	C3A-C2A	-5.30	1.39	1.54
21	B	514	CLA	C3A-C2A	-5.30	1.39	1.54
21	A	362	CLA	C3A-C2A	-5.30	1.39	1.54
21	A	364	CLA	C3A-C2A	-5.30	1.39	1.54
21	C	488	CLA	C3A-C2A	-5.30	1.39	1.54
21	B	518	CLA	C3A-C2A	-5.29	1.39	1.54
21	B	522	CLA	C3A-C2A	-5.29	1.39	1.54
22	A	365	PHO	C3A-C2A	-5.29	1.39	1.54
21	B	520	CLA	C3A-C2A	-5.28	1.39	1.54
21	C	482	CLA	C3A-C2A	-5.28	1.39	1.54
21	B	519	CLA	C3A-C2A	-5.28	1.39	1.54
21	C	480	CLA	C3A-C2A	-5.28	1.39	1.54
21	C	479	CLA	C3A-C2A	-5.28	1.39	1.54
21	B	515	CLA	C3A-C2A	-5.27	1.39	1.54
21	C	481	CLA	C3A-C2A	-5.27	1.39	1.54
21	B	524	CLA	C3A-C2A	-5.27	1.39	1.54
21	C	487	CLA	C3A-C2A	-5.27	1.39	1.54
22	D	355	PHO	C3A-C2A	-5.27	1.39	1.54
21	K	483	CLA	C3A-C2A	-5.26	1.39	1.54
21	A	363	CLA	C3A-C2A	-5.26	1.39	1.54
21	B	525	CLA	C3A-C2A	-5.25	1.39	1.54
21	B	511	CLA	C3A-C2A	-5.25	1.39	1.54
21	C	486	CLA	C3A-C2A	-5.24	1.39	1.54
21	D	354	CLA	C3A-C2A	-5.24	1.39	1.54
21	B	526	CLA	C3A-C2A	-5.23	1.39	1.54
21	C	483	CLA	C3A-C2A	-5.21	1.39	1.54
32	D	357	PL9	C6-C1	-5.15	1.39	1.48
30	T	226	LMT	C4B-C3B	-5.06	1.39	1.52
30	O	274	LMT	C4B-C3B	-5.04	1.39	1.52
30	A	376	LMT	C4B-C3B	-5.01	1.39	1.52
30	D	363	LMT	C4B-C3B	-5.01	1.39	1.52
30	D	536	LMT	C4B-C3B	-5.00	1.39	1.52
30	B	535	LMT	C4B-C3B	-4.99	1.39	1.52
30	I	274	LMT	C4B-C3B	-4.98	1.39	1.52
33	F	85	HEM	C4D-ND	-4.54	1.31	1.36
21	B	518	CLA	C4-C3	-4.44	1.39	1.50
21	B	520	CLA	C4-C3	-4.42	1.39	1.50
21	D	354	CLA	C4-C3	-4.41	1.39	1.50
21	A	362	CLA	C4-C3	-4.41	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	512	CLA	C4-C3	-4.41	1.39	1.50
21	B	517	CLA	C4-C3	-4.40	1.39	1.50
22	D	355	PHO	C4-C3	-4.40	1.39	1.50
21	B	516	CLA	C4-C3	-4.40	1.39	1.50
21	C	482	CLA	C4-C3	-4.39	1.39	1.50
22	A	365	PHO	C4-C3	-4.39	1.39	1.50
21	A	366	CLA	C4-C3	-4.39	1.39	1.50
21	B	519	CLA	C4-C3	-4.38	1.39	1.50
21	B	514	CLA	C4-C3	-4.38	1.39	1.50
21	D	356	CLA	C4-C3	-4.38	1.39	1.50
21	C	481	CLA	C4-C3	-4.37	1.39	1.50
21	B	513	CLA	C4-C3	-4.37	1.39	1.50
21	C	483	CLA	C4-C3	-4.37	1.39	1.50
21	C	479	CLA	C4-C3	-4.37	1.39	1.50
21	B	515	CLA	C4-C3	-4.37	1.39	1.50
21	C	484	CLA	C4-C3	-4.37	1.39	1.50
21	B	523	CLA	C4-C3	-4.37	1.39	1.50
21	B	524	CLA	C4-C3	-4.37	1.39	1.50
21	A	363	CLA	C4-C3	-4.36	1.39	1.50
21	B	511	CLA	C4-C3	-4.36	1.39	1.50
21	A	364	CLA	C4-C3	-4.36	1.39	1.50
21	C	477	CLA	C4-C3	-4.35	1.39	1.50
21	C	480	CLA	C4-C3	-4.35	1.39	1.50
21	C	486	CLA	C4-C3	-4.35	1.39	1.50
21	C	485	CLA	C4-C3	-4.35	1.39	1.50
21	K	483	CLA	C4-C3	-4.35	1.39	1.50
21	C	487	CLA	C4-C3	-4.35	1.39	1.50
21	B	522	CLA	C4-C3	-4.35	1.39	1.50
21	B	526	CLA	C4-C3	-4.35	1.39	1.50
21	C	488	CLA	C4-C3	-4.34	1.39	1.50
21	C	478	CLA	C4-C3	-4.33	1.39	1.50
21	B	525	CLA	C4-C3	-4.33	1.39	1.50
21	B	521	CLA	C4-C3	-4.32	1.39	1.50
21	C	481	CLA	CAA-CBA	-4.26	1.39	1.52
21	B	518	CLA	CAA-CBA	-4.19	1.39	1.52
21	B	517	CLA	CAA-CBA	-4.18	1.39	1.52
21	B	515	CLA	CAA-CBA	-4.18	1.39	1.52
21	C	484	CLA	CAA-CBA	-4.17	1.39	1.52
21	B	519	CLA	CAA-CBA	-4.16	1.39	1.52
21	C	480	CLA	CAA-CBA	-4.16	1.39	1.52
21	C	478	CLA	CAA-CBA	-4.15	1.39	1.52
21	B	522	CLA	CAA-CBA	-4.14	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	479	CLA	CAA-CBA	-4.14	1.39	1.52
21	B	520	CLA	CAA-CBA	-4.14	1.39	1.52
21	C	488	CLA	CAA-CBA	-4.14	1.39	1.52
21	C	477	CLA	CAA-CBA	-4.14	1.39	1.52
22	A	365	PHO	CAA-CBA	-4.13	1.39	1.52
21	B	521	CLA	CAA-CBA	-4.12	1.39	1.52
21	B	512	CLA	CAA-CBA	-4.12	1.39	1.52
21	A	362	CLA	CAA-CBA	-4.12	1.39	1.52
21	K	483	CLA	CAA-CBA	-4.12	1.39	1.52
21	B	524	CLA	CAA-CBA	-4.11	1.39	1.52
21	D	356	CLA	CAA-CBA	-4.11	1.39	1.52
21	B	514	CLA	CAA-CBA	-4.11	1.39	1.52
21	B	523	CLA	CAA-CBA	-4.11	1.39	1.52
21	D	354	CLA	CAA-CBA	-4.10	1.39	1.52
21	C	486	CLA	CAA-CBA	-4.10	1.39	1.52
21	A	364	CLA	CAA-CBA	-4.09	1.39	1.52
21	A	366	CLA	CAA-CBA	-4.08	1.39	1.52
21	B	513	CLA	CAA-CBA	-4.08	1.39	1.52
21	B	516	CLA	CAA-CBA	-4.08	1.39	1.52
21	C	482	CLA	CAA-CBA	-4.08	1.39	1.52
21	C	485	CLA	CAA-CBA	-4.07	1.39	1.52
22	D	355	PHO	CAA-CBA	-4.07	1.39	1.52
21	C	483	CLA	CAA-CBA	-4.07	1.39	1.52
21	B	526	CLA	CAA-CBA	-4.06	1.39	1.52
21	A	363	CLA	CAA-CBA	-4.06	1.39	1.52
21	B	525	CLA	CAA-CBA	-4.04	1.39	1.52
21	B	511	CLA	CAA-CBA	-4.03	1.39	1.52
21	C	487	CLA	CAA-CBA	-4.01	1.39	1.52
26	C	493	DGD	O5D-C6D	-3.52	1.37	1.43
33	V	164	HEM	C3B-CAB	-3.28	1.41	1.47
33	F	85	HEM	CAD-C3D	-3.23	1.46	1.52
32	D	357	PL9	C12-C13	-3.23	1.39	1.50
21	A	364	CLA	C3D-C2D	-3.22	1.32	1.39
32	D	357	PL9	C32-C33	-3.19	1.39	1.50
32	D	357	PL9	C37-C38	-3.17	1.39	1.50
32	D	357	PL9	C27-C28	-3.13	1.39	1.50
33	V	164	HEM	C4D-ND	-3.07	1.33	1.36
26	C	491	DGD	O2E-C2E	-2.99	1.36	1.43
26	C	493	DGD	C5B-C4B	-2.98	1.34	1.51
22	A	365	PHO	C1B-C2B	-2.97	1.39	1.45
33	V	164	HEM	CAD-C3D	-2.94	1.46	1.52
22	D	355	PHO	C1B-C2B	-2.92	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	481	CLA	CAA-C2A	-2.85	1.48	1.54
28	C	475	SQD	C20-C19	-2.81	1.35	1.51
26	C	491	DGD	C5B-C4B	-2.79	1.35	1.51
26	C	492	DGD	O5D-C6D	-2.73	1.38	1.43
28	C	475	SQD	C19-C18	-2.72	1.36	1.51
28	C	475	SQD	C33-C32	-2.72	1.36	1.51
28	F	224	SQD	C14-C13	-2.64	1.36	1.51
28	D	361	SQD	C15-C14	-2.64	1.36	1.51
25	C	489	BCR	C19-C18	-2.63	1.40	1.45
28	L	213	SQD	C12-C11	-2.63	1.36	1.51
28	C	475	SQD	C17-C16	-2.63	1.36	1.51
28	D	361	SQD	C14-C13	-2.62	1.36	1.51
28	F	224	SQD	C13-C12	-2.61	1.36	1.51
28	C	475	SQD	C12-C11	-2.61	1.36	1.51
28	D	361	SQD	C16-C15	-2.60	1.36	1.51
28	D	361	SQD	C12-C11	-2.59	1.36	1.51
28	D	361	SQD	C13-C12	-2.59	1.36	1.51
28	F	224	SQD	C17-C16	-2.58	1.36	1.51
28	L	213	SQD	C16-C15	-2.58	1.36	1.51
28	F	224	SQD	C12-C11	-2.57	1.36	1.51
28	L	213	SQD	C17-C16	-2.56	1.37	1.51
28	F	224	SQD	C15-C14	-2.55	1.37	1.51
28	C	475	SQD	C11-C10	-2.54	1.37	1.51
28	D	361	SQD	C11-C10	-2.54	1.37	1.51
28	C	475	SQD	C32-C31	-2.52	1.37	1.51
28	C	475	SQD	C18-C17	-2.51	1.37	1.51
29	D	359	LMG	C16-C15	-2.50	1.37	1.51
28	L	213	SQD	C11-C10	-2.50	1.37	1.51
26	A	375	DGD	C5B-C4B	-2.49	1.37	1.51
21	D	356	CLA	C3D-C2D	-2.47	1.34	1.39
28	C	475	SQD	C16-C15	-2.47	1.37	1.51
26	C	493	DGD	O2E-C2E	-2.46	1.37	1.43
25	D	358	BCR	C19-C18	-2.46	1.40	1.45
28	F	224	SQD	C16-C15	-2.43	1.37	1.51
26	C	474	DGD	C5B-C4B	-2.41	1.37	1.51
28	L	213	SQD	C13-C12	-2.40	1.37	1.51
28	L	213	SQD	C15-C14	-2.40	1.37	1.51
28	L	213	SQD	C20-C19	-2.38	1.38	1.51
28	C	475	SQD	C13-C12	-2.36	1.38	1.51
28	L	213	SQD	C14-C13	-2.36	1.38	1.51
29	C	494	LMG	C16-C15	-2.35	1.38	1.51
28	C	475	SQD	C15-C14	-2.35	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	493	DGD	C4D-C3D	-2.33	1.46	1.52
25	Z	116	BCR	C23-C22	-2.29	1.40	1.45
28	L	213	SQD	C19-C18	-2.28	1.38	1.51
29	I	220	LMG	C16-C15	-2.28	1.38	1.51
28	C	475	SQD	C14-C13	-2.27	1.38	1.51
29	B	531	LMG	C16-C15	-2.27	1.38	1.51
29	M	217	LMG	C16-C15	-2.22	1.38	1.51
32	D	357	PL9	C36-C37	-2.21	1.46	1.53
21	D	354	CLA	C3D-C2D	-2.20	1.35	1.39
28	F	224	SQD	C11-C10	-2.19	1.39	1.51
26	C	493	DGD	O6E-C5E	-2.17	1.39	1.44
26	C	474	DGD	C4A-C3A	-2.17	1.39	1.51
26	C	492	DGD	C9A-C8A	-2.16	1.39	1.51
26	C	492	DGD	C4A-C3A	-2.16	1.39	1.51
26	B	533	DGD	C4A-C3A	-2.16	1.39	1.51
21	C	482	CLA	C3D-C2D	-2.15	1.35	1.39
29	B	531	LMG	C39-C38	-2.15	1.39	1.51
30	B	535	LMT	C10-C9	-2.14	1.39	1.51
29	C	494	LMG	C34-C33	-2.14	1.39	1.51
26	C	493	DGD	C4A-C3A	-2.14	1.39	1.51
26	B	533	DGD	CEB-CDB	-2.14	1.39	1.51
28	C	475	SQD	C21-C20	-2.14	1.36	1.51
30	D	536	LMT	C10-C9	-2.14	1.39	1.51
25	C	489	BCR	C20-C21	-2.14	1.37	1.43
26	C	493	DGD	CFB-CEB	-2.13	1.39	1.51
29	D	359	LMG	C34-C33	-2.13	1.39	1.51
26	C	493	DGD	CEB-CDB	-2.13	1.39	1.51
26	C	492	DGD	CFB-CEB	-2.13	1.39	1.51
30	T	226	LMT	C10-C9	-2.13	1.39	1.51
30	I	274	LMT	C10-C9	-2.13	1.39	1.51
30	D	536	LMT	C5-C4	-2.13	1.39	1.51
26	C	493	DGD	C9A-C8A	-2.13	1.39	1.51
29	I	220	LMG	C34-C33	-2.12	1.39	1.51
26	C	491	DGD	C4A-C3A	-2.12	1.39	1.51
26	C	493	DGD	C9B-C8B	-2.12	1.39	1.51
30	O	274	LMT	C10-C9	-2.12	1.39	1.51
26	C	493	DGD	CDA-CCA	-2.12	1.39	1.51
30	B	535	LMT	C5-C4	-2.12	1.39	1.51
29	D	359	LMG	C39-C38	-2.12	1.39	1.51
26	B	533	DGD	C5B-C4B	-2.12	1.39	1.51
26	B	533	DGD	CDA-CCA	-2.12	1.39	1.51
29	B	531	LMG	C20-C19	-2.12	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	213	SQD	C18-C17	-2.11	1.39	1.51
29	J	492	LMG	C34-C33	-2.11	1.39	1.51
26	B	533	DGD	C9A-C8A	-2.11	1.39	1.51
28	D	361	SQD	C17-C16	-2.11	1.36	1.51
30	O	274	LMT	C5-C4	-2.11	1.39	1.51
26	B	533	DGD	CFB-CEB	-2.11	1.39	1.51
29	B	531	LMG	C34-C33	-2.11	1.39	1.51
26	D	362	DGD	CEB-CDB	-2.11	1.39	1.51
26	A	375	DGD	C4A-C3A	-2.11	1.39	1.51
26	C	492	DGD	CEB-CDB	-2.11	1.39	1.51
26	D	362	DGD	CFB-CEB	-2.11	1.39	1.51
30	A	376	LMT	C10-C9	-2.11	1.39	1.51
30	A	376	LMT	C5-C4	-2.11	1.39	1.51
26	D	362	DGD	CDA-CCA	-2.10	1.39	1.51
29	M	217	LMG	C34-C33	-2.10	1.39	1.51
29	J	492	LMG	C39-C38	-2.10	1.39	1.51
30	I	274	LMT	C5-C4	-2.10	1.39	1.51
26	C	474	DGD	C9B-C8B	-2.10	1.39	1.51
29	C	494	LMG	C20-C19	-2.10	1.39	1.51
26	C	491	DGD	C9A-C8A	-2.10	1.39	1.51
26	C	474	DGD	C9A-C8A	-2.10	1.39	1.51
29	D	359	LMG	C20-C19	-2.09	1.39	1.51
30	T	226	LMT	C5-C4	-2.09	1.39	1.51
26	A	375	DGD	C9B-C8B	-2.09	1.39	1.51
26	C	492	DGD	C9B-C8B	-2.09	1.39	1.51
26	B	533	DGD	C9B-C8B	-2.09	1.39	1.51
21	K	483	CLA	C3D-C2D	-2.09	1.35	1.39
29	I	220	LMG	C20-C19	-2.08	1.39	1.51
26	D	362	DGD	C9A-C8A	-2.08	1.39	1.51
28	C	475	SQD	C34-C33	-2.08	1.36	1.51
29	J	492	LMG	C20-C19	-2.08	1.39	1.51
29	M	217	LMG	C20-C19	-2.08	1.39	1.51
30	D	363	LMT	C5-C4	-2.07	1.39	1.51
26	D	362	DGD	C5B-C4B	-2.07	1.39	1.51
26	D	362	DGD	C4A-C3A	-2.07	1.39	1.51
26	D	362	DGD	C9B-C8B	-2.06	1.39	1.51
21	B	525	CLA	C3D-C2D	-2.05	1.35	1.39
21	B	525	CLA	C3D-CAD	-2.03	1.40	1.46
25	J	112	BCR	C19-C18	-2.03	1.41	1.45
21	A	362	CLA	C3D-C2D	-2.03	1.35	1.39
26	C	492	DGD	C5B-C4B	-2.03	1.40	1.51
28	F	224	SQD	C18-C17	-2.02	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	518	CLA	C3B-CAB	-2.02	1.43	1.47
27	C	476	LHG	C6-C5	2.00	1.56	1.50
21	B	512	CLA	CMC-C2C	2.00	1.55	1.50
21	C	479	CLA	CMD-C2D	2.00	1.55	1.51
30	B	535	LMT	C3B-C2B	2.00	1.57	1.52
21	B	526	CLA	CMC-C2C	2.01	1.55	1.50
26	B	533	DGD	C2A-C1A	2.01	1.56	1.50
30	A	376	LMT	O5B-C5B	2.02	1.49	1.44
21	C	482	CLA	OBD-CAD	2.02	1.25	1.22
21	B	519	CLA	CMD-C2D	2.02	1.55	1.51
21	C	480	CLA	CBA-CGA	2.03	1.56	1.50
30	I	274	LMT	O5B-C5B	2.03	1.49	1.44
29	I	220	LMG	C1-C2	2.04	1.58	1.52
21	B	523	CLA	C5-C3	2.04	1.55	1.51
21	C	487	CLA	CHC-C1C	2.04	1.41	1.35
25	X	107	BCR	C14-C13	2.05	1.38	1.35
28	D	361	SQD	C44-C45	2.06	1.56	1.50
33	F	85	HEM	C2A-C3A	2.06	1.43	1.37
21	C	482	CLA	CMD-C2D	2.06	1.56	1.51
30	O	274	LMT	C1B-C2B	2.06	1.58	1.52
30	D	536	LMT	C3'-C4'	2.07	1.58	1.52
21	B	518	CLA	CHC-C1C	2.07	1.41	1.35
26	D	362	DGD	C2B-C1B	2.07	1.56	1.50
28	C	475	SQD	C24-C23	2.08	1.56	1.50
21	K	483	CLA	O1D-CGD	2.08	1.26	1.21
21	B	521	CLA	CMC-C2C	2.09	1.55	1.50
21	C	478	CLA	C5-C3	2.11	1.55	1.51
21	B	512	CLA	CHC-C1C	2.11	1.41	1.35
30	D	536	LMT	C1B-C2B	2.11	1.58	1.52
27	A	371	LHG	C6-C5	2.11	1.56	1.50
21	C	486	CLA	C5-C3	2.12	1.55	1.51
28	C	475	SQD	C44-C45	2.12	1.56	1.50
29	M	217	LMG	C11-C10	2.12	1.56	1.50
21	B	511	CLA	CBD-CHA	2.13	1.62	1.52
21	B	520	CLA	CAC-C3C	2.13	1.56	1.51
25	B	530	BCR	C24-C23	2.13	1.39	1.33
29	A	373	LMG	O1-C1	2.13	1.43	1.40
30	T	226	LMT	O5B-C5B	2.14	1.49	1.44
26	B	528	DGD	O3G-C1D	2.15	1.43	1.40
25	J	115	BCR	C24-C23	2.15	1.39	1.33
21	C	478	CLA	CAC-C3C	2.15	1.56	1.51
25	B	530	BCR	C7-C6	2.15	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	115	BCR	C21-C22	2.15	1.38	1.35
29	D	360	LMG	O1-C1	2.16	1.43	1.40
26	B	528	DGD	O5D-C1E	2.17	1.44	1.40
21	C	477	CLA	CBA-CGA	2.18	1.57	1.50
21	B	511	CLA	C5-C3	2.19	1.56	1.51
22	D	355	PHO	O1D-CGD	2.19	1.26	1.21
21	C	483	CLA	CBA-CGA	2.20	1.57	1.50
21	B	515	CLA	O1D-CGD	2.20	1.26	1.21
30	B	535	LMT	C1B-C2B	2.20	1.58	1.52
21	A	363	CLA	C4C-C3C	2.20	1.48	1.45
21	B	518	CLA	OBD-CAD	2.20	1.25	1.22
30	D	536	LMT	O1B-C1B	2.20	1.47	1.41
29	J	492	LMG	C4-C5	2.21	1.57	1.53
21	C	479	CLA	CBA-CGA	2.21	1.57	1.50
30	I	274	LMT	O5'-C5'	2.22	1.49	1.44
25	B	527	BCR	C38-C26	2.22	1.54	1.51
28	L	213	SQD	C24-C23	2.22	1.57	1.50
30	T	226	LMT	C4B-C5B	2.22	1.57	1.53
33	F	85	HEM	C4B-NB	2.23	1.40	1.36
29	J	492	LMG	C11-C10	2.23	1.57	1.50
21	B	524	CLA	CAC-C3C	2.23	1.57	1.51
21	B	511	CLA	CAC-C3C	2.24	1.57	1.51
21	B	525	CLA	CHC-C1C	2.24	1.41	1.35
21	C	483	CLA	OBD-CAD	2.24	1.25	1.22
25	B	530	BCR	C10-C9	2.25	1.38	1.35
25	C	490	BCR	C10-C9	2.25	1.38	1.35
32	D	357	PL9	C5-C4	2.26	1.55	1.47
26	A	375	DGD	C1G-C2G	2.26	1.57	1.50
29	I	220	LMG	O8-C9	2.27	1.50	1.45
26	C	474	DGD	C2A-C1A	2.27	1.57	1.50
21	C	486	CLA	CMC-C2C	2.28	1.55	1.50
25	J	115	BCR	C17-C18	2.28	1.38	1.35
32	D	357	PL9	C23-C24	2.29	1.38	1.33
29	I	220	LMG	O1-C7	2.29	1.47	1.43
21	B	516	CLA	O2A-C1	2.30	1.53	1.46
21	B	522	CLA	CHC-C1C	2.30	1.42	1.35
21	C	479	CLA	CHC-C1C	2.31	1.42	1.35
21	B	511	CLA	CAA-C2A	2.31	1.58	1.54
28	F	224	SQD	C44-C45	2.31	1.57	1.50
21	B	511	CLA	OBD-CAD	2.31	1.25	1.22
21	C	488	CLA	OBD-CAD	2.32	1.25	1.22
25	J	115	BCR	C10-C9	2.32	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	536	LMT	C4B-C5B	2.32	1.58	1.53
30	O	274	LMT	O5'-C5'	2.33	1.50	1.44
32	D	357	PL9	C10-C9	2.33	1.56	1.50
29	C	494	LMG	C7-C8	2.33	1.57	1.50
21	B	521	CLA	CBA-CGA	2.34	1.57	1.50
21	B	518	CLA	C5-C3	2.34	1.56	1.51
21	A	362	CLA	CMC-C2C	2.34	1.56	1.50
26	C	493	DGD	C4E-C3E	2.35	1.58	1.52
21	B	518	CLA	CMC-C2C	2.36	1.56	1.50
29	I	220	LMG	C7-C8	2.37	1.57	1.50
30	D	536	LMT	C4'-C5'	2.37	1.59	1.52
21	C	487	CLA	C2A-C1A	2.37	1.57	1.52
21	C	482	CLA	CHC-C1C	2.37	1.42	1.35
21	B	517	CLA	O2A-C1	2.37	1.53	1.46
21	C	480	CLA	C5-C3	2.37	1.56	1.51
21	C	486	CLA	C4B-CHC	2.38	1.46	1.40
21	B	525	CLA	CMC-C2C	2.39	1.56	1.50
28	D	361	SQD	O5-C1	2.39	1.47	1.41
21	C	488	CLA	CMC-C2C	2.40	1.56	1.50
21	B	523	CLA	CMC-C2C	2.40	1.56	1.50
21	B	525	CLA	CBA-CGA	2.41	1.57	1.50
25	B	529	BCR	C38-C26	2.41	1.55	1.51
21	C	483	CLA	CAC-C3C	2.42	1.57	1.51
30	I	274	LMT	C3B-C2B	2.42	1.58	1.52
30	I	274	LMT	O5'-C1'	2.42	1.47	1.41
21	B	518	CLA	O2A-C1	2.42	1.53	1.46
29	B	531	LMG	O6-C1	2.43	1.47	1.41
29	I	220	LMG	O6-C5	2.43	1.50	1.44
26	B	533	DGD	C2B-C1B	2.43	1.57	1.50
30	I	274	LMT	C1B-C2B	2.43	1.59	1.52
21	D	356	CLA	C5-C3	2.44	1.56	1.51
21	B	514	CLA	O1D-CGD	2.44	1.27	1.21
30	D	363	LMT	O5'-C5'	2.44	1.50	1.44
21	C	480	CLA	CHC-C1C	2.45	1.42	1.35
26	C	493	DGD	O3G-C1D	2.46	1.44	1.40
21	B	526	CLA	CHC-C1C	2.46	1.42	1.35
32	D	357	PL9	C48-C49	2.47	1.39	1.32
21	B	526	CLA	C5-C3	2.48	1.56	1.51
30	O	274	LMT	O5B-C5B	2.48	1.50	1.44
29	D	359	LMG	O6-C1	2.48	1.48	1.41
21	C	482	CLA	CAA-C2A	2.49	1.58	1.54
26	D	362	DGD	O2G-C2G	2.49	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	530	BCR	C38-C26	2.49	1.55	1.51
21	B	517	CLA	C6-C7	2.49	1.63	1.52
22	D	355	PHO	C1D-C2D	2.49	1.51	1.45
21	A	363	CLA	CHC-C1C	2.50	1.42	1.35
21	D	356	CLA	CHC-C1C	2.50	1.42	1.35
21	C	488	CLA	CAC-C3C	2.50	1.57	1.51
21	C	487	CLA	CAC-C3C	2.51	1.57	1.51
25	C	490	BCR	C26-C25	2.51	1.38	1.34
21	B	511	CLA	C1B-CHB	2.51	1.46	1.40
21	C	484	CLA	CAC-C3C	2.51	1.57	1.51
26	C	474	DGD	C3E-C2E	2.51	1.58	1.52
21	C	486	CLA	OBD-CAD	2.52	1.26	1.22
33	F	85	HEM	CMC-C2C	2.52	1.57	1.51
28	L	213	SQD	C44-C45	2.53	1.57	1.50
21	C	486	CLA	CBA-CGA	2.54	1.58	1.50
25	C	489	BCR	C10-C9	2.54	1.39	1.35
26	C	492	DGD	O5D-C1E	2.54	1.44	1.40
28	D	361	SQD	C8-C7	2.55	1.58	1.50
21	C	480	CLA	OBD-CAD	2.55	1.26	1.22
26	D	362	DGD	O6D-C5D	2.55	1.50	1.44
28	L	213	SQD	C8-C7	2.56	1.58	1.50
21	B	515	CLA	CBA-CGA	2.56	1.58	1.50
30	I	274	LMT	O1'-C1'	2.57	1.44	1.40
21	B	524	CLA	CHC-C1C	2.57	1.42	1.35
30	A	376	LMT	C1B-C2B	2.58	1.59	1.52
22	A	365	PHO	O1D-CGD	2.58	1.27	1.21
25	B	529	BCR	C10-C9	2.58	1.39	1.35
29	J	492	LMG	O7-C10	2.58	1.41	1.34
21	B	522	CLA	CMC-C2C	2.59	1.56	1.50
21	C	485	CLA	O1D-CGD	2.59	1.27	1.21
21	B	522	CLA	O1D-CGD	2.59	1.27	1.21
21	C	479	CLA	C5-C3	2.59	1.57	1.51
21	D	354	CLA	O1D-CGD	2.59	1.27	1.21
32	D	357	PL9	C43-C44	2.59	1.39	1.33
32	D	357	PL9	C38-C39	2.60	1.39	1.33
32	D	357	PL9	C18-C19	2.61	1.39	1.33
26	C	491	DGD	O6D-C5D	2.61	1.50	1.44
21	B	513	CLA	CHC-C1C	2.61	1.42	1.35
26	D	362	DGD	C1E-C2E	2.62	1.60	1.52
27	C	476	LHG	C4-C5	2.62	1.58	1.50
33	F	85	HEM	CAA-C2A	2.62	1.56	1.52
21	D	354	CLA	CHC-C1C	2.63	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	220	LMG	O8-C28	2.63	1.41	1.33
26	C	492	DGD	O2G-C1B	2.64	1.41	1.34
25	J	112	BCR	C14-C13	2.64	1.39	1.35
28	F	224	SQD	O6-C1	2.64	1.44	1.40
26	C	491	DGD	C3G-C2G	2.64	1.58	1.50
32	D	357	PL9	C8-C9	2.64	1.39	1.33
21	B	514	CLA	CMC-C2C	2.64	1.56	1.50
21	B	524	CLA	CMC-C2C	2.65	1.56	1.50
30	A	376	LMT	O1'-C1'	2.65	1.44	1.40
29	M	217	LMG	O7-C10	2.65	1.42	1.34
21	B	524	CLA	CBA-CGA	2.66	1.58	1.50
21	D	356	CLA	O1D-CGD	2.66	1.27	1.21
21	C	480	CLA	O1D-CGD	2.66	1.27	1.21
25	X	107	BCR	C5-C6	2.66	1.39	1.34
29	I	220	LMG	C4-C5	2.67	1.58	1.53
26	B	533	DGD	C4E-C3E	2.67	1.59	1.52
29	C	494	LMG	O7-C8	2.67	1.53	1.46
21	C	485	CLA	CHC-C1C	2.68	1.43	1.35
30	D	536	LMT	O5'-C1'	2.68	1.48	1.41
26	A	375	DGD	C2A-C1A	2.68	1.58	1.50
26	D	362	DGD	C3D-C2D	2.68	1.59	1.52
29	M	217	LMG	O7-C8	2.68	1.53	1.46
21	A	364	CLA	CBA-CGA	2.69	1.58	1.50
28	L	213	SQD	O3-C3	2.69	1.49	1.43
21	B	518	CLA	CBA-CGA	2.70	1.58	1.50
29	C	494	LMG	O1-C7	2.70	1.48	1.43
21	B	522	CLA	CAC-C3C	2.71	1.58	1.51
25	J	112	BCR	C26-C25	2.72	1.39	1.34
21	D	356	CLA	CBA-CGA	2.72	1.58	1.50
21	A	363	CLA	CAA-C2A	2.72	1.59	1.54
30	D	363	LMT	C4'-C5'	2.72	1.60	1.52
21	B	513	CLA	CBA-CGA	2.73	1.58	1.50
22	A	365	PHO	CMC-C2C	2.73	1.56	1.50
21	C	483	CLA	CHC-C1C	2.73	1.43	1.35
25	C	489	BCR	C26-C25	2.75	1.39	1.34
32	D	357	PL9	C33-C34	2.75	1.39	1.33
21	B	523	CLA	CHB-C4A	2.75	1.37	1.33
30	T	226	LMT	O5B-C1B	2.75	1.48	1.41
21	B	519	CLA	O1D-CGD	2.75	1.28	1.21
26	D	362	DGD	C3G-C2G	2.75	1.58	1.50
25	D	358	BCR	C5-C6	2.76	1.39	1.34
21	A	362	CLA	CHC-C1C	2.76	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	475	SQD	C8-C7	2.78	1.58	1.50
21	C	484	CLA	OBD-CAD	2.78	1.26	1.22
25	B	529	BCR	C14-C13	2.78	1.39	1.35
21	B	517	CLA	CMC-C2C	2.78	1.56	1.50
28	C	475	SQD	O5-C1	2.79	1.48	1.41
21	A	366	CLA	CHC-C1C	2.80	1.43	1.35
21	B	513	CLA	CMC-C2C	2.82	1.57	1.50
21	A	364	CLA	CMC-C2C	2.82	1.57	1.50
30	T	226	LMT	C1B-C2B	2.82	1.60	1.52
29	J	492	LMG	O6-C1	2.82	1.48	1.41
21	D	354	CLA	CMC-C2C	2.82	1.57	1.50
21	A	364	CLA	O1D-CGD	2.82	1.28	1.21
29	M	217	LMG	O6-C1	2.82	1.48	1.41
21	A	363	CLA	CHB-C4A	2.82	1.37	1.33
25	C	489	BCR	C5-C6	2.83	1.39	1.34
21	B	523	CLA	CHC-C1C	2.83	1.43	1.35
21	C	477	CLA	CMC-C2C	2.85	1.57	1.50
21	A	366	CLA	CMC-C2C	2.85	1.57	1.50
30	O	274	LMT	C4'-C5'	2.85	1.60	1.52
21	B	523	CLA	O1D-CGD	2.86	1.28	1.21
21	B	515	CLA	CHC-C1C	2.86	1.43	1.35
30	D	363	LMT	O5B-C1B	2.87	1.48	1.41
21	C	483	CLA	O1D-CGD	2.87	1.28	1.21
21	C	479	CLA	CMC-C2C	2.87	1.57	1.50
33	V	164	HEM	CMC-C2C	2.88	1.57	1.51
22	A	365	PHO	C1D-C2D	2.88	1.52	1.45
30	O	274	LMT	O1'-C1'	2.89	1.45	1.40
21	B	524	CLA	O1D-CGD	2.89	1.28	1.21
21	C	483	CLA	C5-C3	2.91	1.57	1.51
21	B	520	CLA	O1D-CGD	2.91	1.28	1.21
21	K	483	CLA	CMC-C2C	2.91	1.57	1.50
21	B	516	CLA	O1D-CGD	2.92	1.28	1.21
26	B	533	DGD	O2G-C1B	2.92	1.42	1.34
28	C	475	SQD	O8-S	2.93	1.57	1.47
29	I	220	LMG	O6-C1	2.94	1.49	1.41
26	D	362	DGD	O1G-C1A	2.95	1.42	1.33
26	C	474	DGD	C4E-C3E	2.96	1.59	1.52
30	B	535	LMT	O1B-C4'	2.96	1.51	1.43
28	D	361	SQD	O6-C1	2.97	1.45	1.40
26	C	493	DGD	C3G-C2G	2.98	1.59	1.50
21	A	363	CLA	O1D-CGD	2.98	1.28	1.21
21	B	514	CLA	CBA-CGA	2.98	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	481	CLA	O1D-CGD	2.99	1.28	1.21
21	A	362	CLA	O2A-CGA	2.99	1.42	1.33
21	B	516	CLA	CMC-C2C	2.99	1.57	1.50
21	B	518	CLA	O1D-CGD	3.00	1.28	1.21
21	C	477	CLA	O1D-CGD	3.00	1.28	1.21
21	C	479	CLA	O1D-CGD	3.00	1.28	1.21
25	B	530	BCR	C14-C13	3.00	1.39	1.35
30	A	376	LMT	O5'-C1'	3.00	1.49	1.41
21	B	515	CLA	C4C-C3C	3.01	1.50	1.45
21	A	364	CLA	CHB-C4A	3.02	1.37	1.33
30	I	274	LMT	C4'-C5'	3.02	1.61	1.52
21	C	487	CLA	CBA-CGA	3.03	1.59	1.50
21	B	515	CLA	C5-C3	3.03	1.57	1.51
30	T	226	LMT	O1'-C1'	3.03	1.45	1.40
21	B	513	CLA	O1D-CGD	3.05	1.28	1.21
25	Z	116	BCR	C38-C26	3.05	1.56	1.51
30	A	376	LMT	C4'-C5'	3.05	1.61	1.52
28	F	224	SQD	C24-C23	3.05	1.59	1.50
21	C	484	CLA	O1D-CGD	3.06	1.28	1.21
21	B	525	CLA	O1D-CGD	3.06	1.28	1.21
21	A	363	CLA	CBA-CGA	3.06	1.59	1.50
21	C	478	CLA	O1D-CGD	3.07	1.29	1.21
21	B	525	CLA	C5-C3	3.08	1.58	1.51
21	B	520	CLA	CMC-C2C	3.08	1.57	1.50
21	C	478	CLA	CMC-C2C	3.09	1.57	1.50
25	J	115	BCR	C2-C1	3.10	1.61	1.54
30	I	274	LMT	C3'-C4'	3.10	1.60	1.52
29	C	494	LMG	O6-C1	3.13	1.49	1.41
25	C	490	BCR	C14-C13	3.13	1.39	1.35
21	A	363	CLA	CMC-C2C	3.13	1.57	1.50
26	A	375	DGD	O1G-C1G	3.13	1.52	1.45
21	B	519	CLA	CMC-C2C	3.13	1.57	1.50
21	D	356	CLA	CMC-C2C	3.13	1.57	1.50
26	C	493	DGD	O5D-C1E	3.14	1.45	1.40
25	C	490	BCR	C29-C30	3.14	1.61	1.54
28	D	361	SQD	O3-C3	3.14	1.50	1.43
25	X	107	BCR	C2-C1	3.14	1.61	1.54
25	D	358	BCR	C2-C1	3.15	1.61	1.54
21	B	512	CLA	O1D-CGD	3.15	1.29	1.21
25	X	107	BCR	C1-C6	3.15	1.58	1.53
21	C	482	CLA	CAC-C3C	3.15	1.59	1.51
21	B	517	CLA	O1D-CGD	3.16	1.29	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	485	CLA	CMC-C2C	3.17	1.57	1.50
21	C	488	CLA	CHC-C1C	3.18	1.44	1.35
25	C	489	BCR	C29-C30	3.18	1.61	1.54
21	B	515	CLA	CMC-C2C	3.19	1.57	1.50
22	A	365	PHO	C1C-C2C	3.19	1.52	1.45
21	C	482	CLA	CMC-C2C	3.20	1.57	1.50
21	A	362	CLA	O1D-CGD	3.20	1.29	1.21
25	B	527	BCR	C29-C30	3.21	1.61	1.54
28	F	224	SQD	O5-C1	3.21	1.49	1.41
22	D	355	PHO	CMC-C2C	3.21	1.57	1.50
21	C	481	CLA	CMC-C2C	3.23	1.57	1.50
32	D	357	PL9	C2-C1	3.23	1.53	1.44
21	C	484	CLA	CHC-C1C	3.23	1.44	1.35
28	F	224	SQD	C1-C2	3.23	1.61	1.52
21	C	483	CLA	CMC-C2C	3.24	1.57	1.50
28	F	224	SQD	O8-S	3.24	1.58	1.47
28	F	224	SQD	C8-C7	3.24	1.60	1.50
30	B	535	LMT	O1'-C1'	3.25	1.45	1.40
25	B	527	BCR	C2-C1	3.25	1.61	1.54
28	F	224	SQD	O3-C3	3.26	1.50	1.43
28	D	361	SQD	O48-C23	3.27	1.42	1.33
25	Z	116	BCR	C2-C1	3.29	1.61	1.54
25	A	369	BCR	C29-C30	3.29	1.61	1.54
27	C	476	LHG	O7-C7	3.29	1.43	1.34
21	B	511	CLA	CBA-CGA	3.29	1.60	1.50
28	L	213	SQD	O5-C1	3.30	1.50	1.41
21	B	517	CLA	CHB-C4A	3.30	1.37	1.33
21	C	487	CLA	O1D-CGD	3.30	1.29	1.21
21	B	517	CLA	C5-C3	3.31	1.58	1.51
22	D	355	PHO	C1C-C2C	3.32	1.53	1.45
25	Z	116	BCR	C29-C30	3.33	1.61	1.54
21	C	487	CLA	CAA-C2A	3.33	1.60	1.54
21	C	487	CLA	CMC-C2C	3.34	1.58	1.50
26	D	362	DGD	O6E-C1E	3.34	1.50	1.41
21	B	526	CLA	C1C-C2C	3.35	1.51	1.44
26	D	362	DGD	O1G-C1G	3.36	1.52	1.45
21	A	366	CLA	O1D-CGD	3.36	1.29	1.21
30	O	274	LMT	O5'-C1'	3.38	1.50	1.41
25	J	112	BCR	C29-C30	3.38	1.62	1.54
25	B	527	BCR	C5-C6	3.39	1.40	1.34
28	L	213	SQD	O8-S	3.39	1.58	1.47
26	D	362	DGD	O2G-C1B	3.40	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	357	PL9	C6-C5	3.40	1.53	1.35
21	B	526	CLA	O1D-CGD	3.40	1.29	1.21
25	J	115	BCR	C14-C13	3.40	1.40	1.35
25	Z	116	BCR	C5-C6	3.40	1.40	1.34
21	C	480	CLA	CMC-C2C	3.41	1.58	1.50
25	A	369	BCR	C2-C1	3.42	1.62	1.54
30	O	274	LMT	O1B-C1B	3.42	1.50	1.41
21	B	517	CLA	CHC-C1C	3.44	1.45	1.35
21	B	521	CLA	C5-C3	3.44	1.58	1.51
21	C	481	CLA	CHC-C1C	3.45	1.45	1.35
26	D	362	DGD	C1G-C2G	3.45	1.60	1.50
30	A	376	LMT	O1B-C4'	3.45	1.52	1.43
25	J	115	BCR	C1-C6	3.46	1.58	1.53
33	V	164	HEM	CBC-CAC	3.47	1.53	1.28
25	J	112	BCR	C2-C1	3.48	1.62	1.54
33	F	85	HEM	CBC-CAC	3.48	1.53	1.28
21	B	516	CLA	CHB-C4A	3.48	1.38	1.33
21	C	482	CLA	CBA-CGA	3.48	1.60	1.50
30	T	226	LMT	O5'-C1'	3.51	1.50	1.41
25	J	112	BCR	C1-C6	3.52	1.58	1.53
21	B	511	CLA	CMC-C2C	3.52	1.58	1.50
21	B	522	CLA	CHB-C4A	3.52	1.38	1.33
27	A	371	LHG	O8-C23	3.54	1.43	1.33
21	B	524	CLA	C5-C3	3.54	1.59	1.51
26	A	375	DGD	O6E-C1E	3.54	1.50	1.41
25	C	490	BCR	C2-C1	3.55	1.62	1.54
21	B	516	CLA	C5-C3	3.55	1.59	1.51
22	D	355	PHO	C3B-C4B	3.57	1.51	1.43
25	B	529	BCR	C2-C1	3.57	1.62	1.54
28	C	475	SQD	O6-C1	3.58	1.46	1.40
21	B	525	CLA	C4C-C3C	3.58	1.51	1.45
30	I	274	LMT	O5B-C1B	3.59	1.50	1.41
30	D	363	LMT	O5'-C1'	3.59	1.50	1.41
30	B	535	LMT	O1B-C1B	3.60	1.51	1.41
21	C	488	CLA	O1D-CGD	3.60	1.30	1.21
25	X	107	BCR	C29-C30	3.60	1.62	1.54
21	C	487	CLA	C5-C3	3.61	1.59	1.51
30	D	536	LMT	O5B-C1B	3.61	1.50	1.41
21	C	482	CLA	O1D-CGD	3.63	1.30	1.21
21	C	484	CLA	C4C-C3C	3.63	1.51	1.45
21	B	521	CLA	CHB-C4A	3.64	1.38	1.33
30	B	535	LMT	O5'-C1'	3.64	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	376	LMT	O1B-C1B	3.64	1.51	1.41
28	C	475	SQD	O7-S	3.65	1.55	1.45
22	A	365	PHO	C4C-C3C	3.66	1.51	1.45
21	B	512	CLA	C4C-C3C	3.66	1.51	1.45
21	B	511	CLA	C1C-C2C	3.66	1.51	1.44
28	C	475	SQD	O48-C23	3.67	1.44	1.33
25	C	489	BCR	C2-C1	3.67	1.62	1.54
21	B	511	CLA	O1D-CGD	3.67	1.30	1.21
26	D	362	DGD	C2A-C1A	3.68	1.61	1.50
21	B	522	CLA	C4C-C3C	3.68	1.51	1.45
28	D	361	SQD	O8-S	3.68	1.59	1.47
21	A	363	CLA	O2D-CGD	3.68	1.42	1.33
21	B	512	CLA	CHB-C4A	3.69	1.38	1.33
30	O	274	LMT	O1B-C4'	3.69	1.52	1.43
21	B	521	CLA	O1D-CGD	3.70	1.30	1.21
21	B	513	CLA	C4C-C3C	3.70	1.51	1.45
21	C	486	CLA	O1D-CGD	3.70	1.30	1.21
25	A	369	BCR	C5-C6	3.71	1.40	1.34
21	B	513	CLA	CHB-C4A	3.71	1.38	1.33
21	B	523	CLA	C4C-C3C	3.72	1.51	1.45
21	A	362	CLA	C1C-C2C	3.73	1.51	1.44
26	A	375	DGD	O6E-C5E	3.73	1.53	1.44
21	B	514	CLA	O2D-CGD	3.75	1.42	1.33
22	D	355	PHO	O2D-CGD	3.75	1.42	1.33
26	C	474	DGD	O2G-C1B	3.77	1.45	1.34
21	D	356	CLA	O2D-CGD	3.79	1.42	1.33
21	A	366	CLA	C4C-C3C	3.79	1.51	1.45
21	C	477	CLA	C1C-C2C	3.80	1.51	1.44
25	B	527	BCR	C26-C25	3.80	1.41	1.34
21	A	362	CLA	C4C-C3C	3.80	1.51	1.45
25	A	369	BCR	C26-C25	3.82	1.41	1.34
27	C	476	LHG	O8-C23	3.83	1.44	1.33
21	B	518	CLA	C4C-C3C	3.85	1.51	1.45
28	C	475	SQD	O3-C3	3.86	1.51	1.43
25	D	358	BCR	C1-C6	3.87	1.59	1.53
21	B	521	CLA	C1C-C2C	3.88	1.52	1.44
28	L	213	SQD	O6-C1	3.88	1.47	1.40
21	C	486	CLA	CHC-C1C	3.88	1.46	1.35
21	C	488	CLA	C4C-C3C	3.89	1.51	1.45
21	B	520	CLA	O2A-CGA	3.90	1.44	1.33
26	B	533	DGD	O6E-C1E	3.92	1.51	1.41
21	C	477	CLA	C4C-C3C	3.94	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	481	CLA	O2D-CGD	3.95	1.43	1.33
26	A	375	DGD	O5D-C1E	3.96	1.47	1.40
21	D	354	CLA	O2D-CGD	3.97	1.43	1.33
25	D	358	BCR	C29-C30	3.97	1.63	1.54
21	C	479	CLA	C4C-C3C	3.97	1.52	1.45
25	B	529	BCR	C29-C30	3.97	1.63	1.54
22	D	355	PHO	O2A-CGA	3.98	1.45	1.33
21	B	524	CLA	C4C-C3C	3.98	1.52	1.45
29	J	492	LMG	O7-C8	3.99	1.57	1.46
26	B	533	DGD	O6D-C1D	4.01	1.51	1.41
21	B	512	CLA	C1C-C2C	4.01	1.52	1.44
21	D	354	CLA	CHB-C4A	4.01	1.38	1.33
21	A	364	CLA	C1C-C2C	4.02	1.52	1.44
28	C	475	SQD	C1-C2	4.02	1.64	1.52
25	Z	116	BCR	C26-C25	4.02	1.41	1.34
21	B	518	CLA	O2D-CGD	4.03	1.43	1.33
21	B	516	CLA	CBA-CGA	4.03	1.62	1.50
30	B	535	LMT	O5B-C1B	4.03	1.51	1.41
21	B	515	CLA	CHB-C4A	4.03	1.38	1.33
27	A	371	LHG	O7-C7	4.04	1.46	1.34
25	X	107	BCR	C26-C25	4.04	1.41	1.34
21	B	524	CLA	O2D-CGD	4.05	1.43	1.33
21	C	479	CLA	O2D-CGD	4.06	1.43	1.33
23	A	367	MES	C8-S	4.06	1.83	1.77
21	A	364	CLA	C4C-C3C	4.07	1.52	1.45
28	L	213	SQD	C1-C2	4.07	1.64	1.52
26	C	474	DGD	O6E-C1E	4.07	1.51	1.41
21	B	513	CLA	C1C-C2C	4.08	1.52	1.44
21	B	519	CLA	C4C-C3C	4.08	1.52	1.45
33	F	85	HEM	C1B-NB	4.09	1.41	1.36
26	C	474	DGD	O3G-C1D	4.09	1.47	1.40
26	C	474	DGD	O6D-C5D	4.09	1.54	1.44
21	A	364	CLA	O2D-CGD	4.10	1.43	1.33
21	B	517	CLA	O2D-CGD	4.10	1.43	1.33
21	B	512	CLA	O2D-CGD	4.10	1.43	1.33
21	B	520	CLA	C1C-C2C	4.11	1.52	1.44
26	C	474	DGD	O1G-C1A	4.11	1.45	1.33
21	B	523	CLA	O2D-CGD	4.11	1.43	1.33
21	B	514	CLA	C1C-C2C	4.13	1.52	1.44
28	D	361	SQD	C1-C2	4.14	1.64	1.52
22	A	365	PHO	O2A-CGA	4.14	1.45	1.33
21	B	514	CLA	CHB-C4A	4.16	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	C4C-C3C	4.16	1.52	1.45
21	K	483	CLA	C4C-C3C	4.17	1.52	1.45
21	C	478	CLA	C4C-C3C	4.17	1.52	1.45
21	C	481	CLA	C4C-C3C	4.17	1.52	1.45
25	B	529	BCR	C1-C6	4.18	1.59	1.53
21	B	519	CLA	C1C-C2C	4.19	1.52	1.44
21	B	519	CLA	O2A-CGA	4.20	1.45	1.33
28	L	213	SQD	O48-C23	4.20	1.45	1.33
25	C	490	BCR	C5-C6	4.21	1.41	1.34
25	B	530	BCR	C29-C30	4.23	1.64	1.54
30	D	363	LMT	O1'-C1'	4.23	1.47	1.40
25	C	489	BCR	C30-C25	4.24	1.59	1.53
26	A	375	DGD	C3G-C2G	4.24	1.62	1.50
21	B	516	CLA	C1C-C2C	4.25	1.52	1.44
21	B	515	CLA	O2D-CGD	4.25	1.44	1.33
26	C	474	DGD	C3G-C2G	4.26	1.62	1.50
28	C	475	SQD	O5-C5	4.26	1.54	1.44
21	B	523	CLA	O2A-CGA	4.30	1.46	1.33
28	F	224	SQD	O7-S	4.30	1.57	1.45
21	B	520	CLA	O2D-CGD	4.31	1.44	1.33
21	C	485	CLA	O2A-CGA	4.31	1.46	1.33
22	A	365	PHO	C3B-C4B	4.33	1.52	1.43
21	A	363	CLA	C1C-C2C	4.33	1.52	1.44
21	C	480	CLA	C4C-C3C	4.35	1.52	1.45
21	B	514	CLA	C4C-C3C	4.35	1.52	1.45
21	B	513	CLA	O2D-CGD	4.35	1.44	1.33
21	B	521	CLA	O2A-CGA	4.38	1.46	1.33
28	D	361	SQD	O5-C5	4.38	1.55	1.44
21	A	366	CLA	O2D-CGD	4.39	1.44	1.33
21	C	480	CLA	C1C-C2C	4.39	1.53	1.44
25	J	112	BCR	C5-C6	4.39	1.42	1.34
21	B	518	CLA	C1C-C2C	4.40	1.53	1.44
25	J	115	BCR	C29-C30	4.40	1.64	1.54
28	C	475	SQD	O47-C7	4.41	1.47	1.34
25	B	530	BCR	C2-C1	4.41	1.64	1.54
21	C	480	CLA	O2D-CGD	4.41	1.44	1.33
28	F	224	SQD	O5-C5	4.42	1.55	1.44
21	B	522	CLA	C1C-C2C	4.43	1.53	1.44
27	A	371	LHG	P-O6	4.43	1.78	1.59
26	C	493	DGD	O6D-C1D	4.44	1.52	1.41
25	D	358	BCR	C30-C25	4.44	1.59	1.53
21	K	483	CLA	CHB-C4A	4.44	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	356	CLA	C4C-C3C	4.45	1.52	1.45
21	C	478	CLA	O2D-CGD	4.45	1.44	1.33
28	D	361	SQD	O7-S	4.50	1.58	1.45
25	B	530	BCR	C5-C6	4.52	1.42	1.34
21	B	525	CLA	C1C-C2C	4.53	1.53	1.44
21	D	354	CLA	C1C-C2C	4.53	1.53	1.44
26	C	492	DGD	O6D-C1D	4.53	1.53	1.41
22	A	365	PHO	O2D-CGD	4.54	1.44	1.33
26	A	375	DGD	O6D-C5D	4.55	1.55	1.44
21	B	517	CLA	C1C-C2C	4.55	1.53	1.44
21	D	354	CLA	C4C-C3C	4.59	1.53	1.45
21	K	483	CLA	O2D-CGD	4.59	1.44	1.33
28	L	213	SQD	O47-C7	4.59	1.47	1.34
33	F	85	HEM	C3C-CAC	4.59	1.56	1.47
21	B	522	CLA	O2A-CGA	4.60	1.46	1.33
21	C	478	CLA	C1C-C2C	4.60	1.53	1.44
21	A	362	CLA	O2D-CGD	4.61	1.44	1.33
21	A	366	CLA	O2A-CGA	4.61	1.46	1.33
21	B	521	CLA	C4C-C3C	4.61	1.53	1.45
21	B	526	CLA	C4C-C3C	4.62	1.53	1.45
26	B	533	DGD	O5D-C1E	4.62	1.48	1.40
25	B	530	BCR	C26-C25	4.62	1.42	1.34
21	K	483	CLA	C1C-C2C	4.63	1.53	1.44
21	C	478	CLA	CHB-C4A	4.63	1.39	1.33
21	A	363	CLA	O2A-CGA	4.64	1.47	1.33
30	O	274	LMT	O5B-C1B	4.65	1.53	1.41
21	B	523	CLA	C1C-C2C	4.66	1.53	1.44
21	A	366	CLA	CHB-C4A	4.66	1.39	1.33
21	C	487	CLA	O2D-CGD	4.68	1.45	1.33
26	C	491	DGD	O3G-C1D	4.68	1.48	1.40
21	C	480	CLA	O2A-CGA	4.70	1.47	1.33
25	D	358	BCR	C26-C25	4.71	1.42	1.34
25	B	527	BCR	C30-C25	4.72	1.60	1.53
28	L	213	SQD	O7-S	4.72	1.58	1.45
21	C	488	CLA	O2D-CGD	4.72	1.45	1.33
26	A	375	DGD	O6D-C1D	4.73	1.53	1.41
28	F	224	SQD	O48-C23	4.73	1.47	1.33
21	C	484	CLA	C1C-C2C	4.74	1.53	1.44
21	K	483	CLA	O2A-CGA	4.74	1.47	1.33
21	C	484	CLA	O2A-CGA	4.74	1.47	1.33
21	C	479	CLA	C1C-C2C	4.74	1.53	1.44
28	F	224	SQD	O47-C7	4.75	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	512	CLA	O2A-CGA	4.77	1.47	1.33
33	V	164	HEM	C3C-CAC	4.78	1.57	1.47
21	C	486	CLA	C4C-C3C	4.80	1.53	1.45
21	C	483	CLA	C4C-C3C	4.82	1.53	1.45
21	B	516	CLA	C4C-C3C	4.82	1.53	1.45
25	B	529	BCR	C26-C25	4.84	1.42	1.34
21	A	366	CLA	C1C-C2C	4.85	1.53	1.44
21	B	514	CLA	O2A-CGA	4.85	1.47	1.33
21	B	522	CLA	O2D-CGD	4.87	1.45	1.33
25	B	529	BCR	C5-C6	4.89	1.42	1.34
21	C	483	CLA	O2A-CGA	4.90	1.47	1.33
21	C	486	CLA	O2D-CGD	4.90	1.45	1.33
21	C	488	CLA	O2A-CGA	4.91	1.47	1.33
27	C	476	LHG	P-O6	4.92	1.80	1.59
21	B	525	CLA	O2D-CGD	4.94	1.45	1.33
22	D	355	PHO	C4C-C3C	4.95	1.53	1.45
21	C	485	CLA	O2D-CGD	4.96	1.45	1.33
30	A	376	LMT	O5B-C1B	4.96	1.54	1.41
21	B	516	CLA	O2D-CGD	4.97	1.45	1.33
21	C	483	CLA	C1C-C2C	4.97	1.54	1.44
21	D	356	CLA	O2A-CGA	4.97	1.48	1.33
21	C	485	CLA	C4C-C3C	4.98	1.53	1.45
21	C	488	CLA	C1C-C2C	5.03	1.54	1.44
21	C	485	CLA	C1C-C2C	5.05	1.54	1.44
21	C	478	CLA	O2A-CGA	5.05	1.48	1.33
25	B	527	BCR	C1-C6	5.06	1.60	1.53
21	B	524	CLA	C1C-C2C	5.06	1.54	1.44
21	B	515	CLA	C1C-C2C	5.07	1.54	1.44
21	B	526	CLA	O2D-CGD	5.07	1.46	1.33
28	L	213	SQD	O5-C5	5.08	1.56	1.44
21	D	356	CLA	C1C-C2C	5.09	1.54	1.44
28	D	361	SQD	O47-C7	5.11	1.49	1.34
25	J	115	BCR	C26-C25	5.14	1.43	1.34
21	C	487	CLA	C4C-C3C	5.15	1.54	1.45
21	B	521	CLA	O2D-CGD	5.15	1.46	1.33
21	C	487	CLA	C1C-C2C	5.16	1.54	1.44
26	C	491	DGD	O6D-C1D	5.19	1.54	1.41
21	B	519	CLA	O2D-CGD	5.19	1.46	1.33
26	D	362	DGD	O6D-C1D	5.20	1.54	1.41
21	C	483	CLA	O2D-CGD	5.21	1.46	1.33
21	C	479	CLA	O2A-CGA	5.23	1.48	1.33
25	A	369	BCR	C1-C6	5.24	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	520	CLA	C4C-C3C	5.25	1.54	1.45
21	D	354	CLA	O2A-CGA	5.25	1.48	1.33
26	C	491	DGD	O5D-C1E	5.34	1.49	1.40
21	B	519	CLA	CHB-C4A	5.37	1.40	1.33
21	B	525	CLA	O2A-CGA	5.40	1.49	1.33
26	C	474	DGD	O6D-C1D	5.40	1.55	1.41
21	C	482	CLA	C4C-C3C	5.42	1.54	1.45
27	A	371	LHG	P-O3	5.43	1.82	1.59
21	C	486	CLA	C1C-C2C	5.44	1.55	1.44
21	C	481	CLA	CHB-C4A	5.50	1.40	1.33
21	C	481	CLA	O2A-CGA	5.50	1.49	1.33
21	C	477	CLA	O2A-CGA	5.52	1.49	1.33
21	C	484	CLA	CHB-C4A	5.54	1.40	1.33
21	C	482	CLA	O2A-CGA	5.55	1.49	1.33
21	C	477	CLA	O2D-CGD	5.56	1.47	1.33
21	C	485	CLA	CHB-C4A	5.57	1.40	1.33
25	C	490	BCR	C30-C25	5.57	1.61	1.53
21	A	364	CLA	O2A-CGA	5.63	1.49	1.33
21	B	513	CLA	O2A-CGA	5.63	1.49	1.33
21	B	520	CLA	CHB-C4A	5.66	1.40	1.33
21	C	488	CLA	CHB-C4A	5.66	1.40	1.33
21	C	477	CLA	CHB-C4A	5.69	1.40	1.33
21	C	486	CLA	O2A-CGA	5.72	1.50	1.33
25	Z	116	BCR	C1-C6	5.72	1.61	1.53
21	C	481	CLA	C1C-C2C	5.75	1.55	1.44
21	A	362	CLA	CHB-C4A	5.75	1.40	1.33
21	B	516	CLA	O2A-CGA	5.76	1.50	1.33
21	B	526	CLA	O2A-CGA	5.76	1.50	1.33
25	C	490	BCR	C1-C6	5.83	1.61	1.53
21	B	511	CLA	O2A-CGA	5.85	1.50	1.33
26	D	362	DGD	O3G-C1D	5.87	1.50	1.40
25	J	115	BCR	C5-C6	5.87	1.44	1.34
21	C	482	CLA	O2D-CGD	5.91	1.48	1.33
21	B	522	CLA	C3B-C2B	5.92	1.48	1.40
21	B	518	CLA	CHB-C4A	5.98	1.41	1.33
21	B	517	CLA	C3B-C2B	6.02	1.48	1.40
25	Z	116	BCR	C30-C25	6.03	1.62	1.53
33	V	164	HEM	C3B-C2B	6.06	1.48	1.40
21	B	515	CLA	O2A-CGA	6.07	1.51	1.33
21	C	482	CLA	C1C-C2C	6.08	1.56	1.44
21	C	484	CLA	O2D-CGD	6.08	1.48	1.33
21	D	356	CLA	CHB-C4A	6.16	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	479	CLA	CHB-C4A	6.18	1.41	1.33
21	B	511	CLA	O2D-CGD	6.19	1.48	1.33
21	C	480	CLA	CHB-C4A	6.21	1.41	1.33
26	D	362	DGD	O5D-C1E	6.21	1.51	1.40
26	C	474	DGD	O5D-C1E	6.21	1.51	1.40
25	A	369	BCR	C30-C25	6.22	1.62	1.53
27	C	476	LHG	P-O3	6.23	1.85	1.59
21	C	487	CLA	O2A-CGA	6.30	1.51	1.33
21	C	483	CLA	CHB-C4A	6.37	1.41	1.33
21	C	486	CLA	CHB-C4A	6.39	1.41	1.33
21	B	524	CLA	O2A-CGA	6.46	1.52	1.33
21	B	524	CLA	CHB-C4A	6.48	1.41	1.33
25	J	115	BCR	C30-C25	6.49	1.62	1.53
21	B	511	CLA	C4C-C3C	6.54	1.56	1.45
21	B	517	CLA	O2A-CGA	6.57	1.52	1.33
25	J	112	BCR	C30-C25	6.59	1.62	1.53
21	B	513	CLA	C3B-C2B	6.61	1.49	1.40
21	A	362	CLA	C2-C3	6.61	1.49	1.33
21	B	525	CLA	CHB-C4A	6.62	1.41	1.33
21	B	523	CLA	C3B-C2B	6.64	1.49	1.40
22	D	355	PHO	C2-C3	6.77	1.49	1.33
25	B	530	BCR	C1-C6	6.80	1.63	1.53
26	A	375	DGD	O3G-C1D	6.82	1.52	1.40
25	C	489	BCR	C1-C6	6.83	1.63	1.53
21	B	524	CLA	C3B-C2B	6.86	1.49	1.40
25	B	529	BCR	C30-C25	7.00	1.63	1.53
21	C	482	CLA	CHB-C4A	7.09	1.42	1.33
21	K	483	CLA	C3B-C2B	7.16	1.49	1.40
21	B	521	CLA	C3B-C2B	7.16	1.49	1.40
21	D	356	CLA	C3B-C2B	7.19	1.49	1.40
21	A	362	CLA	C3B-C2B	7.29	1.50	1.40
22	A	365	PHO	C3B-C2B	7.29	1.50	1.37
21	C	477	CLA	C3B-C2B	7.31	1.50	1.40
21	A	364	CLA	C3B-C2B	7.33	1.50	1.40
28	L	213	SQD	C4-C3	7.35	1.71	1.52
21	C	478	CLA	C3B-C2B	7.38	1.50	1.40
21	C	485	CLA	C3B-C2B	7.49	1.50	1.40
21	B	518	CLA	C3B-C2B	7.63	1.50	1.40
21	A	363	CLA	C3B-C2B	7.70	1.50	1.40
21	B	518	CLA	O2A-CGA	7.72	1.56	1.33
21	B	512	CLA	C2-C3	7.73	1.52	1.33
21	B	515	CLA	C3B-C2B	7.73	1.50	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	512	CLA	C3B-C2B	7.74	1.50	1.40
22	D	355	PHO	C3B-C2B	7.76	1.51	1.37
21	A	363	CLA	C2-C3	7.85	1.52	1.33
21	B	513	CLA	C2-C3	7.88	1.52	1.33
21	D	354	CLA	C3B-C2B	7.92	1.50	1.40
28	D	361	SQD	C4-C3	7.93	1.72	1.52
21	B	520	CLA	C3B-C2B	7.97	1.50	1.40
21	A	366	CLA	C2-C3	8.01	1.53	1.33
32	D	357	PL9	C2-C3	8.03	1.56	1.34
27	A	371	LHG	P-O5	8.09	1.81	1.50
21	C	484	CLA	C2-C3	8.09	1.53	1.33
21	C	488	CLA	C2-C3	8.11	1.53	1.33
28	F	224	SQD	C4-C3	8.15	1.73	1.52
21	K	483	CLA	C2-C3	8.19	1.53	1.33
22	A	365	PHO	C2-C3	8.21	1.53	1.33
21	B	516	CLA	C3B-C2B	8.21	1.51	1.40
21	C	486	CLA	C3B-C2B	8.24	1.51	1.40
21	D	354	CLA	C2-C3	8.27	1.53	1.33
21	C	480	CLA	C3B-C2B	8.32	1.51	1.40
27	C	476	LHG	P-O5	8.36	1.82	1.50
21	C	478	CLA	C2-C3	8.36	1.53	1.33
21	B	523	CLA	C2-C3	8.38	1.54	1.33
25	B	530	BCR	C30-C25	8.39	1.65	1.53
21	C	485	CLA	C2-C3	8.40	1.54	1.33
21	B	522	CLA	C2-C3	8.41	1.54	1.33
21	B	525	CLA	C3B-C2B	8.44	1.51	1.40
21	C	483	CLA	C3B-C2B	8.50	1.51	1.40
21	D	356	CLA	C2-C3	8.51	1.54	1.33
21	A	364	CLA	C2-C3	8.56	1.54	1.33
21	B	519	CLA	C3B-C2B	8.63	1.51	1.40
33	F	85	HEM	C3B-C2B	8.68	1.51	1.40
21	C	483	CLA	C2-C3	8.69	1.54	1.33
21	C	487	CLA	CHB-C4A	8.70	1.44	1.33
21	B	526	CLA	CHB-C4A	8.70	1.44	1.33
21	B	514	CLA	C3B-C2B	8.71	1.51	1.40
28	C	475	SQD	C4-C3	8.74	1.74	1.52
21	B	520	CLA	C2-C3	8.77	1.54	1.33
21	B	511	CLA	C2-C3	8.79	1.55	1.33
21	B	526	CLA	C3B-C2B	8.80	1.52	1.40
21	C	488	CLA	C3B-C2B	8.80	1.52	1.40
21	C	480	CLA	C2-C3	8.82	1.55	1.33
21	A	366	CLA	C3B-C2B	8.83	1.52	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	484	CLA	C3B-C2B	8.92	1.52	1.40
21	B	525	CLA	C2-C3	9.01	1.55	1.33
21	C	481	CLA	C2-C3	9.04	1.55	1.33
21	C	479	CLA	C3B-C2B	9.10	1.52	1.40
21	C	479	CLA	C2-C3	9.12	1.55	1.33
21	B	519	CLA	C2-C3	9.13	1.55	1.33
21	C	486	CLA	C2-C3	9.22	1.56	1.33
21	B	516	CLA	C2-C3	9.23	1.56	1.33
21	B	515	CLA	C2-C3	9.26	1.56	1.33
21	B	526	CLA	C2-C3	9.27	1.56	1.33
32	D	357	PL9	C13-C14	9.28	1.56	1.33
21	C	477	CLA	C2-C3	9.31	1.56	1.33
21	C	487	CLA	C3B-C2B	9.33	1.52	1.40
21	B	514	CLA	C2-C3	9.35	1.56	1.33
21	C	487	CLA	C2-C3	9.77	1.57	1.33
21	B	518	CLA	C2-C3	9.81	1.57	1.33
21	B	517	CLA	C2-C3	9.94	1.57	1.33
21	C	482	CLA	C3B-C2B	9.94	1.53	1.40
21	C	481	CLA	C3B-C2B	9.99	1.53	1.40
21	B	521	CLA	C2-C3	10.05	1.58	1.33
21	C	482	CLA	C2-C3	10.12	1.58	1.33
21	B	524	CLA	C2-C3	10.38	1.58	1.33
21	B	511	CLA	CHB-C4A	10.63	1.47	1.33
32	D	357	PL9	C28-C29	10.83	1.60	1.33
21	B	511	CLA	C3B-C2B	12.42	1.56	1.40

All (1202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	115	BCR	C32-C1-C6	-10.59	93.14	110.31
33	F	85	HEM	CMA-C3A-C2A	-9.47	107.09	124.94
25	J	115	BCR	C32-C1-C31	-9.36	79.83	108.50
32	D	357	PL9	C7-C8-C9	-8.97	111.71	126.71
33	V	164	HEM	CMA-C3A-C2A	-8.54	108.84	124.94
33	V	164	HEM	C4A-C3A-C2A	-8.39	101.16	107.00
33	F	85	HEM	C4A-C3A-C2A	-7.64	101.68	107.00
26	D	362	DGD	C3G-O3G-C1D	-7.42	98.55	113.76
28	F	224	SQD	O8-S-C6	-7.40	96.97	106.01
26	C	474	DGD	C6D-C5D-C4D	-6.79	97.53	112.00
25	J	115	BCR	C32-C1-C2	-6.71	82.33	108.80
29	B	531	LMG	C13-C12-C11	-6.68	88.78	113.24
28	L	213	SQD	O8-S-C6	-6.66	97.88	106.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	493	DGD	C6D-O5D-C1E	-6.62	100.17	113.76
26	C	492	DGD	C6D-O5D-C1E	-6.57	100.28	113.76
26	C	491	DGD	O1G-C1G-C2G	-6.46	92.41	108.66
26	C	474	DGD	C1G-O1G-C1A	-6.27	98.27	117.13
29	B	531	LMG	C19-C18-C17	-6.26	82.22	114.45
26	C	493	DGD	C4B-C3B-C2B	-6.16	90.68	113.24
26	C	493	DGD	C6D-C5D-C4D	-6.15	98.89	112.00
21	C	481	CLA	CAA-C2A-C1A	-6.15	91.83	111.97
29	D	359	LMG	C13-C12-C11	-6.11	90.85	113.24
28	D	361	SQD	O8-S-C6	-5.99	98.69	106.01
26	C	493	DGD	C3G-O3G-C1D	-5.88	101.70	113.76
28	C	475	SQD	O8-S-C6	-5.84	98.88	106.01
26	C	474	DGD	O3G-C1D-C2D	-5.82	98.74	108.23
29	B	531	LMG	C17-C16-C15	-5.71	85.05	114.45
29	D	359	LMG	C7-O1-C1	-5.69	102.08	113.76
26	A	375	DGD	C6D-O5D-C1E	-5.59	102.29	113.76
26	C	492	DGD	C4A-C3A-C2A	-5.53	92.99	113.24
32	D	357	PL9	C32-C33-C34	-5.52	113.82	127.68
26	C	491	DGD	C4B-C3B-C2B	-5.48	93.17	113.24
28	D	361	SQD	O9-S-C6	-5.48	102.15	106.83
26	C	492	DGD	C6A-C5A-C4A	-5.45	86.37	114.45
21	C	481	CLA	CAA-CBA-CGA	-5.43	96.99	113.35
32	D	357	PL9	C11-C9-C8	-5.36	110.12	121.10
29	B	531	LMG	C7-O1-C1	-5.36	102.77	113.76
26	C	474	DGD	C6D-O5D-C1E	-5.35	102.79	113.76
29	I	220	LMG	C13-C12-C11	-5.29	93.84	113.24
30	D	536	LMT	C1B-O1B-C4'	-5.28	105.14	118.00
21	C	480	CLA	CAA-C2A-C1A	-5.17	95.05	111.97
26	C	493	DGD	C1D-O6D-C5D	-5.10	104.10	113.72
26	D	362	DGD	C6D-O5D-C1E	-5.09	103.33	113.76
26	C	491	DGD	C6D-C5D-C4D	-5.05	101.24	112.00
26	A	375	DGD	O3G-C1D-C2D	-5.04	100.01	108.23
21	B	518	CLA	CAA-C2A-C1A	-5.04	95.46	111.97
26	A	375	DGD	C4B-C3B-C2B	-5.02	94.84	113.24
26	C	474	DGD	C1D-O6D-C5D	-5.01	104.28	113.72
26	C	492	DGD	C6D-C5D-C4D	-5.00	101.35	112.00
26	A	375	DGD	C6D-C5D-C4D	-4.98	101.39	112.00
26	C	492	DGD	C1D-O6D-C5D	-4.98	104.33	113.72
28	L	213	SQD	O9-S-C6	-4.92	102.63	106.83
29	D	359	LMG	O8-C9-C8	-4.91	96.31	108.66
32	D	357	PL9	C12-C13-C14	-4.91	115.34	127.68
29	B	531	LMG	C9-C8-C7	-4.83	100.95	111.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	492	DGD	C3G-O3G-C1D	-4.79	103.94	113.76
26	C	474	DGD	O3G-C3G-C2G	-4.73	99.74	110.99
32	D	357	PL9	C22-C23-C24	-4.67	115.94	127.68
32	D	357	PL9	C42-C43-C44	-4.63	116.05	127.68
25	X	107	BCR	C12-C13-C14	-4.62	111.86	118.94
29	B	531	LMG	C22-C21-C20	-4.59	90.81	114.45
26	C	492	DGD	C8A-C7A-C6A	-4.50	91.25	114.45
26	C	491	DGD	C6D-O5D-C1E	-4.49	104.55	113.76
25	J	115	BCR	C1-C6-C5	-4.48	116.29	122.59
25	J	115	BCR	C38-C26-C27	-4.48	104.96	113.45
26	C	491	DGD	C4A-C3A-C2A	-4.47	96.86	113.24
29	B	531	LMG	C15-C14-C13	-4.38	91.91	114.45
25	X	107	BCR	C38-C26-C27	-4.37	105.17	113.45
25	B	529	BCR	C33-C5-C4	-4.33	105.23	113.45
25	D	358	BCR	C38-C26-C27	-4.28	105.33	113.45
29	C	494	LMG	C13-C12-C11	-4.27	97.57	113.24
29	I	220	LMG	C9-C8-C7	-4.27	102.22	111.86
30	D	363	LMT	C1B-O1B-C4'	-4.25	107.65	118.00
29	C	494	LMG	O1-C7-C8	-4.24	100.90	110.99
21	B	521	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
26	C	474	DGD	C3A-C2A-C1A	-4.20	98.26	113.58
32	D	357	PL9	C10-C9-C8	-4.16	112.59	123.69
25	J	112	BCR	C33-C5-C4	-4.15	105.58	113.45
25	A	369	BCR	C38-C26-C27	-4.09	105.69	113.45
21	C	486	CLA	C2C-C1C-NC	-4.05	107.44	110.22
25	C	489	BCR	C38-C26-C27	-4.04	105.78	113.45
25	X	107	BCR	C30-C25-C26	-4.02	116.95	122.59
25	D	358	BCR	C33-C5-C4	-4.00	105.86	113.45
25	B	529	BCR	C38-C26-C27	-3.99	105.89	113.45
21	C	481	CLA	C2C-C1C-NC	-3.97	107.50	110.22
25	J	115	BCR	C33-C5-C4	-3.96	105.94	113.45
25	B	530	BCR	C33-C5-C4	-3.93	105.99	113.45
25	C	490	BCR	C33-C5-C4	-3.91	106.04	113.45
26	B	533	DGD	C3A-C2A-C1A	-3.90	99.36	113.58
25	B	527	BCR	C33-C5-C4	-3.87	106.10	113.45
26	C	493	DGD	C6B-C5B-C4B	-3.87	94.49	114.45
26	C	493	DGD	O1G-C1G-C2G	-3.86	98.97	108.66
28	F	224	SQD	O9-S-C6	-3.86	103.53	106.83
26	D	362	DGD	C6D-C5D-C4D	-3.81	103.88	112.00
21	B	515	CLA	CAA-C2A-C1A	-3.78	99.59	111.97
25	B	527	BCR	C38-C26-C27	-3.77	106.30	113.45
21	C	488	CLA	C2C-C1C-NC	-3.77	107.64	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	492	DGD	C3G-C2G-C1G	-3.74	103.43	111.86
21	C	480	CLA	CAA-CBA-CGA	-3.72	102.15	113.35
25	D	358	BCR	C1-C6-C5	-3.70	117.39	122.59
26	B	533	DGD	C1D-O6D-C5D	-3.69	106.76	113.72
25	Z	116	BCR	C33-C5-C4	-3.66	106.51	113.45
25	C	490	BCR	C38-C26-C27	-3.65	106.52	113.45
21	C	488	CLA	CAA-CBA-CGA	-3.64	102.38	113.35
30	D	536	LMT	O1'-C1-C2	-3.64	96.70	109.68
21	C	479	CLA	O1D-CGD-CBD	-3.63	118.09	124.60
25	J	112	BCR	C8-C9-C10	-3.62	113.38	118.94
26	C	491	DGD	C3G-O3G-C1D	-3.61	106.35	113.76
25	C	490	BCR	C23-C22-C21	-3.57	113.46	118.94
29	D	360	LMG	C8-O7-C10	-3.56	109.47	117.88
28	C	475	SQD	O9-S-C6	-3.55	103.79	106.83
29	I	220	LMG	C15-C14-C13	-3.55	96.16	114.45
26	B	528	DGD	C2G-O2G-C1B	-3.54	109.50	117.88
29	A	373	LMG	C8-O7-C10	-3.54	109.51	117.88
21	B	524	CLA	O1D-CGD-CBD	-3.51	118.30	124.60
25	A	369	BCR	C33-C5-C4	-3.51	106.79	113.45
30	B	535	LMT	C1-O1'-C1'	-3.50	107.86	113.87
25	B	530	BCR	C38-C26-C27	-3.47	106.86	113.45
25	Z	116	BCR	C38-C26-C27	-3.47	106.87	113.45
32	D	357	PL9	C20-C19-C18	-3.47	114.43	123.69
25	J	112	BCR	C30-C25-C26	-3.47	117.72	122.59
25	J	112	BCR	C38-C26-C27	-3.46	106.89	113.45
26	A	375	DGD	C3G-C2G-C1G	-3.45	104.07	111.86
29	J	492	LMG	C12-C11-C10	-3.45	101.00	113.58
21	B	524	CLA	CAA-C2A-C1A	-3.43	100.72	111.97
21	A	363	CLA	CAA-C2A-C1A	-3.43	100.73	111.97
25	D	358	BCR	C30-C25-C26	-3.42	117.78	122.59
25	B	527	BCR	C12-C13-C14	-3.42	113.69	118.94
25	X	107	BCR	C33-C5-C4	-3.42	106.97	113.45
25	B	530	BCR	C30-C25-C26	-3.41	117.80	122.59
25	A	369	BCR	C30-C25-C26	-3.41	117.80	122.59
25	J	112	BCR	C1-C6-C5	-3.40	117.81	122.59
21	C	486	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
32	D	357	PL9	C7-C3-C2	-3.36	118.45	123.23
21	C	484	CLA	CAA-C2A-C1A	-3.34	101.02	111.97
30	O	274	LMT	O1'-C1-C2	-3.34	97.76	109.68
21	C	477	CLA	CAA-C2A-C1A	-3.34	101.03	111.97
25	J	115	BCR	C30-C25-C26	-3.32	117.92	122.59
21	B	517	CLA	C2C-C1C-NC	-3.32	107.94	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	518	CLA	CAA-CBA-CGA	-3.26	103.54	113.35
29	J	492	LMG	C14-C13-C12	-3.25	97.72	114.45
21	C	484	CLA	C2C-C1C-NC	-3.24	108.00	110.22
26	A	375	DGD	C6B-C5B-C4B	-3.20	97.98	114.45
26	C	474	DGD	O1G-C1A-O1A	-3.19	115.62	123.55
25	C	489	BCR	C33-C5-C4	-3.19	107.40	113.45
25	X	107	BCR	C1-C6-C5	-3.18	118.12	122.59
28	D	361	SQD	C3-C4-C5	-3.18	104.62	110.22
21	D	354	CLA	C12-C11-C10	-3.18	97.88	113.25
28	C	475	SQD	C3-C4-C5	-3.18	104.62	110.22
29	I	220	LMG	C17-C16-C15	-3.15	98.22	114.45
21	B	519	CLA	CAA-CBA-CGA	-3.11	103.97	113.35
26	C	491	DGD	C6B-C5B-C4B	-3.11	98.44	114.45
25	C	490	BCR	C30-C25-C26	-3.10	118.24	122.59
21	C	478	CLA	O1D-CGD-CBD	-3.10	119.04	124.60
29	C	494	LMG	C31-C30-C29	-3.09	101.93	113.24
22	A	365	PHO	C2A-C1A-NA	-3.08	108.16	111.91
26	C	491	DGD	C1D-O6D-C5D	-3.08	107.91	113.72
21	C	479	CLA	CAA-C2A-C1A	-3.08	101.88	111.97
30	D	536	LMT	C4-C3-C2	-3.07	98.62	114.45
29	J	492	LMG	C9-C8-C7	-3.07	104.93	111.86
25	B	530	BCR	C1-C6-C5	-3.06	118.29	122.59
29	D	359	LMG	C15-C14-C13	-3.06	98.70	114.45
25	B	527	BCR	C30-C25-C26	-3.05	118.30	122.59
22	A	365	PHO	CAB-C3B-C2B	-3.05	118.34	128.56
25	C	489	BCR	C1-C6-C5	-3.03	118.33	122.59
28	F	224	SQD	C3-C4-C5	-3.03	104.88	110.22
25	C	489	BCR	C23-C22-C21	-3.01	114.33	118.94
26	A	375	DGD	O6D-C5D-C4D	-3.01	104.12	109.66
25	C	490	BCR	C1-C6-C5	-3.00	118.38	122.59
25	C	489	BCR	C30-C25-C26	-3.00	118.38	122.59
25	B	527	BCR	C1-C6-C5	-3.00	118.38	122.59
25	Z	116	BCR	C30-C25-C26	-3.00	118.38	122.59
26	C	474	DGD	O1A-C1A-C2A	-2.99	111.86	123.68
21	B	522	CLA	O1D-CGD-CBD	-2.96	119.29	124.60
25	B	529	BCR	C1-C6-C5	-2.94	118.45	122.59
21	B	520	CLA	O1D-CGD-CBD	-2.94	119.31	124.60
32	D	357	PL9	C35-C34-C33	-2.94	115.84	123.69
25	B	527	BCR	C19-C18-C17	-2.92	114.45	118.94
21	B	519	CLA	CAA-C2A-C1A	-2.92	102.40	111.97
21	C	478	CLA	CAA-C2A-C1A	-2.91	102.42	111.97
26	A	375	DGD	O3G-C3G-C2G	-2.91	104.07	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	475	SQD	O8-S-O9	-2.90	104.72	111.37
21	B	516	CLA	CAA-CBA-CGA	-2.90	104.62	113.35
29	C	494	LMG	O8-C9-C8	-2.89	101.40	108.66
21	C	481	CLA	C3D-CAD-CBD	-2.88	103.52	107.60
32	D	357	PL9	C10-C9-C11	-2.88	110.29	115.29
30	I	274	LMT	O1'-C1-C2	-2.87	99.42	109.68
32	D	357	PL9	C15-C14-C13	-2.87	116.04	123.69
21	C	477	CLA	CAA-CBA-CGA	-2.85	104.75	113.35
28	L	213	SQD	C3-C4-C5	-2.85	105.20	110.22
21	B	517	CLA	CAA-C2A-C1A	-2.85	102.65	111.97
30	D	363	LMT	O1'-C1-C2	-2.83	99.57	109.68
30	A	376	LMT	C7-C6-C5	-2.83	99.88	114.45
21	B	513	CLA	O1D-CGD-CBD	-2.83	119.53	124.60
26	C	492	DGD	CBA-CAA-C9A	-2.82	99.90	114.45
21	C	483	CLA	O1D-CGD-CBD	-2.81	119.55	124.60
25	B	529	BCR	C30-C25-C26	-2.81	118.64	122.59
26	C	493	DGD	C8B-C7B-C6B	-2.80	100.02	114.45
21	A	363	CLA	O1D-CGD-CBD	-2.79	119.58	124.60
22	A	365	PHO	CBD-CHA-C4D	-2.79	105.39	108.54
25	D	358	BCR	C23-C22-C21	-2.78	114.68	118.94
26	B	533	DGD	O1G-C1A-O1A	-2.78	116.65	123.55
21	B	521	CLA	CAA-CBA-CGA	-2.77	104.99	113.35
22	D	355	PHO	CAB-C3B-C2B	-2.77	119.29	128.56
22	A	365	PHO	O1D-CGD-CBD	-2.77	119.63	124.60
30	O	274	LMT	C4-C3-C2	-2.74	100.34	114.45
26	C	493	DGD	C8A-C7A-C6A	-2.73	100.37	114.45
30	I	274	LMT	C4-C3-C2	-2.72	100.44	114.45
21	K	483	CLA	O1D-CGD-CBD	-2.70	119.76	124.60
21	D	356	CLA	O1D-CGD-CBD	-2.69	119.77	124.60
25	J	112	BCR	C32-C1-C2	-2.69	98.19	108.80
21	C	485	CLA	O1D-CGD-CBD	-2.69	119.77	124.60
21	C	479	CLA	C3D-CAD-CBD	-2.68	103.81	107.60
32	D	357	PL9	O1-C4-C3	-2.68	117.67	120.71
29	D	359	LMG	C17-C16-C15	-2.68	100.66	114.45
21	B	516	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
25	C	490	BCR	C40-C30-C29	-2.66	98.31	108.80
21	D	356	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
30	A	376	LMT	C4-C3-C2	-2.65	100.79	114.45
29	C	494	LMG	C6-C5-C4	-2.65	106.81	113.00
21	B	513	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
21	C	480	CLA	O1D-CGD-CBD	-2.64	119.86	124.60
21	B	513	CLA	CAA-C2A-C3A	-2.62	105.61	112.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	I	274	LMT	C7-C6-C5	-2.62	100.94	114.45
21	B	516	CLA	CAA-C2A-C3A	-2.62	105.63	112.81
26	B	533	DGD	C6D-C5D-C4D	-2.62	106.42	112.00
21	C	484	CLA	C3D-CAD-CBD	-2.61	103.90	107.60
21	A	363	CLA	C2C-C1C-NC	-2.61	108.43	110.22
21	C	478	CLA	C3D-CAD-CBD	-2.60	103.92	107.60
30	D	536	LMT	C7-C6-C5	-2.60	101.07	114.45
21	B	524	CLA	C3D-CAD-CBD	-2.59	103.93	107.60
29	D	359	LMG	O7-C8-C9	-2.58	99.04	108.44
21	C	488	CLA	CAA-C2A-C1A	-2.57	103.55	111.97
25	Z	116	BCR	C19-C18-C17	-2.57	115.00	118.94
29	I	220	LMG	C19-C18-C17	-2.57	101.21	114.45
21	C	482	CLA	O1D-CGD-CBD	-2.57	119.99	124.60
22	D	355	PHO	C3A-C4A-NA	-2.56	108.65	113.06
21	C	482	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
26	B	528	DGD	C1G-O1G-C1A	-2.55	109.47	117.13
29	D	360	LMG	C9-O8-C28	-2.54	109.50	117.13
33	V	164	HEM	C4C-C3C-C2C	-2.53	105.13	106.90
26	A	375	DGD	C1D-O6D-C5D	-2.53	108.94	113.72
21	B	515	CLA	O1D-CGD-CBD	-2.53	120.05	124.60
21	B	511	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
29	A	373	LMG	C9-O8-C28	-2.53	109.53	117.13
21	B	516	CLA	C3D-CAD-CBD	-2.53	104.03	107.60
21	B	515	CLA	C2C-C1C-NC	-2.52	108.49	110.22
30	T	226	LMT	C1-O1'-C1'	-2.52	109.54	113.87
30	D	536	LMT	O1'-C1'-C2'	-2.51	104.14	108.23
21	C	487	CLA	CHA-C1A-NA	-2.50	120.36	126.18
21	B	511	CLA	O1D-CGD-CBD	-2.50	120.11	124.60
29	M	217	LMG	O8-C9-C8	-2.50	102.39	108.66
26	C	493	DGD	CBA-CAA-C9A	-2.50	101.60	114.45
30	A	376	LMT	C1B-O1B-C4'	-2.49	111.92	118.00
26	B	533	DGD	O3G-C3G-C2G	-2.49	105.06	110.99
29	J	492	LMG	C34-C33-C32	-2.49	101.63	114.45
21	A	364	CLA	CAA-C2A-C1A	-2.49	103.83	111.97
33	F	85	HEM	CBD-CAD-C3D	-2.48	107.73	112.47
21	B	519	CLA	O1D-CGD-CBD	-2.47	120.16	124.60
21	C	480	CLA	C3D-CAD-CBD	-2.47	104.11	107.60
30	O	274	LMT	O1'-C1'-C2'	-2.46	104.22	108.23
26	A	375	DGD	C6E-C5E-C4E	-2.46	107.26	113.00
21	A	363	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
21	C	486	CLA	C3B-C4B-NB	-2.45	106.04	109.21
21	B	514	CLA	C3D-CAD-CBD	-2.45	104.13	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	M	217	LMG	C12-C11-C10	-2.44	104.68	113.58
21	C	483	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
21	B	511	CLA	OBD-CAD-CBD	-2.44	122.26	125.94
32	D	357	PL9	C25-C24-C23	-2.44	117.19	123.69
21	D	354	CLA	O1D-CGD-CBD	-2.43	120.24	124.60
21	B	517	CLA	O1D-CGD-CBD	-2.42	120.26	124.60
21	B	518	CLA	C3D-CAD-CBD	-2.42	104.18	107.60
21	C	487	CLA	O1D-CGD-CBD	-2.41	120.26	124.60
21	A	364	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
21	B	523	CLA	O1D-CGD-CBD	-2.41	120.27	124.60
26	B	533	DGD	O2G-C1B-O1B	-2.40	117.68	123.68
21	C	484	CLA	O1D-CGD-CBD	-2.40	120.29	124.60
21	B	514	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
21	C	484	CLA	C3B-C4B-NB	-2.40	106.11	109.21
21	D	354	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
21	B	512	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
21	B	520	CLA	C3D-CAD-CBD	-2.37	104.25	107.60
25	J	112	BCR	C12-C13-C14	-2.37	115.31	118.94
21	B	516	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
21	D	356	CLA	OBD-CAD-CBD	-2.36	122.38	125.94
29	M	217	LMG	O7-C10-O9	-2.36	117.79	123.68
26	C	493	DGD	CFB-CEB-CDB	-2.35	102.33	114.45
22	A	365	PHO	C3A-C4A-NA	-2.35	109.01	113.06
26	C	474	DGD	O1B-C1B-C2B	-2.34	114.42	123.68
21	B	524	CLA	C2C-C1C-NC	-2.34	108.61	110.22
21	B	517	CLA	C3B-C4B-NB	-2.34	106.18	109.21
21	B	525	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
21	C	483	CLA	C3D-CAD-CBD	-2.34	104.29	107.60
29	D	359	LMG	C6-C5-C4	-2.34	107.53	113.00
30	D	363	LMT	O1'-C1'-C2'	-2.34	104.42	108.23
21	C	477	CLA	O1D-CGD-CBD	-2.34	120.41	124.60
26	D	362	DGD	CBA-CAA-C9A	-2.33	102.47	114.45
26	B	533	DGD	C3G-C2G-C1G	-2.32	106.62	111.86
21	B	518	CLA	O1D-CGD-CBD	-2.32	120.44	124.60
29	C	494	LMG	C19-C18-C17	-2.32	102.52	114.45
25	X	107	BCR	C19-C18-C17	-2.32	115.39	118.94
21	B	523	CLA	C3D-CAD-CBD	-2.31	104.33	107.60
21	B	518	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
21	D	354	CLA	C2C-C1C-NC	-2.30	108.64	110.22
21	B	517	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
21	C	482	CLA	C3D-CAD-CBD	-2.30	104.35	107.60
26	A	375	DGD	C8B-C7B-C6B	-2.29	102.64	114.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	491	DGD	C4E-C3E-C2E	-2.29	106.81	110.84
21	A	364	CLA	O1D-CGD-CBD	-2.28	120.50	124.60
21	D	354	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
21	B	526	CLA	OBD-CAD-CBD	-2.28	122.50	125.94
25	D	358	BCR	C12-C13-C14	-2.28	115.44	118.94
26	D	362	DGD	O2G-C2G-C3G	-2.28	100.15	108.44
21	B	512	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
29	D	359	LMG	O7-C10-C11	-2.27	106.85	111.55
21	B	516	CLA	C12-C11-C10	-2.26	102.30	113.25
26	D	362	DGD	C8A-C7A-C6A	-2.26	102.80	114.45
21	B	523	CLA	C3B-C4B-NB	-2.26	106.29	109.21
21	C	483	CLA	C3B-C4B-NB	-2.26	106.29	109.21
21	C	481	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
21	B	521	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
21	B	525	CLA	C2C-C1C-NC	-2.25	108.68	110.22
21	C	488	CLA	C3B-C4B-NB	-2.25	106.30	109.21
21	C	484	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
21	C	482	CLA	C3B-C4B-NB	-2.25	106.31	109.21
21	B	517	CLA	C3D-CAD-CBD	-2.25	104.42	107.60
21	B	516	CLA	O1D-CGD-CBD	-2.24	120.57	124.60
29	D	360	LMG	C1-O6-C5	-2.24	109.49	113.72
25	A	369	BCR	C23-C22-C21	-2.24	115.50	118.94
30	A	376	LMT	O1'-C1'-C2'	-2.24	104.58	108.23
21	B	522	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
29	A	373	LMG	C1-O6-C5	-2.24	109.50	113.72
21	A	363	CLA	OBD-CAD-CBD	-2.23	122.56	125.94
21	B	519	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
29	M	217	LMG	C14-C13-C12	-2.23	102.95	114.45
26	B	528	DGD	C1D-O6D-C5D	-2.23	109.51	113.72
26	B	528	DGD	C1E-O6E-C5E	-2.23	109.52	113.72
26	B	533	DGD	C3G-O3G-C1D	-2.22	109.20	113.76
21	B	526	CLA	O1D-CGD-CBD	-2.22	120.62	124.60
21	A	366	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
22	D	355	PHO	O1D-CGD-CBD	-2.21	120.62	124.60
21	B	520	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
26	B	533	DGD	C7A-C6A-C5A	-2.20	103.10	114.45
29	C	494	LMG	C17-C16-C15	-2.20	103.11	114.45
29	J	492	LMG	O7-C10-O9	-2.20	118.19	123.68
21	B	513	CLA	C3D-CAD-CBD	-2.20	104.49	107.60
25	Z	116	BCR	C1-C6-C5	-2.20	119.50	122.59
26	C	493	DGD	C6A-C5A-C4A	-2.19	103.15	114.45
21	B	524	CLA	CAA-CBA-CGA	-2.19	106.75	113.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	116	BCR	C12-C13-C14	-2.19	115.58	118.94
21	C	488	CLA	CMB-C2B-C1B	-2.19	125.11	128.46
21	B	523	CLA	C2C-C1C-NC	-2.18	108.72	110.22
21	B	521	CLA	C4-C3-C5	-2.18	111.50	115.29
26	B	533	DGD	C5B-C4B-C3B	-2.18	103.21	114.45
21	C	486	CLA	OBD-CAD-CBD	-2.18	122.65	125.94
26	C	493	DGD	CDB-CCB-CBB	-2.18	103.24	114.45
21	A	362	CLA	C7-C6-C5	-2.18	107.06	113.11
28	D	361	SQD	O8-S-O9	-2.17	106.39	111.37
21	A	366	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
21	B	522	CLA	C2C-C1C-NC	-2.17	108.73	110.22
21	C	479	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
21	B	511	CLA	O2D-CGD-O1D	-2.17	119.46	123.82
21	A	362	CLA	C3D-CAD-CBD	-2.16	104.54	107.60
25	B	530	BCR	C12-C13-C14	-2.16	115.62	118.94
21	B	525	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
25	C	490	BCR	C12-C13-C14	-2.15	115.64	118.94
30	D	363	LMT	C4-C3-C2	-2.15	103.39	114.45
21	B	522	CLA	C3D-CAD-CBD	-2.15	104.56	107.60
21	B	522	CLA	C3B-C4B-NB	-2.14	106.44	109.21
21	C	482	CLA	C2C-C1C-NC	-2.14	108.75	110.22
21	C	488	CLA	C3D-CAD-CBD	-2.14	104.57	107.60
30	A	376	LMT	C9-C8-C7	-2.13	103.46	114.45
26	B	533	DGD	CDA-CCA-CBA	-2.13	103.47	114.45
26	D	362	DGD	C4A-C3A-C2A	-2.13	105.44	113.24
21	K	483	CLA	C12-C11-C10	-2.13	102.97	113.25
21	B	514	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
21	A	362	CLA	C2C-C1C-NC	-2.12	108.77	110.22
21	C	485	CLA	C3D-CAD-CBD	-2.12	104.60	107.60
21	A	362	CLA	O1D-CGD-CBD	-2.12	120.80	124.60
29	I	220	LMG	O1-C7-C8	-2.12	105.95	110.99
21	B	517	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
25	A	369	BCR	C12-C13-C14	-2.11	115.70	118.94
21	A	362	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
21	A	363	CLA	C3D-CAD-CBD	-2.10	104.62	107.60
30	A	376	LMT	C1'-O5'-C5'	-2.10	109.76	113.72
25	X	107	BCR	C23-C22-C21	-2.10	115.72	118.94
29	D	360	LMG	C7-O1-C1	-2.10	109.45	113.76
21	B	513	CLA	C3B-C4B-NB	-2.09	106.50	109.21
29	J	492	LMG	O9-C10-C11	-2.09	115.42	123.68
28	L	213	SQD	O8-S-O9	-2.09	106.58	111.37
28	F	224	SQD	O48-C23-O10	-2.09	118.36	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	112	BCR	C40-C30-C29	-2.09	100.56	108.80
22	D	355	PHO	CBD-CHA-C4D	-2.09	106.19	108.54
26	B	528	DGD	C6D-O5D-C1E	-2.09	109.48	113.76
29	M	217	LMG	C7-O1-C1	-2.08	109.49	113.76
21	C	482	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
26	B	528	DGD	C3G-O3G-C1D	-2.08	109.49	113.76
21	B	517	CLA	C9-C8-C7	-2.08	103.78	111.36
26	C	493	DGD	O6D-C1D-C2D	-2.08	106.29	110.30
29	A	373	LMG	C7-O1-C1	-2.07	109.51	113.76
28	D	361	SQD	C46-C45-C44	-2.07	107.19	111.86
21	B	513	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
21	B	524	CLA	C3B-C4B-NB	-2.06	106.55	109.21
21	C	487	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
21	C	481	CLA	O1D-CGD-CBD	-2.05	120.91	124.60
21	B	519	CLA	C3D-CAD-CBD	-2.05	104.70	107.60
21	B	515	CLA	C3D-CAD-CBD	-2.05	104.70	107.60
21	B	514	CLA	OBD-CAD-CBD	-2.04	122.85	125.94
21	C	481	CLA	C3B-C4B-NB	-2.04	106.57	109.21
29	D	359	LMG	C32-C31-C30	-2.04	103.95	114.45
21	C	486	CLA	C3D-CAD-CBD	-2.04	104.72	107.60
21	B	525	CLA	C3B-C4B-NB	-2.04	106.58	109.21
21	B	517	CLA	C12-C11-C10	-2.04	103.41	113.25
21	C	480	CLA	OBD-CAD-CBD	-2.03	122.87	125.94
21	A	364	CLA	C3D-CAD-CBD	-2.03	104.73	107.60
29	C	494	LMG	O1-C1-C2	-2.03	104.93	108.23
26	B	533	DGD	O1B-C1B-C2B	-2.02	115.69	123.68
21	D	356	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
21	B	511	CLA	CHA-C1A-NA	-2.02	121.49	126.18
21	C	484	CLA	C12-C11-C10	-2.02	103.50	113.25
21	A	366	CLA	C3B-C4B-NB	-2.02	106.60	109.21
21	B	518	CLA	C4-C3-C5	-2.02	111.79	115.29
21	B	517	CLA	C9-C8-C10	-2.00	104.05	111.36
21	B	523	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
21	K	483	CLA	C3D-CAD-CBD	-2.00	104.77	107.60
21	C	486	CLA	C12-C11-C10	-2.00	103.57	113.25
21	K	483	CLA	C1D-CHD-C4C	2.00	125.22	122.48
26	D	362	DGD	C5A-C4A-C3A	2.00	124.77	114.45
28	L	213	SQD	C19-C18-C17	2.00	124.78	114.45
26	C	493	DGD	O2G-C2G-C3G	2.00	115.72	108.44
21	C	477	CLA	OBD-CAD-C3D	2.00	131.72	128.03
28	L	213	SQD	C13-C12-C11	2.01	124.80	114.45
25	D	358	BCR	C11-C10-C9	2.01	130.18	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	369	BCR	C1-C6-C7	2.02	121.41	115.73
29	I	220	LMG	C16-C15-C14	2.02	124.87	114.45
25	B	530	BCR	C36-C18-C19	2.02	121.32	118.10
25	A	369	BCR	C8-C7-C6	2.02	132.92	127.25
21	C	479	CLA	O2A-CGA-CBA	2.03	117.81	111.90
21	C	477	CLA	C1-C2-C3	2.03	129.70	125.96
29	J	492	LMG	C35-C34-C33	2.04	124.95	114.45
22	A	365	PHO	C1C-NC-C4C	2.04	110.55	106.52
26	C	491	DGD	C3G-C2G-C1G	2.04	116.45	111.86
21	A	366	CLA	CED-O2D-CGD	2.04	120.75	115.97
21	B	520	CLA	C1D-CHD-C4C	2.04	125.28	122.48
26	D	362	DGD	C3A-C2A-C1A	2.04	121.05	113.58
30	I	274	LMT	O5'-C5'-C6'	2.05	111.32	106.41
21	A	366	CLA	C1D-CHD-C4C	2.06	125.30	122.48
25	Z	116	BCR	C28-C27-C26	2.06	117.33	113.78
28	C	475	SQD	O8-S-O7	2.06	116.10	111.37
21	B	518	CLA	C11-C12-C13	2.06	122.51	115.73
22	D	355	PHO	CAA-C2A-C1A	2.07	117.62	112.28
21	B	516	CLA	O2D-CGD-CBD	2.07	114.99	111.30
26	C	493	DGD	C5B-C4B-C3B	2.07	125.11	114.45
21	B	518	CLA	CMB-C2B-C3B	2.07	128.73	124.89
21	B	518	CLA	C16-C15-C13	2.07	122.53	115.73
21	B	524	CLA	C1D-CHD-C4C	2.07	125.31	122.48
22	D	355	PHO	C1-C2-C3	2.08	129.78	125.96
26	B	533	DGD	C4B-C3B-C2B	2.08	120.85	113.24
21	C	481	CLA	CED-O2D-CGD	2.08	120.86	115.97
21	B	512	CLA	C1D-CHD-C4C	2.09	125.34	122.48
26	C	493	DGD	C4D-C3D-C2D	2.09	114.52	110.84
33	F	85	HEM	CAD-CBD-CGD	2.09	116.23	112.66
21	C	479	CLA	OBD-CAD-C3D	2.10	131.89	128.03
21	A	364	CLA	OBD-CAD-C3D	2.10	131.90	128.03
21	B	526	CLA	CBA-CAA-C2A	2.11	120.10	113.80
21	B	514	CLA	CMB-C2B-C3B	2.11	128.80	124.89
25	Z	116	BCR	C40-C30-C25	2.11	113.73	110.31
21	A	363	CLA	CMB-C2B-C3B	2.11	128.81	124.89
25	J	112	BCR	C36-C18-C19	2.11	121.46	118.10
21	B	521	CLA	C11-C12-C13	2.11	122.66	115.73
28	F	224	SQD	O47-C7-C8	2.12	115.94	111.55
26	C	491	DGD	C5A-C4A-C3A	2.12	125.36	114.45
25	A	369	BCR	C21-C20-C19	2.12	129.73	123.23
21	C	479	CLA	C2A-C1A-CHA	2.12	127.67	123.92
29	C	494	LMG	C30-C29-C28	2.12	121.33	113.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	107	BCR	C36-C18-C19	2.12	121.48	118.10
22	D	355	PHO	CBD-CHA-C1A	2.13	131.38	126.36
25	A	369	BCR	C40-C30-C25	2.13	113.77	110.31
22	D	355	PHO	C1C-NC-C4C	2.13	110.74	106.52
26	C	492	DGD	O3D-C3D-C2D	2.14	115.00	110.36
25	J	115	BCR	C28-C27-C26	2.14	117.46	113.78
30	O	274	LMT	O5B-C5B-C6B	2.14	111.53	106.41
25	B	530	BCR	C1-C6-C7	2.14	121.74	115.73
28	F	224	SQD	C32-C31-C30	2.14	130.13	113.42
28	D	361	SQD	C15-C14-C13	2.15	125.51	114.45
29	I	220	LMG	O6-C1-O1	2.15	115.12	110.02
25	B	530	BCR	C32-C1-C6	2.16	113.81	110.31
28	F	224	SQD	C17-C16-C15	2.16	125.58	114.45
21	B	512	CLA	CED-O2D-CGD	2.16	121.04	115.97
25	Z	116	BCR	C1-C6-C7	2.16	121.81	115.73
21	C	484	CLA	OBD-CAD-C3D	2.17	132.03	128.03
33	V	164	HEM	CAD-C3D-C2D	2.17	135.21	129.00
21	C	484	CLA	C1D-CHD-C4C	2.17	125.46	122.48
21	B	514	CLA	C5-C3-C2	2.18	125.56	121.10
25	J	112	BCR	C28-C27-C26	2.18	117.53	113.78
25	X	107	BCR	C1-C6-C7	2.19	121.88	115.73
21	C	480	CLA	C1D-CHD-C4C	2.19	125.47	122.48
21	B	514	CLA	C1D-CHD-C4C	2.19	125.47	122.48
26	C	474	DGD	O6E-C5E-C4E	2.19	113.70	109.66
29	I	220	LMG	C14-C13-C12	2.19	125.76	114.45
21	D	356	CLA	OBD-CAD-C3D	2.20	132.07	128.03
25	A	369	BCR	C32-C1-C6	2.20	113.87	110.31
25	B	529	BCR	C32-C1-C6	2.20	113.87	110.31
28	C	475	SQD	O47-C7-C8	2.20	116.12	111.55
21	C	485	CLA	OBD-CAD-C3D	2.20	132.08	128.03
21	D	356	CLA	CED-O2D-CGD	2.20	121.13	115.97
29	C	494	LMG	C12-C11-C10	2.20	121.62	113.58
22	A	365	PHO	C1B-NB-C4B	2.20	110.88	106.52
25	B	529	BCR	C16-C15-C14	2.20	128.17	123.46
25	B	529	BCR	C7-C8-C9	2.20	129.52	126.21
26	C	492	DGD	C7A-C6A-C5A	2.21	125.83	114.45
21	C	477	CLA	C1D-CHD-C4C	2.21	125.50	122.48
21	B	525	CLA	CED-O2D-CGD	2.21	121.16	115.97
21	B	524	CLA	OBD-CAD-C3D	2.21	132.10	128.03
25	D	358	BCR	C40-C30-C25	2.21	113.90	110.31
28	C	475	SQD	C17-C16-C15	2.22	125.89	114.45
21	C	485	CLA	C1D-CHD-C4C	2.22	125.52	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	489	BCR	C7-C8-C9	2.22	129.55	126.21
21	D	354	CLA	C11-C10-C8	2.22	123.04	115.73
28	F	224	SQD	O8-S-O7	2.23	116.47	111.37
25	B	527	BCR	C34-C9-C8	2.23	121.64	118.10
26	B	533	DGD	O5D-C6D-C5D	2.23	112.67	108.94
21	B	526	CLA	OBD-CAD-C3D	2.23	132.13	128.03
21	C	488	CLA	CBA-CAA-C2A	2.24	120.49	113.80
30	O	274	LMT	O1B-C1B-C2B	2.24	113.15	108.11
21	C	478	CLA	C1-C2-C3	2.24	130.09	125.96
26	C	491	DGD	O6E-C5E-C4E	2.24	113.79	109.66
21	B	518	CLA	CED-O2D-CGD	2.25	121.24	115.97
21	C	478	CLA	OBD-CAD-C3D	2.25	132.18	128.03
25	Z	116	BCR	C36-C18-C19	2.26	121.69	118.10
22	D	355	PHO	C1B-NB-C4B	2.26	111.00	106.52
25	B	530	BCR	C40-C30-C25	2.26	113.98	110.31
21	C	479	CLA	C1D-CHD-C4C	2.27	125.59	122.48
21	B	511	CLA	OBD-CAD-C3D	2.27	132.21	128.03
21	B	516	CLA	CMB-C2B-C3B	2.27	129.11	124.89
25	J	112	BCR	C37-C22-C23	2.28	121.73	118.10
21	C	482	CLA	C2A-C1A-CHA	2.28	127.96	123.92
21	B	515	CLA	OBD-CAD-C3D	2.29	132.24	128.03
21	C	478	CLA	C1D-CHD-C4C	2.29	125.62	122.48
25	A	369	BCR	C2-C1-C6	2.29	114.06	110.48
25	J	115	BCR	C40-C30-C25	2.29	114.03	110.31
25	J	112	BCR	C16-C17-C18	2.30	130.59	127.31
25	B	527	BCR	C32-C1-C6	2.30	114.03	110.31
25	C	490	BCR	C28-C27-C26	2.30	117.74	113.78
26	A	375	DGD	O6E-C5E-C6E	2.30	111.92	106.41
25	B	527	BCR	C15-C14-C13	2.30	130.59	127.31
25	C	490	BCR	C32-C1-C6	2.30	114.04	110.31
25	Z	116	BCR	C35-C13-C12	2.31	121.78	118.10
25	B	529	BCR	C28-C27-C26	2.31	117.76	113.78
27	C	476	LHG	C6-C5-C4	2.31	117.08	111.86
26	C	474	DGD	O2D-C2D-C1D	2.32	114.87	110.03
21	B	512	CLA	C2A-C1A-CHA	2.32	128.03	123.92
25	J	115	BCR	C31-C1-C2	2.32	117.95	108.80
28	L	213	SQD	C17-C16-C15	2.32	126.41	114.45
21	K	483	CLA	CED-O2D-CGD	2.32	121.42	115.97
26	D	362	DGD	O3D-C3D-C2D	2.33	115.42	110.36
21	B	519	CLA	C1D-CHD-C4C	2.33	125.67	122.48
25	B	530	BCR	C16-C17-C18	2.33	130.64	127.31
28	L	213	SQD	O8-S-O7	2.33	116.72	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	354	CLA	C2A-C1A-CHA	2.33	128.06	123.92
21	B	514	CLA	C2A-C1A-CHA	2.33	128.06	123.92
25	X	107	BCR	C37-C22-C23	2.34	121.82	118.10
21	C	487	CLA	C3A-C2A-C1A	2.34	104.84	101.34
21	C	479	CLA	C6-C5-C3	2.34	117.96	112.66
21	D	354	CLA	OBD-CAD-C3D	2.35	132.35	128.03
22	A	365	PHO	CED-O2D-CGD	2.35	121.48	115.97
32	D	357	PL9	C53-C6-C1	2.35	119.84	114.84
25	A	369	BCR	C35-C13-C12	2.35	121.85	118.10
25	B	530	BCR	C34-C9-C8	2.35	121.85	118.10
28	F	224	SQD	C15-C14-C13	2.36	126.60	114.45
25	B	530	BCR	C37-C22-C23	2.36	121.86	118.10
29	J	492	LMG	O8-C28-C29	2.36	118.77	111.90
25	J	112	BCR	C40-C30-C25	2.37	114.16	110.31
21	D	354	CLA	CED-O2D-CGD	2.37	121.53	115.97
29	B	531	LMG	O8-C28-C29	2.37	118.81	111.90
21	C	480	CLA	C2A-C1A-CHA	2.38	128.14	123.92
21	B	525	CLA	C1D-CHD-C4C	2.39	125.75	122.48
26	C	493	DGD	O6E-C5E-C4E	2.39	114.07	109.66
21	B	516	CLA	C1D-CHD-C4C	2.40	125.77	122.48
25	B	530	BCR	C35-C13-C12	2.40	121.92	118.10
25	B	530	BCR	C28-C27-C26	2.40	117.91	113.78
25	B	530	BCR	C30-C25-C24	2.40	122.48	115.73
25	A	369	BCR	C30-C25-C24	2.41	122.50	115.73
21	B	514	CLA	C4A-NA-C1A	2.41	109.44	106.45
21	A	362	CLA	OBD-CAD-C3D	2.42	132.48	128.03
21	B	513	CLA	OBD-CAD-C3D	2.43	132.50	128.03
28	L	213	SQD	O47-C7-C8	2.43	116.60	111.55
21	D	356	CLA	C1-C2-C3	2.43	130.44	125.96
26	C	491	DGD	C3A-C2A-C1A	2.43	122.47	113.58
21	B	518	CLA	OBD-CAD-C3D	2.44	132.52	128.03
25	B	529	BCR	C40-C30-C25	2.44	114.26	110.31
28	L	213	SQD	C45-O47-C7	2.44	123.65	117.88
25	C	490	BCR	C23-C24-C25	2.44	134.09	127.25
29	J	492	LMG	C13-C12-C11	2.44	122.20	113.24
28	D	361	SQD	C31-C30-C29	2.45	132.52	113.42
21	B	511	CLA	C3A-C2A-C1A	2.45	105.00	101.34
32	D	357	PL9	C40-C39-C41	2.45	119.54	115.29
21	B	516	CLA	OBD-CAD-C3D	2.46	132.55	128.03
25	D	358	BCR	C16-C17-C18	2.47	130.84	127.31
21	B	513	CLA	CED-O2D-CGD	2.48	121.77	115.97
21	C	486	CLA	C2A-C1A-CHA	2.48	128.31	123.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	522	CLA	C1-C2-C3	2.48	130.52	125.96
21	D	356	CLA	C1D-CHD-C4C	2.48	125.88	122.48
26	C	491	DGD	O2G-C2G-C3G	2.49	117.48	108.44
21	C	485	CLA	C1-C2-C3	2.49	130.54	125.96
28	C	475	SQD	C15-C14-C13	2.49	127.29	114.45
21	B	518	CLA	C2A-C1A-CHA	2.49	128.34	123.92
21	C	486	CLA	OBD-CAD-C3D	2.49	132.62	128.03
21	B	513	CLA	C1D-CHD-C4C	2.50	125.90	122.48
21	D	354	CLA	C3A-C2A-C1A	2.50	105.09	101.34
25	Z	116	BCR	C15-C14-C13	2.50	130.88	127.31
28	C	475	SQD	C45-O47-C7	2.51	123.80	117.88
25	A	369	BCR	C7-C8-C9	2.51	129.98	126.21
26	C	491	DGD	O6D-C1D-O3G	2.51	115.99	110.02
25	C	489	BCR	C40-C30-C25	2.52	114.40	110.31
21	B	521	CLA	C1D-CHD-C4C	2.53	125.94	122.48
29	J	492	LMG	C39-C38-C37	2.53	127.48	114.45
21	C	486	CLA	O2D-CGD-CBD	2.53	115.82	111.30
21	B	511	CLA	C1C-NC-C4C	2.53	108.51	107.06
26	C	474	DGD	C4D-C3D-C2D	2.54	115.31	110.84
21	B	512	CLA	OBD-CAD-C3D	2.54	132.71	128.03
25	B	529	BCR	C16-C17-C18	2.54	130.94	127.31
21	C	482	CLA	C5-C3-C2	2.55	126.33	121.10
21	B	520	CLA	OBD-CAD-C3D	2.55	132.73	128.03
29	J	492	LMG	C9-O8-C28	2.55	124.81	117.13
21	C	483	CLA	CED-O2D-CGD	2.56	121.96	115.97
21	A	364	CLA	C1D-CHD-C4C	2.56	125.98	122.48
21	A	362	CLA	CED-O2D-CGD	2.56	121.97	115.97
21	B	517	CLA	C11-C12-C13	2.56	124.15	115.73
25	D	358	BCR	C35-C13-C12	2.57	122.19	118.10
29	B	531	LMG	C14-C13-C12	2.57	127.69	114.45
26	B	533	DGD	C4A-C3A-C2A	2.57	122.66	113.24
22	D	355	PHO	C3A-C2A-C1A	2.57	104.71	101.68
26	D	362	DGD	O6E-C1E-O5D	2.57	116.13	110.02
28	L	213	SQD	C31-C30-C29	2.57	133.51	113.42
25	B	527	BCR	C24-C23-C22	2.57	130.08	126.21
21	B	523	CLA	CED-O2D-CGD	2.58	122.02	115.97
25	J	115	BCR	C21-C20-C19	2.59	131.17	123.23
26	A	375	DGD	O1G-C1A-C2A	2.59	119.43	111.90
21	B	511	CLA	C1-C2-C3	2.59	130.73	125.96
30	I	274	LMT	C1-O1'-C1'	2.59	118.32	113.87
22	D	355	PHO	C3A-C4A-CHB	2.59	126.14	121.75
25	B	527	BCR	C36-C18-C19	2.59	122.23	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	511	CLA	CED-O2D-CGD	2.60	122.06	115.97
21	B	526	CLA	C1D-CHD-C4C	2.60	126.03	122.48
21	A	363	CLA	OBD-CAD-C3D	2.60	132.81	128.03
21	D	354	CLA	C4A-NA-C1A	2.60	109.68	106.45
21	A	364	CLA	CED-O2D-CGD	2.60	122.07	115.97
21	A	362	CLA	C2A-C1A-CHA	2.60	128.53	123.92
21	B	518	CLA	C1D-CHD-C4C	2.61	126.05	122.48
22	D	355	PHO	CAB-C3B-C4B	2.62	136.19	126.11
21	C	482	CLA	C1D-CHD-C4C	2.62	126.07	122.48
21	B	515	CLA	CED-O2D-CGD	2.63	122.12	115.97
25	J	112	BCR	C34-C9-C8	2.63	122.28	118.10
21	C	478	CLA	CED-O2D-CGD	2.63	122.13	115.97
21	B	522	CLA	OBD-CAD-C3D	2.63	132.88	128.03
21	C	477	CLA	CBA-CAA-C2A	2.64	121.68	113.80
21	C	488	CLA	CED-O2D-CGD	2.64	122.15	115.97
21	A	364	CLA	C1-C2-C3	2.64	130.82	125.96
27	A	371	LHG	O8-C6-C5	2.64	115.29	108.66
25	C	489	BCR	C1-C6-C7	2.64	123.15	115.73
26	C	492	DGD	O2G-C2G-C3G	2.64	118.04	108.44
28	L	213	SQD	C15-C14-C13	2.65	128.09	114.45
25	J	112	BCR	C35-C13-C12	2.65	122.32	118.10
32	D	357	PL9	C2-C1-C6	2.65	122.27	117.82
25	C	490	BCR	C37-C22-C23	2.65	122.32	118.10
26	B	528	DGD	O1G-C1A-C2A	2.65	119.62	111.90
29	D	359	LMG	C38-C37-C36	2.66	128.16	114.45
21	B	511	CLA	C2A-C1A-CHA	2.66	128.64	123.92
26	A	375	DGD	C1G-O1G-C1A	2.66	125.14	117.13
21	C	478	CLA	C2A-C1A-CHA	2.67	128.65	123.92
21	B	525	CLA	C1-C2-C3	2.67	130.87	125.96
29	A	373	LMG	O8-C28-C29	2.67	119.67	111.90
29	C	494	LMG	C9-C8-C7	2.67	117.88	111.86
21	B	517	CLA	CBA-CAA-C2A	2.67	121.79	113.80
29	D	360	LMG	O8-C28-C29	2.68	119.69	111.90
25	B	530	BCR	C3-C4-C5	2.68	118.39	113.78
21	C	487	CLA	C1D-CHD-C4C	2.68	126.15	122.48
25	A	369	BCR	C37-C22-C23	2.68	122.37	118.10
27	A	371	LHG	O7-C7-C8	2.68	117.12	111.55
21	C	483	CLA	C1D-CHD-C4C	2.69	126.16	122.48
25	J	112	BCR	C8-C7-C6	2.69	134.78	127.25
29	J	492	LMG	O7-C8-C9	2.69	118.21	108.44
21	B	514	CLA	OBD-CAD-C3D	2.70	133.00	128.03
21	B	526	CLA	CED-O2D-CGD	2.70	122.31	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	536	LMT	O1B-C1B-C2B	2.70	114.20	108.11
21	C	480	CLA	OBD-CAD-C3D	2.70	133.01	128.03
21	C	481	CLA	C4A-NA-C1A	2.71	109.82	106.45
21	C	479	CLA	C3A-C2A-C1A	2.72	105.41	101.34
21	B	523	CLA	C1-C2-C3	2.72	130.96	125.96
21	B	520	CLA	C2A-C1A-CHA	2.72	128.74	123.92
21	B	521	CLA	CED-O2D-CGD	2.73	122.36	115.97
25	B	529	BCR	C11-C10-C9	2.73	131.21	127.31
25	C	490	BCR	C30-C25-C24	2.75	123.46	115.73
26	D	362	DGD	O2G-C2G-C1G	2.75	118.44	108.44
21	B	517	CLA	OBD-CAD-C3D	2.75	133.10	128.03
21	B	521	CLA	C2A-C1A-CHA	2.75	128.80	123.92
25	C	490	BCR	C35-C13-C12	2.76	122.50	118.10
21	B	524	CLA	C4A-NA-C1A	2.76	109.88	106.45
23	A	367	MES	O3S-S-C8	2.77	109.46	106.06
21	B	511	CLA	C1D-CHD-C4C	2.78	126.28	122.48
21	B	522	CLA	O2D-CGD-CBD	2.78	116.26	111.30
21	B	514	CLA	C3A-C2A-C1A	2.78	105.50	101.34
21	C	488	CLA	O2D-CGD-CBD	2.79	116.28	111.30
21	C	485	CLA	O2D-CGD-CBD	2.80	116.30	111.30
26	C	492	DGD	O6E-C1E-C2E	2.81	115.71	110.30
25	B	527	BCR	C11-C10-C9	2.81	131.32	127.31
21	B	518	CLA	C5-C3-C2	2.81	126.86	121.10
21	B	519	CLA	CED-O2D-CGD	2.81	122.56	115.97
25	C	489	BCR	C37-C22-C23	2.82	122.59	118.10
25	D	358	BCR	C20-C21-C22	2.82	131.33	127.31
21	C	488	CLA	C2A-C3A-C4A	2.82	106.42	101.87
21	B	513	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	B	529	BCR	C24-C23-C22	2.83	130.46	126.21
22	A	365	PHO	CAB-C3B-C4B	2.83	137.02	126.11
25	C	490	BCR	C15-C14-C13	2.84	131.36	127.31
26	C	474	DGD	C4A-C3A-C2A	2.84	123.66	113.24
21	C	486	CLA	CED-O2D-CGD	2.85	122.64	115.97
25	Z	116	BCR	C32-C1-C6	2.85	114.93	110.31
21	B	517	CLA	O2A-CGA-CBA	2.86	120.22	111.90
21	B	517	CLA	C4A-NA-C1A	2.86	110.00	106.45
21	C	481	CLA	OBD-CAD-C3D	2.86	133.30	128.03
21	A	362	CLA	C1D-CHD-C4C	2.87	126.40	122.48
25	B	529	BCR	C21-C20-C19	2.87	132.02	123.23
26	C	493	DGD	O6E-C1E-C2E	2.87	115.83	110.30
25	D	358	BCR	C37-C22-C23	2.87	122.67	118.10
26	C	491	DGD	O3G-C3G-C2G	2.87	117.81	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	520	CLA	C1-C2-C3	2.87	131.25	125.96
21	B	524	CLA	C3A-C2A-C1A	2.87	105.64	101.34
21	C	477	CLA	CED-O2D-CGD	2.88	122.71	115.97
21	A	363	CLA	C4A-NA-C1A	2.88	110.03	106.45
25	C	490	BCR	C20-C21-C22	2.88	131.42	127.31
21	B	523	CLA	C4A-NA-C1A	2.88	110.03	106.45
21	B	512	CLA	C4A-NA-C1A	2.88	110.03	106.45
30	D	536	LMT	C1-O1'-C1'	2.89	118.82	113.87
25	Z	116	BCR	C2-C1-C6	2.89	115.00	110.48
21	B	523	CLA	C2A-C1A-CHA	2.90	129.05	123.92
21	B	516	CLA	C1-C2-C3	2.90	131.29	125.96
25	B	527	BCR	C23-C24-C25	2.90	135.37	127.25
21	A	363	CLA	C2A-C1A-CHA	2.91	129.07	123.92
21	C	480	CLA	C2A-C3A-C4A	2.91	106.57	101.87
21	A	366	CLA	C1C-NC-C4C	2.92	108.73	107.06
21	B	519	CLA	C1C-NC-C4C	2.92	108.73	107.06
28	C	475	SQD	C32-C31-C30	2.92	129.51	114.45
28	D	361	SQD	O47-C7-C8	2.92	117.62	111.55
21	C	485	CLA	CED-O2D-CGD	2.92	122.83	115.97
25	C	489	BCR	C32-C1-C6	2.94	115.08	110.31
22	A	365	PHO	CBD-CHA-C1A	2.95	133.30	126.36
21	B	519	CLA	C4A-NA-C1A	2.95	110.12	106.45
21	B	523	CLA	C2A-C3A-C4A	2.96	106.64	101.87
21	B	516	CLA	C1C-NC-C4C	2.96	108.76	107.06
21	C	482	CLA	O2D-CGD-CBD	2.97	116.60	111.30
21	B	514	CLA	O2D-CGD-CBD	2.97	116.61	111.30
29	B	531	LMG	C21-C20-C19	2.98	129.81	114.45
22	A	365	PHO	C2A-C3A-C4A	2.99	107.31	101.33
26	C	491	DGD	O6E-C1E-O5D	2.99	117.12	110.02
25	B	529	BCR	C2-C1-C6	3.00	115.16	110.48
26	C	493	DGD	O3G-C3G-C2G	3.00	118.14	110.99
26	C	493	DGD	C3B-C2B-C1B	3.01	124.56	113.58
25	J	112	BCR	C30-C25-C24	3.01	124.18	115.73
25	C	489	BCR	C2-C1-C6	3.01	115.18	110.48
21	K	483	CLA	C2A-C1A-CHA	3.01	129.25	123.92
21	B	522	CLA	C2A-C3A-C4A	3.01	106.73	101.87
33	F	85	HEM	CAD-C3D-C2D	3.02	137.62	129.00
21	B	521	CLA	C4A-NA-C1A	3.02	110.20	106.45
21	B	515	CLA	C4A-NA-C1A	3.02	110.20	106.45
21	C	484	CLA	C2A-C3A-C4A	3.02	106.75	101.87
26	C	492	DGD	C5A-C4A-C3A	3.03	130.04	114.45
21	B	523	CLA	O2D-CGD-CBD	3.03	116.71	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	494	LMG	C7-O1-C1	3.03	119.97	113.76
21	B	521	CLA	C5-C3-C2	3.03	127.30	121.10
21	K	483	CLA	C1C-NC-C4C	3.03	108.80	107.06
21	C	478	CLA	C4A-NA-C1A	3.03	110.21	106.45
21	C	483	CLA	C1-C2-C3	3.03	131.55	125.96
21	C	486	CLA	C4A-NA-C1A	3.04	110.22	106.45
21	B	512	CLA	C3A-C2A-C1A	3.04	105.90	101.34
25	B	527	BCR	C35-C13-C12	3.04	122.95	118.10
30	O	274	LMT	C1-O1'-C1'	3.05	119.09	113.87
21	B	524	CLA	C1-C2-C3	3.05	131.57	125.96
25	D	358	BCR	C8-C7-C6	3.05	135.80	127.25
21	B	523	CLA	C3A-C2A-C1A	3.05	105.91	101.34
28	D	361	SQD	C45-O47-C7	3.06	125.11	117.88
25	B	529	BCR	C23-C24-C25	3.08	135.88	127.25
21	B	516	CLA	CED-O2D-CGD	3.08	123.20	115.97
21	C	487	CLA	C1C-NC-C4C	3.08	108.83	107.06
28	F	224	SQD	C45-O47-C7	3.08	125.16	117.88
22	D	355	PHO	C2A-C3A-C4A	3.09	107.50	101.33
21	B	519	CLA	C2A-C3A-C4A	3.10	106.87	101.87
26	D	362	DGD	O6D-C5D-C4D	3.10	115.36	109.66
25	X	107	BCR	C23-C24-C25	3.10	135.93	127.25
21	B	521	CLA	C6-C5-C3	3.10	119.69	112.66
21	B	520	CLA	C3A-C2A-C1A	3.11	105.99	101.34
21	C	485	CLA	C1C-NC-C4C	3.11	108.84	107.06
21	C	484	CLA	CED-O2D-CGD	3.11	123.26	115.97
21	C	482	CLA	C3A-C2A-C1A	3.11	106.00	101.34
26	A	375	DGD	C3B-C2B-C1B	3.12	124.96	113.58
21	B	522	CLA	C4A-NA-C1A	3.12	110.32	106.45
21	B	514	CLA	CBA-CAA-C2A	3.12	123.13	113.80
23	A	367	MES	O1S-S-C8	3.12	109.48	106.79
21	C	488	CLA	C1D-CHD-C4C	3.13	126.76	122.48
25	J	112	BCR	C24-C23-C22	3.13	130.91	126.21
25	C	490	BCR	C2-C1-C6	3.13	115.37	110.48
21	C	488	CLA	C1-C2-C3	3.13	131.72	125.96
21	B	522	CLA	CED-O2D-CGD	3.13	123.32	115.97
25	B	529	BCR	C8-C7-C6	3.14	136.03	127.25
21	C	486	CLA	C1D-CHD-C4C	3.14	126.77	122.48
21	C	482	CLA	C1C-NC-C4C	3.14	108.86	107.06
21	C	482	CLA	CED-O2D-CGD	3.14	123.33	115.97
23	A	367	MES	O2S-S-C8	3.15	109.50	106.79
21	B	520	CLA	C4A-NA-C1A	3.15	110.36	106.45
21	C	478	CLA	C1C-NC-C4C	3.15	108.87	107.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	484	CLA	C4A-NA-C1A	3.15	110.37	106.45
21	C	478	CLA	CBA-CAA-C2A	3.16	123.26	113.80
25	D	358	BCR	C23-C24-C25	3.16	136.11	127.25
21	B	522	CLA	C2A-C1A-CHA	3.16	129.53	123.92
21	C	483	CLA	C3A-C2A-C1A	3.16	106.08	101.34
21	B	512	CLA	C2A-C3A-C4A	3.17	106.98	101.87
21	C	483	CLA	C2A-C3A-C4A	3.17	106.99	101.87
26	C	474	DGD	O2G-C2G-C1G	3.17	119.96	108.44
21	B	520	CLA	C1C-NC-C4C	3.17	108.88	107.06
21	C	486	CLA	C2A-C3A-C4A	3.17	106.99	101.87
21	C	485	CLA	C2A-C3A-C4A	3.17	107.00	101.87
21	B	521	CLA	C3A-C2A-C1A	3.18	106.09	101.34
21	C	480	CLA	C4A-NA-C1A	3.18	110.39	106.45
21	C	486	CLA	C3A-C2A-C1A	3.18	106.11	101.34
21	B	518	CLA	C11-C10-C8	3.19	126.19	115.73
21	A	362	CLA	C4A-NA-C1A	3.19	110.42	106.45
21	B	519	CLA	C2A-C1A-CHA	3.20	129.59	123.92
25	X	107	BCR	C24-C23-C22	3.20	131.03	126.21
21	A	364	CLA	C4A-NA-C1A	3.21	110.44	106.45
30	I	274	LMT	O1B-C4'-C3'	3.21	114.92	107.19
26	C	493	DGD	O3D-C3D-C2D	3.22	117.35	110.36
29	J	492	LMG	O8-C9-C8	3.22	116.73	108.66
25	C	489	BCR	C35-C13-C12	3.22	123.23	118.10
21	C	484	CLA	C1-C2-C3	3.22	131.89	125.96
21	A	364	CLA	O2D-CGD-CBD	3.23	117.06	111.30
21	C	483	CLA	C1C-NC-C4C	3.23	108.91	107.06
26	C	491	DGD	C3B-C2B-C1B	3.23	125.36	113.58
25	B	530	BCR	C24-C23-C22	3.23	131.06	126.21
25	A	369	BCR	C29-C30-C25	3.23	115.53	110.48
21	D	356	CLA	C3A-C2A-C1A	3.23	106.18	101.34
21	A	366	CLA	C2A-C3A-C4A	3.24	107.10	101.87
21	B	514	CLA	C2A-C3A-C4A	3.24	107.10	101.87
21	C	481	CLA	C2A-C3A-C4A	3.24	107.11	101.87
21	K	483	CLA	C4A-NA-C1A	3.25	110.49	106.45
21	B	519	CLA	O2D-CGD-CBD	3.26	117.12	111.30
26	A	375	DGD	O2G-C2G-C3G	3.26	120.30	108.44
21	C	483	CLA	C4A-NA-C1A	3.26	110.50	106.45
21	C	484	CLA	O2D-CGD-CBD	3.27	117.14	111.30
29	I	220	LMG	O8-C28-C29	3.27	121.42	111.90
21	B	514	CLA	C1C-NC-C4C	3.28	108.94	107.06
21	C	477	CLA	C2A-C3A-C4A	3.28	107.17	101.87
21	A	363	CLA	C2A-C3A-C4A	3.28	107.17	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	356	CLA	C2A-C1A-CHA	3.29	129.75	123.92
25	Z	116	BCR	C16-C17-C18	3.29	132.00	127.31
29	B	531	LMG	O1-C7-C8	3.29	118.81	110.99
21	B	521	CLA	C2A-C3A-C4A	3.29	107.18	101.87
25	X	107	BCR	C35-C13-C12	3.29	123.34	118.10
21	D	354	CLA	C2A-C3A-C4A	3.29	107.19	101.87
21	D	354	CLA	C1D-CHD-C4C	3.29	126.98	122.48
21	A	363	CLA	C3A-C2A-C1A	3.29	106.27	101.34
25	Z	116	BCR	C8-C7-C6	3.30	136.49	127.25
21	B	516	CLA	C2A-C3A-C4A	3.30	107.20	101.87
21	B	525	CLA	C3A-C2A-C1A	3.31	106.30	101.34
21	C	481	CLA	O2D-CGD-CBD	3.31	117.21	111.30
21	K	483	CLA	C2A-C3A-C4A	3.31	107.22	101.87
21	B	515	CLA	C2A-C3A-C4A	3.32	107.23	101.87
21	A	362	CLA	C3A-C2A-C1A	3.32	106.31	101.34
21	B	513	CLA	C4A-NA-C1A	3.32	110.58	106.45
21	B	524	CLA	C2A-C3A-C4A	3.32	107.24	101.87
21	B	511	CLA	C4A-NA-C1A	3.33	110.58	106.45
26	C	492	DGD	O6E-C1E-O5D	3.33	117.92	110.02
21	B	521	CLA	C1C-NC-C4C	3.33	108.97	107.06
21	D	356	CLA	CBA-CAA-C2A	3.33	123.77	113.80
21	C	482	CLA	C2A-C3A-C4A	3.33	107.25	101.87
21	B	521	CLA	O2D-CGD-CBD	3.34	117.27	111.30
21	C	485	CLA	C4A-NA-C1A	3.34	110.60	106.45
21	C	479	CLA	C1C-NC-C4C	3.34	108.98	107.06
21	C	484	CLA	CBA-CAA-C2A	3.34	123.80	113.80
21	A	364	CLA	C2A-C3A-C4A	3.34	107.27	101.87
21	A	364	CLA	C3A-C2A-C1A	3.35	106.35	101.34
25	C	490	BCR	C8-C7-C6	3.35	136.63	127.25
21	B	517	CLA	C1D-CHD-C4C	3.35	127.07	122.48
29	I	220	LMG	O8-C9-C8	3.36	117.09	108.66
25	X	107	BCR	C16-C17-C18	3.36	132.11	127.31
29	B	531	LMG	C16-C15-C14	3.37	131.80	114.45
21	D	356	CLA	C1C-NC-C4C	3.37	108.99	107.06
25	B	529	BCR	C29-C30-C25	3.37	115.75	110.48
21	B	526	CLA	C4A-NA-C1A	3.37	110.64	106.45
27	C	476	LHG	O8-C23-C24	3.37	121.71	111.90
21	B	517	CLA	C2A-C3A-C4A	3.37	107.32	101.87
21	C	483	CLA	C2A-C1A-CHA	3.37	129.90	123.92
25	D	358	BCR	C29-C30-C25	3.38	115.76	110.48
21	B	517	CLA	C2A-C1A-CHA	3.38	129.91	123.92
21	C	478	CLA	C2A-C3A-C4A	3.38	107.33	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	T	226	LMT	C3B-C4B-C5B	3.38	116.18	110.22
29	C	494	LMG	C38-C37-C36	3.39	131.93	114.45
21	B	526	CLA	C2A-C1A-CHA	3.40	129.95	123.92
21	B	513	CLA	O2D-CGD-CBD	3.41	117.39	111.30
25	C	489	BCR	C29-C30-C25	3.42	115.82	110.48
21	B	515	CLA	C3A-C2A-C1A	3.42	106.46	101.34
25	B	530	BCR	C2-C1-C6	3.42	115.82	110.48
21	C	482	CLA	C4A-NA-C1A	3.42	110.70	106.45
21	C	488	CLA	C4A-NA-C1A	3.43	110.70	106.45
21	C	487	CLA	C1-C2-C3	3.43	132.28	125.96
21	C	488	CLA	C2A-C1A-CHA	3.44	130.02	123.92
21	B	519	CLA	C1-C2-C3	3.44	132.30	125.96
21	K	483	CLA	C3A-C2A-C1A	3.44	106.50	101.34
21	C	479	CLA	C2A-C3A-C4A	3.45	107.44	101.87
21	B	526	CLA	C3A-C2A-C1A	3.45	106.51	101.34
32	D	357	PL9	C26-C27-C28	3.45	123.82	111.97
21	C	479	CLA	C4A-NA-C1A	3.46	110.74	106.45
21	D	356	CLA	C2A-C3A-C4A	3.46	107.46	101.87
21	A	366	CLA	C3A-C2A-C1A	3.46	106.53	101.34
21	C	484	CLA	C3A-C2A-C1A	3.46	106.53	101.34
21	B	526	CLA	C2A-C3A-C4A	3.47	107.47	101.87
25	Z	116	BCR	C23-C24-C25	3.47	136.96	127.25
29	C	494	LMG	O7-C8-C7	3.47	121.04	108.44
21	B	512	CLA	O2D-CGD-CBD	3.47	117.50	111.30
21	C	485	CLA	C3A-C2A-C1A	3.47	106.54	101.34
21	B	525	CLA	C2A-C3A-C4A	3.47	107.48	101.87
26	C	493	DGD	C1G-O1G-C1A	3.48	127.59	117.13
21	A	362	CLA	C2A-C3A-C4A	3.48	107.49	101.87
26	A	375	DGD	O6D-C5D-C6D	3.48	113.59	106.64
21	B	524	CLA	C1C-NC-C4C	3.49	109.06	107.06
29	J	492	LMG	C38-C37-C36	3.49	132.44	114.45
26	C	492	DGD	O6D-C5D-C4D	3.49	116.10	109.66
21	B	516	CLA	CBA-CAA-C2A	3.50	124.26	113.80
21	B	517	CLA	C1-C2-C3	3.50	132.40	125.96
21	B	520	CLA	C2A-C3A-C4A	3.50	107.53	101.87
21	A	366	CLA	C4A-NA-C1A	3.52	110.82	106.45
21	B	519	CLA	C3A-C2A-C1A	3.52	106.61	101.34
29	B	531	LMG	C12-C11-C10	3.53	126.46	113.58
29	B	531	LMG	C38-C37-C36	3.53	132.64	114.45
25	J	115	BCR	C29-C30-C25	3.53	116.00	110.48
21	C	478	CLA	C3A-C2A-C1A	3.53	106.63	101.34
29	D	359	LMG	C12-C11-C10	3.54	126.50	113.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	363	LMT	C3B-C4B-C5B	3.54	116.45	110.22
21	B	515	CLA	O2D-CGD-CBD	3.54	117.63	111.30
21	D	356	CLA	C4A-NA-C1A	3.55	110.86	106.45
21	B	522	CLA	C3A-C2A-C1A	3.55	106.65	101.34
21	A	364	CLA	CBA-CAA-C2A	3.55	124.42	113.80
29	J	492	LMG	C8-O7-C10	3.55	126.27	117.88
21	B	513	CLA	C1C-NC-C4C	3.55	109.10	107.06
21	B	516	CLA	C4A-NA-C1A	3.55	110.86	106.45
21	C	479	CLA	CBA-CAA-C2A	3.55	124.43	113.80
25	X	107	BCR	C2-C1-C6	3.57	116.05	110.48
21	C	477	CLA	C4A-NA-C1A	3.57	110.89	106.45
21	C	477	CLA	C1C-NC-C4C	3.57	109.11	107.06
30	D	536	LMT	C3B-C4B-C5B	3.59	116.54	110.22
25	B	527	BCR	C2-C1-C6	3.59	116.09	110.48
25	B	530	BCR	C29-C30-C25	3.59	116.09	110.48
25	B	530	BCR	C23-C24-C25	3.60	137.34	127.25
21	K	483	CLA	C1-C2-C3	3.60	132.59	125.96
21	B	526	CLA	O2D-CGD-CBD	3.60	117.74	111.30
21	B	526	CLA	C1-C2-C3	3.61	132.60	125.96
21	C	486	CLA	C1-C2-C3	3.61	132.61	125.96
28	C	475	SQD	C11-C10-C9	3.62	133.11	114.45
28	D	361	SQD	O48-C23-C24	3.62	122.44	111.90
28	C	475	SQD	C31-C30-C29	3.62	133.12	114.45
32	D	357	PL9	C25-C24-C26	3.62	121.58	115.29
27	C	476	LHG	O7-C7-C8	3.63	119.10	111.55
21	A	363	CLA	C1-C2-C3	3.65	132.67	125.96
21	C	477	CLA	C2A-C1A-CHA	3.65	130.40	123.92
21	B	518	CLA	C2A-C3A-C4A	3.66	107.78	101.87
21	A	366	CLA	C2A-C1A-CHA	3.67	130.42	123.92
25	J	112	BCR	C29-C30-C25	3.67	116.22	110.48
21	B	513	CLA	C3A-C2A-C1A	3.67	106.84	101.34
29	I	220	LMG	C12-C11-C10	3.67	127.00	113.58
28	L	213	SQD	O48-C23-C24	3.68	122.59	111.90
21	B	517	CLA	C3A-C2A-C1A	3.68	106.85	101.34
21	B	523	CLA	C1C-NC-C4C	3.69	109.17	107.06
30	I	274	LMT	C3B-C4B-C5B	3.69	116.72	110.22
30	A	376	LMT	C3B-C4B-C5B	3.70	116.73	110.22
21	B	525	CLA	C4A-NA-C1A	3.70	111.05	106.45
21	B	511	CLA	C2A-C3A-C4A	3.70	107.85	101.87
28	L	213	SQD	C11-C10-C9	3.71	133.57	114.45
25	B	527	BCR	C29-C30-C25	3.72	116.29	110.48
21	B	513	CLA	C2A-C3A-C4A	3.73	107.89	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	478	CLA	O2D-CGD-CBD	3.73	117.96	111.30
30	B	535	LMT	C3B-C4B-C5B	3.73	116.79	110.22
28	F	224	SQD	C44-O6-C1	3.73	121.41	113.76
21	C	487	CLA	C4A-NA-C1A	3.73	111.09	106.45
21	C	487	CLA	O2D-CGD-CBD	3.74	117.99	111.30
21	A	362	CLA	O2D-CGD-CBD	3.76	118.02	111.30
26	C	474	DGD	O6E-C1E-O5D	3.76	118.95	110.02
25	C	489	BCR	C33-C5-C6	3.76	128.72	124.51
25	B	527	BCR	C16-C17-C18	3.77	132.69	127.31
32	D	357	PL9	C35-C34-C36	3.77	121.83	115.29
29	B	531	LMG	C20-C19-C18	3.77	133.89	114.45
21	B	519	CLA	CBA-CAA-C2A	3.78	125.10	113.80
21	C	477	CLA	O2D-CGD-CBD	3.78	118.05	111.30
28	D	361	SQD	C11-C10-C9	3.78	133.93	114.45
30	O	274	LMT	C3B-C4B-C5B	3.78	116.88	110.22
29	I	220	LMG	O7-C8-C7	3.79	122.21	108.44
21	A	364	CLA	C2A-C1A-CHA	3.79	130.64	123.92
21	B	515	CLA	CBA-CAA-C2A	3.80	125.16	113.80
25	D	358	BCR	C2-C1-C6	3.80	116.43	110.48
21	A	366	CLA	O2D-CGD-CBD	3.80	118.10	111.30
27	A	371	LHG	O8-C23-C24	3.81	122.97	111.90
26	D	362	DGD	C2G-O2G-C1B	3.81	126.88	117.88
21	C	481	CLA	C1D-CHD-C4C	3.83	127.72	122.48
26	C	492	DGD	O2G-C2G-C1G	3.84	122.38	108.44
21	C	482	CLA	CBA-CAA-C2A	3.84	125.28	113.80
26	D	362	DGD	O2G-C1B-C2B	3.84	119.53	111.55
21	B	518	CLA	C3A-C2A-C1A	3.85	107.10	101.34
21	B	525	CLA	O2D-CGD-CBD	3.85	118.18	111.30
29	D	360	LMG	O7-C10-C11	3.85	119.55	111.55
22	D	355	PHO	C4D-C3D-CAD	3.86	112.58	105.41
21	B	522	CLA	C1C-NC-C4C	3.87	109.28	107.06
25	C	490	BCR	C29-C30-C25	3.87	116.53	110.48
21	C	485	CLA	C2A-C1A-CHA	3.88	130.80	123.92
26	B	528	DGD	O2G-C1B-C2B	3.89	119.63	111.55
21	C	481	CLA	C3A-C2A-C1A	3.89	107.17	101.34
21	C	480	CLA	C1C-NC-C4C	3.89	109.29	107.06
28	C	475	SQD	C44-O6-C1	3.89	121.75	113.76
29	A	373	LMG	O7-C10-C11	3.90	119.64	111.55
25	J	112	BCR	C23-C24-C25	3.90	138.17	127.25
25	X	107	BCR	C8-C7-C6	3.90	138.18	127.25
21	B	525	CLA	C1C-NC-C4C	3.91	109.30	107.06
32	D	357	PL9	C30-C29-C31	3.92	122.08	115.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	525	CLA	C2A-C1A-CHA	3.92	130.86	123.92
26	D	362	DGD	C3G-C2G-C1G	3.92	120.69	111.86
25	Z	116	BCR	C29-C30-C25	3.93	116.62	110.48
21	B	518	CLA	O2D-CGD-CBD	3.93	118.32	111.30
21	B	526	CLA	C1C-NC-C4C	3.93	109.31	107.06
21	B	518	CLA	C4A-NA-C1A	3.94	111.34	106.45
32	D	357	PL9	C15-C14-C16	3.95	122.13	115.29
21	C	483	CLA	O2D-CGD-CBD	3.96	118.38	111.30
21	C	486	CLA	CBA-CAA-C2A	4.00	125.75	113.80
21	C	480	CLA	C3A-C2A-C1A	4.00	107.33	101.34
21	C	487	CLA	C2A-C3A-C4A	4.00	108.33	101.87
21	D	354	CLA	O2D-CGD-CBD	4.00	118.45	111.30
21	B	516	CLA	C3A-C2A-C1A	4.02	107.35	101.34
21	C	479	CLA	C1-C2-C3	4.03	133.37	125.96
32	D	357	PL9	C20-C19-C21	4.03	122.28	115.29
22	A	365	PHO	O2D-CGD-CBD	4.05	118.53	111.30
22	A	365	PHO	C3A-C2A-C1A	4.05	106.45	101.68
32	D	357	PL9	C3-C4-C5	4.06	124.08	118.63
21	B	518	CLA	C1C-NC-C4C	4.06	109.39	107.06
28	F	224	SQD	C11-C10-C9	4.08	135.49	114.45
26	B	533	DGD	O6E-C1E-O5D	4.08	119.71	110.02
21	B	512	CLA	C1C-NC-C4C	4.09	109.41	107.06
21	D	356	CLA	O2D-CGD-CBD	4.09	118.61	111.30
28	D	361	SQD	C44-O6-C1	4.09	122.15	113.76
26	B	533	DGD	O5D-C1E-C2E	4.09	114.91	108.23
29	B	531	LMG	C18-C17-C16	4.10	135.58	114.45
28	F	224	SQD	O48-C23-C24	4.10	123.83	111.90
21	C	484	CLA	C1C-NC-C4C	4.11	109.42	107.06
21	B	515	CLA	C1C-NC-C4C	4.12	109.42	107.06
22	D	355	PHO	O2D-CGD-CBD	4.12	118.67	111.30
21	B	517	CLA	O2D-CGD-CBD	4.14	118.69	111.30
25	D	358	BCR	C24-C23-C22	4.14	132.43	126.21
21	A	364	CLA	C1C-NC-C4C	4.18	109.46	107.06
28	C	475	SQD	O48-C23-C24	4.19	124.08	111.90
25	X	107	BCR	C29-C30-C25	4.19	117.03	110.48
21	B	513	CLA	C2A-C1A-CHA	4.20	131.35	123.92
25	J	112	BCR	C7-C8-C9	4.20	132.52	126.21
29	D	359	LMG	O7-C8-C7	4.20	123.71	108.44
26	B	533	DGD	O1G-C1A-C2A	4.22	124.19	111.90
30	D	363	LMT	C1-O1'-C1'	4.23	121.13	113.87
26	A	375	DGD	O6D-C1D-O3G	4.23	120.06	110.02
25	J	112	BCR	C11-C10-C9	4.29	133.44	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	480	CLA	O2D-CGD-CBD	4.30	118.98	111.30
21	A	363	CLA	O2D-CGD-CBD	4.32	119.01	111.30
21	C	487	CLA	C2A-C1A-CHA	4.32	131.57	123.92
25	C	490	BCR	C24-C23-C22	4.33	132.72	126.21
22	A	365	PHO	C4D-C3D-CAD	4.34	113.47	105.41
26	C	493	DGD	O6D-C5D-C4D	4.35	117.68	109.66
25	J	115	BCR	C8-C7-C6	4.36	139.45	127.25
29	D	359	LMG	C9-O8-C28	4.37	130.28	117.13
21	B	520	CLA	O2D-CGD-CBD	4.38	119.13	111.30
21	C	477	CLA	C3A-C2A-C1A	4.40	107.93	101.34
25	J	112	BCR	C2-C1-C6	4.41	117.37	110.48
21	B	518	CLA	CBA-CAA-C2A	4.41	127.00	113.80
26	B	533	DGD	O6D-C5D-C6D	4.47	115.56	106.64
21	B	517	CLA	C11-C10-C8	4.48	130.44	115.73
26	C	493	DGD	O6E-C1E-O5D	4.49	120.67	110.02
21	A	363	CLA	CBA-CAA-C2A	4.52	127.31	113.80
30	A	376	LMT	O1B-C1B-C2B	4.54	118.33	108.11
21	B	521	CLA	CBA-CAA-C2A	4.55	127.41	113.80
26	C	474	DGD	C3G-C2G-C1G	4.55	122.12	111.86
25	C	489	BCR	C24-C23-C22	4.56	133.06	126.21
33	F	85	HEM	CAA-CBA-CGA	4.56	120.45	112.66
21	K	483	CLA	O2D-CGD-CBD	4.61	119.54	111.30
29	D	359	LMG	C9-C8-C7	4.62	122.27	111.86
21	B	516	CLA	C2A-C1A-CHA	4.65	132.16	123.92
21	A	363	CLA	C1C-NC-C4C	4.65	109.73	107.06
21	C	488	CLA	C3A-C2A-C1A	4.68	108.35	101.34
25	B	530	BCR	C7-C8-C9	4.69	133.26	126.21
29	B	531	LMG	O7-C8-C7	4.70	125.52	108.44
29	M	217	LMG	C9-O8-C28	4.72	131.33	117.13
25	X	107	BCR	C33-C5-C6	4.77	129.85	124.51
21	B	524	CLA	CBA-CAA-C2A	4.78	128.10	113.80
26	A	375	DGD	O5D-C1E-C2E	4.79	116.05	108.23
21	C	479	CLA	O2D-CGD-CBD	4.89	120.03	111.30
33	V	164	HEM	CBA-CAA-C2A	4.90	121.85	112.48
25	J	112	BCR	C38-C26-C25	4.92	130.02	124.51
25	B	530	BCR	C33-C5-C6	4.93	130.02	124.51
28	L	213	SQD	C44-O6-C1	4.93	123.87	113.76
25	C	490	BCR	C38-C26-C25	4.97	130.07	124.51
25	A	369	BCR	C33-C5-C6	4.99	130.09	124.51
25	J	115	BCR	C23-C24-C25	5.00	141.25	127.25
26	A	375	DGD	C3G-O3G-C1D	5.08	124.17	113.76
26	C	474	DGD	C3G-O3G-C1D	5.08	124.17	113.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	527	BCR	C8-C7-C6	5.10	141.54	127.25
21	B	511	CLA	O2D-CGD-CBD	5.11	120.43	111.30
25	A	369	BCR	C24-C23-C22	5.13	133.92	126.21
29	D	359	LMG	O1-C7-C8	5.13	123.20	110.99
25	Z	116	BCR	C33-C5-C6	5.16	130.28	124.51
25	X	107	BCR	C15-C14-C13	5.17	134.69	127.31
21	B	524	CLA	O2D-CGD-CBD	5.32	120.81	111.30
26	A	375	DGD	O5D-C6D-C5D	5.33	117.87	108.94
25	B	530	BCR	C38-C26-C25	5.41	130.56	124.51
26	D	362	DGD	C1G-O1G-C1A	5.43	133.47	117.13
25	J	115	BCR	C31-C1-C6	5.43	119.12	110.31
21	A	362	CLA	C1C-NC-C4C	5.49	110.21	107.06
25	C	489	BCR	C38-C26-C25	5.57	130.74	124.51
25	C	490	BCR	C33-C5-C6	5.59	130.77	124.51
21	C	480	CLA	CBA-CAA-C2A	5.60	130.57	113.80
28	C	475	SQD	C25-C24-C23	5.61	134.07	113.58
29	C	494	LMG	C9-O8-C28	5.63	134.05	117.13
26	C	492	DGD	O2G-C1B-C2B	5.70	123.39	111.55
21	C	481	CLA	CBA-CAA-C2A	5.83	131.24	113.80
26	D	362	DGD	O6D-C5D-C6D	5.85	118.32	106.64
28	F	224	SQD	O6-C1-C2	5.86	117.79	108.23
25	D	358	BCR	C33-C5-C6	5.88	131.09	124.51
25	Z	116	BCR	C38-C26-C25	5.89	131.10	124.51
28	L	213	SQD	C25-C24-C23	5.95	135.31	113.58
25	B	527	BCR	C33-C5-C6	5.97	131.19	124.51
28	L	213	SQD	C10-C9-C8	6.00	135.21	113.24
26	D	362	DGD	O3G-C3G-C2G	6.01	125.28	110.99
28	F	224	SQD	C25-C24-C23	6.05	135.67	113.58
25	B	527	BCR	C38-C26-C25	6.09	131.33	124.51
32	D	357	PL9	C46-C47-C48	6.11	132.92	111.97
28	C	475	SQD	C10-C9-C8	6.11	135.62	113.24
25	B	529	BCR	C33-C5-C6	6.11	131.35	124.51
25	J	115	BCR	C33-C5-C6	6.11	131.35	124.51
26	C	474	DGD	O6D-C1D-O3G	6.13	124.58	110.02
28	D	361	SQD	C10-C9-C8	6.15	135.77	113.24
28	D	361	SQD	C25-C24-C23	6.16	136.06	113.58
28	F	224	SQD	C10-C9-C8	6.16	135.81	113.24
27	A	371	LHG	C25-C24-C23	6.20	136.21	113.58
25	J	115	BCR	C38-C26-C25	6.24	131.49	124.51
25	B	529	BCR	C38-C26-C25	6.24	131.49	124.51
25	A	369	BCR	C38-C26-C25	6.26	131.52	124.51
25	J	112	BCR	C33-C5-C6	6.36	131.63	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	476	LHG	C25-C24-C23	6.38	136.87	113.58
29	M	217	LMG	O7-C10-C11	6.49	125.03	111.55
28	L	213	SQD	O6-C1-C2	6.53	118.89	108.23
25	D	358	BCR	C38-C26-C25	6.53	131.82	124.51
25	J	115	BCR	C2-C1-C6	6.59	120.79	110.48
28	D	361	SQD	O6-C1-C2	6.68	119.13	108.23
21	B	517	CLA	C1C-NC-C4C	6.73	110.92	107.06
25	X	107	BCR	C38-C26-C25	6.73	132.04	124.51
21	D	354	CLA	C1C-NC-C4C	6.79	110.96	107.06
21	C	488	CLA	C1C-NC-C4C	6.81	110.97	107.06
26	C	491	DGD	C1G-O1G-C1A	6.85	137.74	117.13
28	C	475	SQD	O6-C1-C2	6.86	119.43	108.23
26	C	474	DGD	O2G-C1B-C2B	6.90	125.88	111.55
28	C	475	SQD	C5-C6-S	7.04	124.14	114.34
26	C	474	DGD	O1G-C1A-C2A	7.08	132.49	111.90
29	J	492	LMG	O7-C10-C11	7.14	126.39	111.55
21	C	486	CLA	C1C-NC-C4C	7.17	111.18	107.06
26	C	492	DGD	O6D-C5D-C6D	7.18	120.97	106.64
26	B	533	DGD	O2G-C1B-C2B	7.26	126.63	111.55
26	C	491	DGD	O6D-C5D-C6D	7.46	121.54	106.64
33	V	164	HEM	CMA-C3A-C4A	7.64	140.21	128.46
21	C	481	CLA	C1C-NC-C4C	7.76	111.52	107.06
26	C	493	DGD	C2G-O2G-C1B	7.95	136.66	117.88
28	C	475	SQD	O5-C1-O6	8.17	129.41	110.02
28	D	361	SQD	O5-C1-O6	8.22	129.54	110.02
29	I	220	LMG	C8-O7-C10	8.35	137.60	117.88
26	C	492	DGD	O5D-C6D-C5D	8.43	123.05	108.94
26	C	493	DGD	O6D-C5D-C6D	8.51	123.63	106.64
32	D	357	PL9	C7-C3-C4	8.52	123.80	116.88
33	F	85	HEM	CMA-C3A-C4A	8.56	141.62	128.46
26	C	474	DGD	O6D-C5D-C6D	8.67	123.95	106.64
26	C	474	DGD	O5D-C1E-C2E	8.69	122.41	108.23
26	C	491	DGD	C2G-O2G-C1B	8.78	138.62	117.88
28	D	361	SQD	C5-C6-S	8.79	126.58	114.34
28	F	224	SQD	O5-C1-O6	8.82	130.97	110.02
26	D	362	DGD	O5D-C6D-C5D	8.95	123.92	108.94
26	C	491	DGD	O5D-C6D-C5D	8.97	123.95	108.94
26	A	375	DGD	C2G-O2G-C1B	9.00	139.15	117.88
29	B	531	LMG	C8-O7-C10	9.03	139.20	117.88
28	L	213	SQD	O5-C1-O6	9.15	131.75	110.02
26	C	493	DGD	O5D-C1E-C2E	9.35	123.49	108.23
28	F	224	SQD	C5-C6-S	9.44	127.48	114.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	362	DGD	O5D-C1E-C2E	9.45	123.66	108.23
28	L	213	SQD	C5-C6-S	9.48	127.53	114.34
29	C	494	LMG	C8-O7-C10	9.55	140.44	117.88
29	D	359	LMG	C8-O7-C10	9.78	140.99	117.88
26	C	491	DGD	O5D-C1E-C2E	9.92	124.41	108.23
26	C	492	DGD	O5D-C1E-C2E	10.15	124.80	108.23
26	C	474	DGD	O5D-C6D-C5D	11.22	127.71	108.94
28	F	224	SQD	O7-S-C6	11.36	116.53	106.83
28	L	213	SQD	O7-S-C6	11.49	116.64	106.83
28	C	475	SQD	O7-S-C6	11.70	116.83	106.83
26	C	493	DGD	O5D-C6D-C5D	12.05	129.11	108.94
28	D	361	SQD	O7-S-C6	12.39	117.42	106.83
26	C	474	DGD	O1G-C1G-C2G	14.25	144.47	108.66

All (144) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	479	CLA	C8
21	C	479	CLA	NC
21	C	479	CLA	ND
21	C	479	CLA	NA
21	C	480	CLA	C8
21	C	480	CLA	NC
21	C	480	CLA	ND
21	C	480	CLA	NA
21	A	363	CLA	C8
21	A	363	CLA	NC
21	A	363	CLA	ND
21	A	363	CLA	NA
22	D	355	PHO	C8
21	B	516	CLA	C8
21	B	516	CLA	NC
21	B	516	CLA	ND
21	B	516	CLA	NA
21	B	523	CLA	C8
21	B	523	CLA	NC
21	B	523	CLA	ND
21	B	523	CLA	NA
21	B	526	CLA	C8
21	B	526	CLA	NC
21	B	526	CLA	ND
21	B	526	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	B	511	CLA	C8
21	B	511	CLA	NC
21	B	511	CLA	ND
21	B	511	CLA	NA
22	A	365	PHO	C8
21	B	525	CLA	C8
21	B	525	CLA	NC
21	B	525	CLA	ND
21	B	525	CLA	NA
21	C	485	CLA	C8
21	C	485	CLA	NC
21	C	485	CLA	ND
21	C	485	CLA	NA
21	A	362	CLA	C8
21	A	362	CLA	NC
21	A	362	CLA	ND
21	A	362	CLA	NA
21	B	513	CLA	C8
21	B	513	CLA	NC
21	B	513	CLA	ND
21	B	513	CLA	NA
21	B	519	CLA	C8
21	B	519	CLA	NC
21	B	519	CLA	ND
21	B	519	CLA	NA
21	C	481	CLA	C8
21	C	481	CLA	NC
21	C	481	CLA	ND
21	C	481	CLA	NA
21	B	522	CLA	C8
21	B	522	CLA	NC
21	B	522	CLA	ND
21	B	522	CLA	NA
21	C	483	CLA	C8
21	C	483	CLA	NC
21	C	483	CLA	ND
21	C	483	CLA	NA
21	B	517	CLA	C8
21	B	517	CLA	NC
21	B	517	CLA	ND
21	B	517	CLA	NA
21	D	354	CLA	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	D	354	CLA	NC
21	D	354	CLA	ND
21	D	354	CLA	NA
26	C	493	DGD	C1E
21	A	366	CLA	C8
21	A	366	CLA	NC
21	A	366	CLA	ND
21	A	366	CLA	NA
21	B	515	CLA	C8
21	B	515	CLA	NC
21	B	515	CLA	ND
21	B	515	CLA	NA
21	C	487	CLA	C8
21	C	487	CLA	NC
21	C	487	CLA	ND
21	C	487	CLA	NA
21	C	486	CLA	C8
21	C	486	CLA	NC
21	C	486	CLA	ND
21	C	486	CLA	NA
21	C	478	CLA	C8
21	C	478	CLA	NC
21	C	478	CLA	ND
21	C	478	CLA	NA
21	B	520	CLA	C8
21	B	520	CLA	NC
21	B	520	CLA	ND
21	B	520	CLA	NA
21	K	483	CLA	C8
21	K	483	CLA	NC
21	K	483	CLA	ND
21	K	483	CLA	NA
21	C	488	CLA	C8
21	C	488	CLA	NC
21	C	488	CLA	ND
21	C	488	CLA	NA
21	C	482	CLA	C8
21	C	482	CLA	NC
21	C	482	CLA	ND
21	C	482	CLA	NA
21	D	356	CLA	C8
21	D	356	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	D	356	CLA	ND
21	D	356	CLA	NA
21	B	524	CLA	C8
21	B	524	CLA	NC
21	B	524	CLA	ND
21	B	524	CLA	NA
26	C	492	DGD	C1E
21	B	512	CLA	C8
21	B	512	CLA	NC
21	B	512	CLA	ND
21	B	512	CLA	NA
21	B	514	CLA	C8
21	B	514	CLA	NC
21	B	514	CLA	ND
21	B	514	CLA	NA
21	C	477	CLA	C8
21	C	477	CLA	NC
21	C	477	CLA	ND
21	C	477	CLA	NA
21	A	364	CLA	C8
21	A	364	CLA	NC
21	A	364	CLA	ND
21	A	364	CLA	NA
21	B	518	CLA	C8
21	B	518	CLA	NC
21	B	518	CLA	ND
21	B	518	CLA	NA
21	B	521	CLA	C8
21	B	521	CLA	NC
21	B	521	CLA	ND
21	B	521	CLA	NA
21	C	484	CLA	C8
21	C	484	CLA	NC
21	C	484	CLA	ND
21	C	484	CLA	NA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	D	357	PL9	C29-C28-C27-C26
32	D	357	PL9	C49-C48-C47-C46
28	D	361	SQD	C45-O47-C7-O49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	361	SQD	C45-O47-C7-C8

There are no ring outliers.

76 monomers are involved in 704 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	362	CLA	20	0
21	A	363	CLA	14	0
21	A	364	CLA	6	0
22	A	365	PHO	8	0
21	A	366	CLA	10	0
23	A	367	MES	13	0
25	A	369	BCR	8	0
27	A	371	LHG	7	0
29	A	373	LMG	40	0
26	A	375	DGD	1	0
21	B	511	CLA	6	0
21	B	512	CLA	9	0
21	B	513	CLA	24	0
21	B	514	CLA	10	0
21	B	515	CLA	10	0
21	B	516	CLA	6	0
21	B	517	CLA	20	0
21	B	518	CLA	15	0
21	B	519	CLA	8	0
21	B	520	CLA	7	0
21	B	521	CLA	12	0
21	B	522	CLA	13	0
21	B	523	CLA	7	0
21	B	524	CLA	5	0
21	B	525	CLA	7	0
21	B	526	CLA	6	0
26	B	528	DGD	23	0
25	B	529	BCR	5	0
25	B	530	BCR	2	0
29	B	531	LMG	6	0
26	B	533	DGD	19	0
30	B	535	LMT	2	0
26	C	474	DGD	8	0
28	C	475	SQD	5	0
27	C	476	LHG	5	0
21	C	477	CLA	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	478	CLA	16	0
21	C	479	CLA	18	0
21	C	480	CLA	11	0
21	C	481	CLA	17	0
21	C	482	CLA	6	0
21	C	483	CLA	13	0
21	C	484	CLA	15	0
21	C	485	CLA	5	0
21	C	486	CLA	24	0
21	C	487	CLA	15	0
21	C	488	CLA	7	0
25	C	489	BCR	18	0
25	C	490	BCR	8	0
26	C	491	DGD	17	0
26	C	492	DGD	14	0
26	C	493	DGD	39	0
29	C	494	LMG	6	0
21	D	354	CLA	15	0
22	D	355	PHO	12	0
21	D	356	CLA	5	0
32	D	357	PL9	31	0
25	D	358	BCR	8	0
29	D	359	LMG	6	0
29	D	360	LMG	30	0
28	D	361	SQD	9	0
30	D	363	LMT	2	0
30	D	536	LMT	1	0
33	F	85	HEM	6	0
30	I	274	LMT	2	0
25	J	112	BCR	12	0
25	J	115	BCR	7	0
29	J	492	LMG	4	0
21	K	483	CLA	15	0
28	L	213	SQD	2	0
29	M	217	LMG	3	0
30	O	274	LMT	1	0
30	T	226	LMT	1	0
33	V	164	HEM	5	0
25	X	107	BCR	6	0
25	Z	116	BCR	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.07	20 (5%) 23 16	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.05	14 (2%) 52 38	129, 158, 178, 180	0
3	C	448/461 (97%)	0.04	19 (4%) 37 26	136, 168, 180, 180	0
4	D	340/352 (96%)	0.20	24 (7%) 17 12	126, 154, 179, 180	0
5	E	77/83 (92%)	0.14	2 (2%) 56 42	138, 157, 179, 180	0
6	F	38/44 (86%)	0.20	6 (15%) 2 2	138, 157, 169, 177	0
7	H	65/65 (100%)	0.05	3 (4%) 33 24	139, 164, 177, 180	0
8	I	35/38 (92%)	0.26	5 (14%) 3 3	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.41	0 100 100	141, 155, 169, 171	0
10	K	37/37 (100%)	-0.09	1 (2%) 55 41	156, 166, 179, 180	0
11	L	37/37 (100%)	0.26	3 (8%) 13 10	152, 168, 180, 180	0
12	M	34/36 (94%)	0.73	8 (23%) 1 1	153, 165, 180, 180	0
13	O	243/246 (98%)	0.38	20 (8%) 12 10	143, 174, 180, 180	0
14	T	30/32 (93%)	0.14	2 (6%) 19 13	152, 169, 180, 180	0
15	U	97/104 (93%)	0.17	3 (3%) 49 36	141, 160, 171, 179	0
16	V	137/137 (100%)	0.09	5 (3%) 43 32	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.07	2 (7%) 17 12	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.13	4 (11%) 6 5	144, 156, 174, 178	0
19	Z	62/62 (100%)	0.08	4 (6%) 20 14	166, 178, 180, 180	0
All	All	2597/2714 (95%)	0.10	145 (5%) 25 18	126, 164, 180, 180	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	M	1	MET	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	K	46	ARG	5.2
7	H	2	ALA	4.9
2	B	85	GLY	4.9
8	I	26	GLY	4.8
12	M	2	GLU	4.7
1	A	18	CYS	4.6
4	D	241	GLU	4.5
3	C	135	ARG	4.5
13	O	234	THR	4.3
1	A	230	THR	4.2
3	C	473	ASP	4.2
13	O	113	VAL	4.2
1	A	231	GLU	4.1
11	L	2	GLU	4.0
3	C	27	ASP	4.0
4	D	227	GLU	4.0
12	M	33	GLN	4.0
13	O	51	THR	3.9
3	C	460	ASP	3.9
5	E	84	LYS	3.9
1	A	12	ASN	3.9
13	O	167	ASP	3.8
4	D	65	SER	3.8
16	V	125	ASP	3.7
12	M	32	GLN	3.6
5	E	17	VAL	3.6
1	A	11	ALA	3.6
3	C	101	PRO	3.6
1	A	266	ASN	3.6
4	D	239	GLN	3.5
19	Z	62	VAL	3.5
4	D	76	VAL	3.4
2	B	485	GLU	3.4
6	F	14	PRO	3.4
3	C	142	GLU	3.4
4	D	13	GLY	3.3
13	O	54	GLY	3.3
4	D	79	SER	3.3
12	M	31	SER	3.3
3	C	260	ALA	3.3
18	X	45	LYS	3.3
6	F	12	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	30	THR	3.2
3	C	204	LEU	3.1
3	C	461	ARG	3.1
1	A	15	GLU	3.1
12	M	30	GLU	3.1
4	D	71	CYS	3.1
1	A	232	SER	3.1
11	L	11	GLU	3.0
13	O	271	PRO	3.0
14	T	22	PHE	3.0
3	C	147	PHE	3.0
3	C	203	THR	3.0
3	C	30	SER	3.0
7	H	24	GLY	3.0
15	U	39	LEU	3.0
8	I	34	ARG	2.9
2	B	322	GLY	2.9
18	X	42	GLN	2.9
2	B	84	THR	2.9
3	C	28	GLN	2.9
16	V	103	LYS	2.9
16	V	113	GLU	2.8
4	D	240	ALA	2.8
3	C	463	SER	2.8
1	A	228	THR	2.7
19	Z	27	TYR	2.7
2	B	2	GLY	2.7
4	D	234	ALA	2.7
1	A	253	GLY	2.6
4	D	246	MET	2.6
13	O	155	THR	2.6
13	O	62	GLN	2.6
12	M	3	VAL	2.6
13	O	84	ASN	2.6
4	D	233	ARG	2.6
15	U	38	GLU	2.6
3	C	352	GLY	2.6
2	B	3	LEU	2.6
6	F	42	PHE	2.6
13	O	236	GLU	2.6
19	Z	29	SER	2.5
3	C	228	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	V	135	GLU	2.5
13	O	112	LYS	2.5
13	O	114	ASN	2.5
2	B	338	GLN	2.5
2	B	180	PRO	2.5
4	D	295	SER	2.5
3	C	375	LEU	2.5
17	y	42	ARG	2.5
13	O	173	ASN	2.5
16	V	104	ASN	2.5
1	A	25	ASP	2.4
1	A	243	GLU	2.4
1	A	14	TRP	2.4
12	M	34	LYS	2.4
3	C	100	GLY	2.4
4	D	263	ASN	2.4
13	O	47	THR	2.4
6	F	13	TYR	2.4
6	F	15	ILE	2.4
4	D	235	PHE	2.4
4	D	237	PRO	2.4
8	I	33	LYS	2.3
2	B	350	GLU	2.3
4	D	232	PHE	2.3
14	T	26	PRO	2.3
17	y	45	ASN	2.3
2	B	336	ILE	2.3
4	D	80	THR	2.3
4	D	226	GLY	2.3
13	O	83	LYS	2.3
4	D	225	ASP	2.3
8	I	27	ASP	2.3
18	X	38	ILE	2.3
4	D	172	SER	2.3
11	L	3	PRO	2.3
19	Z	28	ALA	2.3
3	C	106	VAL	2.2
13	O	82	PRO	2.2
15	U	54	LYS	2.2
2	B	78	TRP	2.2
1	A	229	GLU	2.2
18	X	44	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	165	SER	2.2
2	B	484	PRO	2.1
1	A	134	SER	2.1
7	H	15	ASN	2.1
2	B	218	LEU	2.1
6	F	11	VAL	2.1
1	A	227	THR	2.1
13	O	32	THR	2.1
8	I	25	SER	2.1
13	O	31	LEU	2.1
13	O	118	SER	2.1
1	A	19	ASN	2.1
4	D	238	THR	2.0
2	B	116	VAL	2.0
4	D	242	GLU	2.0
1	A	315	ASN	2.0
1	A	250	ALA	2.0
1	A	242	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	BCR	X	107	40/40	0.81	0.55	6.83	154,158,161,163	0
25	BCR	B	529	40/40	0.74	0.53	5.72	166,169,173,174	0
25	BCR	J	115	40/40	0.66	0.72	4.62	171,180,180,180	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	B	526	65/65	0.67	0.51	4.23	167,177,180,180	0
25	BCR	B	527	40/40	0.79	0.71	4.07	161,169,176,178	0
25	BCR	B	530	40/40	0.42	0.85	3.57	173,180,180,180	0
30	LMT	I	274	35/35	0.73	0.64	3.30	170,180,180,180	0
21	CLA	B	511	65/65	0.73	0.55	3.26	148,179,180,180	0
29	LMG	J	492	48/55	0.73	0.51	3.20	155,175,180,180	0
21	CLA	A	363	65/65	0.78	0.43	3.13	154,161,175,177	0
30	LMT	A	376	35/35	0.72	0.46	2.92	162,180,180,180	0
26	DGD	D	362	63/66	0.70	0.54	2.81	177,180,180,180	0
28	SQD	F	224	45/54	0.55	0.79	2.63	152,179,180,180	0
30	LMT	D	363	31/35	0.69	0.72	2.53	170,180,180,180	0
26	DGD	C	474	56/66	0.69	0.43	2.38	158,180,180,180	0
21	CLA	D	354	65/65	0.86	0.37	2.25	135,154,164,168	0
29	LMG	D	360	48/55	0.67	0.51	2.16	140,169,176,177	0
21	CLA	A	366	65/65	0.76	0.39	2.06	152,162,164,166	0
21	CLA	B	518	65/65	0.90	0.33	1.99	150,164,167,169	0
21	CLA	B	522	65/65	0.92	0.29	1.87	134,144,163,165	0
26	DGD	C	493	66/66	0.81	0.34	1.87	159,174,180,180	0
30	LMT	D	536	35/35	0.74	0.37	1.84	168,173,180,180	0
28	SQD	L	213	47/54	0.71	0.61	1.82	155,178,180,180	0
25	BCR	J	112	40/40	0.83	0.31	1.67	157,160,172,173	0
26	DGD	B	528	58/66	0.82	0.36	1.60	126,136,172,173	0
32	PL9	D	357	55/55	0.65	0.44	1.56	146,153,161,162	0
26	DGD	C	492	62/66	0.77	0.36	1.48	153,171,180,180	0
25	BCR	C	490	40/40	0.79	0.49	1.46	164,169,180,180	0
21	CLA	C	484	65/65	0.88	0.29	1.45	168,177,180,180	0
21	CLA	B	524	65/65	0.80	0.53	1.43	157,180,180,180	0
21	CLA	D	356	65/65	0.83	0.34	1.41	149,154,162,164	0
25	BCR	A	369	40/40	0.82	0.40	1.38	164,171,178,178	0
22	PHO	D	355	64/64	0.91	0.39	1.37	140,162,169,171	0
29	LMG	C	494	45/55	0.69	0.59	1.36	168,180,180,180	0
21	CLA	B	520	65/65	0.93	0.38	1.33	150,162,165,167	0
21	CLA	C	477	65/65	0.88	0.30	1.27	163,169,179,180	0
26	DGD	B	533	66/66	0.78	0.35	1.20	166,179,180,180	0
21	CLA	C	478	65/65	0.87	0.33	1.15	153,155,166,170	0
28	SQD	D	361	43/54	0.86	0.30	1.10	160,173,180,180	0
21	CLA	A	362	65/65	0.90	0.28	0.98	149,154,159,163	0
21	CLA	B	515	65/65	0.93	0.32	0.95	142,162,168,170	0
22	PHO	A	365	64/64	0.92	0.29	0.91	143,154,162,164	0
21	CLA	B	525	65/65	0.84	0.37	0.88	148,167,180,180	0
21	CLA	C	483	65/65	0.88	0.37	0.85	164,180,180,180	0
25	BCR	Z	116	40/40	0.79	0.45	0.85	163,165,170,171	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	LMG	M	217	42/55	0.65	0.77	0.79	166,180,180,180	0
21	CLA	C	482	65/65	0.73	0.46	0.74	148,179,180,180	0
25	BCR	D	358	40/40	0.88	0.28	0.70	135,151,162,162	0
29	LMG	D	359	46/55	0.84	0.33	0.68	142,163,180,180	0
21	CLA	K	483	65/65	0.92	0.38	0.64	155,160,174,176	0
29	LMG	A	373	51/55	0.71	0.44	0.63	169,174,180,180	0
21	CLA	B	519	65/65	0.85	0.31	0.60	152,157,158,159	0
26	DGD	C	491	53/66	0.87	0.29	0.58	155,160,166,168	0
21	CLA	C	480	65/65	0.90	0.27	0.56	151,159,180,180	0
21	CLA	B	521	65/65	0.93	0.26	0.54	149,169,175,179	0
25	BCR	C	489	40/40	0.77	0.33	0.53	152,169,171,171	0
21	CLA	C	485	65/65	0.88	0.29	0.52	170,176,178,180	0
21	CLA	B	513	65/65	0.94	0.26	0.52	133,170,171,172	0
28	SQD	C	475	51/54	0.74	0.43	0.51	156,172,180,180	0
21	CLA	A	364	65/65	0.88	0.31	0.48	126,141,175,177	0
29	LMG	B	531	49/55	0.80	0.35	0.47	160,167,175,176	0
21	CLA	B	514	65/65	0.91	0.30	0.45	139,146,168,169	0
21	CLA	B	523	65/65	0.94	0.23	0.37	134,142,169,170	0
33	HEM	F	85	43/43	0.94	0.39	0.36	154,159,162,163	0
21	CLA	C	481	65/65	0.86	0.28	0.28	152,180,180,180	0
21	CLA	B	516	65/65	0.89	0.27	0.23	152,155,180,180	0
21	CLA	C	487	65/65	0.85	0.34	0.22	176,180,180,180	0
27	LHG	A	371	39/49	0.87	0.31	0.21	156,175,179,180	0
33	HEM	V	164	43/43	0.95	0.29	0.14	89,102,122,129	0
21	CLA	B	512	65/65	0.93	0.24	0.11	142,165,172,173	0
21	CLA	C	486	65/65	0.83	0.31	-0.12	143,180,180,180	0
21	CLA	C	488	65/65	0.79	0.34	-0.14	169,176,179,180	0
21	CLA	C	479	65/65	0.89	0.25	-0.29	162,180,180,180	0
21	CLA	B	517	65/65	0.87	0.26	-0.43	144,160,164,167	0
31	BCT	D	353	4/4	0.96	0.27	-0.54	169,170,170,171	0
24	OEC	A	368	5/9	0.89	0.24	-0.73	118,138,151,154	0
23	MES	A	367	12/12	0.93	0.20	-0.92	136,144,152,153	0
20	FE2	A	361	1/1	0.96	0.18	-1.09	160,160,160,160	0
34	CA	O	273	1/1	0.33	0.68	-	180,180,180,180	0
30	LMT	O	274	35/35	0.70	0.39	-	180,180,180,180	0
30	LMT	T	226	35/35	0.65	0.96	-	156,180,180,180	0
27	LHG	C	476	37/49	0.53	0.45	-	143,176,180,180	0
26	DGD	A	375	52/66	0.78	0.64	-	164,180,180,180	0
30	LMT	B	535	35/35	0.77	0.73	-	163,180,180,180	0
34	CA	K	56	1/1	0.81	0.42	-	180,180,180,180	0
34	CA	F	225	1/1	0.88	0.43	-	142,142,142,142	0
29	LMG	I	220	43/55	0.63	0.84	-	158,180,180,180	0

6.5 Other polymers [i](#)

There are no such residues in this entry.