



Full wwPDB X-ray Structure Validation Report

Jun 17, 2014 – 04:54 AM BST

PDB ID : 4V62
Title : Crystal Structure of cyanobacterial Photosystem II
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

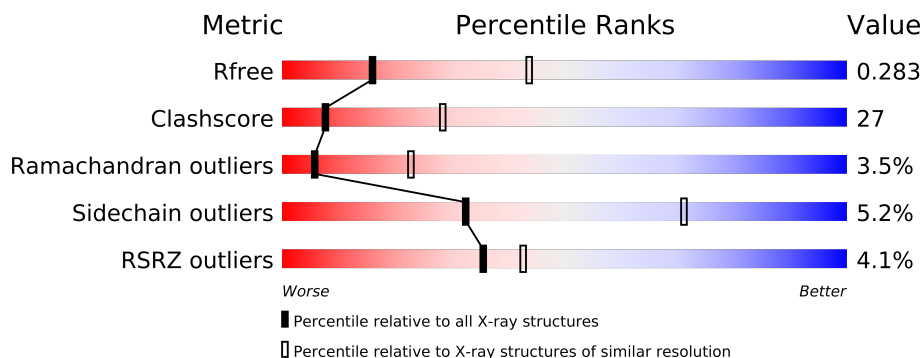
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	344	
1	BA	344	
2	AB	510	
2	BB	510	
3	AC	473	
3	BC	473	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	

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Mol	Chain	Length	Quality of chain
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	50	
18	BX	50	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	AA	406	-	X
22	CLA	AB	601	-	X
22	CLA	AB	604	-	X
22	CLA	AB	614	-	X
22	CLA	AC	504	-	X
22	CLA	AC	507	-	X
22	CLA	AC	512	-	X
22	CLA	AC	513	-	X
22	CLA	AD	404	-	X
22	CLA	BA	405	-	X
22	CLA	BA	407	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	BB	612	-	X
22	CLA	BC	513	-	X
23	PHO	BD	403	-	X
24	PL9	AA	407	-	X
24	PL9	AJ	101	-	X
24	PL9	BA	408	-	X
24	PL9	BJ	101	-	X
26	BCR	AH	101	-	X
26	BCR	AJ	102	-	X
26	BCR	AK	102	-	X
26	BCR	AZ	101	-	X
26	BCR	BB	622	-	X
26	BCR	BC	514	-	X
26	BCR	BJ	102	-	X
26	BCR	BK	102	-	X
26	BCR	BZ	101	-	X
27	DGD	AB	626	-	X
27	DGD	AD	410	-	X
27	DGD	BA	411	-	X
27	DGD	BB	602	-	X
27	DGD	BD	410	-	X
28	LHG	AC	521	-	X
28	LHG	BC	521	-	X
29	SQD	AA	415	-	X
29	SQD	AF	101	-	X
29	SQD	BA	401	-	X
29	SQD	BF	101	-	X
30	LMG	AA	416	-	X
30	LMG	AB	623	-	X
30	LMG	AC	520	-	X
30	LMG	AD	408	-	X
30	LMG	AI	101	-	X
30	LMG	BB	623	-	X
30	LMG	BC	519	-	X
30	LMG	BC	520	-	X
30	LMG	BD	407	-	X
30	LMG	BD	408	-	X
30	LMG	BE	102	-	X
30	LMG	BI	101	-	X
31	CL	AA	414	-	X
31	CL	BA	415	-	X
32	LMT	AB	624	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	LMT	AB	625	-	X
32	LMT	AB	627	-	X
32	LMT	AD	411	-	X
32	LMT	AI	102	-	X
32	LMT	AT	101	-	X
32	LMT	BB	625	-	X
32	LMT	BB	626	-	X
32	LMT	BD	411	-	X
32	LMT	BI	102	-	X
32	LMT	BT	101	-	X
33	BCT	AD	401	-	X
35	CA	BO	301	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50234 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	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	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
AC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
AC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
AC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
AC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
AC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8
BC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
BC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
BC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
BC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
BC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
BC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
BC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	BD	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	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	BH	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	AI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	BI	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	AJ	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	BJ	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	AK	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	BK	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	AL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	BL	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	AM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	BM	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	AO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	BO	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	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AU	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	BU	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	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Protein ycf12.

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

- Molecule 18 is a protein called Photosystem II PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	BX	37	Total	C	N	O	0	0	0
			270	182	41	47			

- Molecule 19 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	BY	28	Total	C	N	O	0	0	0
			140	84	28	28			

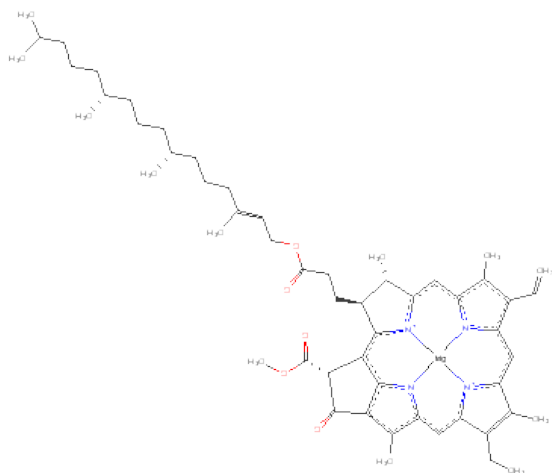
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BA	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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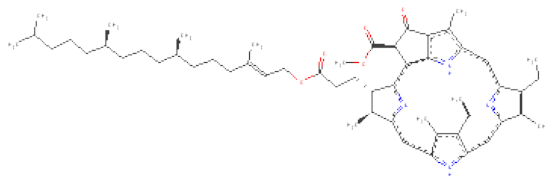
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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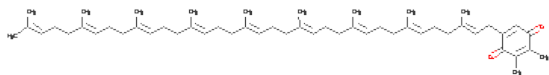
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



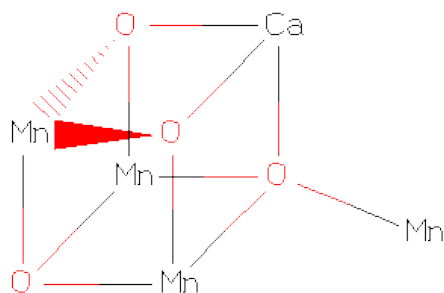
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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: C₅₃H₈₀O₂).



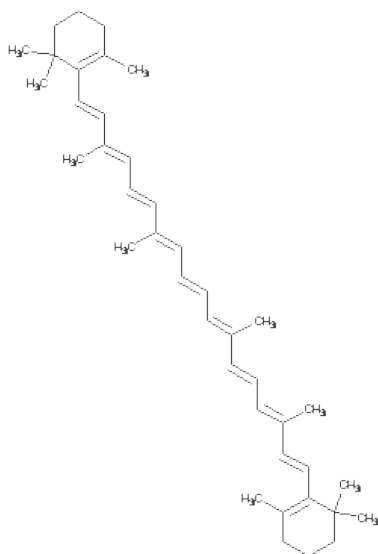
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	AA	1	Total	C	O	0	0
			45	43	2		
24	AD	1	Total	C	O	0	0
			55	53	2		
24	AJ	1	Total	C	O	0	0
			35	33	2		
24	BA	1	Total	C	O	0	0
			45	43	2		
24	BD	1	Total	C	O	0	0
			55	53	2		
24	BJ	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	AA	1	Total	Ca	Mn	0	0
			5	1	4		
25	BA	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	AA	1	Total	C	0	0
			40	40		
26	AB	1	Total	C	0	0
			40	40		

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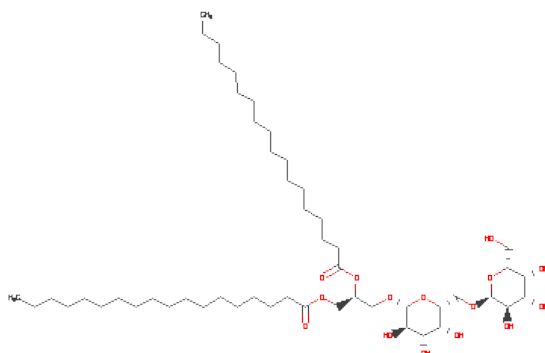
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BD	1	Total C 40 40	0	0
26	BJ	1	Total C 40 40	0	0
26	BK	1	Total C 40 40	0	0
26	BX	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	BZ	1	Total C 40 40	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



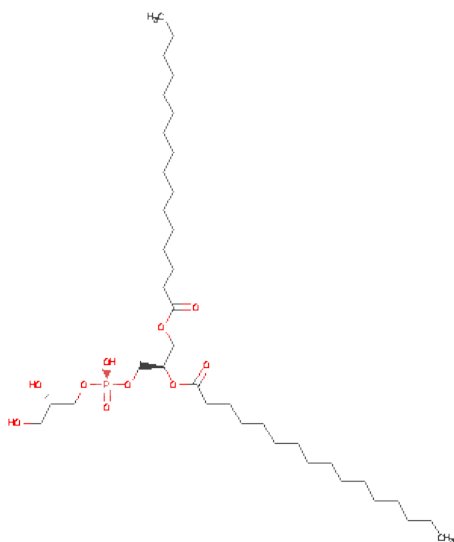
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0
27	AB	1	Total C O 52 37 15	0	0
27	AC	1	Total C O 53 38 15	0	0
27	AC	1	Total C O 62 47 15	0	0
27	AC	1	Total C O 66 51 15	0	0
27	AD	1	Total C O 63 48 15	0	0
27	AH	1	Total C O 58 43 15	0	0
27	BA	1	Total C O 56 41 15	0	0
27	BB	1	Total C O 52 37 15	0	0
27	BC	1	Total C O 53 38 15	0	0

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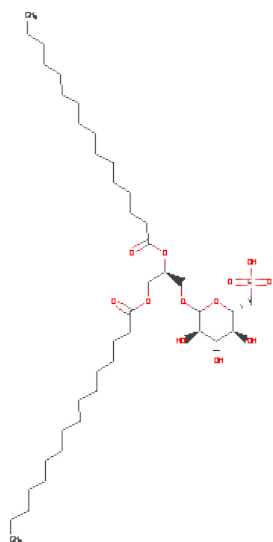
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	BC	1	Total	C	O	0	0
			62	47	15		
27	BC	1	Total	C	O	0	0
			66	51	15		
27	BD	1	Total	C	O	0	0
			63	48	15		
27	BH	1	Total	C	O	0	0
			58	43	15		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



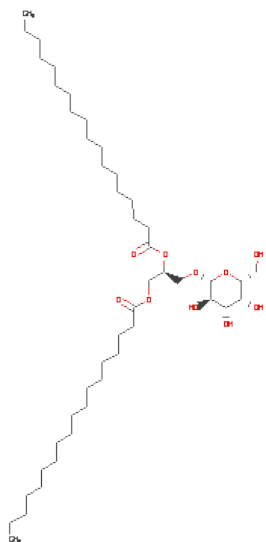
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	AA	1	Total	C	O	P	0	0
			39	28	10	1		
28	AC	1	Total	C	O	P	0	0
			37	26	10	1		
28	BA	1	Total	C	O	P	0	0
			39	28	10	1		
28	BC	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 29 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
29	AA	1	Total	C	O	S	0	0
			51	38	12	1		
29	AA	1	Total	C	O	S	0	0
			54	41	12	1		
29	AD	1	Total	C	O	S	0	0
			43	30	12	1		
29	AF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BA	1	Total	C	O	S	0	0
			54	41	12	1		
29	BA	1	Total	C	O	S	0	0
			51	38	12	1		
29	BB	1	Total	C	O	S	0	0
			47	34	12	1		
29	BD	1	Total	C	O	S	0	0
			43	30	12	1		
29	BF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BL	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	AA	1	Total	C	O	0	0
			51	41	10		
30	AA	1	Total	C	O	0	0
			42	32	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			42	32	10		
30	AC	1	Total	C	O	0	0
			48	38	10		
30	AC	1	Total	C	O	0	0
			45	35	10		
30	AD	1	Total	C	O	0	0
			46	36	10		
30	AD	1	Total	C	O	0	0
			48	38	10		
30	AE	1	Total	C	O	0	0
			44	34	10		
30	AI	1	Total	C	O	0	0
			43	33	10		
30	AM	1	Total	C	O	0	0
			42	32	10		
30	BA	1	Total	C	O	0	0
			51	41	10		
30	BB	1	Total	C	O	0	0
			49	39	10		

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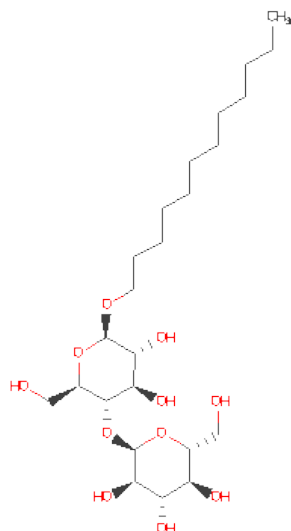
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	BB	1	Total	C	O	0	0
			49	39	10		
30	BC	1	Total	C	O	0	0
			48	38	10		
30	BC	1	Total	C	O	0	0
			45	35	10		
30	BD	1	Total	C	O	0	0
			46	36	10		
30	BD	1	Total	C	O	0	0
			48	38	10		
30	BE	1	Total	C	O	0	0
			44	34	10		
30	BI	1	Total	C	O	0	0
			43	33	10		
30	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

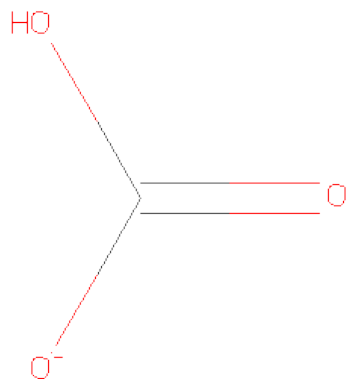
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	AA	1	Total	Cl	0	0
			1	1		
31	BA	1	Total	Cl	0	0
			1	1		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



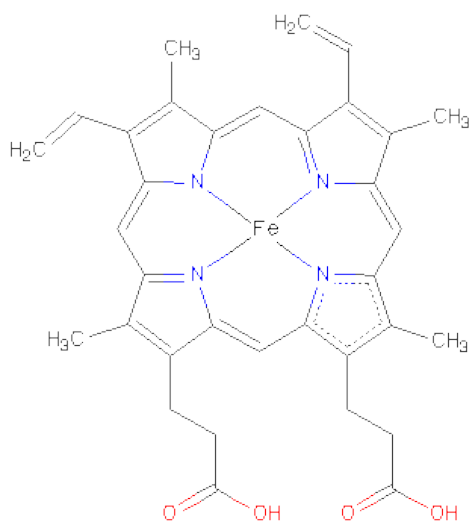
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AD	1	Total C O 31 20 11	0	0
32	AI	1	Total C O 35 24 11	0	0
32	AM	1	Total C O 35 24 11	0	0
32	AT	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BD	1	Total C O 31 20 11	0	0
32	BI	1	Total C O 35 24 11	0	0
32	BM	1	Total C O 35 24 11	0	0
32	BT	1	Total C O 35 24 11	0	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	AD	1	Total	C	O	0	0
			4	1	3		
33	BD	1	Total	C	O	0	0
			4	1	3		

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
34	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	BE	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	BV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

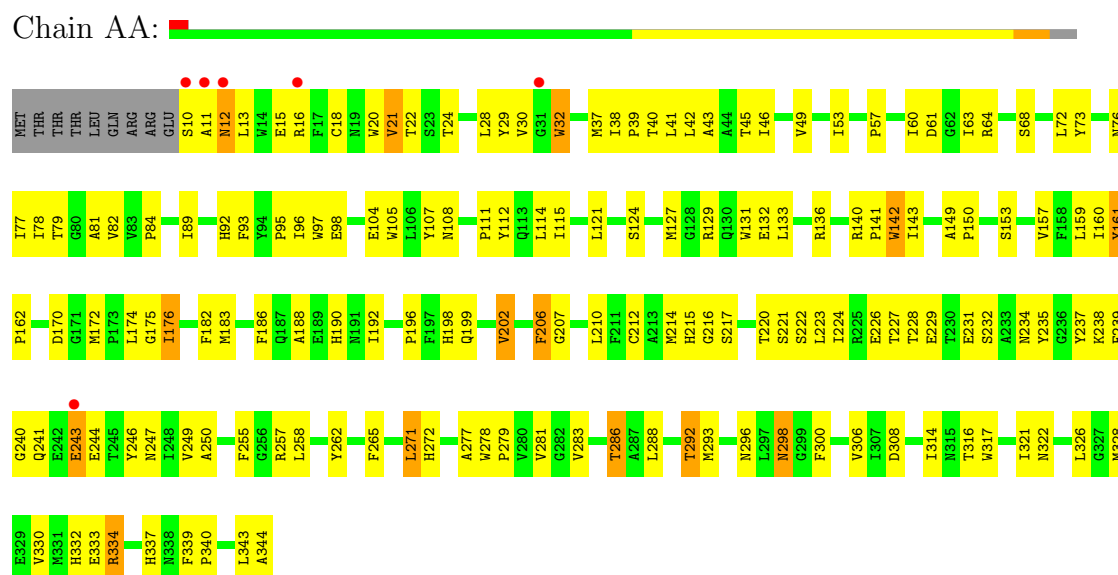
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	AO	1	Total 1	Ca 1	0	0
35	BO	1	Total 1	Ca 1	0	0
35	AK	1	Total 1	Ca 1	0	0
35	BK	1	Total 1	Ca 1	0	0

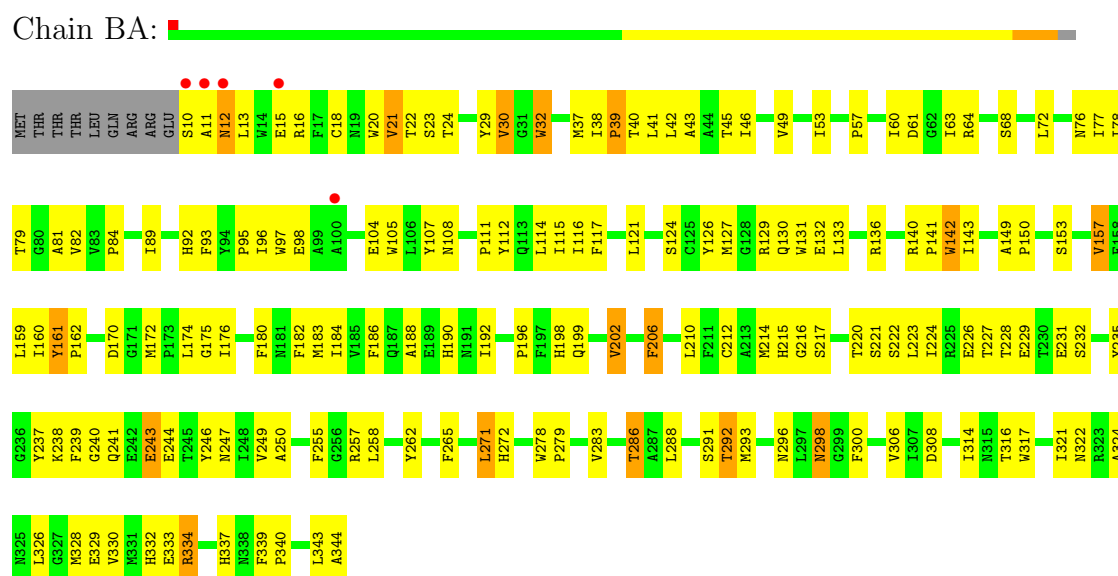
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein

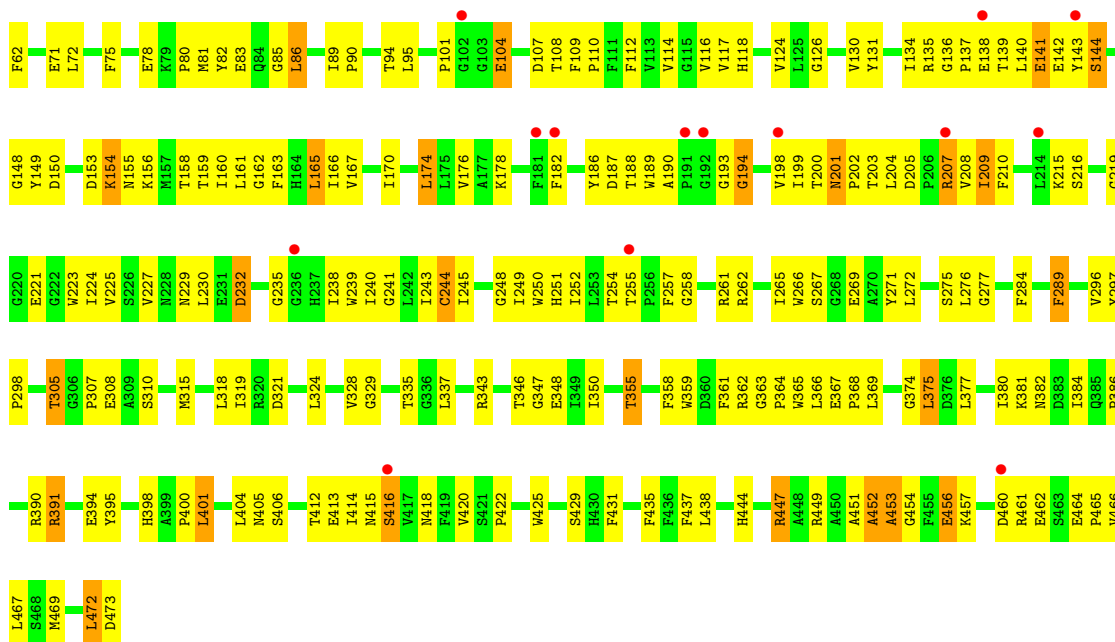


• Molecule 1: Photosystem Q(B) protein



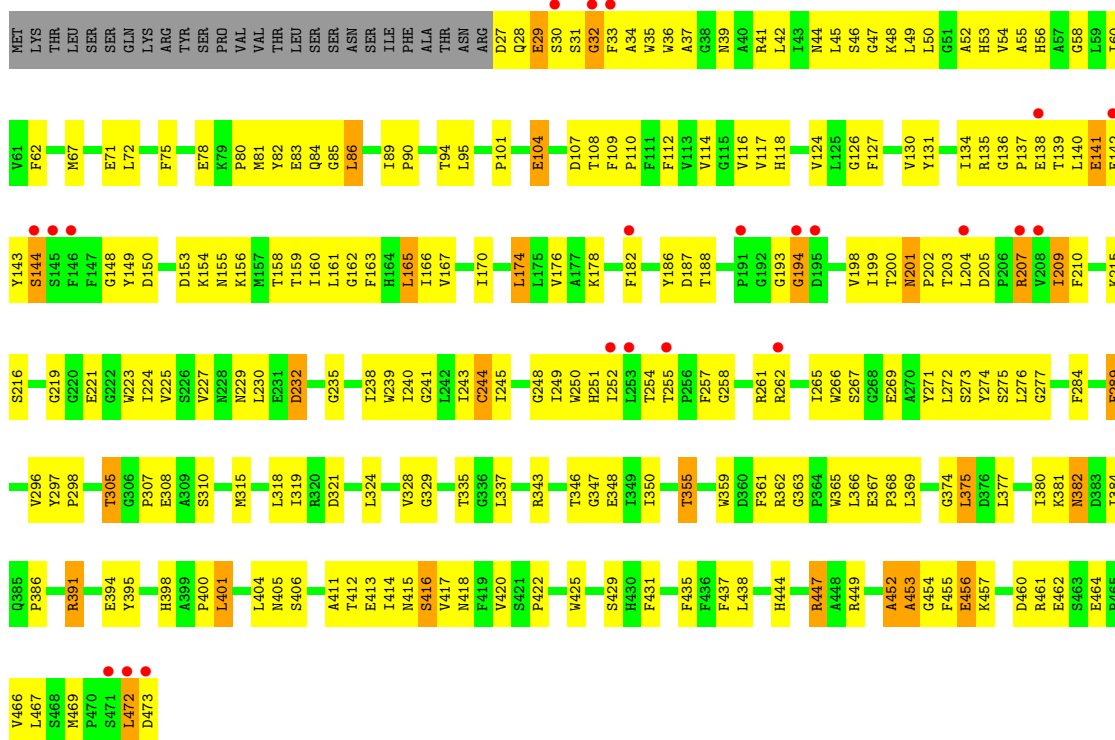
• Molecule 2: Photosystem II core light harvesting protein





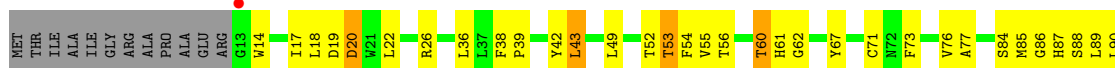
• Molecule 3: Photosystem II CP43 protein

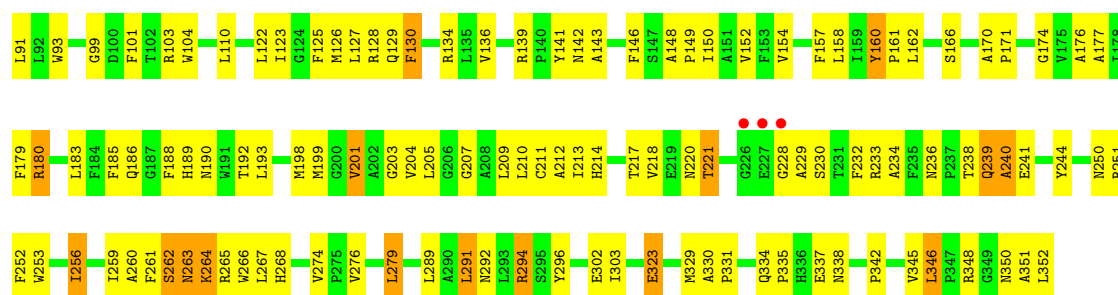
Chain BC:



• Molecule 4: Photosystem II reaction center D2 protein

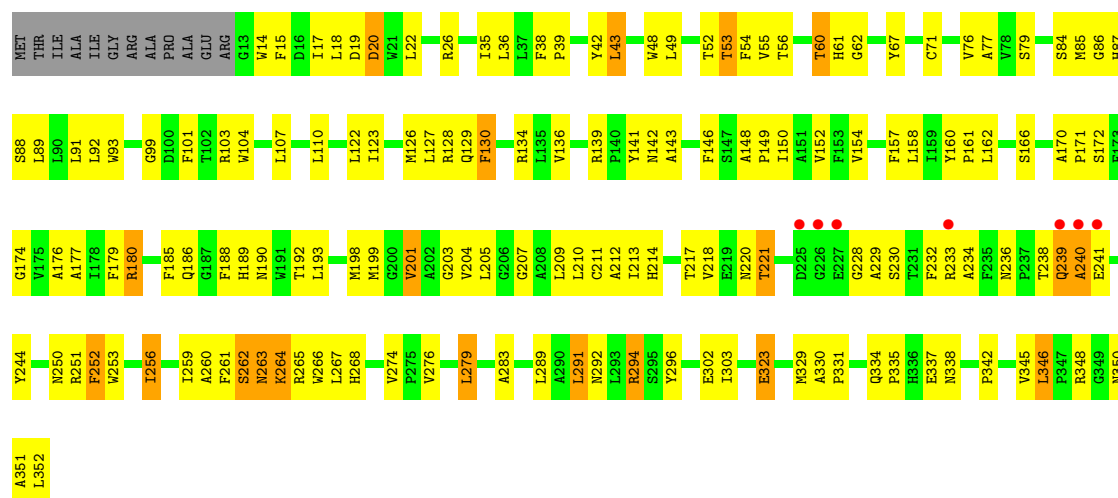
Chain AD:





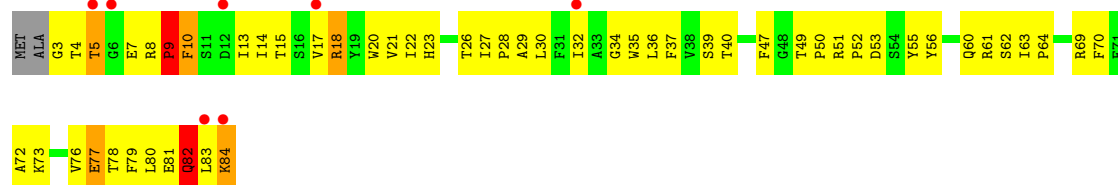
• Molecule 4: Photosystem II reaction center D2 protein

Chain BD:



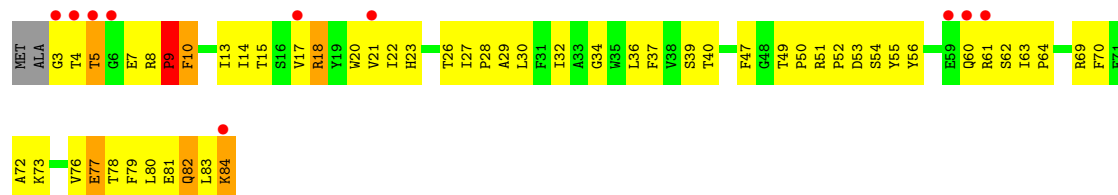
• Molecule 5: Cytochrome b559 subunit alpha

Chain AE:



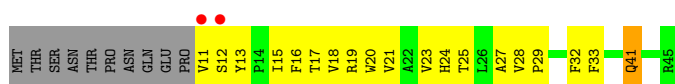
• Molecule 5: Cytochrome b559 subunit alpha

Chain BE:



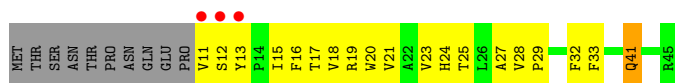
• Molecule 6: Cytochrome b559 subunit beta

Chain AF:



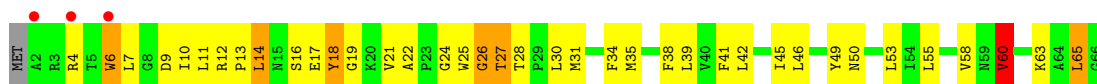
- Molecule 6: Cytochrome b559 subunit beta

Chain BF:



- Molecule 7: Photosystem II reaction center protein H

Chain AH:



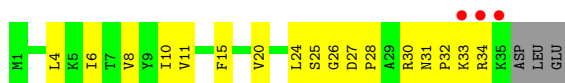
- Molecule 7: Photosystem II reaction center protein H

Chain BH:



- Molecule 8: Photosystem II reaction center protein I

Chain AI:



- Molecule 8: Photosystem II reaction center protein I

Chain BI:



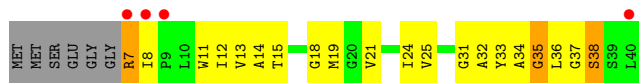
- Molecule 9: Photosystem II reaction center protein J

Chain AJ:



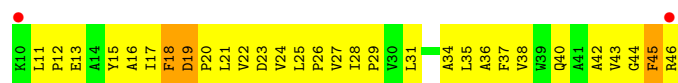
- Molecule 9: Photosystem II reaction center protein J

Chain BJ:



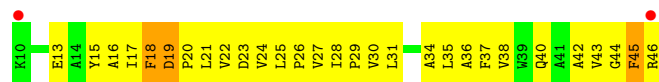
- Molecule 10: Photosystem II reaction center protein K

Chain AK:



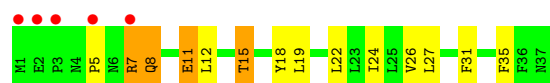
- Molecule 10: Photosystem II reaction center protein K

Chain BK:



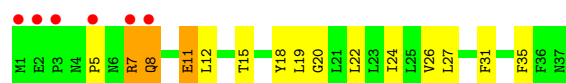
- Molecule 11: Photosystem II reaction center protein L

Chain AL:



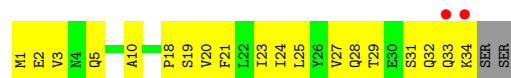
- Molecule 11: Photosystem II reaction center protein L

Chain BL:



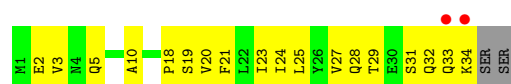
- Molecule 12: Photosystem II reaction center protein M

Chain AM:



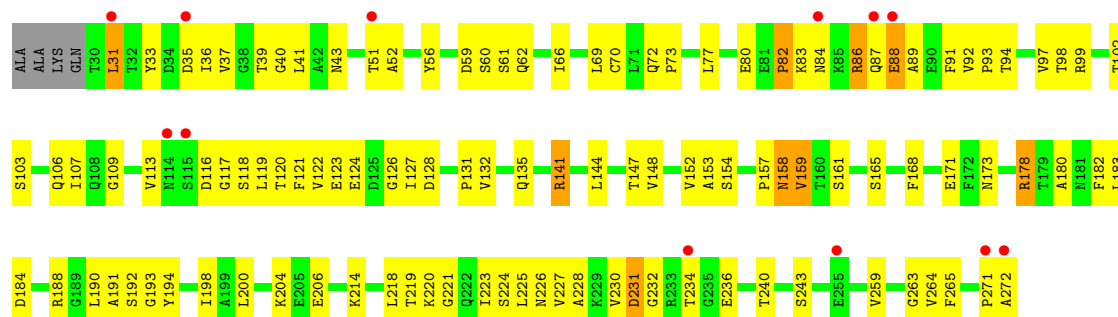
- Molecule 12: Photosystem II reaction center protein M

Chain BM:

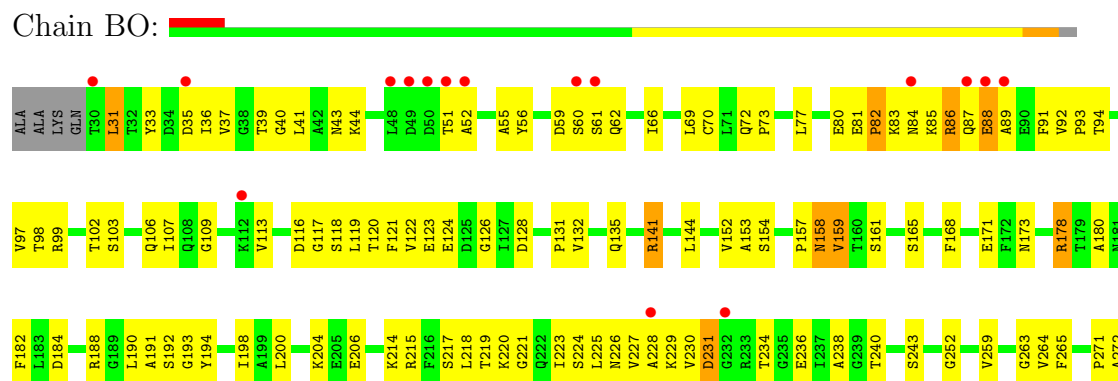


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



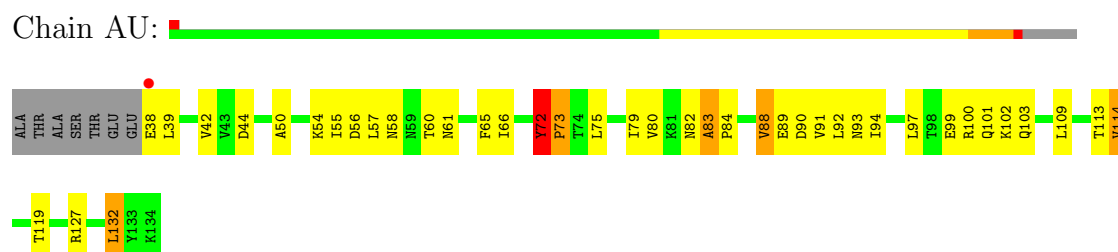
- Molecule 14: Photosystem II reaction center protein T



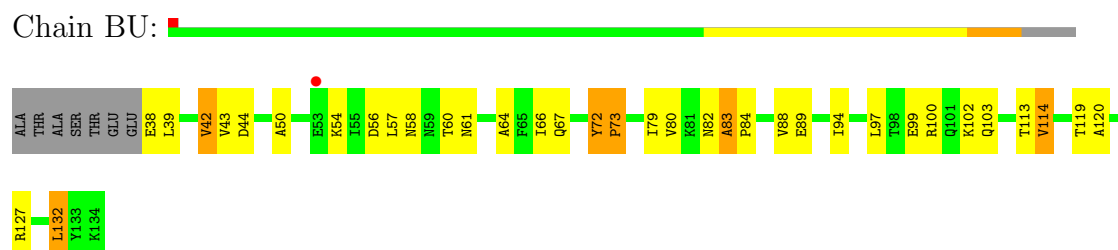
- Molecule 14: Photosystem II reaction center protein T



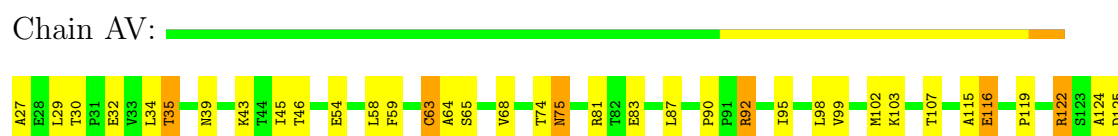
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550





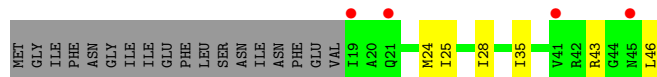
• Molecule 16: Cytochrome c-550

Chain BV:



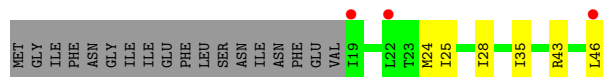
• Molecule 17: Protein ycf12

Chain Ay:



• Molecule 17: Protein ycf12

Chain By:



• Molecule 18: Photosystem II PsbX protein

Chain AX:



• Molecule 18: Photosystem II PsbX protein

Chain BX:



• Molecule 19: Photosystem II protein Y

Chain AY:



• Molecule 19: Photosystem II protein Y

Chain BY:



- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:

- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 99.3 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292 0.250 , 0.283	Depositor DCC
R_{free} test set	3869 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 193457 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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	AA	0.44	0/2713	0.66	0/3700
1	BA	0.43	0/2713	0.65	0/3700
2	AB	0.44	0/3986	0.67	3/5433 (0.1%)
2	BB	0.43	0/3986	0.66	3/5433 (0.1%)
3	AC	0.41	0/3556	0.64	1/4842 (0.0%)
3	BC	0.39	0/3556	0.63	1/4842 (0.0%)
4	AD	0.47	0/2801	0.65	0/3818
4	BD	0.45	0/2801	0.65	0/3818
5	AE	0.45	0/685	0.71	0/933
5	BE	0.45	0/685	0.70	0/933
6	AF	0.45	0/291	0.59	0/397
6	BF	0.47	0/291	0.57	0/397
7	AH	0.42	0/520	0.73	1/709 (0.1%)
7	BH	0.40	0/520	0.72	1/709 (0.1%)
8	AI	0.51	0/293	0.68	0/395
8	BI	0.50	0/293	0.67	0/395
9	AJ	0.43	0/255	0.69	0/346
9	BJ	0.45	0/255	0.66	0/346
10	AK	0.43	0/303	0.63	0/416
10	BK	0.44	0/303	0.61	0/416
11	AL	0.39	0/311	0.65	0/422
11	BL	0.41	0/311	0.65	0/422
12	AM	0.44	0/270	0.70	0/367
12	BM	0.45	0/270	0.67	0/367
13	AO	0.44	0/1876	0.70	0/2548
13	BO	0.43	0/1876	0.70	0/2548
14	AT	0.50	0/284	0.62	0/381
14	BT	0.48	0/284	0.62	0/381
15	AU	0.42	0/785	0.73	1/1064 (0.1%)
15	BU	0.40	0/785	0.73	0/1064
16	AV	0.38	0/1081	0.65	0/1468
16	BV	0.37	0/1081	0.64	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ay	0.46	0/202	0.73	0/272
17	By	0.41	0/202	0.74	0/272
18	AX	0.43	0/273	0.63	0/370
18	BX	0.41	0/273	0.63	0/370
20	AZ	0.45	0/490	0.69	0/669
20	BZ	0.47	0/490	0.70	0/669
All	All	0.43	0/41950	0.66	11/57100 (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	AA	0	1
1	BA	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	486	LEU	CA-CB-CG	7.12	131.67	115.30
2	AB	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	AB	488	PRO	N-CA-C	5.86	127.33	112.10
2	AB	489	GLU	N-CA-C	5.76	126.56	111.00
7	AH	65	LEU	CA-CB-CG	5.72	128.45	115.30
7	BH	65	LEU	CA-CB-CG	5.72	128.45	115.30
2	BB	488	PRO	N-CA-C	5.71	126.94	112.10
2	BB	489	GLU	N-CA-C	5.65	126.25	111.00
3	AC	32	GLY	N-CA-C	-5.54	99.24	113.10
3	BC	32	GLY	N-CA-C	-5.09	100.37	113.10
15	AU	72	TYR	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	161	TYR	Sidechain
1	BA	161	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2628	0	2524	179	0
1	BA	2628	0	2524	179	0
2	AB	3850	0	3718	224	0
2	BB	3850	0	3718	227	0
3	AC	3444	0	3365	258	0
3	BC	3444	0	3365	263	0
4	AD	2706	0	2608	177	0
4	BD	2706	0	2608	184	0
5	AE	666	0	651	71	0
5	BE	666	0	651	74	0
6	AF	282	0	291	28	0
6	BF	282	0	291	29	0
7	AH	507	0	521	52	0
7	BH	507	0	521	50	0
8	AI	286	0	308	15	0
8	BI	286	0	308	18	0
9	AJ	249	0	262	28	0
9	BJ	249	0	262	26	0
10	AK	293	0	305	42	0
10	BK	293	0	305	44	0
11	AL	304	0	316	15	0
11	BL	304	0	316	17	0
12	AM	267	0	289	27	0
12	BM	267	0	289	26	0
13	AO	1845	0	1801	115	0
13	BO	1845	0	1801	118	0
14	AT	275	0	288	21	0
14	BT	275	0	288	20	0
15	AU	774	0	773	46	0
15	BU	774	0	773	42	0
16	AV	1060	0	1068	42	0
16	BV	1060	0	1068	39	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	BX	270	0	299	25	0
19	AY	140	0	32	4	0
19	BY	140	0	32	6	0
20	AZ	479	0	516	54	0
20	BZ	479	0	516	55	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0
22	AA	260	0	288	18	0
22	AB	1040	0	1152	77	0
22	AC	845	0	936	61	0
22	AD	130	0	144	11	0
22	BA	260	0	288	18	0
22	BB	1040	0	1152	83	0
22	BC	845	0	936	62	0
22	BD	130	0	144	12	0
23	AA	64	0	74	5	0
23	AD	64	0	74	2	0
23	BA	64	0	74	5	0
23	BD	64	0	74	5	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	10	0
26	AC	80	0	112	15	0
26	AD	40	0	56	3	0
26	AH	40	0	56	5	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	8	0
26	AZ	40	0	56	5	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	17	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BX	40	0	56	6	0
26	BZ	40	0	56	5	0
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	21	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	6	0
32	AD	31	0	35	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0
32	AT	35	0	46	3	0
32	BB	105	0	138	5	0
32	BD	31	0	35	1	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2715	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (2715) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:AV:63:CYS:SG	34:AV:201:HEM:HAB	1.85	1.16
15:BU:83:ALA:HB1	15:BU:84:PRO:HD2	1.23	1.16
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.23	1.16
16:BV:63:CYS:SG	34:BV:201:HEM:HAB	1.85	1.15
9:BJ:15:THR:HG21	10:BK:38:VAL:HG13	1.24	1.13
2:BB:68:ARG:HH22	22:BB:607:CLA:HED1	1.13	1.11
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.22	1.09
2:AB:68:ARG:HH22	22:AB:604:CLA:HED1	1.12	1.07
1:AA:129:ARG:HH21	4:AD:256:ILE:HD12	1.19	1.06
2:BB:121:GLU:HG2	7:BH:4:ARG:HG2	1.36	1.05
2:AB:121:GLU:HG2	7:AH:4:ARG:HG2	1.36	1.04
13:BO:178:ARG:HG3	13:BO:178:ARG:HH11	1.17	1.04
13:AO:178:ARG:HG3	13:AO:178:ARG:HH11	1.18	1.04
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.37	1.03
3:BC:254:THR:HG22	3:BC:255:THR:H	1.23	1.03
3:AC:254:THR:HG22	3:AC:255:THR:H	1.18	1.03
1:BA:317:TRP:CZ3	4:BD:180:ARG:HD3	1.96	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:129:ARG:HH21	4:BD:256:ILE:HD12	1.20	1.00
13:BO:82:PRO:HG3	13:BO:89:ALA:HB2	1.40	1.00
2:AB:149:LEU:HG	22:AB:603:CLA:HBC1	1.44	1.00
1:AA:317:TRP:CZ3	4:AD:180:ARG:HD3	1.95	0.99
12:AM:33:GLN:HB3	12:BM:33:GLN:HB3	1.43	0.97
4:AD:26:ARG:HD3	6:AF:18:VAL:HG11	1.47	0.97
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.30	0.97
2:BB:149:LEU:HG	22:BB:606:CLA:HBC1	1.45	0.96
13:BO:230:VAL:HG12	13:BO:231:ASP:H	1.32	0.94
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.49	0.94
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	1.98	0.93
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.33	0.92
4:BD:26:ARG:HD3	6:BF:18:VAL:HG11	1.48	0.92
2:BB:271:THR:HG22	2:BB:273:TYR:H	1.35	0.92
15:BU:83:ALA:HB1	15:BU:84:PRO:CD	2.00	0.91
13:BO:69:LEU:HB3	13:BO:107:ILE:HB	1.51	0.91
2:BB:414:PRO:HB2	2:BB:415:PRO:HD3	1.53	0.90
14:BT:29:ILE:H	14:BT:29:ILE:HD12	1.34	0.90
2:BB:68:ARG:NH2	22:BB:607:CLA:HED1	1.87	0.90
13:BO:178:ARG:CG	13:BO:178:ARG:HH11	1.84	0.90
3:BC:473:ASP:HB2	14:BT:26:PRO:HB3	1.54	0.90
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.53	0.89
1:AA:72:LEU:HD13	30:AA:416:LMG:H111	1.55	0.89
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.37	0.89
22:BB:611:CLA:HMD1	22:BB:613:CLA:HAB	1.53	0.89
22:AD:404:CLA:H42	18:AX:26:GLY:HA3	1.53	0.89
13:BO:69:LEU:HD12	13:BO:70:CYS:H	1.37	0.88
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.73	0.88
22:BD:404:CLA:H42	18:BX:26:GLY:HA3	1.56	0.88
2:AB:68:ARG:NH2	22:AB:604:CLA:HED1	1.88	0.88
13:AO:178:ARG:HH11	13:AO:178:ARG:CG	1.88	0.87
5:BE:18:ARG:HD2	5:BE:22:ILE:HD11	1.55	0.87
7:BH:12:ARG:HD3	7:BH:12:ARG:O	1.74	0.87
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.57	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.55	0.87
22:AB:608:CLA:HMD1	22:AB:610:CLA:HAB	1.55	0.86
22:AB:608:CLA:HAB	4:AD:123:ILE:HG23	1.58	0.86
11:BL:5:PRO:HA	11:BL:7:ARG:HH22	1.38	0.86
2:AB:271:THR:HG22	2:AB:273:TYR:H	1.39	0.86
3:AC:305:THR:HG22	3:AC:308:GLU:H	1.40	0.86
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	1.92	0.85
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.39	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:317:TRP:HZ3	4:BD:180:ARG:HD3	1.36	0.85
3:BC:155:ASN:HD21	3:BC:255:THR:HB	1.39	0.85
3:AC:447:ARG:HH11	3:AC:447:ARG:HG2	1.40	0.85
18:AX:12:ILE:HG12	18:AX:16:LEU:HD12	1.56	0.85
3:BC:224:ILE:O	3:BC:227:VAL:HG23	1.76	0.85
7:AH:12:ARG:O	7:AH:12:ARG:HD3	1.76	0.84
34:BE:101:HEM:HBC2	6:BF:27:ALA:HB1	1.58	0.84
11:BL:8:GLN:N	11:BL:8:GLN:HE21	1.74	0.84
2:BB:120:LEU:HD13	22:BB:619:CLA:HMD2	1.60	0.84
34:AE:101:HEM:HBC2	6:AF:27:ALA:HB1	1.59	0.84
3:BC:447:ARG:HH11	3:BC:447:ARG:HG2	1.40	0.84
5:AE:18:ARG:HD2	5:AE:22:ILE:HD11	1.60	0.84
11:AL:5:PRO:HA	11:AL:7:ARG:HH22	1.39	0.84
3:BC:39:ASN:HB2	22:BC:508:CLA:HBA1	1.57	0.84
3:BC:305:THR:HG23	3:BC:307:PRO:HD2	1.59	0.84
3:BC:449:ARG:HE	22:BC:505:CLA:HED1	1.42	0.84
3:AC:155:ASN:HD21	3:AC:255:THR:HB	1.40	0.84
22:BB:611:CLA:HAB	4:BD:123:ILE:HG23	1.60	0.84
3:AC:305:THR:HG23	3:AC:307:PRO:HD2	1.60	0.84
3:BC:305:THR:HG22	3:BC:308:GLU:H	1.40	0.84
15:BU:72:TYR:HB3	15:BU:73:PRO:HD3	1.59	0.83
4:BD:148:ALA:HB3	4:BD:149:PRO:HD3	1.60	0.83
20:BZ:36:SER:HA	20:BZ:39:LEU:HG	1.60	0.83
11:AL:8:GLN:HE21	11:AL:8:GLN:N	1.75	0.83
3:AC:39:ASN:HB2	22:AC:508:CLA:HBA1	1.58	0.83
22:BA:403:CLA:H152	23:BA:406:PHO:H51	1.60	0.83
3:BC:166:ILE:HG23	3:BC:245:ILE:HG23	1.60	0.83
3:AC:449:ARG:HE	22:AC:505:CLA:HED1	1.43	0.83
2:BB:68:ARG:HH22	22:BB:607:CLA:CED	1.91	0.83
2:AB:68:ARG:HH22	22:AB:604:CLA:CED	1.92	0.83
2:BB:124:ARG:HE	2:BB:131:PRO:HD3	1.42	0.83
1:BA:41:LEU:HD13	23:BA:406:PHO:H2	1.61	0.82
18:BX:12:ILE:HG12	18:BX:16:LEU:HD12	1.61	0.82
2:AB:124:ARG:HE	2:AB:131:PRO:HD3	1.43	0.82
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.61	0.81
2:BB:489:GLU:HB2	5:BE:3:GLY:N	1.95	0.81
4:BD:129:GLN:NE2	4:BD:143:ALA:HA	1.97	0.80
2:AB:489:GLU:HB2	5:AE:3:GLY:N	1.96	0.80
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.46	0.80
22:AA:402:CLA:H152	23:AA:405:PHO:H51	1.63	0.80
26:AD:406:BCR:H403	9:AJ:25:VAL:HG21	1.64	0.80
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:41:LEU:HD13	23:AA:405:PHO:H2	1.62	0.79
3:AC:254:THR:HG22	3:AC:255:THR:N	1.96	0.79
1:BA:258:LEU:HD12	4:BD:128:ARG:HD3	1.65	0.79
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.63	0.79
13:AO:230:VAL:HG12	13:AO:231:ASP:N	1.98	0.79
13:BO:218:LEU:HD22	15:BU:119:THR:HG21	1.65	0.79
2:AB:348:ASN:HB3	2:AB:354:LEU:HD21	1.65	0.78
2:AB:187:PRO:HB3	22:AB:601:CLA:HMB2	1.65	0.78
2:AB:24:LEU:HD21	22:AB:616:CLA:HAB	1.65	0.78
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.49	0.78
5:AE:84:LYS:HB2	5:AE:84:LYS:NZ	1.97	0.78
4:BD:60:THR:HG23	4:BD:61:HIS:CD2	2.18	0.78
2:AB:271:THR:HG22	2:AB:273:TYR:N	1.98	0.78
13:BO:83:LYS:HG2	13:BO:84:ASN:H	1.47	0.78
13:BO:31:LEU:HB2	13:BO:36:ILE:HD11	1.66	0.78
1:BA:12:ASN:HD22	1:BA:15:GLU:HB2	1.49	0.78
2:AB:120:LEU:HD13	22:AB:616:CLA:HMD2	1.64	0.78
2:BB:271:THR:HG22	2:BB:273:TYR:N	1.98	0.78
11:BL:5:PRO:HA	11:BL:7:ARG:NH2	1.99	0.78
24:BA:408:PL9:H33	4:BD:38:PHE:HD1	1.47	0.77
1:BA:192:ILE:HA	1:BA:293:MET:HE3	1.67	0.77
2:BB:124:ARG:HH11	2:BB:124:ARG:HG3	1.49	0.77
26:BD:406:BCR:H403	9:BJ:25:VAL:HG21	1.64	0.77
2:BB:187:PRO:HB3	22:BB:604:CLA:HMB2	1.65	0.77
24:AA:407:PL9:H33	4:AD:38:PHE:HD1	1.48	0.77
2:BB:24:LEU:HD21	22:BB:619:CLA:HAB	1.67	0.76
22:BC:501:CLA:HMB3	26:BC:515:BCR:H403	1.67	0.76
2:AB:329:PRO:HB3	22:AB:607:CLA:HED1	1.65	0.76
26:BC:514:BCR:H353	26:BK:102:BCR:H321	1.68	0.76
5:BE:84:LYS:NZ	5:BE:84:LYS:HB2	2.00	0.76
2:BB:329:PRO:HB3	22:BB:610:CLA:HED1	1.67	0.76
2:BB:188:ASP:HA	7:BH:58:VAL:HG23	1.68	0.76
13:AO:31:LEU:HB2	13:AO:36:ILE:HD11	1.67	0.76
1:AA:258:LEU:HD12	4:AD:128:ARG:HD3	1.66	0.76
3:AC:42:LEU:HD13	22:AC:511:CLA:HMA3	1.68	0.76
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.66	0.76
20:AZ:32:ASP:HB2	20:AZ:35:ARG:HG2	1.67	0.76
3:BC:42:LEU:HD13	22:BC:511:CLA:HMA3	1.67	0.75
2:AB:134:ASP:OD2	2:AB:137:LYS:HE3	1.86	0.75
4:BD:244:TYR:OH	4:BD:264:LYS:HE3	1.86	0.75
1:AA:192:ILE:HA	1:AA:293:MET:HE3	1.68	0.75
3:AC:391:ARG:NH1	3:AC:391:ARG:HB2	2.02	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:18:ARG:HB3	5:BE:18:ARG:HH11	1.50	0.75
18:AX:12:ILE:O	18:AX:12:ILE:HG23	1.85	0.75
2:BB:134:ASP:OD2	2:BB:137:LYS:HE3	1.87	0.75
1:BA:57:PRO:HG3	1:BA:68:SER:HB3	1.68	0.75
22:AC:501:CLA:HMB3	26:AC:515:BCR:H403	1.69	0.75
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.07	0.75
3:BC:254:THR:HG22	3:BC:255:THR:N	2.00	0.75
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.86	0.75
2:BB:150:CYS:HB2	22:BB:606:CLA:HMC3	1.68	0.74
1:BA:214:MET:CE	1:BA:214:MET:HA	2.17	0.74
11:AL:5:PRO:HA	11:AL:7:ARG:NH2	2.00	0.74
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.69	0.74
13:BO:230:VAL:HG12	13:BO:231:ASP:N	2.02	0.74
3:AC:241:GLY:O	3:AC:245:ILE:HG13	1.88	0.74
1:AA:214:MET:HA	1:AA:214:MET:CE	2.17	0.74
2:AB:137:LYS:HD2	7:AH:14:LEU:O	1.87	0.74
4:AD:244:TYR:OH	4:AD:264:LYS:HE3	1.88	0.74
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.70	0.74
5:BE:17:VAL:O	5:BE:21:VAL:HG23	1.87	0.74
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.53	0.74
2:AB:135:LEU:HD23	2:AB:138:MET:HE3	1.70	0.74
5:AE:18:ARG:HH11	5:AE:18:ARG:HB3	1.52	0.73
13:BO:69:LEU:HD12	13:BO:70:CYS:N	2.03	0.73
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.88	0.73
4:AD:60:THR:HG23	4:AD:61:HIS:CD2	2.23	0.73
26:AC:514:BCR:H353	26:AK:102:BCR:H321	1.69	0.73
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.69	0.73
3:BC:155:ASN:HA	3:BC:158:THR:HG22	1.70	0.73
3:BC:241:GLY:O	3:BC:245:ILE:HG13	1.87	0.73
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.17	0.73
2:BB:286:ARG:HG2	2:BB:286:ARG:HH11	1.54	0.73
4:BD:88:SER:HB2	5:BE:69:ARG:NH2	2.02	0.73
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.19	0.73
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.88	0.73
12:AM:20:VAL:HG21	12:BM:20:VAL:HG21	1.69	0.73
2:BB:483:ASP:CG	2:BB:484:PRO:HD2	2.08	0.73
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.88	0.73
2:BB:135:LEU:HA	2:BB:138:MET:HE3	1.70	0.73
13:BO:35:ASP:C	13:BO:36:ILE:HD12	2.09	0.73
2:BB:348:ASN:HB3	2:BB:354:LEU:HD21	1.71	0.73
22:BD:404:CLA:H43	18:BX:23:LEU:HA	1.71	0.73
3:AC:254:THR:CG2	3:AC:255:THR:H	2.00	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:41:LEU:O	1:AA:45:THR:HG22	1.88	0.72
16:BV:63:CYS:SG	34:BV:201:HEM:CAB	2.74	0.72
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.02	0.72
20:BZ:32:ASP:CG	20:BZ:33:TRP:H	1.92	0.72
20:BZ:32:ASP:HB2	20:BZ:35:ARG:HG2	1.71	0.72
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.89	0.72
3:AC:405:ASN:HD22	27:AC:518:DGD:HD5	1.54	0.72
3:BC:240:ILE:O	3:BC:244:CYS:HB2	1.89	0.72
1:AA:129:ARG:NH2	4:AD:256:ILE:HD12	2.01	0.72
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.90	0.72
3:BC:391:ARG:HB2	3:BC:391:ARG:NH1	2.04	0.72
1:BA:41:LEU:O	1:BA:45:THR:HG22	1.89	0.72
3:AC:361:PHE:HA	27:AC:516:DGD:HE61	1.72	0.72
3:BC:305:THR:CG2	3:BC:308:GLU:H	2.02	0.72
2:BB:483:ASP:CB	2:BB:484:PRO:HD2	2.19	0.72
13:AO:69:LEU:HD12	13:AO:70:CYS:N	2.05	0.72
13:AO:86:ARG:NH1	13:AO:87:GLN:HA	2.05	0.72
13:BO:86:ARG:NH1	13:BO:87:GLN:HA	2.05	0.72
3:AC:391:ARG:HH11	3:AC:391:ARG:HB2	1.55	0.71
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	2.04	0.71
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.72	0.71
2:AB:68:ARG:NH1	2:AB:262:THR:HG23	2.04	0.71
2:AB:188:ASP:HA	7:AH:58:VAL:HG23	1.72	0.71
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.90	0.71
12:AM:33:GLN:HB3	12:BM:33:GLN:CB	2.19	0.71
3:BC:405:ASN:HD22	27:BC:518:DGD:HD5	1.55	0.71
22:AD:404:CLA:H43	18:AX:23:LEU:HA	1.71	0.71
13:BO:92:VAL:CG1	13:BO:93:PRO:HD2	2.20	0.71
2:AB:124:ARG:HG3	2:AB:124:ARG:HH11	1.55	0.71
14:AT:29:ILE:CD1	14:AT:29:ILE:H	1.95	0.71
1:BA:129:ARG:NH2	4:BD:256:ILE:HA	2.06	0.71
2:BB:68:ARG:NH1	2:BB:262:THR:HG23	2.06	0.70
3:BC:29:GLU:HB3	10:BK:46:ARG:NH1	2.06	0.70
2:AB:150:CYS:HB2	22:AB:603:CLA:HMC3	1.72	0.70
4:BD:148:ALA:HB2	4:BD:276:VAL:HG13	1.71	0.70
3:AC:348:GLU:OE2	13:AO:37:VAL:HA	1.91	0.70
3:AC:187:ASP:HB2	3:AC:230:LEU:HD12	1.73	0.70
7:AH:38:PHE:HB2	26:AH:101:BCR:H10C	1.74	0.70
13:BO:77:LEU:HD23	13:BO:93:PRO:HA	1.72	0.70
15:AU:38:GLU:HG2	15:AU:39:LEU:N	2.05	0.70
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.06	0.70
16:AV:63:CYS:SG	34:AV:201:HEM:CAB	2.74	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:27:THR:HG22	2:BB:107:LEU:HD13	1.72	0.70
1:BA:93:PHE:CD2	1:BA:95:PRO:HD3	2.26	0.70
4:BD:192:THR:HG23	22:BD:402:CLA:HBC2	1.74	0.70
3:BC:158:THR:O	3:BC:251:HIS:HB3	1.92	0.70
5:BE:26:THR:HB	34:BE:101:HEM:HBB2	1.74	0.70
13:AO:77:LEU:HD23	13:AO:93:PRO:HA	1.74	0.70
4:BD:39:PRO:O	4:BD:43:LEU:HD22	1.91	0.70
13:AO:35:ASP:C	13:AO:36:ILE:HD12	2.12	0.70
13:AO:87:GLN:O	13:AO:88:GLU:HB3	1.91	0.70
18:BX:12:ILE:O	18:BX:12:ILE:HG23	1.89	0.70
16:AV:115:ALA:CB	16:AV:122:ARG:HD2	2.22	0.70
2:BB:137:LYS:HD2	7:BH:14:LEU:O	1.92	0.69
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.26	0.69
30:AB:623:LMG:H111	1:BA:72:LEU:HD13	1.74	0.69
3:BC:85:GLY:N	27:BC:517:DGD:HE4	2.06	0.69
1:BA:332:HIS:CD2	1:BA:333:GLU:HG3	2.27	0.69
6:BF:17:THR:HG23	6:BF:20:TRP:H	1.57	0.69
4:AD:55:VAL:HG21	4:AD:110:LEU:HD12	1.74	0.69
7:BH:38:PHE:HB2	26:BX:101:BCR:H10C	1.73	0.69
4:AD:152:VAL:HG21	4:AD:279:LEU:HD12	1.72	0.69
4:AD:122:LEU:HD11	23:AD:403:PHO:H92	1.74	0.69
13:AO:33:TYR:O	13:AO:37:VAL:HG23	1.92	0.69
5:BE:56:TYR:O	16:BV:27:ALA:HB2	1.92	0.69
4:BD:152:VAL:HG21	4:BD:279:LEU:HD12	1.74	0.69
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.92	0.69
5:AE:26:THR:HB	34:AE:101:HEM:HBB2	1.74	0.69
3:AC:85:GLY:N	27:AC:517:DGD:HE4	2.07	0.69
5:AE:81:GLU:O	5:AE:83:LEU:N	2.24	0.69
18:BX:34:PHE:O	18:BX:38:ILE:HG12	1.91	0.69
16:BV:115:ALA:CB	16:BV:122:ARG:HD2	2.23	0.69
3:BC:254:THR:CG2	3:BC:255:THR:H	2.04	0.69
12:AM:33:GLN:CB	12:BM:33:GLN:HB3	2.19	0.69
2:BB:135:LEU:HD23	2:BB:138:MET:HE3	1.74	0.69
4:AD:39:PRO:O	4:AD:43:LEU:HD22	1.93	0.69
3:BC:348:GLU:OE2	13:BO:37:VAL:HA	1.93	0.69
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.55	0.69
13:BO:33:TYR:O	13:BO:37:VAL:HG23	1.92	0.69
4:AD:87:HIS:HD2	4:AD:162:LEU:HD23	1.58	0.69
2:BB:264:PRO:HG2	2:BB:267:LEU:HD12	1.74	0.69
15:BU:54:LYS:HB2	15:BU:113:THR:HG23	1.75	0.68
13:BO:178:ARG:CG	13:BO:178:ARG:NH1	2.53	0.68
4:AD:261:PHE:HB2	24:AD:405:PL9:H522	1.74	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:BU:38:GLU:HG2	15:BU:39:LEU:N	2.08	0.68
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.92	0.68
1:BA:129:ARG:NH2	4:BD:256:ILE:HD12	2.02	0.68
20:AZ:30:PRO:HG3	20:AZ:33:TRP:HZ3	1.58	0.68
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.27	0.68
4:AD:192:THR:HG23	22:AD:402:CLA:HBC2	1.74	0.68
1:AA:40:THR:HG21	1:AA:121:LEU:HD23	1.73	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HD2	1.74	0.68
20:AZ:32:ASP:HB3	20:AZ:35:ARG:NH1	2.08	0.68
2:BB:284:ILE:HG12	2:BB:309:LEU:CD1	2.23	0.68
10:AK:19:ASP:N	10:AK:20:PRO:HD2	2.09	0.68
3:BC:166:ILE:O	3:BC:170:ILE:HG13	1.93	0.68
2:AB:135:LEU:HA	2:AB:138:MET:HE3	1.74	0.68
13:AO:206:GLU:H	13:AO:206:GLU:CD	1.97	0.68
2:BB:135:LEU:HB2	2:BB:136:PRO:HD3	1.75	0.68
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.27	0.68
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.76	0.68
4:BD:122:LEU:HD11	23:BD:403:PHO:H92	1.76	0.68
2:BB:103:LEU:HD21	22:BB:608:CLA:HMC3	1.75	0.68
22:AA:404:CLA:HAB	22:AD:402:CLA:H72	1.76	0.68
20:AZ:28:ALA:O	20:AZ:30:PRO:HD3	1.93	0.68
2:BB:315:ILE:HG22	2:BB:426:PHE:HB3	1.76	0.68
2:BB:4:PRO:HD2	2:BB:7:ARG:HD2	1.74	0.68
12:BM:31:SER:HB3	30:BM:102:LMG:HC71	1.76	0.68
2:AB:284:ILE:HG12	2:AB:309:LEU:CD1	2.23	0.68
22:BA:405:CLA:HAB	22:BD:402:CLA:H72	1.76	0.68
4:AD:279:LEU:HG	23:AD:403:PHO:HBC3	1.76	0.68
2:BB:135:LEU:HD23	2:BB:138:MET:CE	2.24	0.68
3:BC:415:ASN:O	3:BC:416:SER:HB3	1.94	0.68
4:BD:250:ASN:HD22	4:BD:262:SER:HB3	1.58	0.67
3:BC:305:THR:HG22	3:BC:308:GLU:CB	2.24	0.67
5:AE:81:GLU:C	5:AE:83:LEU:H	1.96	0.67
5:BE:81:GLU:C	5:BE:83:LEU:H	1.97	0.67
4:BD:180:ARG:HH11	4:BD:180:ARG:CG	2.07	0.67
4:AD:180:ARG:CG	4:AD:180:ARG:HH11	2.08	0.67
20:BZ:33:TRP:O	20:BZ:37:LYS:HB2	1.93	0.67
2:BB:331:ASN:HB3	2:BB:437:LEU:HD12	1.75	0.67
3:AC:42:LEU:HD21	22:AC:511:CLA:H2A	1.74	0.67
3:BC:361:PHE:HA	27:BC:516:DGD:HE61	1.77	0.67
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.48	0.67
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	1.94	0.67
2:AB:264:PRO:HG2	2:AB:267:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:BK:19:ASP:N	10:BK:20:PRO:HD2	2.10	0.67
2:AB:135:LEU:HD23	2:AB:138:MET:CE	2.25	0.67
7:BH:6:TRP:CE2	7:BH:10:ILE:HD11	2.29	0.67
6:BF:11:VAL:HG12	6:BF:12:SER:N	2.09	0.67
24:BA:408:PL9:H33	4:BD:38:PHE:CD1	2.29	0.67
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.59	0.67
5:BE:27:ILE:HB	5:BE:28:PRO:HD3	1.77	0.67
13:BO:206:GLU:CD	13:BO:206:GLU:H	1.97	0.67
3:AC:472:LEU:HD12	3:AC:473:ASP:H	1.59	0.67
3:BC:215:LYS:HB3	3:BC:223:TRP:HA	1.77	0.67
3:AC:166:ILE:O	3:AC:170:ILE:HG13	1.94	0.67
1:AA:183:MET:HA	22:AA:402:CLA:HMD2	1.76	0.67
3:BC:391:ARG:HB2	3:BC:391:ARG:HH11	1.59	0.67
3:BC:75:PHE:HD1	3:BC:86:LEU:HD21	1.60	0.67
12:AM:31:SER:HB3	30:AM:101:LMG:HC71	1.77	0.67
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.59	0.67
1:BA:174:LEU:HD22	23:BA:406:PHO:H151	1.75	0.67
4:BD:186:GLN:HB2	22:BD:402:CLA:HBC1	1.77	0.67
3:BC:155:ASN:HD21	3:BC:255:THR:CB	2.07	0.67
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.77	0.67
2:AB:271:THR:CG2	2:AB:273:TYR:H	2.08	0.67
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.24	0.67
22:AB:602:CLA:H42	7:AH:45:ILE:HD11	1.76	0.67
2:BB:356:VAL:HG22	2:BB:370:LEU:HD21	1.77	0.67
3:AC:377:LEU:O	3:AC:381:LYS:HB2	1.95	0.67
5:AE:78:THR:O	5:AE:81:GLU:HB2	1.94	0.67
1:BA:32:TRP:HA	1:BA:32:TRP:CE3	2.30	0.67
3:BC:161:LEU:HG	3:BC:165:LEU:HD12	1.77	0.66
3:BC:449:ARG:HE	22:BC:505:CLA:CED	2.07	0.66
2:BB:483:ASP:OD2	2:BB:484:PRO:HD2	1.95	0.66
13:BO:92:VAL:HG12	13:BO:93:PRO:HD2	1.78	0.66
5:BE:81:GLU:O	5:BE:83:LEU:N	2.27	0.66
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
3:BC:377:LEU:O	3:BC:381:LYS:HB2	1.94	0.66
3:AC:75:PHE:HD1	3:AC:86:LEU:HD21	1.59	0.66
2:BB:284:ILE:HG23	2:BB:305:ILE:HD12	1.76	0.66
6:BF:11:VAL:HG12	6:BF:12:SER:H	1.59	0.66
3:BC:42:LEU:HD21	22:BC:511:CLA:H2A	1.77	0.66
22:AC:507:CLA:H112	26:AC:515:BCR:H362	1.78	0.66
12:AM:23:ILE:HD13	30:AM:101:LMG:H182	1.78	0.66
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.66
2:AB:141:ILE:CG2	22:AB:615:CLA:HBB1	2.26	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:AC:505:CLA:HBA1	22:AC:505:CLA:HBD	1.77	0.66
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.14	0.66
1:BA:183:MET:HA	22:BA:403:CLA:HMD2	1.76	0.66
5:BE:18:ARG:O	5:BE:22:ILE:HG13	1.95	0.66
5:BE:84:LYS:HZ2	5:BE:84:LYS:HB2	1.61	0.66
5:BE:15:THR:HG23	9:BJ:8:ILE:O	1.95	0.66
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.09	0.66
1:BA:238:LYS:HD2	14:BT:32:LYS:HB3	1.76	0.66
11:BL:7:ARG:O	11:BL:7:ARG:HD2	1.96	0.66
3:AC:305:THR:HG22	3:AC:308:GLU:CB	2.26	0.66
3:BC:114:VAL:HG22	30:BC:520:LMG:H152	1.77	0.66
3:BC:30:SER:HB2	10:BK:46:ARG:O	1.95	0.66
1:BA:40:THR:HG21	1:BA:121:LEU:HD23	1.77	0.66
3:BC:89:ILE:N	3:BC:90:PRO:HD2	2.11	0.66
1:BA:343:LEU:O	1:BA:344:ALA:HB2	1.96	0.66
20:BZ:30:PRO:HG3	20:BZ:33:TRP:HZ3	1.60	0.66
3:AC:277:GLY:C	22:AC:505:CLA:HBC2	2.15	0.66
4:BD:279:LEU:HG	23:BD:403:PHO:HBC3	1.76	0.66
3:BC:277:GLY:C	22:BC:505:CLA:HBC2	2.16	0.66
2:BB:133:LEU:HB3	2:BB:138:MET:CE	2.26	0.66
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.26	0.66
13:BO:120:THR:HG22	13:BO:154:SER:OG	1.96	0.66
1:BA:77:ILE:HD11	14:BT:6:TYR:HB3	1.78	0.66
22:BC:505:CLA:HBA1	22:BC:505:CLA:HBD	1.78	0.65
2:BB:490:GLN:O	2:BB:490:GLN:OE1	2.15	0.65
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.62	0.65
2:BB:327:THR:HG22	22:BB:610:CLA:H12	1.78	0.65
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	1.95	0.65
24:AA:407:PL9:H33	4:AD:38:PHE:CD1	2.31	0.65
5:BE:78:THR:O	5:BE:81:GLU:HB2	1.96	0.65
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.78	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.96	0.65
3:AC:161:LEU:HG	3:AC:165:LEU:HD12	1.78	0.65
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.11	0.65
3:AC:55:ALA:HB1	26:AC:514:BCR:H373	1.78	0.65
20:BZ:33:TRP:CD1	20:BZ:33:TRP:O	2.50	0.65
1:AA:32:TRP:HA	1:AA:32:TRP:CE3	2.31	0.65
2:BB:247:PHE:HE1	22:BB:605:CLA:H101	1.61	0.65
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.78	0.65
2:AB:331:ASN:HB3	2:AB:437:LEU:HD12	1.79	0.65
2:BB:86:ILE:O	2:BB:86:ILE:HD12	1.96	0.65
2:BB:270:PRO:HG3	2:BB:312:TYR:HD2	1.61	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:386:ALA:HB3	15:BU:132:LEU:HD11	1.79	0.65
3:AC:155:ASN:HD21	3:AC:255:THR:CB	2.07	0.65
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.78	0.65
3:AC:30:SER:HB2	10:AK:46:ARG:O	1.95	0.65
2:BB:356:VAL:HG22	2:BB:370:LEU:CD2	2.27	0.65
4:BD:103:ARG:HG3	5:BE:73:LYS:HG3	1.78	0.65
20:BZ:49:ALA:O	20:BZ:53:VAL:HG23	1.96	0.65
9:AJ:14:ALA:CB	26:AK:102:BCR:H393	2.27	0.65
4:BD:261:PHE:HB2	24:BD:405:PL9:H522	1.78	0.65
22:BC:507:CLA:H112	26:BC:515:BCR:H362	1.78	0.65
13:BO:87:GLN:O	13:BO:88:GLU:HB3	1.96	0.65
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.61	0.65
2:AB:271:THR:HB	2:AB:274:GLN:HG3	1.78	0.65
22:BC:512:CLA:H143	22:BC:513:CLA:H162	1.79	0.65
20:BZ:28:ALA:O	20:BZ:30:PRO:HD3	1.97	0.65
2:AB:248:ALA:HA	22:AB:603:CLA:H42	1.79	0.65
11:AL:7:ARG:HD2	11:AL:7:ARG:O	1.97	0.65
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.96	0.65
3:BC:187:ASP:HB2	3:BC:230:LEU:HD12	1.78	0.65
2:AB:490:GLN:O	2:AB:490:GLN:OE1	2.15	0.65
2:AB:247:PHE:HE1	22:AB:602:CLA:H101	1.62	0.64
22:BC:511:CLA:H151	20:BZ:20:VAL:HG13	1.78	0.64
27:BC:518:DGD:HD2	9:BJ:32:ALA:O	1.97	0.64
3:BC:55:ALA:HB1	26:BC:514:BCR:H373	1.77	0.64
14:BT:29:ILE:HD12	14:BT:29:ILE:N	2.10	0.64
3:AC:186:TYR:HE2	3:AC:188:THR:HG22	1.62	0.64
2:AB:86:ILE:HD12	2:AB:86:ILE:O	1.97	0.64
2:BB:271:THR:CG2	2:BB:273:TYR:H	2.08	0.64
22:BB:611:CLA:HMA1	4:BD:130:PHE:CE1	2.32	0.64
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	2.11	0.64
2:AB:139:PHE:CZ	2:AB:143:LEU:HD22	2.32	0.64
4:BD:87:HIS:HD2	4:BD:162:LEU:HD23	1.62	0.64
3:AC:449:ARG:HE	22:AC:505:CLA:CED	2.08	0.64
15:BU:94:ILE:O	15:BU:97:LEU:HG	1.98	0.64
3:BC:472:LEU:HD12	3:BC:473:ASP:H	1.62	0.64
3:BC:156:LYS:O	3:BC:160:ILE:HG13	1.97	0.64
13:AO:86:ARG:C	13:AO:86:ARG:HD2	2.18	0.64
2:AB:103:LEU:HD21	22:AB:605:CLA:HMC3	1.78	0.64
2:BB:271:THR:HB	2:BB:274:GLN:HG3	1.80	0.64
2:AB:327:THR:HG22	22:AB:607:CLA:H12	1.78	0.64
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.79	0.64
15:BU:58:ASN:ND2	15:BU:114:VAL:HG13	2.13	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:AC:511:CLA:H151	20:AZ:20:VAL:HG13	1.78	0.64
5:BE:26:THR:O	5:BE:29:ALA:HB3	1.97	0.64
4:BD:129:GLN:HE22	4:BD:143:ALA:HA	1.61	0.64
1:AA:174:LEU:HD22	23:AA:405:PHO:H151	1.78	0.64
22:BC:511:CLA:H171	20:BZ:20:VAL:HA	1.80	0.64
15:AU:66:ILE:O	15:AU:66:ILE:HG22	1.98	0.64
22:BC:505:CLA:CMD	22:BC:507:CLA:HAB	2.28	0.64
15:BU:66:ILE:HG22	15:BU:66:ILE:O	1.97	0.64
7:AH:35:MET:HE2	26:AH:101:BCR:HC21	1.80	0.64
13:AO:36:ILE:HG23	13:AO:41:LEU:HB3	1.80	0.64
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.28	0.64
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.64
13:AO:117:GLY:O	13:AO:159:VAL:HG12	1.98	0.64
2:AB:286:ARG:HH11	2:AB:286:ARG:HG2	1.62	0.64
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.80	0.63
16:AV:143:GLY:O	16:AV:147:VAL:HG23	1.97	0.63
2:BB:379:ALA:HA	2:BB:390:TYR:HB3	1.79	0.63
12:BM:23:ILE:HD13	30:BM:102:LMG:H182	1.79	0.63
3:BC:204:LEU:HD21	3:BC:238:ILE:HG21	1.79	0.63
3:AC:209:ILE:HG23	26:AC:515:BCR:H382	1.81	0.63
3:BC:141:GLU:H	3:BC:141:GLU:CD	2.02	0.63
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.98	0.63
13:BO:144:LEU:HD13	13:BO:259:VAL:HG11	1.80	0.63
2:BB:141:ILE:CG2	22:BB:618:CLA:HBB1	2.27	0.63
2:AB:386:ALA:HB3	15:AU:132:LEU:HD11	1.80	0.63
2:BB:139:PHE:CZ	2:BB:143:LEU:HD22	2.32	0.63
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.98	0.63
3:BC:223:TRP:CD2	3:BC:224:ILE:HG13	2.34	0.63
4:AD:186:GLN:HB2	22:AD:402:CLA:HBC1	1.80	0.63
22:AB:602:CLA:H61	7:AH:46:LEU:HD13	1.80	0.63
2:AB:486:LEU:HD13	2:AB:486:LEU:O	1.98	0.63
3:BC:150:ASP:HB3	3:BC:153:ASP:HB2	1.78	0.63
9:BJ:14:ALA:CB	26:BK:102:BCR:H393	2.28	0.63
29:AA:412:SQD:H311	22:AC:508:CLA:H71	1.81	0.63
27:AC:518:DGD:HD2	9:AJ:32:ALA:O	1.99	0.63
22:AC:511:CLA:H171	20:AZ:20:VAL:HA	1.79	0.63
10:BK:18:PHE:HD2	10:BK:18:PHE:N	1.96	0.63
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	1.99	0.63
13:BO:36:ILE:HG23	13:BO:41:LEU:HB3	1.79	0.63
1:BA:81:ALA:HB2	1:BA:175:GLY:HA3	1.80	0.63
2:AB:297:THR:OG1	2:AB:300:GLU:HG3	1.98	0.63
10:AK:18:PHE:HD2	10:AK:18:PHE:N	1.97	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:79:PHE:O	5:BE:84:LYS:HB3	1.99	0.63
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.81	0.63
13:BO:86:ARG:HD2	13:BO:86:ARG:C	2.19	0.63
5:BE:36:LEU:O	5:BE:40:THR:HG23	1.99	0.63
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.10	0.62
22:AB:605:CLA:HMB3	22:AB:606:CLA:H11	1.81	0.62
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.80	0.62
7:BH:19:GLY:O	7:BH:21:VAL:HG13	1.98	0.62
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.62
1:BA:57:PRO:HG3	1:BA:68:SER:CB	2.29	0.62
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.81	0.62
7:AH:19:GLY:O	7:AH:21:VAL:HG13	1.99	0.62
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.34	0.62
20:BZ:32:ASP:HB3	20:BZ:35:ARG:NH1	2.13	0.62
2:BB:124:ARG:NE	2:BB:131:PRO:HD3	2.14	0.62
1:BA:89:ILE:HD11	1:BA:108:ASN:HB3	1.81	0.62
26:BK:102:BCR:HC8	26:BK:102:BCR:H331	1.82	0.62
26:BC:514:BCR:H312	20:BZ:9:LEU:HD11	1.80	0.62
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.82	0.62
22:AC:505:CLA:CMD	22:AC:507:CLA:HAB	2.29	0.62
2:BB:224:ARG:HG2	7:BH:24:GLY:O	1.99	0.62
14:AT:29:ILE:N	14:AT:29:ILE:HD12	2.10	0.62
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	1.99	0.62
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.81	0.62
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.30	0.62
3:BC:186:TYR:HE2	3:BC:188:THR:HG22	1.65	0.62
18:AX:11:THR:HG23	18:AX:12:ILE:HG22	1.81	0.62
2:AB:124:ARG:NE	2:AB:131:PRO:HD3	2.13	0.62
30:AD:408:LMG:HC62	11:AL:15:THR:HG21	1.82	0.62
5:AE:64:PRO:HB3	5:AE:84:LYS:HE2	1.82	0.62
22:BB:605:CLA:H42	7:BH:45:ILE:HD11	1.82	0.62
1:BA:29:TYR:CG	1:BA:133:LEU:HD13	2.34	0.62
12:AM:28:GLN:HB3	12:BM:27:VAL:HG12	1.81	0.62
3:BC:310:SER:OG	3:BC:355:THR:HG23	2.00	0.62
6:BF:28:VAL:HB	6:BF:29:PRO:HD3	1.81	0.62
2:BB:222:PRO:HG3	7:BH:27:THR:H	1.63	0.62
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.20	0.62
4:AD:267:LEU:C	4:AD:267:LEU:HD23	2.20	0.62
4:AD:26:ARG:CD	6:AF:18:VAL:HG11	2.27	0.62
26:AC:514:BCR:H312	20:AZ:9:LEU:HD11	1.80	0.61
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.15	0.61
5:BE:64:PRO:HB3	5:BE:84:LYS:HE2	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:AH:58:VAL:O	7:AH:58:VAL:HG13	2.00	0.61
15:AU:94:ILE:O	15:AU:97:LEU:HG	2.00	0.61
1:BA:93:PHE:HZ	22:BA:407:CLA:HAA1	1.65	0.61
1:AA:93:PHE:HZ	22:AA:406:CLA:HAA1	1.64	0.61
1:AA:18:CYS:O	1:AA:22:THR:HG22	2.00	0.61
16:AV:102:MET:HE3	16:AV:141:ILE:HG21	1.81	0.61
1:BA:142:TRP:HB2	4:BD:220:ASN:OD1	2.01	0.61
15:AU:54:LYS:HB2	15:AU:113:THR:HG23	1.82	0.61
3:BC:209:ILE:HG23	26:BC:515:BCR:H382	1.81	0.61
12:AM:27:VAL:HG12	12:BM:28:GLN:HB3	1.80	0.61
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.65	0.61
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.82	0.61
1:BA:228:THR:HG22	1:BA:229:GLU:H	1.66	0.61
1:BA:161:TYR:HB3	1:BA:162:PRO:HD3	1.82	0.61
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.81	0.61
1:BA:257:ARG:HG3	1:BA:257:ARG:HH11	1.65	0.61
3:BC:107:ASP:OD2	3:BC:110:PRO:HD3	1.99	0.61
22:AC:512:CLA:H143	22:AC:513:CLA:H162	1.82	0.61
3:AC:44:ASN:O	3:AC:45:LEU:HD12	1.99	0.61
20:BZ:55:GLY:HA2	26:BZ:101:BCR:H312	1.83	0.61
3:AC:248:GLY:O	3:AC:252:ILE:HG12	2.00	0.61
16:BV:143:GLY:O	16:BV:147:VAL:HG23	2.00	0.61
1:AA:89:ILE:HD11	1:AA:108:ASN:HB3	1.81	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.00	0.61
2:BB:471:ALA:HB2	4:BD:130:PHE:CZ	2.36	0.61
4:BD:55:VAL:HG21	4:BD:110:LEU:HD12	1.81	0.61
3:BC:318:LEU:HG	3:BC:328:VAL:HG11	1.83	0.61
16:BV:81:ARG:CZ	16:BV:157:GLY:HA3	2.30	0.61
2:BB:371:THR:HG22	2:BB:377:VAL:HA	1.82	0.61
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.82	0.61
10:BK:17:ILE:HD12	10:BK:17:ILE:N	2.16	0.61
15:AU:97:LEU:O	15:AU:102:LYS:HE2	2.01	0.61
3:AC:52:ALA:HA	22:AC:511:CLA:HMB3	1.82	0.61
2:AB:264:PRO:CG	2:AB:267:LEU:HD12	2.31	0.61
4:AD:342:PRO:O	4:AD:345:VAL:HG12	2.01	0.61
2:BB:172:TYR:O	2:BB:174:LEU:HG	2.00	0.61
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.01	0.61
3:BC:337:LEU:HD12	13:BO:131:PRO:HG3	1.83	0.61
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.83	0.61
4:AD:209:LEU:C	4:AD:209:LEU:HD23	2.21	0.61
30:BD:408:LMG:HC62	11:BL:15:THR:HG21	1.82	0.61
5:BE:18:ARG:NH1	5:BE:18:ARG:HB3	2.14	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.36	0.61
5:AE:18:ARG:O	5:AE:22:ILE:HG13	2.00	0.60
2:BB:486:LEU:O	2:BB:486:LEU:HD13	2.01	0.60
10:BK:18:PHE:N	10:BK:18:PHE:CD2	2.68	0.60
2:BB:68:ARG:HH11	2:BB:262:THR:HG23	1.67	0.60
1:BA:202:VAL:HG11	22:BA:405:CLA:OBD	1.99	0.60
3:BC:112:PHE:O	3:BC:116:VAL:HG13	2.01	0.60
10:AK:17:ILE:N	10:AK:17:ILE:HD12	2.17	0.60
29:BA:413:SQD:H311	22:BC:508:CLA:H71	1.83	0.60
18:BX:11:THR:HG23	18:BX:12:ILE:HG22	1.82	0.60
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	2.01	0.60
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.83	0.60
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	2.00	0.60
1:AA:60:ILE:HD12	1:AA:84:PRO:HD2	1.83	0.60
4:BD:250:ASN:ND2	4:BD:262:SER:HB3	2.17	0.60
3:AC:391:ARG:HD2	3:AC:395:TYR:CE2	2.36	0.60
5:BE:4:THR:HG22	5:BE:5:THR:N	2.16	0.60
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.00	0.60
3:AC:461:ARG:HH11	3:AC:461:ARG:HG3	1.65	0.60
5:AE:23:HIS:HA	5:AE:26:THR:OG1	2.00	0.60
7:BH:12:ARG:HD3	7:BH:12:ARG:C	2.22	0.60
2:AB:471:ALA:HB2	4:AD:130:PHE:CZ	2.36	0.60
4:AD:199:MET:HB3	24:AD:405:PL9:H28	1.84	0.60
26:AK:102:BCR:H331	26:AK:102:BCR:HC8	1.83	0.60
3:BC:305:THR:HG22	3:BC:308:GLU:HB2	1.83	0.60
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.01	0.60
20:AZ:32:ASP:CB	20:AZ:35:ARG:HG2	2.30	0.60
2:BB:222:PRO:HG3	7:BH:26:GLY:HA3	1.83	0.60
1:BA:29:TYR:CD2	1:BA:133:LEU:HD13	2.37	0.60
1:BA:214:MET:HE3	1:BA:214:MET:HA	1.82	0.60
12:AM:20:VAL:HG22	12:BM:20:VAL:HG11	1.84	0.60
2:AB:208:VAL:HG21	22:AB:602:CLA:HMC1	1.84	0.60
2:BB:208:VAL:HG21	22:BB:605:CLA:HMC1	1.83	0.60
3:BC:143:TYR:O	3:BC:144:SER:HB2	2.01	0.60
2:AB:213:GLY:O	2:AB:217:ILE:HG13	2.02	0.60
5:AE:4:THR:HG22	5:AE:5:THR:N	2.17	0.60
3:BC:52:ALA:HA	22:BC:511:CLA:HMB3	1.84	0.60
13:AO:31:LEU:HD12	13:AO:31:LEU:N	2.17	0.60
3:AC:186:TYR:CE2	3:AC:188:THR:HG22	2.37	0.60
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	1.82	0.60
1:BA:306:VAL:HG13	1:BA:314:ILE:O	2.01	0.60
2:AB:41:GLU:OE1	2:AB:63:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.82	0.60
20:AZ:33:TRP:HD1	20:AZ:33:TRP:O	1.84	0.60
13:BO:39:THR:OG1	13:BO:41:LEU:HB2	2.02	0.60
13:BO:117:GLY:O	13:BO:159:VAL:HG12	2.01	0.60
4:BD:239:GLN:O	4:BD:240:ALA:HB3	2.02	0.60
3:AC:114:VAL:HG22	30:AC:520:LMG:H152	1.83	0.60
1:AA:153:SER:CB	22:AA:402:CLA:H11	2.32	0.60
1:AA:202:VAL:HG11	22:AA:404:CLA:OBD	2.02	0.60
16:BV:90:PRO:O	16:BV:92:ARG:HD3	2.02	0.60
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.84	0.60
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.37	0.59
2:BB:213:GLY:O	2:BB:217:ILE:HG13	2.02	0.59
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.01	0.59
4:BD:267:LEU:C	4:BD:267:LEU:HD23	2.21	0.59
5:AE:79:PHE:O	5:AE:84:LYS:HB3	2.01	0.59
1:AA:214:MET:HE3	1:AA:214:MET:HA	1.83	0.59
12:AM:20:VAL:HG11	12:BM:20:VAL:HG22	1.83	0.59
5:AE:18:ARG:NH1	5:AE:18:ARG:HB3	2.17	0.59
15:BU:97:LEU:O	15:BU:102:LYS:HE2	2.02	0.59
3:BC:155:ASN:O	3:BC:158:THR:HG22	2.03	0.59
5:BE:26:THR:HB	34:BE:101:HEM:CBB	2.32	0.59
22:AD:404:CLA:HMD2	32:AD:411:LMT:H22	1.85	0.59
22:AC:502:CLA:H111	22:AC:503:CLA:HMB2	1.84	0.59
3:BC:461:ARG:HH11	3:BC:461:ARG:HG3	1.68	0.59
15:BU:113:THR:O	15:BU:114:VAL:HG23	2.02	0.59
10:AK:21:LEU:HD11	26:AK:102:BCR:HC32	1.84	0.59
10:AK:18:PHE:CD2	10:AK:18:PHE:N	2.69	0.59
26:AT:102:BCR:H393	22:BB:610:CLA:HAC2	1.83	0.59
1:BA:13:LEU:HD12	1:BA:13:LEU:H	1.68	0.59
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.83	0.59
4:BD:87:HIS:CD2	4:BD:162:LEU:HD23	2.38	0.59
4:BD:209:LEU:HD23	4:BD:209:LEU:C	2.23	0.59
1:BA:153:SER:CB	22:BA:403:CLA:H11	2.33	0.59
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.83	0.59
16:BV:125:ASP:HA	16:BV:131:ARG:HH21	1.68	0.59
1:AA:257:ARG:HH11	1:AA:257:ARG:HG3	1.66	0.59
11:AL:7:ARG:C	11:AL:8:GLN:HE21	2.06	0.59
22:BC:502:CLA:H111	22:BC:503:CLA:HMB2	1.84	0.59
5:BE:76:VAL:O	5:BE:80:LEU:HD22	2.03	0.59
1:BA:272:HIS:CD2	4:BD:218:VAL:HG21	2.38	0.59
2:AB:68:ARG:HH11	2:AB:262:THR:HG23	1.68	0.59
3:AC:124:VAL:HB	26:AZ:101:BCR:H362	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:343:ARG:NH1	3:BC:347:GLY:O	2.35	0.59
15:BU:83:ALA:CB	15:BU:84:PRO:CD	2.78	0.59
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.02	0.59
22:BB:605:CLA:H61	7:BH:46:LEU:HD13	1.84	0.59
4:BD:274:VAL:HA	24:BD:405:PL9:H253	1.85	0.59
5:AE:26:THR:HB	34:AE:101:HEM:CBB	2.33	0.59
3:BC:124:VAL:HB	26:BZ:101:BCR:H362	1.84	0.59
20:BZ:32:ASP:CB	20:BZ:35:ARG:HG2	2.32	0.59
2:BB:264:PRO:CG	2:BB:267:LEU:HD12	2.32	0.59
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.03	0.59
13:BO:123:GLU:HG2	13:BO:124:GLU:N	2.17	0.59
7:BH:35:MET:HE2	26:BX:101:BCR:HC21	1.85	0.58
20:BZ:33:TRP:HD1	20:BZ:33:TRP:O	1.86	0.58
20:BZ:36:SER:OG	20:BZ:39:LEU:HD12	2.03	0.58
2:BB:192:PRO:HD2	7:BH:60:VAL:HG12	1.85	0.58
4:AD:55:VAL:HG21	4:AD:110:LEU:CD1	2.33	0.58
4:BD:18:LEU:HD22	18:BX:38:ILE:CD1	2.32	0.58
22:AB:615:CLA:H143	22:AB:616:CLA:HMA3	1.85	0.58
11:BL:7:ARG:C	11:BL:8:GLN:HE21	2.04	0.58
3:BC:248:GLY:O	3:BC:252:ILE:HG12	2.02	0.58
3:BC:318:LEU:HD23	3:BC:318:LEU:C	2.23	0.58
3:AC:305:THR:HG23	3:AC:307:PRO:CD	2.32	0.58
1:AA:13:LEU:HD12	1:AA:13:LEU:H	1.69	0.58
10:BK:40:GLN:HA	10:BK:43:VAL:HG12	1.85	0.58
3:AC:318:LEU:C	3:AC:318:LEU:HD23	2.24	0.58
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.84	0.58
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.18	0.58
2:AB:212:ALA:HB2	22:AB:609:CLA:HMC3	1.85	0.58
3:AC:112:PHE:O	3:AC:116:VAL:HG13	2.03	0.58
16:BV:135:GLU:O	16:BV:139:VAL:HG23	2.03	0.58
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.05	0.58
10:BK:18:PHE:CE1	20:BZ:9:LEU:HG	2.39	0.58
1:BA:82:VAL:HB	1:BA:174:LEU:HB2	1.85	0.58
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.03	0.58
2:BB:112:CYS:HB3	26:BB:622:BCR:H393	1.85	0.58
32:BB:626:LMT:H102	7:BH:35:MET:SD	2.43	0.58
3:BC:165:LEU:HD21	22:BC:506:CLA:HHC	1.85	0.58
22:AB:607:CLA:HAC2	26:AB:618:BCR:H393	1.84	0.58
1:BA:143:ILE:HD11	4:BD:217:THR:HA	1.86	0.58
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	2.03	0.58
15:AU:38:GLU:HG2	15:AU:39:LEU:H	1.68	0.58
4:BD:342:PRO:O	4:BD:345:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:249:VAL:HG11	2:BB:486:LEU:HD23	1.86	0.58
22:BD:404:CLA:HMD2	32:BD:411:LMT:H22	1.84	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
7:BH:58:VAL:HG13	7:BH:58:VAL:O	2.02	0.58
4:BD:18:LEU:O	4:BD:22:LEU:HG	2.02	0.58
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	1.85	0.58
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.85	0.58
1:BA:49:VAL:O	1:BA:53:ILE:HG13	2.04	0.58
7:AH:12:ARG:HD3	7:AH:12:ARG:C	2.24	0.58
4:BD:160:TYR:HB3	4:BD:161:PRO:CD	2.33	0.58
22:BC:505:CLA:H92	22:BC:505:CLA:HAB	1.85	0.58
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.68	0.58
2:AB:329:PRO:HD3	22:AB:607:CLA:HED2	1.86	0.58
2:BB:188:ASP:OD1	7:BH:58:VAL:HA	2.04	0.58
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.34	0.58
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.03	0.58
1:BA:60:ILE:HD12	1:BA:84:PRO:HD2	1.86	0.58
20:AZ:16:SER:O	20:AZ:20:VAL:HG23	2.04	0.58
4:AD:87:HIS:CD2	4:AD:162:LEU:HD23	2.37	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.04	0.58
3:BC:44:ASN:O	3:BC:45:LEU:HD12	2.04	0.58
15:BU:57:LEU:HD22	15:BU:79:ILE:HG21	1.86	0.58
3:AC:447:ARG:NH1	3:AC:447:ARG:HG2	2.16	0.57
5:AE:84:LYS:HB2	5:AE:84:LYS:HZ2	1.68	0.57
1:BA:190:HIS:HB3	1:BA:293:MET:HE2	1.86	0.57
2:BB:133:LEU:HB3	2:BB:138:MET:HE2	1.86	0.57
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.03	0.57
20:BZ:5:PHE:HA	20:BZ:57:LEU:CD2	2.34	0.57
2:AB:6:TYR:HA	22:AB:611:CLA:H11	1.85	0.57
10:BK:31:LEU:O	10:BK:34:ALA:HB3	2.04	0.57
2:AB:149:LEU:HG	22:AB:603:CLA:CBC	2.29	0.57
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.02	0.57
16:AV:81:ARG:CZ	16:AV:157:GLY:HA3	2.34	0.57
13:BO:180:ALA:HB1	13:BO:191:ALA:HB2	1.86	0.57
4:AD:188:PHE:HE2	4:AD:329:MET:CE	2.17	0.57
1:BA:140:ARG:HH22	28:BA:412:LHG:P	2.27	0.57
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.05	0.57
11:AL:11:GLU:HG2	11:AL:12:LEU:N	2.19	0.57
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	2.04	0.57
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.69	0.57
20:BZ:16:SER:O	20:BZ:20:VAL:HG23	2.04	0.57
22:BB:618:CLA:H143	22:BB:619:CLA:HMA3	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:BF:19:ARG:O	6:BF:23:VAL:HG23	2.04	0.57
18:AX:45:LYS:N	18:AX:45:LYS:HD3	2.20	0.57
3:AC:130:VAL:O	3:AC:134:ILE:HG12	2.04	0.57
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.04	0.57
4:AD:252:PHE:O	4:AD:256:ILE:HG22	2.05	0.57
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.05	0.57
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.05	0.57
4:AD:18:LEU:O	4:AD:22:LEU:HG	2.05	0.57
4:BD:36:LEU:O	4:BD:39:PRO:HD2	2.05	0.57
13:BO:118:SER:HB3	13:BO:157:PRO:HA	1.87	0.57
4:BD:188:PHE:HE2	4:BD:329:MET:CE	2.17	0.57
15:AU:57:LEU:HD22	15:AU:79:ILE:HG21	1.87	0.57
3:AC:37:ALA:HA	22:AC:508:CLA:O1A	2.04	0.57
22:AC:505:CLA:HAB	22:AC:505:CLA:H92	1.87	0.57
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.53	0.57
2:AB:133:LEU:HB3	2:AB:138:MET:HE2	1.86	0.57
3:BC:44:ASN:C	3:BC:45:LEU:HD12	2.25	0.57
4:BD:346:LEU:O	4:BD:348:ARG:HG3	2.05	0.57
2:BB:248:ALA:HA	22:BB:606:CLA:H42	1.86	0.57
12:AM:29:THR:O	12:AM:32:GLN:HG3	2.05	0.57
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.05	0.57
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.40	0.57
5:AE:7:GLU:CD	5:AE:7:GLU:H	2.07	0.57
20:BZ:36:SER:HA	20:BZ:39:LEU:CG	2.31	0.57
2:AB:174:LEU:HD23	2:AB:308:LYS:HG2	1.87	0.57
3:BC:130:VAL:O	3:BC:134:ILE:HG12	2.04	0.57
10:BK:26:PRO:O	10:BK:29:PRO:HD2	2.04	0.57
3:BC:37:ALA:HA	22:BC:508:CLA:O1A	2.05	0.57
4:BD:18:LEU:HD22	18:BX:38:ILE:HD13	1.85	0.57
2:AB:256:MET:HA	2:AB:263:THR:HG21	1.87	0.57
4:BD:56:THR:HG21	5:BE:50:PRO:HD3	1.86	0.57
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.57
5:AE:84:LYS:HZ3	5:AE:84:LYS:HB2	1.70	0.57
18:BX:45:LYS:N	18:BX:45:LYS:HD3	2.19	0.57
2:BB:41:GLU:OE1	2:BB:63:LEU:HB2	2.04	0.57
4:BD:199:MET:HB3	24:BD:405:PL9:H28	1.86	0.56
22:BB:608:CLA:HMB3	22:BB:609:CLA:H11	1.86	0.56
13:BO:230:VAL:CG1	13:BO:231:ASP:H	2.12	0.56
3:AC:165:LEU:HD21	22:AC:506:CLA:HH3	1.85	0.56
4:AD:266:TRP:CD1	30:AD:408:LMG:HC3	2.40	0.56
24:AD:405:PL9:H13	30:AD:408:LMG:H132	1.87	0.56
13:BO:31:LEU:HD12	13:BO:31:LEU:N	2.19	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:391:ARG:HD2	3:BC:395:TYR:CE2	2.40	0.56
2:AB:191:ASN:ND2	7:AH:60:VAL:HA	2.20	0.56
3:BC:186:TYR:CE2	3:BC:188:THR:HG22	2.39	0.56
4:BD:157:PHE:CE1	4:BD:171:PRO:HG2	2.40	0.56
15:BU:100:ARG:HH11	15:BU:103:GLN:HG2	1.70	0.56
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.09	0.56
2:BB:414:PRO:HB2	2:BB:415:PRO:CD	2.33	0.56
2:BB:212:ALA:HB2	22:BB:612:CLA:HMC3	1.86	0.56
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.05	0.56
3:BC:305:THR:HG22	3:BC:308:GLU:N	2.16	0.56
20:BZ:29:SER:HB2	20:BZ:31:GLN:HG3	1.88	0.56
1:AA:249:VAL:HG11	2:AB:486:LEU:HD23	1.87	0.56
6:BF:21:VAL:O	6:BF:25:THR:HG23	2.06	0.56
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.40	0.56
5:BE:23:HIS:HA	5:BE:26:THR:OG1	2.05	0.56
2:AB:61:PHE:CE1	22:AB:607:CLA:HMB3	2.41	0.56
2:BB:286:ARG:HG2	2:BB:286:ARG:NH1	2.17	0.56
2:BB:297:THR:OG1	2:BB:300:GLU:HG3	2.04	0.56
20:BZ:26:ALA:CB	20:BZ:40:ILE:HD11	2.36	0.56
16:AV:87:LEU:HD12	16:AV:87:LEU:N	2.20	0.56
9:BJ:14:ALA:HB3	26:BK:102:BCR:H393	1.88	0.56
10:BK:21:LEU:HD11	26:BK:102:BCR:HC32	1.87	0.56
13:BO:80:GLU:O	13:BO:89:ALA:HB1	2.05	0.56
30:AA:416:LMG:H112	2:BB:43:ALA:HA	1.87	0.56
3:BC:305:THR:HG23	3:BC:307:PRO:CD	2.32	0.56
20:AZ:55:GLY:HA2	26:AZ:101:BCR:H312	1.87	0.56
4:AD:274:VAL:HA	24:AD:405:PL9:H253	1.86	0.56
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.41	0.56
26:AA:409:BCR:H321	29:AA:415:SQD:H321	1.87	0.56
22:BC:501:CLA:H42	22:BC:502:CLA:HMD1	1.88	0.56
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.86	0.56
4:BD:85:MET:CE	5:BE:69:ARG:HA	2.35	0.56
13:BO:154:SER:O	13:BO:168:PHE:HA	2.05	0.56
20:BZ:23:VAL:O	20:BZ:26:ALA:HB3	2.06	0.56
1:BA:18:CYS:O	1:BA:22:THR:HG22	2.05	0.56
12:BM:29:THR:O	12:BM:32:GLN:HG3	2.06	0.56
16:BV:59:PHE:HA	16:BV:63:CYS:SG	2.46	0.56
10:BK:24:VAL:O	10:BK:27:VAL:HG12	2.06	0.56
30:BD:408:LMG:H111	11:BL:19:LEU:HD21	1.87	0.56
13:BO:178:ARG:HG3	13:BO:178:ARG:NH1	2.00	0.56
2:BB:12:LEU:HB2	22:BB:615:CLA:HMC2	1.88	0.56
4:AD:152:VAL:HG21	4:AD:279:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.53	0.56
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.70	0.56
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.56
4:BD:26:ARG:CD	6:BF:18:VAL:HG11	2.29	0.56
1:AA:140:ARG:HH22	28:AA:411:LHG:P	2.28	0.56
3:BC:239:TRP:CE3	3:BC:243:ILE:HD11	2.40	0.56
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.88	0.56
13:BO:141:ARG:HH11	13:BO:141:ARG:HG2	1.71	0.56
3:BC:429:SER:HB3	27:BC:517:DGD:HA81	1.88	0.56
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.88	0.56
4:AD:199:MET:HG2	24:AD:405:PL9:H322	1.86	0.56
1:BA:265:PHE:CD1	1:BA:271:LEU:HA	2.41	0.56
2:AB:191:ASN:HD21	7:AH:60:VAL:HA	1.70	0.56
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.40	0.56
2:BB:434:THR:HG23	13:BO:204:LYS:HE3	1.86	0.56
3:BC:374:GLY:O	3:BC:375:LEU:C	2.44	0.56
2:AB:112:CYS:HB3	26:AB:620:BCR:H393	1.88	0.56
22:BB:611:CLA:H42	4:BD:127:LEU:HD11	1.86	0.56
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.87	0.56
18:AX:12:ILE:HG12	18:AX:16:LEU:CD1	2.31	0.56
20:AZ:29:SER:HB2	20:AZ:31:GLN:HG3	1.88	0.56
1:BA:11:ALA:O	1:BA:12:ASN:CB	2.53	0.56
2:BB:191:ASN:HB2	7:BH:58:VAL:CG2	2.36	0.56
13:AO:31:LEU:H	13:AO:31:LEU:HD12	1.71	0.56
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.36	0.56
2:BB:170:ASP:HB2	2:BB:171:PRO:CD	2.36	0.56
9:AJ:14:ALA:HB1	26:AK:102:BCR:H393	1.88	0.56
29:BA:413:SQD:H223	27:BC:518:DGD:HAE1	1.88	0.56
10:BK:17:ILE:HD12	10:BK:17:ILE:H	1.71	0.56
16:AV:125:ASP:HA	16:AV:131:ARG:HH21	1.70	0.56
1:AA:104:GLU:OE2	13:AO:99:ARG:HD3	2.06	0.56
16:BV:102:MET:HE3	16:BV:141:ILE:HG21	1.88	0.56
4:BD:60:THR:HG23	4:BD:61:HIS:HD2	1.70	0.55
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.07	0.55
16:BV:29:LEU:HD11	16:BV:34:LEU:HD21	1.87	0.55
3:AC:199:ILE:N	3:AC:199:ILE:HD12	2.22	0.55
8:AI:11:VAL:O	8:AI:15:PHE:HD2	1.89	0.55
24:BD:405:PL9:H13	30:BD:408:LMG:H132	1.87	0.55
14:AT:7:VAL:HG12	32:AT:101:LMT:H122	1.89	0.55
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.21	0.55
13:BO:83:LYS:HG2	13:BO:84:ASN:N	2.20	0.55
2:AB:43:ALA:HA	30:AB:623:LMG:H112	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:267:LEU:O	4:AD:267:LEU:HD23	2.06	0.55
20:BZ:5:PHE:HA	20:BZ:57:LEU:HD21	1.88	0.55
20:AZ:26:ALA:CB	20:AZ:40:ILE:HD11	2.36	0.55
3:AC:305:THR:HG22	3:AC:308:GLU:N	2.16	0.55
13:AO:83:LYS:HE2	2:BB:338:GLN:HA	1.87	0.55
4:BD:221:THR:HG23	4:BD:244:TYR:HB2	1.87	0.55
15:BU:38:GLU:HG2	15:BU:39:LEU:H	1.71	0.55
4:BD:267:LEU:HD23	4:BD:267:LEU:O	2.07	0.55
1:BA:104:GLU:OE2	13:BO:99:ARG:HD3	2.06	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CD2	2.41	0.55
13:BO:86:ARG:HH11	13:BO:87:GLN:HA	1.71	0.55
6:BF:16:PHE:CD2	29:BF:101:SQD:H262	2.41	0.55
4:BD:49:LEU:O	4:BD:53:THR:HG23	2.06	0.55
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.36	0.55
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.88	0.55
3:BC:350:ILE:HG21	3:BC:359:TRP:HB2	1.89	0.55
1:BA:140:ARG:NH2	1:BA:142:TRP:HZ3	2.05	0.55
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.41	0.55
3:BC:107:ASP:OD2	3:BC:109:PHE:HB3	2.06	0.55
2:BB:6:TYR:HA	22:BB:614:CLA:H11	1.88	0.55
1:BA:238:LYS:O	1:BA:241:GLN:HG3	2.07	0.55
30:AD:407:LMG:O3	9:AJ:37:GLY:HA3	2.07	0.55
1:BA:244:GLU:HG3	1:BA:246:TYR:H	1.71	0.55
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.42	0.55
4:AD:157:PHE:CE1	4:AD:171:PRO:HG2	2.41	0.55
3:BC:346:THR:O	13:BO:40:GLY:HA2	2.07	0.55
1:BA:131:TRP:CE3	1:BA:132:GLU:N	2.74	0.55
22:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.88	0.55
3:AC:95:LEU:HD13	22:AC:502:CLA:H143	1.89	0.55
18:BX:12:ILE:CG1	18:BX:16:LEU:HD12	2.36	0.55
1:AA:37:MET:HG2	1:AA:41:LEU:HD12	1.89	0.55
5:AE:55:TYR:O	5:AE:84:LYS:HE3	2.07	0.55
2:BB:174:LEU:HD23	2:BB:308:LYS:HG2	1.87	0.55
2:BB:183:PRO:HB2	2:BB:185:TRP:CH2	2.41	0.55
20:BZ:21:ILE:O	20:BZ:25:VAL:HG22	2.07	0.55
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.75	0.55
1:BA:64:ARG:NH1	13:BO:98:THR:HG21	2.22	0.55
4:BD:77:ALA:HB2	4:BD:174:GLY:HA3	1.88	0.55
3:AC:45:LEU:HD23	3:AC:48:LYS:HD2	1.89	0.55
13:BO:66:ILE:HD12	13:BO:121:PHE:CD1	2.41	0.55
20:AZ:36:SER:HA	20:AZ:39:LEU:CG	2.35	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CE2	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.88	0.55
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.47	0.55
4:BD:152:VAL:HG21	4:BD:279:LEU:CD1	2.36	0.55
4:AD:180:ARG:CG	4:AD:180:ARG:NH1	2.70	0.55
3:BC:239:TRP:HE3	3:BC:243:ILE:HD11	1.71	0.55
3:AC:107:ASP:OD2	3:AC:109:PHE:HB3	2.06	0.55
4:BD:88:SER:HB2	5:BE:69:ARG:CZ	2.36	0.55
18:AX:32:LEU:N	18:AX:32:LEU:HD23	2.22	0.55
9:AJ:14:ALA:HB3	26:AK:102:BCR:H393	1.89	0.54
3:BC:425:TRP:CE2	22:BC:504:CLA:HBA1	2.42	0.54
1:BA:38:ILE:O	1:BA:42:LEU:HG	2.06	0.54
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.54
4:BD:199:MET:HG2	24:BD:405:PL9:H322	1.89	0.54
2:BB:154:GLY:O	2:BB:159:THR:HG23	2.07	0.54
4:BD:334:GLN:N	4:BD:335:PRO:HD3	2.22	0.54
16:BV:35:THR:HG23	16:BV:46:THR:OG1	2.07	0.54
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.89	0.54
4:BD:180:ARG:NH1	4:BD:180:ARG:HG3	2.22	0.54
3:BC:473:ASP:HB2	14:BT:26:PRO:CB	2.33	0.54
3:BC:95:LEU:HD13	22:BC:502:CLA:H143	1.88	0.54
4:BD:76:VAL:O	4:BD:77:ALA:HB2	2.07	0.54
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.70	0.54
11:BL:11:GLU:HG2	11:BL:12:LEU:N	2.22	0.54
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.89	0.54
5:AE:8:ARG:NE	5:AE:13:ILE:HG12	2.22	0.54
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.07	0.54
22:BA:404:CLA:HED1	24:BD:405:PL9:H372	1.89	0.54
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.22	0.54
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.07	0.54
15:BU:66:ILE:O	15:BU:66:ILE:CG2	2.56	0.54
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	2.07	0.54
2:BB:224:ARG:NE	7:BH:25:TRP:NE1	2.55	0.54
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.08	0.54
15:AU:100:ARG:O	15:AU:103:GLN:HB3	2.07	0.54
3:BC:158:THR:HG21	3:BC:254:THR:O	2.08	0.54
3:AC:425:TRP:CE2	22:AC:504:CLA:HBA1	2.42	0.54
3:BC:149:TYR:HA	3:BC:156:LYS:HD3	1.89	0.54
3:BC:135:ARG:HB2	20:BZ:27:TYR:HB3	1.90	0.54
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.42	0.54
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.89	0.54
3:BC:369:LEU:HD21	3:BC:384:ILE:HD13	1.89	0.54
13:AO:227:VAL:HG12	13:AO:228:ALA:N	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:235:GLU:HG2	2:AB:235:GLU:O	2.08	0.54
13:AO:141:ARG:HH11	13:AO:141:ARG:HG2	1.71	0.54
2:AB:150:CYS:HA	22:AB:603:CLA:HBC2	1.89	0.54
2:BB:12:LEU:HD22	2:BB:18:ARG:HB2	1.89	0.54
20:BZ:32:ASP:C	20:BZ:34:ASP:N	2.60	0.54
3:AC:135:ARG:HB2	20:AZ:27:TYR:HB3	1.89	0.54
13:AO:86:ARG:C	13:AO:86:ARG:HH11	2.11	0.54
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.90	0.54
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	2.07	0.54
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.88	0.54
1:BA:217:SER:HA	1:BA:220:THR:HG22	1.90	0.54
13:BO:271:PRO:HG2	13:BO:272:ALA:H	1.73	0.54
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.23	0.54
1:AA:76:ASN:OD1	1:AA:79:THR:HG23	2.07	0.54
27:BB:602:DGD:HD3	32:BB:603:LMT:H32	1.89	0.54
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.54
5:BE:55:TYR:O	5:BE:84:LYS:HE3	2.07	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
15:BU:100:ARG:O	15:BU:103:GLN:HB3	2.08	0.54
3:BC:453:ALA:O	8:BI:34:ARG:HB2	2.07	0.54
2:BB:487:SER:N	2:BB:488:PRO:HD2	2.22	0.54
9:BJ:15:THR:O	9:BJ:19:MET:HG3	2.08	0.54
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.23	0.54
2:BB:230:ARG:O	2:BB:233:ASN:HB3	2.08	0.54
2:BB:191:ASN:HD21	7:BH:60:VAL:HA	1.72	0.54
4:BD:239:GLN:O	4:BD:240:ALA:CB	2.56	0.54
5:BE:8:ARG:NE	5:BE:13:ILE:HG12	2.23	0.54
16:AV:35:THR:HG23	16:AV:46:THR:OG1	2.08	0.54
30:AD:408:LMG:H111	11:AL:19:LEU:HD21	1.88	0.54
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.60	0.54
3:BC:45:LEU:HD23	3:BC:48:LYS:HD2	1.90	0.54
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	1.90	0.54
3:BC:276:LEU:HD11	3:BC:444:HIS:HD2	1.73	0.54
3:BC:36:TRP:O	22:BC:508:CLA:H11	2.08	0.53
10:BK:37:PHE:HB3	26:BK:102:BCR:C40	2.39	0.53
3:AC:276:LEU:HD11	3:AC:444:HIS:HD2	1.73	0.53
3:BC:118:HIS:CE1	30:BC:520:LMG:H192	2.42	0.53
3:BC:135:ARG:HE	20:BZ:33:TRP:HE1	1.56	0.53
20:AZ:36:SER:OG	20:AZ:39:LEU:HD12	2.07	0.53
2:BB:191:ASN:ND2	7:BH:60:VAL:HA	2.23	0.53
3:AC:30:SER:OG	4:AD:233:ARG:NH2	2.40	0.53
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:238:THR:O	4:BD:239:GLN:O	2.26	0.53
3:BC:380:ILE:HA	3:BC:384:ILE:HD11	1.88	0.53
20:BZ:14:ILE:O	20:BZ:18:VAL:HG23	2.08	0.53
16:AV:116:GLU:HG3	16:AV:116:GLU:O	2.08	0.53
3:BC:447:ARG:NH1	3:BC:447:ARG:HG2	2.16	0.53
4:BD:266:TRP:CD1	30:BD:408:LMG:HC3	2.42	0.53
6:BF:18:VAL:HG13	6:BF:19:ARG:N	2.23	0.53
1:BA:240:GLY:HA3	14:BT:29:ILE:HG22	1.90	0.53
7:BH:12:ARG:N	7:BH:13:PRO:HD2	2.23	0.53
2:BB:329:PRO:HD3	22:BB:610:CLA:HED2	1.91	0.53
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.90	0.53
10:BK:43:VAL:HG13	10:BK:43:VAL:O	2.08	0.53
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.08	0.53
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.08	0.53
8:BI:11:VAL:O	8:BI:15:PHE:HD2	1.91	0.53
3:AC:42:LEU:CD1	22:AC:511:CLA:HMA3	2.37	0.53
4:AD:279:LEU:HD11	22:AD:402:CLA:O1A	2.09	0.53
22:BB:610:CLA:H42	30:BB:624:LMG:H131	1.90	0.53
7:BH:58:VAL:O	7:BH:58:VAL:CG1	2.56	0.53
4:BD:189:HIS:HA	4:BD:294:ARG:HD2	1.90	0.53
15:BU:58:ASN:OD1	15:BU:84:PRO:HA	2.07	0.53
3:BC:418:ASN:HD21	27:BC:517:DGD:HD4	1.74	0.53
13:BO:178:ARG:HD2	13:BO:182:PHE:CD1	2.43	0.53
3:AC:118:HIS:CE1	30:AC:520:LMG:H192	2.43	0.53
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.19	0.53
3:BC:30:SER:OG	4:BD:233:ARG:NH2	2.41	0.53
2:AB:434:THR:HG23	13:AO:204:LYS:HE3	1.91	0.53
3:BC:137:PRO:HB2	3:BC:139:THR:O	2.09	0.53
20:BZ:3:ILE:O	20:BZ:7:LEU:HG	2.08	0.53
16:BV:87:LEU:HD12	16:BV:87:LEU:N	2.22	0.53
2:BB:341:LYS:HD2	2:BB:429:ILE:HG22	1.90	0.53
1:BA:283:VAL:O	1:BA:286:THR:HG22	2.08	0.53
4:AD:180:ARG:NH1	4:AD:180:ARG:HG3	2.23	0.53
3:AC:473:ASP:HB2	14:AT:26:PRO:CB	2.33	0.53
3:AC:36:TRP:O	22:AC:508:CLA:H11	2.08	0.53
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.55	0.53
3:BC:178:LYS:HA	3:BC:182:PHE:HB2	1.89	0.53
14:BT:29:ILE:H	14:BT:29:ILE:CD1	1.98	0.53
22:BB:612:CLA:HMC2	26:BX:101:BCR:H343	1.91	0.53
3:BC:131:TYR:HE1	3:BC:135:ARG:HD2	1.74	0.53
3:AC:174:LEU:HG	22:AC:512:CLA:H92	1.90	0.53
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:28:PRO:O	5:BE:32:ILE:HG13	2.08	0.53
1:BA:322:ASN:OD1	3:BC:412:THR:HA	2.08	0.53
13:BO:227:VAL:HG12	13:BO:228:ALA:N	2.23	0.53
13:AO:178:ARG:NH1	13:AO:178:ARG:CG	2.55	0.53
5:BE:7:GLU:CD	5:BE:7:GLU:H	2.12	0.53
27:AC:517:DGD:HB62	26:AJ:102:BCR:H352	1.91	0.53
3:BC:117:VAL:HG12	30:BC:520:LMG:H191	1.91	0.53
13:BO:31:LEU:HB2	13:BO:36:ILE:CD1	2.37	0.53
3:BC:337:LEU:CD1	13:BO:131:PRO:HG3	2.38	0.53
1:BA:107:TYR:CD1	13:BO:141:ARG:NH1	2.77	0.53
1:BA:76:ASN:OD1	1:BA:79:THR:HG23	2.08	0.53
9:BJ:14:ALA:HB1	26:BK:102:BCR:H393	1.91	0.53
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.56	0.53
2:BB:235:GLU:HG2	2:BB:235:GLU:O	2.09	0.53
3:BC:33:PHE:CE1	4:BD:229:ALA:CB	2.92	0.53
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.91	0.53
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.08	0.53
10:AK:37:PHE:HB3	26:AK:102:BCR:C40	2.39	0.53
3:BC:117:VAL:CG1	30:BC:520:LMG:H191	2.39	0.53
20:BZ:35:ARG:O	20:BZ:38:GLN:HB3	2.09	0.53
22:AC:501:CLA:H42	22:AC:502:CLA:HMD1	1.90	0.53
4:BD:161:PRO:HG3	4:BD:170:ALA:HB2	1.91	0.53
4:AD:238:THR:O	4:AD:239:GLN:O	2.27	0.53
27:AB:626:DGD:HD3	32:AB:627:LMT:H32	1.90	0.53
15:BU:89:GLU:CD	15:BU:89:GLU:H	2.11	0.53
26:AA:409:BCR:H312	8:AI:15:PHE:CE1	2.44	0.53
22:AB:608:CLA:H12	4:AD:127:LEU:HD21	1.91	0.53
20:BZ:30:PRO:C	20:BZ:32:ASP:H	2.12	0.53
13:BO:92:VAL:HG13	13:BO:93:PRO:HD2	1.92	0.53
6:AF:21:VAL:O	6:AF:25:THR:HG23	2.09	0.53
3:BC:167:VAL:HG12	22:BC:512:CLA:H2	1.89	0.52
18:BX:12:ILE:HG12	18:BX:16:LEU:CD1	2.35	0.52
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.52
3:AC:391:ARG:HH11	3:AC:391:ARG:CB	2.19	0.52
7:AH:55:LEU:O	7:AH:58:VAL:HG12	2.09	0.52
3:BC:71:GLU:OE1	3:BC:89:ILE:HG13	2.08	0.52
4:BD:55:VAL:HG21	4:BD:110:LEU:CD1	2.39	0.52
15:AU:100:ARG:HH11	15:AU:103:GLN:HG2	1.73	0.52
1:BA:43:ALA:HB1	26:BA:410:BCR:H362	1.91	0.52
1:BA:300:PHE:CZ	3:BC:404:LEU:HD23	2.45	0.52
2:AB:341:LYS:HD2	2:AB:429:ILE:HG22	1.90	0.52
15:BU:72:TYR:CB	15:BU:73:PRO:HD3	2.34	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:60:ILE:HG23	22:AC:510:CLA:HMC2	1.91	0.52
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.91	0.52
4:AD:71:CYS:HB2	4:AD:76:VAL:HG12	1.91	0.52
3:AC:80:PRO:HB2	3:AC:83:GLU:HG3	1.90	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.24	0.52
1:AA:196:PRO:HA	1:AA:199:GLN:OE1	2.09	0.52
3:AC:466:VAL:HG13	4:AD:251:ARG:HD2	1.90	0.52
1:AA:49:VAL:O	1:AA:53:ILE:HG13	2.10	0.52
13:BO:234:THR:OG1	13:BO:236:GLU:HG2	2.09	0.52
1:BA:232:SER:HB3	1:BA:235:TYR:CD1	2.44	0.52
6:AF:18:VAL:HG13	6:AF:19:ARG:N	2.25	0.52
15:AU:66:ILE:HG13	15:AU:72:TYR:CD1	2.44	0.52
4:AD:161:PRO:HG3	4:AD:170:ALA:HB2	1.91	0.52
1:AA:22:THR:HG21	8:AI:30:ARG:HD3	1.90	0.52
16:BV:74:THR:O	16:BV:75:ASN:HB2	2.09	0.52
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.92	0.52
15:BU:83:ALA:CB	15:BU:84:PRO:HD2	2.15	0.52
3:BC:269:GLU:OE1	22:BC:508:CLA:HED1	2.08	0.52
30:BD:407:LMG:O3	9:BJ:37:GLY:HA3	2.09	0.52
3:AC:429:SER:HB3	27:AC:517:DGD:HA81	1.91	0.52
2:BB:133:LEU:HB3	2:BB:138:MET:HE1	1.90	0.52
14:BT:7:VAL:HG12	32:BT:101:LMT:H122	1.91	0.52
13:AO:141:ARG:HG2	13:AO:141:ARG:NH1	2.24	0.52
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
16:AV:135:GLU:O	16:AV:139:VAL:HG23	2.08	0.52
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.91	0.52
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.90	0.52
9:BJ:18:GLY:HA3	26:BK:102:BCR:H371	1.92	0.52
2:AB:10:THR:C	2:AB:12:LEU:H	2.12	0.52
3:BC:116:VAL:HG21	26:BZ:101:BCR:H323	1.91	0.52
3:AC:163:PHE:CD1	22:AC:512:CLA:HAB	2.45	0.52
26:AT:102:BCR:C40	2:BB:36:SER:HB2	2.40	0.52
4:AD:85:MET:HE2	5:AE:69:ARG:HA	1.90	0.52
4:BD:87:HIS:CD2	4:BD:162:LEU:HA	2.45	0.52
1:BA:81:ALA:CB	1:BA:175:GLY:HA3	2.39	0.52
2:BB:220:ARG:HB3	2:BB:221:PRO:HD2	1.92	0.52
22:BC:504:CLA:H202	27:BC:518:DGD:HAF2	1.92	0.52
27:BC:517:DGD:HB62	26:BJ:102:BCR:H352	1.91	0.52
10:AK:24:VAL:O	10:AK:27:VAL:HG12	2.10	0.52
30:AD:408:LMG:H392	26:AT:102:BCR:HC32	1.92	0.52
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.45	0.52
1:BA:317:TRP:CD1	4:BD:177:ALA:HB2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:269:GLU:OE1	3:AC:447:ARG:HG2	2.10	0.52
20:BZ:31:GLN:O	20:BZ:32:ASP:HB3	2.10	0.52
3:BC:29:GLU:HB3	10:BK:46:ARG:HH11	1.74	0.52
13:AO:223:ILE:HG13	13:AO:243:SER:HB3	1.92	0.52
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.39	0.52
3:BC:466:VAL:HG13	4:BD:251:ARG:HD2	1.92	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:CD1	2.45	0.52
22:AB:604:CLA:H101	22:AB:615:CLA:H42	1.91	0.52
3:BC:155:ASN:CA	3:BC:158:THR:HG22	2.39	0.52
2:BB:10:THR:C	2:BB:12:LEU:H	2.11	0.52
3:BC:163:PHE:CD1	22:BC:512:CLA:HAB	2.44	0.52
10:AK:43:VAL:HG13	10:AK:43:VAL:O	2.09	0.52
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.40	0.52
16:AV:147:VAL:O	16:AV:150:LYS:HB2	2.10	0.52
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.10	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.52
3:AC:415:ASN:O	3:AC:416:SER:CB	2.57	0.52
12:BM:25:LEU:O	12:BM:28:GLN:HG3	2.10	0.52
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.09	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:HD1	1.75	0.52
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.52
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.10	0.52
3:BC:47:GLY:O	3:BC:50:LEU:HB3	2.10	0.52
3:BC:199:ILE:N	3:BC:199:ILE:HD12	2.25	0.52
20:AZ:17:PHE:CE2	20:AZ:21:ILE:HD11	2.45	0.52
20:BZ:17:PHE:CE2	20:BZ:21:ILE:HD11	2.45	0.52
18:AX:17:LYS:O	18:AX:21:ILE:HG13	2.10	0.52
4:AD:266:TRP:HD1	30:AD:408:LMG:HC3	1.74	0.52
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.52
13:BO:31:LEU:HD12	13:BO:31:LEU:H	1.75	0.52
2:AB:224:ARG:NE	7:AH:25:TRP:NE1	2.58	0.52
13:BO:59:ASP:C	13:BO:61:SER:H	2.13	0.52
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.92	0.52
3:BC:296:VAL:HG23	3:BC:297:TYR:CD2	2.45	0.52
22:BB:607:CLA:H101	22:BB:618:CLA:H42	1.91	0.51
4:BD:252:PHE:O	4:BD:256:ILE:HG22	2.10	0.51
22:AB:603:CLA:H193	7:AH:42:LEU:HD12	1.92	0.51
22:BB:611:CLA:H12	4:BD:127:LEU:HD21	1.92	0.51
1:AA:227:THR:HA	1:AA:231:GLU:OE2	2.10	0.51
1:BA:22:THR:HG21	8:BI:30:ARG:HD3	1.91	0.51
13:BO:141:ARG:NH1	13:BO:141:ARG:HG2	2.24	0.51
4:BD:350:ASN:O	4:BD:352:LEU:N	2.42	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:279:PRO:CG	4:AD:212:ALA:HB2	2.40	0.51
1:AA:43:ALA:HB1	26:AA:409:BCR:H362	1.92	0.51
13:AO:178:ARG:HG3	13:AO:178:ARG:NH1	2.01	0.51
3:AC:418:ASN:HD21	27:AC:517:DGD:HD4	1.74	0.51
28:AC:521:LHG:H162	26:AJ:102:BCR:H313	1.91	0.51
3:BC:116:VAL:CG2	26:BZ:101:BCR:H323	2.41	0.51
20:AZ:3:ILE:O	20:AZ:7:LEU:HG	2.09	0.51
4:BD:136:VAL:HG12	4:BD:136:VAL:O	2.10	0.51
10:BK:35:LEU:HA	10:BK:38:VAL:HG23	1.92	0.51
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.74	0.51
2:BB:61:PHE:CE1	22:BB:610:CLA:HMB3	2.45	0.51
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.51
1:BA:190:HIS:O	1:BA:298:ASN:HB3	2.11	0.51
3:BC:391:ARG:CB	3:BC:391:ARG:HH11	2.22	0.51
2:BB:9:HIS:HB2	22:BB:614:CLA:HBA1	1.91	0.51
4:AD:85:MET:CE	5:AE:69:ARG:HA	2.41	0.51
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.25	0.51
10:BK:20:PRO:O	10:BK:23:ASP:HB2	2.10	0.51
1:AA:140:ARG:NH2	1:AA:142:TRP:HZ3	2.07	0.51
20:BZ:32:ASP:CG	20:BZ:33:TRP:N	2.62	0.51
4:AD:221:THR:HG23	4:AD:221:THR:O	2.10	0.51
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.10	0.51
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.11	0.51
4:AD:87:HIS:CD2	4:AD:162:LEU:HA	2.45	0.51
1:BA:20:TRP:O	1:BA:21:VAL:C	2.49	0.51
20:BZ:5:PHE:CE1	20:BZ:54:VAL:HG13	2.46	0.51
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.51
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.76	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
3:AC:250:TRP:CD1	3:AC:250:TRP:C	2.84	0.51
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.11	0.51
2:BB:434:THR:CG2	13:BO:204:LYS:HE3	2.40	0.51
26:BA:410:BCR:H312	8:BI:15:PHE:CE1	2.45	0.51
4:AD:136:VAL:O	4:AD:136:VAL:HG12	2.10	0.51
2:BB:150:CYS:HA	22:BB:606:CLA:HBC2	1.91	0.51
22:BB:613:CLA:H12	22:BB:613:CLA:H112	1.92	0.51
2:AB:12:LEU:CD2	2:AB:18:ARG:HB2	2.40	0.51
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.76	0.51
16:BV:95:ILE:O	16:BV:99:VAL:HG23	2.09	0.51
2:AB:125:ASP:OD2	2:AB:127:ARG:HB3	2.11	0.51
3:AC:117:VAL:HG12	30:AC:520:LMG:H191	1.92	0.51
2:AB:36:SER:HB2	26:AB:618:BCR:C40	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:BH:55:LEU:HB2	7:BH:58:VAL:HG12	1.93	0.51
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.40	0.51
13:BO:223:ILE:HG12	13:BO:224:SER:N	2.25	0.51
1:BA:196:PRO:HA	1:BA:199:GLN:OE1	2.10	0.51
2:BB:55:MET:CE	2:BB:80:ILE:HD12	2.41	0.51
3:BC:72:LEU:HD11	3:BC:108:THR:HB	1.93	0.51
26:BC:514:BCR:H391	10:BK:36:ALA:HB2	1.93	0.51
22:AB:610:CLA:H112	22:AB:610:CLA:H12	1.93	0.51
20:BZ:32:ASP:OD1	20:BZ:36:SER:HB2	2.11	0.51
22:AC:513:CLA:HMC2	26:AZ:101:BCR:H372	1.93	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.92	0.51
3:BC:62:PHE:HE2	10:BK:29:PRO:HD3	1.75	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB3	1.93	0.51
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.91	0.51
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.46	0.51
3:BC:155:ASN:HA	3:BC:158:THR:CG2	2.38	0.51
32:AB:625:LMT:H102	7:AH:35:MET:SD	2.51	0.51
18:AX:16:LEU:C	18:AX:16:LEU:HD13	2.31	0.51
18:AX:12:ILE:CG1	18:AX:16:LEU:HD12	2.33	0.51
4:BD:221:THR:O	4:BD:221:THR:HG23	2.10	0.51
1:BA:306:VAL:HG11	1:BA:316:THR:HG23	1.92	0.51
4:BD:86:GLY:O	4:BD:166:SER:HB2	2.11	0.51
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.93	0.51
6:AF:16:PHE:CD2	29:AF:101:SQD:H262	2.46	0.51
3:BC:269:GLU:OE1	3:BC:447:ARG:HG2	2.11	0.51
2:BB:256:MET:HA	2:BB:263:THR:HG21	1.93	0.51
1:AA:29:TYR:OH	1:AA:132:GLU:OE2	2.25	0.51
2:AB:12:LEU:HB2	22:AB:612:CLA:HMC2	1.93	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.46	0.51
3:BC:447:ARG:HH11	3:BC:447:ARG:CG	2.14	0.50
3:BC:42:LEU:CD1	22:BC:511:CLA:HMA3	2.38	0.50
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.77	0.50
3:BC:135:ARG:HB2	20:BZ:27:TYR:CG	2.46	0.50
3:AC:116:VAL:HG21	26:AZ:101:BCR:H323	1.92	0.50
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.46	0.50
24:BA:408:PL9:H301	4:BD:42:TYR:HA	1.94	0.50
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.74	0.50
3:BC:80:PRO:HB2	3:BC:83:GLU:HG3	1.91	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.24	0.50
29:BA:413:SQD:H5	4:BD:232:PHE:HB3	1.93	0.50
22:BC:504:CLA:HED1	30:BC:519:LMG:O3	2.11	0.50
3:AC:158:THR:HG21	3:AC:254:THR:O	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:116:VAL:CG2	26:AZ:101:BCR:H323	2.41	0.50
16:BV:147:VAL:O	16:BV:150:LYS:HB2	2.11	0.50
2:BB:63:LEU:N	2:BB:64:PRO:HD2	2.27	0.50
1:AA:149:ALA:HB3	1:AA:150:PRO:CD	2.41	0.50
20:AZ:5:PHE:HA	20:AZ:57:LEU:CD2	2.40	0.50
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.10	0.50
13:BO:190:LEU:HB2	13:BO:214:LYS:HB2	1.93	0.50
3:BC:193:GLY:O	3:BC:194:GLY:C	2.48	0.50
2:BB:149:LEU:HG	22:BB:606:CLA:CBC	2.30	0.50
18:AX:12:ILE:O	18:AX:12:ILE:CG2	2.58	0.50
3:AC:167:VAL:HG12	22:AC:512:CLA:H2	1.94	0.50
1:AA:283:VAL:O	1:AA:286:THR:HG22	2.11	0.50
4:BD:62:GLY:HA3	5:BE:63:ILE:HD13	1.94	0.50
13:AO:86:ARG:HH11	13:AO:87:GLN:HA	1.75	0.50
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.27	0.50
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.93	0.50
1:BA:232:SER:HB3	1:BA:235:TYR:HD1	1.75	0.50
8:BI:27:ASP:N	8:BI:28:PRO:CD	2.74	0.50
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.50
22:AC:504:CLA:H202	27:AC:518:DGD:HAF2	1.94	0.50
3:AC:159:THR:HG23	3:AC:252:ILE:HD13	1.93	0.50
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.47	0.50
5:BE:8:ARG:HB2	6:BF:13:TYR:HB3	1.92	0.50
18:BX:17:LYS:O	18:BX:21:ILE:HG13	2.11	0.50
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	2.11	0.50
22:AB:605:CLA:HBB1	22:AB:606:CLA:H51	1.92	0.50
4:BD:134:ARG:HA	4:BD:134:ARG:HE	1.76	0.50
29:AA:412:SQD:H223	27:AC:518:DGD:HAE1	1.92	0.50
3:AC:418:ASN:HB2	27:AC:518:DGD:HE2	1.92	0.50
22:AB:607:CLA:H42	30:AB:622:LMG:H131	1.92	0.50
3:BC:413:GLU:HG3	3:BC:414:ILE:N	2.27	0.50
13:BO:223:ILE:HG13	13:BO:243:SER:HB3	1.93	0.50
3:AC:81:MET:CE	3:AC:89:ILE:HG22	2.42	0.50
20:AZ:5:PHE:CE1	20:AZ:54:VAL:HG13	2.46	0.50
18:BX:32:LEU:HD23	18:BX:32:LEU:N	2.26	0.50
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.46	0.50
20:AZ:12:LEU:HB2	20:AZ:50:LEU:HD22	1.93	0.50
28:BA:412:LHG:HC12	22:BC:508:CLA:O1D	2.12	0.50
30:AI:101:LMG:H181	32:AI:102:LMT:H42	1.94	0.50
34:BE:101:HEM:HBC2	6:BF:27:ALA:CB	2.37	0.50
22:BB:611:CLA:H151	22:BB:612:CLA:H203	1.93	0.50
2:BB:471:ALA:HB2	4:BD:130:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:AB:612:CLA:H171	22:AB:613:CLA:HBB2	1.94	0.50
22:AB:609:CLA:HMC2	26:AH:101:BCR:H343	1.92	0.50
2:BB:12:LEU:CD2	2:BB:18:ARG:HB2	2.41	0.50
22:AA:403:CLA:HED2	4:AD:198:MET:SD	2.51	0.50
2:AB:9:HIS:HB2	22:AB:611:CLA:HBA1	1.93	0.50
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.11	0.50
3:BC:154:LYS:HE2	3:BC:261:ARG:HD2	1.93	0.50
1:AA:63:ILE:HB	3:AC:335:THR:HG21	1.92	0.50
18:BX:43:ILE:HG22	18:BX:43:ILE:O	2.11	0.50
29:AA:415:SQD:H2	22:BB:619:CLA:H43	1.94	0.50
22:AC:505:CLA:HMD1	22:AC:507:CLA:HAB	1.92	0.50
3:AC:117:VAL:CG1	30:AC:520:LMG:H191	2.41	0.50
2:BB:124:ARG:NH1	2:BB:124:ARG:HG3	2.22	0.50
4:BD:217:THR:O	4:BD:221:THR:HB	2.11	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.50
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.11	0.50
2:AB:55:MET:CE	2:AB:80:ILE:HD12	2.42	0.50
13:AO:59:ASP:HB3	13:AO:62:GLN:HB3	1.93	0.50
27:BC:517:DGD:HBV1	28:BC:521:LHG:H151	1.93	0.50
22:AB:616:CLA:H43	29:BA:401:SQD:H2	1.94	0.50
22:BC:505:CLA:HMD1	22:BC:507:CLA:HAB	1.92	0.50
5:AE:81:GLU:C	5:AE:83:LEU:N	2.64	0.50
2:AB:286:ARG:NH1	2:AB:286:ARG:HG2	2.26	0.50
16:AV:95:ILE:O	16:AV:99:VAL:HG23	2.12	0.50
3:BC:275:SER:HB3	22:BC:509:CLA:HED3	1.94	0.50
30:AI:101:LMG:HC2	32:BB:603:LMT:H11	1.93	0.50
2:AB:141:ILE:HG23	22:AB:615:CLA:HBB1	1.92	0.50
2:BB:96:VAL:HG22	22:BB:609:CLA:HBA1	1.94	0.50
3:AC:269:GLU:OE1	22:AC:508:CLA:HED1	2.12	0.50
3:BC:250:TRP:C	3:BC:250:TRP:CD1	2.85	0.50
3:AC:265:ILE:HG12	22:AC:505:CLA:HED1	1.94	0.50
16:BV:45:ILE:HG12	16:BV:46:THR:N	2.26	0.50
32:AB:627:LMT:H11	30:BI:101:LMG:HC2	1.93	0.50
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.50
1:BA:221:SER:HB3	4:BD:141:TYR:HB2	1.94	0.50
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.46	0.50
2:BB:246:PHE:C	2:BB:246:PHE:CD1	2.85	0.50
1:BA:206:PHE:CE2	22:BD:402:CLA:HBA1	2.47	0.49
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.12	0.49
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.25	0.49
1:BA:330:VAL:HG12	4:BD:348:ARG:HA	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.80	0.49
5:BE:8:ARG:HB2	6:BF:13:TYR:CB	2.42	0.49
1:BA:96:ILE:HG12	1:BA:105:TRP:CE2	2.47	0.49
1:AA:96:ILE:HG12	1:AA:105:TRP:CE2	2.47	0.49
9:AJ:18:GLY:HA3	26:AK:102:BCR:H371	1.93	0.49
3:BC:418:ASN:HB2	27:BC:518:DGD:HE2	1.93	0.49
4:BD:180:ARG:NH1	4:BD:180:ARG:CG	2.69	0.49
2:AB:471:ALA:HB2	4:AD:130:PHE:HZ	1.78	0.49
13:AO:31:LEU:HB2	13:AO:36:ILE:CD1	2.38	0.49
3:AC:391:ARG:HD2	3:AC:395:TYR:CZ	2.47	0.49
4:BD:85:MET:HE2	5:BE:69:ARG:HA	1.94	0.49
1:BA:84:PRO:HA	1:BA:112:TYR:CG	2.47	0.49
3:BC:452:ALA:O	3:BC:454:GLY:N	2.44	0.49
18:BX:32:LEU:O	18:BX:36:VAL:HG23	2.11	0.49
3:AC:315:MET:O	3:AC:319:ILE:HG13	2.12	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
3:AC:72:LEU:HD11	3:AC:108:THR:HB	1.93	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.12	0.49
22:BC:504:CLA:H151	27:BC:517:DGD:HBW1	1.93	0.49
3:AC:473:ASP:CB	14:AT:26:PRO:HB3	2.36	0.49
2:AB:462:PHE:CZ	22:AB:613:CLA:HMB3	2.47	0.49
3:AC:135:ARG:HE	20:AZ:33:TRP:HE1	1.59	0.49
4:BD:54:PHE:HB3	5:BE:47:PHE:CD2	2.47	0.49
3:AC:275:SER:HB3	22:AC:509:CLA:HED3	1.94	0.49
16:AV:29:LEU:HD11	16:AV:34:LEU:HD21	1.92	0.49
1:AA:224:ILE:O	1:AA:226:GLU:OE2	2.30	0.49
2:AB:220:ARG:HB3	2:AB:221:PRO:HD2	1.93	0.49
4:BD:279:LEU:HD11	22:BD:402:CLA:O1A	2.13	0.49
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.60	0.49
14:BT:25:GLU:O	14:BT:26:PRO:C	2.50	0.49
32:BB:626:LMT:H3'	29:BD:409:SQD:H62	1.95	0.49
7:AH:35:MET:HE2	26:AH:101:BCR:H322	1.93	0.49
3:BC:116:VAL:HG23	3:BC:117:VAL:N	2.28	0.49
20:BZ:29:SER:C	20:BZ:31:GLN:H	2.16	0.49
11:AL:12:LEU:HD22	12:AM:25:LEU:HD12	1.93	0.49
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.95	0.49
10:BK:25:LEU:HB2	10:BK:26:PRO:HD3	1.94	0.49
5:BE:34:GLY:HA2	6:BF:32:PHE:CE1	2.48	0.49
4:BD:176:ALA:HA	4:BD:179:PHE:CD2	2.47	0.49
26:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.95	0.49
26:BC:514:BCR:HC22	10:BK:18:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:24:LEU:HB3	2:BB:111:ALA:HB2	1.94	0.49
22:AB:608:CLA:H151	22:AB:609:CLA:H203	1.93	0.49
3:BC:174:LEU:HG	22:BC:512:CLA:H92	1.93	0.49
3:AC:109:PHE:HB3	3:AC:110:PRO:HD3	1.94	0.49
5:BE:4:THR:CG2	5:BE:5:THR:N	2.76	0.49
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.93	0.49
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.49
2:BB:134:ASP:OD2	2:BB:137:LYS:HB2	2.12	0.49
4:BD:266:TRP:HD1	30:BD:408:LMG:HC3	1.76	0.49
22:AB:608:CLA:H51	22:AB:609:CLA:H101	1.94	0.49
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.28	0.49
13:BO:43:ASN:OD1	13:BO:103:SER:HB2	2.11	0.49
13:AO:43:ASN:OD1	13:AO:103:SER:HB2	2.12	0.49
8:BI:30:ARG:O	8:BI:31:ASN:HB3	2.13	0.49
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.12	0.49
9:BJ:34:ALA:O	9:BJ:35:GLY:O	2.31	0.49
1:BA:124:SER:O	1:BA:127:MET:HB3	2.12	0.49
2:AB:137:LYS:O	2:AB:141:ILE:HG13	2.11	0.49
22:BB:608:CLA:HMA1	22:BB:609:CLA:HBA2	1.94	0.49
3:BC:473:ASP:CB	14:BT:26:PRO:HB3	2.37	0.49
22:AD:404:CLA:C4	18:AX:26:GLY:HA3	2.34	0.49
3:AC:405:ASN:HD22	27:AC:518:DGD:C5D	2.25	0.49
24:AA:407:PL9:H301	4:AD:42:TYR:HA	1.94	0.49
1:BA:32:TRP:HA	1:BA:32:TRP:HE3	1.75	0.49
3:BC:90:PRO:O	3:BC:94:THR:HG23	2.12	0.49
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.12	0.49
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.94	0.49
29:BL:101:SQD:H45	14:BT:23:PHE:CD1	2.47	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.34	0.49
3:AC:135:ARG:HB2	20:AZ:27:TYR:CG	2.48	0.49
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.49
4:BD:87:HIS:ND1	27:BH:101:DGD:HD2	2.27	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
5:BE:9:PRO:HB3	30:BE:102:LMG:HC4	1.95	0.49
1:AA:300:PHE:CZ	3:AC:404:LEU:HD23	2.48	0.49
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.12	0.49
8:AI:6:ILE:O	8:AI:10:ILE:HG12	2.13	0.49
22:BB:608:CLA:HBB1	22:BB:609:CLA:H51	1.95	0.49
3:AC:447:ARG:CG	3:AC:447:ARG:NH1	2.74	0.49
5:BE:81:GLU:C	5:BE:83:LEU:N	2.65	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.28	0.49
2:AB:55:MET:HE2	2:AB:80:ILE:HD12	1.94	0.49
2:BB:293:ALA:C	2:BB:295:GLY:H	2.15	0.49
1:BA:114:LEU:C	1:BA:114:LEU:HD23	2.33	0.49
5:AE:9:PRO:HB3	30:AE:102:LMG:HC4	1.95	0.49
9:AJ:11:TRP:CG	10:AK:42:ALA:HA	2.48	0.49
10:BK:18:PHE:O	10:BK:22:VAL:HG23	2.13	0.49
1:AA:28:LEU:HD12	29:AA:415:SQD:H111	1.94	0.49
2:AB:69:LEU:HD21	22:AB:603:CLA:HED3	1.95	0.49
5:BE:22:ILE:O	5:BE:26:THR:HG23	2.13	0.49
3:AC:405:ASN:HB2	27:AC:518:DGD:HG31	1.95	0.49
22:AA:403:CLA:HED1	24:AD:405:PL9:H372	1.95	0.49
1:AA:13:LEU:HD12	1:AA:13:LEU:N	2.28	0.49
4:BD:67:TYR:CE1	4:BD:76:VAL:HG11	2.47	0.49
13:BO:92:VAL:HG12	13:BO:93:PRO:CD	2.43	0.49
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.43	0.49
3:BC:94:THR:HG22	3:BC:298:PRO:HD2	1.95	0.49
3:AC:90:PRO:O	3:AC:94:THR:HG23	2.12	0.49
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.95	0.49
4:BD:86:GLY:HA2	4:BD:166:SER:HB3	1.94	0.49
10:AK:15:TYR:HE2	20:AZ:62:VAL:HG21	1.78	0.49
3:BC:35:TRP:CG	3:BC:36:TRP:N	2.81	0.48
1:BA:283:VAL:HG21	23:BA:406:PHO:HBC3	1.95	0.48
2:AB:69:LEU:HD12	22:AB:605:CLA:HBA1	1.95	0.48
3:BC:60:ILE:HG23	22:BC:510:CLA:HMC2	1.94	0.48
3:BC:135:ARG:NE	20:BZ:33:TRP:HE1	2.11	0.48
4:BD:71:CYS:HB2	4:BD:76:VAL:HG12	1.95	0.48
1:BA:228:THR:HG22	1:BA:229:GLU:N	2.27	0.48
13:AO:94:THR:HB	13:AO:135:GLN:O	2.12	0.48
1:BA:278:TRP:HB3	1:BA:279:PRO:CD	2.42	0.48
2:BB:35:GLY:O	2:BB:38:ALA:HB3	2.12	0.48
7:AH:30:LEU:HD11	7:AH:34:PHE:HE1	1.78	0.48
1:BA:37:MET:HG2	1:BA:41:LEU:HD12	1.94	0.48
32:AB:625:LMT:H3'	29:AD:409:SQD:H62	1.95	0.48
3:BC:159:THR:HG23	3:BC:252:ILE:HD13	1.94	0.48
22:BC:503:CLA:H172	22:BC:510:CLA:HBB2	1.94	0.48
18:BX:16:LEU:HD13	18:BX:16:LEU:C	2.33	0.48
22:AA:402:CLA:H202	22:AA:403:CLA:H93	1.96	0.48
1:BA:13:LEU:HD12	1:BA:13:LEU:N	2.27	0.48
4:BD:49:LEU:HD13	26:BD:406:BCR:C15	2.43	0.48
3:BC:89:ILE:N	3:BC:90:PRO:CD	2.74	0.48
13:AO:159:VAL:O	13:AO:159:VAL:HG13	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:55:MET:HE2	2:BB:80:ILE:HD12	1.94	0.48
20:AZ:5:PHE:HA	20:AZ:57:LEU:HD21	1.95	0.48
26:AB:617:BCR:HC31	12:AM:10:ALA:HB2	1.94	0.48
2:BB:125:ASP:OD2	2:BB:127:ARG:HB3	2.13	0.48
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.13	0.48
13:BO:240:THR:HA	13:BO:264:VAL:HA	1.95	0.48
3:BC:425:TRP:CZ2	22:BC:504:CLA:HBA1	2.48	0.48
9:BJ:11:TRP:CG	10:BK:42:ALA:HA	2.48	0.48
1:BA:45:THR:HG23	1:BA:46:ILE:N	2.28	0.48
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.48
4:AD:134:ARG:HE	4:AD:134:ARG:HA	1.78	0.48
7:AH:35:MET:HE2	26:AH:101:BCR:C32	2.44	0.48
5:AE:28:PRO:O	5:AE:32:ILE:HG13	2.13	0.48
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.48	0.48
1:BA:326:LEU:HD21	3:BC:412:THR:HB	1.94	0.48
3:BC:33:PHE:CD1	4:BD:229:ALA:HB3	2.48	0.48
13:BO:59:ASP:HB3	13:BO:62:GLN:HB3	1.95	0.48
7:BH:30:LEU:HD11	7:BH:34:PHE:HE1	1.78	0.48
13:BO:73:PRO:HG2	13:BO:102:THR:HB	1.95	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
3:BC:258:GLY:CA	3:BC:262:ARG:HH12	2.26	0.48
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.13	0.48
3:AC:425:TRP:CZ2	22:AC:504:CLA:HBA1	2.48	0.48
22:AC:504:CLA:H151	27:AC:517:DGD:HBW1	1.95	0.48
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	1.96	0.48
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.79	0.48
2:AB:256:MET:O	2:AB:448:ARG:NH1	2.42	0.48
1:AA:221:SER:HB2	4:AD:139:ARG:O	2.13	0.48
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.44	0.48
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.13	0.48
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
13:AO:226:ASN:N	13:AO:226:ASN:HD22	2.11	0.48
4:AD:193:LEU:O	4:AD:193:LEU:HG	2.14	0.48
34:AV:201:HEM:HHA	34:AV:201:HEM:HAD2	1.61	0.48
10:BK:17:ILE:CD1	10:BK:17:ILE:H	2.26	0.48
26:AA:409:BCR:H312	8:AI:15:PHE:HE1	1.79	0.48
2:BB:141:ILE:HG23	22:BB:618:CLA:HBB1	1.94	0.48
2:BB:262:THR:HG22	2:BB:263:THR:HG23	1.96	0.48
22:AC:504:CLA:HED1	30:AC:519:LMG:O3	2.13	0.48
20:BZ:35:ARG:HG3	20:BZ:36:SER:N	2.28	0.48
4:AD:62:GLY:HA3	5:AE:63:ILE:HD13	1.96	0.48
13:BO:86:ARG:HH11	13:BO:86:ARG:C	2.16	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:72:LEU:HD21	32:BT:101:LMT:H31	1.96	0.48
3:AC:71:GLU:OE1	3:AC:89:ILE:HG13	2.13	0.48
1:BA:243:GLU:CD	1:BA:243:GLU:H	2.12	0.48
1:BA:63:ILE:HB	3:BC:335:THR:HG21	1.94	0.48
22:BB:606:CLA:H193	7:BH:42:LEU:HD12	1.95	0.48
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.13	0.48
1:BA:190:HIS:HB3	1:BA:293:MET:CE	2.42	0.48
7:BH:55:LEU:O	7:BH:58:VAL:HG12	2.12	0.48
13:AO:86:ARG:O	13:AO:86:ARG:NH1	2.37	0.48
13:BO:159:VAL:O	13:BO:159:VAL:HG13	2.13	0.48
3:BC:216:SER:HB3	3:BC:221:GLU:HB2	1.95	0.48
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.48
20:BZ:47:TRP:O	20:BZ:50:LEU:HB2	2.13	0.48
16:BV:148:GLU:OE1	16:BV:148:GLU:HA	2.13	0.48
28:BC:521:LHG:H271	28:BC:521:LHG:H101	1.95	0.48
2:AB:137:LYS:HZ1	7:AH:17:GLU:H	1.61	0.48
15:BU:72:TYR:HB3	15:BU:73:PRO:CD	2.37	0.48
1:BA:258:LEU:HD12	4:BD:128:ARG:CD	2.42	0.48
1:BA:214:MET:HE2	1:BA:214:MET:HA	1.96	0.48
10:BK:46:ARG:NH1	10:BK:46:ARG:HB2	2.28	0.48
1:BA:343:LEU:O	1:BA:344:ALA:CB	2.60	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.48	0.48
3:AC:315:MET:CE	3:AC:366:LEU:HD13	2.44	0.48
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.95	0.48
2:BB:137:LYS:O	2:BB:141:ILE:HG13	2.14	0.48
6:BF:23:VAL:O	6:BF:27:ALA:CB	2.61	0.48
15:BU:66:ILE:HG13	15:BU:72:TYR:CD1	2.49	0.48
3:AC:48:LYS:HD2	3:AC:138:GLU:HG3	1.94	0.48
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.95	0.48
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.48
5:BE:10:PHE:HB2	30:BE:102:LMG:O2	2.14	0.48
13:AO:194:TYR:CE1	13:AO:198:ILE:HD13	2.49	0.48
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.49	0.48
13:BO:173:ASN:ND2	13:BO:220:LYS:HD3	2.29	0.48
3:BC:308:GLU:HB2	3:BC:361:PHE:CE1	2.49	0.48
22:AC:503:CLA:H172	22:AC:510:CLA:HBB2	1.95	0.48
1:AA:13:LEU:H	1:AA:13:LEU:CD1	2.27	0.48
13:BO:36:ILE:HD12	13:BO:36:ILE:N	2.29	0.48
3:BC:126:GLY:O	3:BC:130:VAL:HG23	2.13	0.48
2:AB:434:THR:CG2	13:AO:204:LYS:HE3	2.44	0.48
13:AO:225:LEU:C	13:AO:226:ASN:HD22	2.17	0.48
11:BL:22:LEU:O	11:BL:26:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:AL:24:ILE:HD12	11:AL:24:ILE:N	2.29	0.48
1:AA:114:LEU:HD23	1:AA:114:LEU:C	2.34	0.48
10:BK:37:PHE:HB3	26:BK:102:BCR:H402	1.95	0.48
3:BC:265:ILE:HG12	22:BC:505:CLA:HED1	1.95	0.48
4:AD:126:MET:CE	4:AD:150:ILE:HG13	2.43	0.48
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.48
2:AB:329:PRO:CB	22:AB:607:CLA:HED1	2.39	0.48
5:BE:15:THR:O	9:BJ:8:ILE:HD12	2.14	0.48
4:AD:87:HIS:ND1	27:AH:102:DGD:HD2	2.29	0.48
3:BC:81:MET:CE	3:BC:89:ILE:HG22	2.44	0.48
4:BD:210:LEU:HA	4:BD:213:ILE:HG22	1.96	0.48
1:AA:111:PRO:O	1:AA:115:ILE:HG13	2.14	0.48
29:BL:101:SQD:H45	14:BT:23:PHE:HD1	1.79	0.48
10:BK:15:TYR:HE2	20:BZ:62:VAL:HG21	1.77	0.48
4:BD:126:MET:CE	4:BD:150:ILE:HG13	2.44	0.47
4:BD:261:PHE:O	4:BD:262:SER:HB3	2.14	0.47
30:BD:408:LMG:O10	11:BL:18:TYR:HB3	2.13	0.47
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.28	0.47
1:BA:13:LEU:CD1	1:BA:13:LEU:H	2.26	0.47
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.47
16:BV:81:ARG:HH11	16:BV:81:ARG:HG2	1.78	0.47
13:BO:157:PRO:O	13:BO:158:ASN:O	2.32	0.47
3:BC:266:TRP:HB3	3:BC:271:TYR:OH	2.14	0.47
1:BA:279:PRO:CG	4:BD:212:ALA:HB2	2.44	0.47
20:BZ:12:LEU:HB2	20:BZ:50:LEU:HD22	1.96	0.47
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.14	0.47
13:AO:36:ILE:HD12	13:AO:36:ILE:N	2.29	0.47
2:BB:349:LYS:HG3	2:BB:350:GLU:OE1	2.14	0.47
2:BB:27:THR:HG22	2:BB:107:LEU:CD1	2.40	0.47
2:BB:224:ARG:HG3	7:BH:25:TRP:CD1	2.48	0.47
18:AX:32:LEU:O	18:AX:36:VAL:HG23	2.13	0.47
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.95	0.47
8:BI:6:ILE:O	8:BI:10:ILE:HG12	2.14	0.47
1:BA:188:ALA:HB2	1:BA:328:MET:HB2	1.94	0.47
5:BE:51:ARG:O	5:BE:53:ASP:N	2.47	0.47
5:AE:22:ILE:O	5:AE:26:THR:HG23	2.14	0.47
2:BB:462:PHE:CZ	22:BB:616:CLA:HMB3	2.49	0.47
3:BC:391:ARG:HD2	3:BC:395:TYR:CZ	2.49	0.47
1:BA:78:ILE:O	1:BA:176:ILE:HB	2.13	0.47
2:AB:246:PHE:CD1	2:AB:246:PHE:C	2.88	0.47
2:BB:256:MET:O	2:BB:448:ARG:NH1	2.45	0.47
28:AA:411:LHG:HC12	22:AC:508:CLA:O1D	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:124:ARG:HD3	2:BB:131:PRO:N	2.30	0.47
3:BC:347:GLY:HA3	13:BO:43:ASN:HB2	1.95	0.47
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.30	0.47
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.47	0.47
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.49	0.47
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.47	0.47
4:BD:93:TRP:HA	4:BD:99:GLY:H	1.80	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
19:BY:11:UNK:C	19:BY:13:UNK:N	2.76	0.47
3:BC:55:ALA:HB1	26:BC:514:BCR:C37	2.44	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.96	0.47
2:AB:124:ARG:HG3	2:AB:124:ARG:NH1	2.26	0.47
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.47
1:AA:12:ASN:O	1:AA:16:ARG:HG3	2.15	0.47
3:BC:413:GLU:HG3	3:BC:414:ILE:H	1.80	0.47
20:AZ:5:PHE:HE1	20:AZ:54:VAL:HG13	1.80	0.47
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.47
14:AT:23:PHE:CD1	29:BB:601:SQD:H45	2.49	0.47
3:BC:367:GLU:HB2	3:BC:368:PRO:HD3	1.97	0.47
1:AA:124:SER:O	1:AA:127:MET:HB3	2.15	0.47
28:BC:521:LHG:H162	26:BJ:102:BCR:H313	1.95	0.47
2:AB:141:ILE:HG21	22:AB:615:CLA:HBB1	1.97	0.47
4:BD:263:ASN:O	4:BD:266:TRP:N	2.47	0.47
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.14	0.47
3:AC:135:ARG:NE	20:AZ:33:TRP:HE1	2.12	0.47
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.47
7:BH:25:TRP:O	7:BH:26:GLY:C	2.53	0.47
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.14	0.47
3:BC:62:PHE:CE2	10:BK:29:PRO:HD3	2.49	0.47
15:BU:100:ARG:NH1	15:BU:103:GLN:HG2	2.29	0.47
2:BB:235:GLU:OE1	2:BB:472:ARG:NH1	2.48	0.47
2:AB:458:PHE:HB3	22:AB:604:CLA:HBC2	1.97	0.47
2:BB:69:LEU:HD12	22:BB:608:CLA:HBA1	1.97	0.47
5:BE:7:GLU:HB3	6:BF:19:ARG:CZ	2.45	0.47
22:BB:615:CLA:H171	22:BB:616:CLA:HBB2	1.96	0.47
22:BC:513:CLA:HMC2	26:BZ:101:BCR:H372	1.96	0.47
3:AC:250:TRP:HE1	22:AC:506:CLA:HED1	1.80	0.47
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.30	0.47
1:AA:206:PHE:CE2	22:AD:402:CLA:HBA1	2.50	0.47
3:BC:365:TRP:CB	3:BC:391:ARG:HG2	2.44	0.47
2:AB:7:ARG:NH2	30:AB:621:LMG:O3	2.46	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:BH:18:TYR:CG	7:BH:19:GLY:N	2.83	0.47
6:AF:41:GLN:OE1	9:AJ:31:GLY:HA3	2.15	0.47
2:BB:341:LYS:HA	2:BB:405:GLU:HB2	1.97	0.47
3:BC:205:ASP:OD1	3:BC:207:ARG:HB3	2.15	0.47
4:BD:185:PHE:CE2	4:BD:289:LEU:HD12	2.49	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
13:BO:194:TYR:CE1	13:BO:198:ILE:HD13	2.50	0.47
1:BA:296:ASN:HB2	3:BC:400:PRO:O	2.14	0.47
2:BB:175:THR:O	2:BB:176:GLY:O	2.33	0.47
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.80	0.47
22:AB:605:CLA:HMA1	22:AB:606:CLA:HBA2	1.96	0.47
29:AA:412:SQD:H5	4:AD:232:PHE:HB3	1.96	0.47
3:BC:109:PHE:HB3	3:BC:110:PRO:HD3	1.96	0.47
4:AD:49:LEU:HD13	26:AD:406:BCR:C15	2.45	0.47
1:AA:190:HIS:HB3	1:AA:293:MET:CE	2.43	0.47
2:BB:173:GLY:HA3	2:BB:265:ILE:HD11	1.95	0.47
5:AE:4:THR:CG2	5:AE:5:THR:N	2.77	0.47
1:BA:107:TYR:HD1	13:BO:141:ARG:NH1	2.13	0.47
13:BO:135:GLN:HG2	13:BO:141:ARG:HG3	1.96	0.47
5:BE:14:ILE:CG2	9:BJ:13:VAL:HG11	2.45	0.47
16:BV:130:MET:SD	16:BV:133:LEU:HD12	2.54	0.47
16:BV:39:ASN:HD21	16:BV:43:LYS:HB3	1.79	0.47
3:AC:27:ASP:OD1	3:AC:28:GLN:HG2	2.14	0.47
14:AT:4:ILE:HD13	26:AT:102:BCR:C38	2.44	0.47
22:AB:607:CLA:H193	11:AL:27:LEU:HD11	1.95	0.47
3:AC:365:TRP:CB	3:AC:391:ARG:HG2	2.45	0.47
5:AE:15:THR:O	9:AJ:8:ILE:HD12	2.15	0.47
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.15	0.47
30:BI:101:LMG:H181	32:BI:102:LMT:H42	1.97	0.47
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.27	0.47
3:AC:229:ASN:ND2	3:AC:232:ASP:OD1	2.44	0.47
4:BD:303:ILE:CD1	12:BM:2:GLU:HG2	2.45	0.47
3:BC:34:ALA:HB2	4:BD:230:SER:CB	2.44	0.47
4:AD:176:ALA:HA	4:AD:179:PHE:CD2	2.49	0.47
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.47
3:BC:405:ASN:HB2	27:BC:518:DGD:HG31	1.97	0.47
1:BA:317:TRP:O	1:BA:321:ILE:HG13	2.15	0.47
15:BU:72:TYR:O	15:BU:73:PRO:C	2.51	0.47
1:BA:258:LEU:O	4:BD:128:ARG:NH1	2.48	0.47
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.45	0.47
4:AD:261:PHE:O	4:AD:262:SER:HB3	2.14	0.47
4:AD:274:VAL:HG13	24:AD:405:PL9:H211	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:11:ALA:HB1	1:BA:15:GLU:OE1	2.15	0.47
1:BA:12:ASN:O	1:BA:16:ARG:HG3	2.14	0.47
1:AA:306:VAL:HG11	1:AA:316:THR:HG23	1.96	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.80	0.47
4:BD:89:LEU:HG	7:BH:50:ASN:OD1	2.15	0.47
2:BB:458:PHE:HB3	22:BB:607:CLA:HBC2	1.97	0.46
3:AC:53:HIS:HB3	22:AC:512:CLA:OBD	2.15	0.46
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.43	0.46
4:AD:14:TRP:CE3	18:AX:38:ILE:HD12	2.50	0.46
13:BO:77:LEU:HB3	13:BO:91:PHE:HB3	1.97	0.46
1:AA:32:TRP:HA	1:AA:32:TRP:HE3	1.76	0.46
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.45	0.46
3:BC:315:MET:HE1	3:BC:369:LEU:HD12	1.97	0.46
30:BE:102:LMG:HC71	30:BE:102:LMG:O9	2.15	0.46
1:BA:40:THR:HG23	22:BA:407:CLA:HBB1	1.96	0.46
6:BF:11:VAL:CG1	6:BF:12:SER:N	2.77	0.46
1:BA:60:ILE:HG23	1:BA:61:ASP:N	2.30	0.46
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	1.97	0.46
3:AC:258:GLY:CA	3:AC:262:ARG:HH12	2.28	0.46
13:BO:225:LEU:C	13:BO:226:ASN:HD22	2.18	0.46
4:BD:122:LEU:HB3	4:BD:150:ILE:CD1	2.46	0.46
22:AB:606:CLA:H72	26:AB:620:BCR:H311	1.97	0.46
22:BB:611:CLA:H51	22:BB:612:CLA:H101	1.97	0.46
2:AB:216:HIS:HE1	22:AB:609:CLA:C1A	2.29	0.46
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.23	0.46
4:AD:60:THR:HG23	4:AD:61:HIS:HD2	1.75	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.31	0.46
16:BV:98:LEU:O	16:BV:102:MET:HG3	2.16	0.46
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.46
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.46
3:BC:258:GLY:HA3	3:BC:262:ARG:HH12	1.80	0.46
13:BO:72:GLN:O	13:BO:263:GLY:HA3	2.14	0.46
26:BB:620:BCR:HC31	12:BM:10:ALA:HB2	1.97	0.46
1:BA:92:HIS:CD2	3:BC:219:GLY:HA3	2.49	0.46
16:AV:68:VAL:HG13	16:AV:68:VAL:O	2.15	0.46
27:BB:602:DGD:HE1	27:BB:602:DGD:HD5	1.66	0.46
2:AB:462:PHE:CE1	22:AB:613:CLA:HMB3	2.50	0.46
2:AB:474:LEU:O	4:AD:134:ARG:NH1	2.48	0.46
27:AC:517:DGD:HBV1	28:AC:521:LHG:H151	1.98	0.46
3:BC:114:VAL:HG13	22:BC:503:CLA:HMA3	1.97	0.46
4:AD:146:PHE:O	4:AD:150:ILE:HG12	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.46
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.46
4:BD:14:TRP:CE3	18:BX:38:ILE:HD12	2.51	0.46
13:BO:94:THR:HB	13:BO:135:GLN:O	2.14	0.46
1:AA:334:ARG:NH1	13:AO:184:ASP:C	2.69	0.46
2:BB:201:HIS:HD2	2:BB:202:HIS:ND1	2.13	0.46
2:BB:422:ARG:HG2	2:BB:422:ARG:HH11	1.80	0.46
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.96	0.46
22:BA:403:CLA:H202	22:BA:404:CLA:H93	1.98	0.46
1:AA:239:PHE:O	14:AT:29:ILE:HA	2.14	0.46
22:BD:404:CLA:C4	18:BX:26:GLY:HA3	2.36	0.46
2:BB:462:PHE:CE1	22:BB:616:CLA:HMB3	2.51	0.46
1:AA:283:VAL:HG21	23:AA:405:PHO:HBC3	1.97	0.46
5:BE:78:THR:HA	5:BE:81:GLU:HG2	1.98	0.46
13:BO:120:THR:HA	13:BO:153:ALA:O	2.15	0.46
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.46
2:BB:265:ILE:HG13	2:BB:266:GLU:N	2.30	0.46
2:AB:341:LYS:HA	2:AB:405:GLU:HB2	1.98	0.46
13:BO:226:ASN:HD22	13:BO:226:ASN:N	2.13	0.46
1:BA:149:ALA:HB3	1:BA:150:PRO:CD	2.45	0.46
13:BO:113:VAL:HA	13:BO:119:LEU:HD23	1.98	0.46
12:AM:24:ILE:HG12	12:BM:24:ILE:HG12	1.98	0.46
1:BA:216:GLY:O	1:BA:220:THR:HG22	2.16	0.46
5:BE:64:PRO:HD3	5:BE:84:LYS:HE2	1.97	0.46
3:BC:460:ASP:O	3:BC:461:ARG:C	2.54	0.46
3:BC:315:MET:O	3:BC:319:ILE:HG13	2.16	0.46
3:BC:33:PHE:HE1	4:BD:229:ALA:CB	2.28	0.46
13:AO:113:VAL:HA	13:AO:119:LEU:HD23	1.97	0.46
15:BU:56:ASP:HB3	15:BU:60:THR:H	1.80	0.46
4:BD:26:ARG:HD3	6:BF:18:VAL:CG1	2.34	0.46
7:BH:35:MET:HE2	26:BX:101:BCR:H322	1.96	0.46
2:AB:10:THR:O	2:AB:13:ILE:HG13	2.16	0.46
3:BC:223:TRP:CE3	3:BC:224:ILE:HG13	2.51	0.46
20:AZ:35:ARG:HG3	20:AZ:36:SER:N	2.30	0.46
1:BA:10:SER:C	1:BA:12:ASN:H	2.19	0.46
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.16	0.46
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.97	0.46
2:BB:7:ARG:NH2	30:BB:623:LMG:O3	2.49	0.46
3:AC:258:GLY:HA3	3:AC:262:ARG:HH12	1.81	0.46
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.46	0.46
3:BC:405:ASN:HD22	27:BC:518:DGD:C5D	2.25	0.46
2:AB:96:VAL:HG22	22:AB:606:CLA:HBA1	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.46
20:BZ:32:ASP:C	20:BZ:34:ASP:H	2.17	0.46
4:AD:217:THR:O	4:AD:221:THR:HB	2.15	0.46
2:AB:59:GLY:HA3	22:AB:607:CLA:HED1	1.98	0.46
3:BC:318:LEU:HD23	3:BC:318:LEU:O	2.16	0.46
3:BC:328:VAL:HG23	3:BC:329:GLY:N	2.30	0.46
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.97	0.46
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.16	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
10:AK:37:PHE:HB3	26:AK:102:BCR:H402	1.97	0.46
2:BB:141:ILE:O	2:BB:144:PHE:HB3	2.16	0.46
2:BB:12:LEU:O	2:BB:14:ASN:N	2.49	0.46
1:AA:40:THR:HG23	22:AA:406:CLA:HBB1	1.98	0.46
3:BC:202:PRO:HB2	3:BC:235:GLY:HA2	1.97	0.46
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.30	0.46
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.98	0.46
1:BA:221:SER:HB2	4:BD:139:ARG:O	2.15	0.46
22:AC:509:CLA:H121	22:AC:509:CLA:HBD	1.97	0.46
3:BC:101:PRO:O	3:BC:104:GLU:HB2	2.16	0.46
16:BV:54:GLU:OE1	16:BV:54:GLU:HA	2.15	0.46
16:AV:54:GLU:OE1	16:AV:54:GLU:HA	2.16	0.46
2:AB:71:VAL:HG21	2:AB:96:VAL:HG21	1.98	0.46
22:BB:609:CLA:H3A	22:BB:609:CLA:HBA2	1.55	0.46
7:BH:35:MET:HE2	26:BX:101:BCR:C32	2.46	0.46
15:BU:72:TYR:CB	15:BU:73:PRO:CD	2.94	0.46
2:AB:329:PRO:HD3	22:AB:607:CLA:CED	2.46	0.46
2:AB:444:ARG:HG3	2:AB:444:ARG:HH11	1.81	0.46
3:BC:315:MET:CE	3:BC:366:LEU:HD13	2.46	0.46
14:AT:23:PHE:HD1	29:BB:601:SQD:H45	1.81	0.46
4:BD:154:VAL:O	4:BD:158:LEU:HB2	2.16	0.46
1:BA:42:LEU:HD23	29:BA:401:SQD:H192	1.98	0.45
4:BD:274:VAL:HG13	24:BD:405:PL9:H211	1.97	0.45
22:AB:608:CLA:H92	29:AD:409:SQD:H172	1.97	0.45
3:BC:163:PHE:CD1	3:BC:252:ILE:HD11	2.51	0.45
1:AA:214:MET:CE	4:AD:142:ASN:ND2	2.79	0.45
13:AO:86:ARG:HD2	13:AO:87:GLN:N	2.31	0.45
3:BC:235:GLY:O	3:BC:238:ILE:HB	2.15	0.45
7:BH:21:VAL:HG23	7:BH:22:ALA:O	2.15	0.45
18:BX:44:ASP:O	18:BX:45:LYS:HB3	2.16	0.45
3:BC:82:TYR:HA	3:BC:422:PRO:HG2	1.98	0.45
1:AA:262:TYR:O	30:AE:102:LMG:H112	2.16	0.45
8:BI:24:LEU:O	8:BI:26:GLY:N	2.41	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:435:PHE:O	3:BC:438:LEU:N	2.47	0.45
22:BB:609:CLA:H72	26:BB:622:BCR:H311	1.98	0.45
3:AC:114:VAL:HG13	22:AC:503:CLA:HMA3	1.97	0.45
2:AB:450:TRP:NE1	22:AB:607:CLA:HBA1	2.32	0.45
4:BD:221:THR:CG2	4:BD:244:TYR:HB2	2.45	0.45
2:BB:484:PRO:O	2:BB:485:GLU:HG2	2.16	0.45
7:AH:21:VAL:HG23	7:AH:22:ALA:O	2.16	0.45
3:AC:318:LEU:HD23	3:AC:318:LEU:O	2.16	0.45
4:BD:213:ILE:HG23	4:BD:214:HIS:N	2.32	0.45
22:BC:509:CLA:HBD	22:BC:509:CLA:H121	1.97	0.45
1:BA:334:ARG:NH1	13:BO:184:ASP:C	2.69	0.45
2:BB:444:ARG:HH11	2:BB:444:ARG:HG3	1.82	0.45
22:BA:403:CLA:HBB1	22:BD:402:CLA:NC	2.32	0.45
34:BE:101:HEM:CBC	6:BF:27:ALA:HB1	2.39	0.45
20:BZ:36:SER:C	20:BZ:38:GLN:N	2.70	0.45
3:AC:210:PHE:HZ	3:AC:243:ILE:HD11	1.81	0.45
3:AC:49:LEU:O	3:AC:53:HIS:ND1	2.43	0.45
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.45
1:BA:214:MET:CE	4:BD:142:ASN:ND2	2.79	0.45
15:AU:99:GLU:HA	15:AU:102:LYS:HE3	1.99	0.45
13:BO:116:ASP:OD1	13:BO:157:PRO:HB3	2.16	0.45
14:BT:22:PHE:C	14:BT:23:PHE:HD2	2.20	0.45
13:BO:56:TYR:O	13:BO:161:SER:HA	2.17	0.45
11:AL:31:PHE:HB3	11:AL:35:PHE:CE1	2.51	0.45
2:BB:289:GLN:OE1	2:BB:292:LEU:HD12	2.17	0.45
2:AB:241:SER:HB3	22:AB:612:CLA:HED3	1.97	0.45
1:AA:258:LEU:HD12	4:AD:128:ARG:CD	2.42	0.45
26:AJ:102:BCR:H361	26:AJ:102:BCR:H20C	1.83	0.45
3:BC:53:HIS:HB3	22:BC:512:CLA:OBD	2.16	0.45
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.31	0.45
30:AD:408:LMG:O10	11:AL:18:TYR:HB3	2.16	0.45
1:BA:10:SER:OG	1:BA:13:LEU:HD12	2.16	0.45
2:BB:270:PRO:HG3	2:BB:312:TYR:CD2	2.45	0.45
2:BB:172:TYR:O	2:BB:173:GLY:C	2.52	0.45
5:BE:77:GLU:HA	5:BE:80:LEU:HD23	1.97	0.45
26:BA:410:BCR:H312	8:BI:15:PHE:HE1	1.82	0.45
3:BC:406:SER:HA	3:BC:420:VAL:CG2	2.46	0.45
12:AM:3:VAL:HG11	14:AT:2:GLU:HG2	1.99	0.45
10:BK:21:LEU:HD11	26:BK:102:BCR:C3	2.46	0.45
2:BB:141:ILE:HG21	22:BB:618:CLA:HBB1	1.97	0.45
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.52	0.45
5:AE:7:GLU:HB3	6:AF:19:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:70:CYS:O	13:BO:265:PHE:HB2	2.15	0.45
13:BO:86:ARG:O	13:BO:86:ARG:HG3	2.16	0.45
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.45	0.45
1:BA:159:LEU:C	1:BA:162:PRO:HD2	2.37	0.45
4:AD:213:ILE:HG23	4:AD:214:HIS:N	2.30	0.45
15:AU:100:ARG:NH1	15:AU:103:GLN:HG2	2.31	0.45
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.97	0.45
5:AE:10:PHE:HB2	30:AE:102:LMG:O2	2.16	0.45
4:BD:303:ILE:HD13	12:BM:2:GLU:HG2	1.99	0.45
13:BO:184:ASP:OD2	13:BO:188:ARG:HB2	2.16	0.45
5:BE:61:ARG:HH22	16:BV:153:GLY:HA3	1.82	0.45
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.52	0.45
11:BL:31:PHE:HB3	11:BL:35:PHE:CE1	2.51	0.45
16:BV:116:GLU:HG3	16:BV:116:GLU:O	2.16	0.45
4:BD:302:GLU:OE1	4:BD:302:GLU:HA	2.17	0.45
15:BU:58:ASN:HD22	15:BU:114:VAL:HG13	1.82	0.45
3:AC:284:PHE:HB3	27:AC:516:DGD:HA51	1.99	0.45
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.51	0.45
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.17	0.45
2:BB:59:GLY:HA3	22:BB:610:CLA:HED1	1.98	0.45
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.17	0.45
13:BO:120:THR:HG22	13:BO:154:SER:CB	2.47	0.45
13:AO:132:VAL:O	13:AO:144:LEU:HD23	2.17	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.31	0.45
13:BO:126:GLY:O	13:BO:128:ASP:N	2.50	0.45
1:AA:212:CYS:HB2	4:AD:211:CYS:HB2	1.99	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
1:BA:227:THR:HA	1:BA:231:GLU:OE2	2.17	0.45
11:BL:24:ILE:HD12	11:BL:24:ILE:N	2.31	0.45
10:AK:18:PHE:O	10:AK:22:VAL:HG23	2.16	0.45
7:AH:9:ASP:O	7:AH:12:ARG:HB3	2.17	0.45
1:AA:317:TRP:HZ3	4:AD:180:ARG:CD	2.19	0.45
2:BB:216:HIS:HE1	22:BB:612:CLA:C1A	2.30	0.45
2:BB:229:LEU:O	2:BB:231:MET:N	2.50	0.45
2:BB:474:LEU:O	4:BD:134:ARG:NH1	2.49	0.45
1:AA:258:LEU:O	4:AD:128:ARG:NH1	2.49	0.45
5:BE:17:VAL:HG22	9:BJ:8:ILE:HD11	1.98	0.45
2:BB:284:ILE:HG23	2:BB:305:ILE:CD1	2.44	0.45
30:BA:414:LMG:H421	22:BB:614:CLA:H142	1.99	0.45
2:AB:306:PRO:HG2	2:AB:309:LEU:HB2	1.98	0.45
3:BC:176:VAL:HG11	3:BC:238:ILE:HG12	1.99	0.45
5:BE:72:ALA:O	5:BE:76:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:182:PHE:O	1:BA:186:PHE:HB2	2.17	0.45
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.45
3:BC:457:LYS:HE3	4:BD:228:GLY:O	2.17	0.45
22:BA:404:CLA:HED2	4:BD:198:MET:SD	2.57	0.45
6:BF:23:VAL:O	6:BF:27:ALA:HB2	2.17	0.45
1:AA:72:LEU:HD21	32:AT:101:LMT:H31	1.99	0.45
2:BB:10:THR:C	2:BB:12:LEU:N	2.70	0.45
3:BC:49:LEU:O	3:BC:53:HIS:ND1	2.43	0.45
20:BZ:36:SER:HA	20:BZ:39:LEU:CD1	2.46	0.45
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.45
4:AD:36:LEU:C	4:AD:39:PRO:HD2	2.37	0.45
2:BB:306:PRO:HG2	2:BB:309:LEU:HB2	1.99	0.45
12:AM:28:GLN:CB	12:BM:27:VAL:HG12	2.47	0.45
3:BC:143:TYR:O	3:BC:144:SER:CB	2.65	0.45
3:AC:176:VAL:HG11	3:AC:238:ILE:HG12	1.99	0.45
20:BZ:5:PHE:HE1	20:BZ:54:VAL:HG13	1.80	0.45
3:BC:193:GLY:O	3:BC:194:GLY:O	2.34	0.45
14:BT:22:PHE:C	14:BT:23:PHE:CD2	2.89	0.45
4:BD:337:GLU:O	4:BD:338:ASN:C	2.55	0.45
4:AD:90:LEU:HD23	4:AD:90:LEU:HA	1.79	0.45
30:BC:519:LMG:H172	10:BK:27:VAL:HG11	1.99	0.45
4:BD:146:PHE:O	4:BD:150:ILE:HG12	2.17	0.45
15:AU:72:TYR:HB3	15:AU:73:PRO:CD	2.34	0.45
2:AB:474:LEU:HD11	22:AB:608:CLA:HAA1	1.98	0.45
2:BB:10:THR:O	2:BB:13:ILE:HG13	2.17	0.45
3:BC:284:PHE:HB3	27:BC:516:DGD:HA51	1.99	0.45
3:AC:245:ILE:O	3:AC:249:ILE:HG12	2.16	0.45
22:AB:607:CLA:HBA2	22:AB:607:CLA:H3A	1.68	0.45
4:BD:239:GLN:HB3	4:BD:240:ALA:H	1.34	0.45
1:BA:222:SER:O	1:BA:246:TYR:HB2	2.16	0.45
1:BA:235:TYR:C	1:BA:237:TYR:H	2.20	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.82	0.45
3:AC:457:LYS:HE3	4:AD:228:GLY:O	2.17	0.45
7:BH:63:LYS:O	7:BH:64:ALA:HB3	2.17	0.45
4:AD:303:ILE:HD13	12:AM:2:GLU:HG2	1.97	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
3:BC:27:ASP:OD1	3:BC:28:GLN:HG2	2.17	0.45
2:AB:141:ILE:O	2:AB:144:PHE:HB3	2.17	0.45
4:BD:253:TRP:HB2	4:BD:260:ALA:HB2	1.99	0.45
12:BM:33:GLN:HG2	12:BM:34:LYS:N	2.30	0.45
2:BB:237:VAL:HG22	22:BB:613:CLA:HBC2	2.00	0.45
2:BB:329:PRO:HD3	22:BB:610:CLA:CED	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:63:ILE:HG23	5:BE:64:PRO:HD2	1.99	0.45
5:BE:69:ARG:HG3	5:BE:70:PHE:N	2.32	0.45
13:AO:120:THR:HG22	13:AO:154:SER:CB	2.47	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
2:AB:169:SER:O	7:AH:65:LEU:HG	2.16	0.45
3:AC:225:VAL:HG13	3:AC:289:PHE:HA	1.99	0.45
16:AV:119:PRO:HG3	16:AV:127:PHE:CD1	2.52	0.45
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.44
3:BC:425:TRP:HE1	27:BC:517:DGD:HE62	1.82	0.44
26:BJ:102:BCR:H20C	26:BJ:102:BCR:H361	1.81	0.44
27:BB:602:DGD:HA21	32:BB:603:LMT:H121	1.98	0.44
3:AC:35:TRP:CG	3:AC:36:TRP:N	2.84	0.44
3:AC:110:PRO:O	3:AC:114:VAL:HG23	2.17	0.44
1:AA:183:MET:HG2	22:AA:403:CLA:HBC1	1.98	0.44
5:AE:64:PRO:HD3	5:AE:84:LYS:HE2	1.98	0.44
1:BA:238:LYS:HA	1:BA:238:LYS:HD3	1.86	0.44
15:BU:82:ASN:ND2	15:BU:94:ILE:HG23	2.32	0.44
3:BC:452:ALA:C	3:BC:454:GLY:N	2.68	0.44
1:BA:262:TYR:O	30:BE:102:LMG:H112	2.17	0.44
5:BE:9:PRO:O	5:BE:10:PHE:C	2.55	0.44
1:BA:210:LEU:HG	23:BD:403:PHO:NC	2.33	0.44
3:BC:243:ILE:O	22:BC:506:CLA:HMC1	2.17	0.44
22:AC:505:CLA:H42	26:AC:515:BCR:H342	1.99	0.44
5:AE:63:ILE:HG23	5:AE:64:PRO:HD2	1.99	0.44
2:BB:191:ASN:HB2	7:BH:58:VAL:HG22	1.98	0.44
2:AB:191:ASN:HB2	7:AH:58:VAL:HG22	1.98	0.44
6:BF:11:VAL:CG1	6:BF:12:SER:H	2.25	0.44
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.44
5:BE:51:ARG:O	5:BE:54:SER:N	2.50	0.44
4:BD:201:VAL:O	4:BD:205:LEU:HB2	2.17	0.44
13:BO:109:GLY:HA3	13:BO:122:VAL:O	2.16	0.44
8:AI:4:LEU:O	8:AI:8:VAL:HG23	2.17	0.44
16:AV:39:ASN:HD21	16:AV:43:LYS:HB3	1.82	0.44
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.32	0.44
3:BC:56:HIS:C	3:BC:58:GLY:N	2.70	0.44
26:BC:514:BCR:H11C	26:BK:102:BCR:H322	1.99	0.44
3:AC:276:LEU:CD1	3:AC:444:HIS:HD2	2.30	0.44
3:AC:425:TRP:HE1	27:AC:517:DGD:HE62	1.81	0.44
30:AC:519:LMG:H172	10:AK:27:VAL:HG11	1.99	0.44
18:AX:16:LEU:HD11	18:AX:20:PHE:CE2	2.53	0.44
3:BC:210:PHE:HZ	3:BC:243:ILE:HD11	1.82	0.44
3:AC:170:ILE:HD13	22:AC:513:CLA:H201	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:AA:402:CLA:HBB1	22:AD:402:CLA:NC	2.32	0.44
2:BB:450:TRP:NE1	22:BB:610:CLA:HBA1	2.33	0.44
13:AO:218:LEU:HD22	15:AU:119:THR:CG2	2.45	0.44
13:AO:86:ARG:O	13:AO:86:ARG:HG3	2.18	0.44
13:BO:132:VAL:O	13:BO:144:LEU:HD23	2.17	0.44
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.17	0.44
3:BC:50:LEU:O	3:BC:54:VAL:HG23	2.18	0.44
1:AA:328:MET:HE1	4:AD:183:LEU:HD22	1.98	0.44
22:BB:617:CLA:H51	26:BB:620:BCR:H372	2.00	0.44
2:BB:435:GLU:O	2:BB:436:THR:C	2.56	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
13:BO:171:GLU:HA	13:BO:221:GLY:O	2.17	0.44
1:AA:243:GLU:CD	1:AA:243:GLU:H	2.16	0.44
2:AB:283:GLU:OE1	2:AB:283:GLU:HA	2.17	0.44
22:BC:508:CLA:H172	27:BC:517:DGD:HBW2	2.00	0.44
7:BH:53:LEU:HD21	7:BH:55:LEU:HD21	1.99	0.44
10:BK:43:VAL:O	10:BK:46:ARG:HG3	2.18	0.44
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.53	0.44
22:AB:614:CLA:H51	26:AB:617:BCR:H372	1.99	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
4:BD:330:ALA:HB3	4:BD:331:PRO:HD3	1.99	0.44
1:BA:224:ILE:O	1:BA:226:GLU:OE2	2.36	0.44
8:AI:11:VAL:HG22	32:AI:102:LMT:H82	2.00	0.44
2:AB:71:VAL:HG21	2:AB:96:VAL:CG2	2.47	0.44
12:BM:33:GLN:CG	12:BM:34:LYS:N	2.81	0.44
3:AC:243:ILE:O	22:AC:506:CLA:HMC1	2.18	0.44
3:AC:449:ARG:NE	22:AC:505:CLA:HED1	2.22	0.44
1:BA:214:MET:HE1	4:BD:142:ASN:ND2	2.33	0.44
1:BA:39:PRO:HB2	22:BA:407:CLA:CBB	2.48	0.44
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.18	0.44
13:AO:116:ASP:OD1	13:AO:157:PRO:HB3	2.18	0.44
3:BC:363:GLY:O	3:BC:367:GLU:HG2	2.17	0.44
7:AH:28:THR:O	7:AH:31:MET:HB3	2.18	0.44
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.17	0.44
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.44
16:AV:59:PHE:CD1	16:AV:63:CYS:SG	3.08	0.44
13:BO:178:ARG:HD2	13:BO:182:PHE:CG	2.53	0.44
4:BD:180:ARG:HH11	4:BD:180:ARG:HG3	1.78	0.44
4:BD:253:TRP:HA	4:BD:256:ILE:HG23	1.99	0.44
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.70	0.44
13:BO:69:LEU:HB3	13:BO:107:ILE:CB	2.36	0.44
2:AB:18:ARG:HD2	2:AB:115:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:271:THR:CG2	2:AB:273:TYR:HB2	2.48	0.44
28:AC:521:LHG:H101	28:AC:521:LHG:H271	2.00	0.44
26:AJ:102:BCR:H371	26:AJ:102:BCR:H24C	1.79	0.44
3:AC:163:PHE:CD1	3:AC:252:ILE:HD11	2.52	0.44
22:BB:610:CLA:H193	11:BL:27:LEU:HD11	1.99	0.44
2:BB:329:PRO:CB	22:BB:610:CLA:HED1	2.43	0.44
1:BA:215:HIS:O	1:BA:216:GLY:C	2.56	0.44
13:BO:86:ARG:CD	13:BO:86:ARG:C	2.84	0.44
1:BA:21:VAL:HG11	1:BA:32:TRP:CE3	2.53	0.44
1:BA:77:ILE:HG12	14:BT:6:TYR:CD1	2.53	0.44
2:BB:86:ILE:C	2:BB:86:ILE:HD12	2.37	0.44
4:AD:209:LEU:O	4:AD:213:ILE:HG22	2.18	0.44
6:AF:16:PHE:O	29:AF:101:SQD:H461	2.18	0.44
2:AB:25:MET:HE2	26:AB:617:BCR:H393	1.98	0.44
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.44
3:BC:225:VAL:HG13	3:BC:289:PHE:HA	1.99	0.44
3:AC:55:ALA:HB1	26:AC:514:BCR:C37	2.46	0.44
2:BB:145:LEU:CD1	22:BB:618:CLA:HMB2	2.47	0.44
1:BA:153:SER:HB2	22:BA:403:CLA:H43	2.00	0.44
2:BB:413:ASP:O	2:BB:414:PRO:C	2.55	0.44
5:BE:20:TRP:HD1	9:BJ:8:ILE:HD13	1.83	0.44
13:BO:86:ARG:HD2	13:BO:87:GLN:N	2.32	0.44
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.45	0.44
4:BD:36:LEU:C	4:BD:39:PRO:HD2	2.37	0.44
2:BB:7:ARG:HG2	22:BB:614:CLA:CED	2.48	0.44
1:AA:107:TYR:HD1	13:AO:141:ARG:NH1	2.16	0.44
2:BB:25:MET:HE2	26:BB:620:BCR:H393	2.00	0.44
4:BD:101:PHE:O	4:BD:104:TRP:HB3	2.17	0.44
7:BH:39:LEU:C	7:BH:39:LEU:HD23	2.38	0.44
26:AC:514:BCR:H11C	26:AK:102:BCR:H322	2.00	0.44
3:BC:245:ILE:O	3:BC:249:ILE:HG12	2.18	0.44
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.44
2:AB:185:TRP:CE3	22:AB:601:CLA:H61	2.53	0.44
3:AC:143:TYR:O	3:AC:144:SER:CB	2.64	0.44
2:AB:263:THR:HB	2:AB:448:ARG:HH12	1.82	0.44
3:AC:50:LEU:O	3:AC:54:VAL:HG23	2.17	0.44
5:BE:34:GLY:O	5:BE:37:PHE:HB3	2.17	0.44
10:BK:44:GLY:O	10:BK:45:PHE:C	2.56	0.44
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.18	0.44
2:AB:422:ARG:HG2	2:AB:422:ARG:HH11	1.81	0.44
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	2.00	0.44
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.18	0.44
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.44
2:BB:59:GLY:HA3	22:BB:610:CLA:CED	2.48	0.44
1:BA:12:ASN:O	1:BA:15:GLU:HB3	2.18	0.44
1:BA:214:MET:O	1:BA:215:HIS:C	2.54	0.44
1:AA:220:THR:O	1:AA:223:LEU:HG	2.18	0.44
3:BC:140:LEU:HB2	3:BC:148:GLY:HA2	2.00	0.44
16:AV:81:ARG:HH11	16:AV:81:ARG:HG2	1.83	0.44
30:BI:101:LMG:H132	32:BI:102:LMT:O2'	2.18	0.44
3:AC:82:TYR:HA	3:AC:422:PRO:HG2	2.00	0.44
3:BC:258:GLY:C	3:BC:262:ARG:NH1	2.71	0.44
3:BC:229:ASN:ND2	3:BC:232:ASP:OD1	2.43	0.44
1:AA:247:ASN:HB3	1:AA:250:ALA:HB3	2.00	0.44
2:AB:298:LEU:HA	2:AB:298:LEU:HD12	1.75	0.44
10:AK:17:ILE:C	10:AK:18:PHE:HD2	2.21	0.43
1:BA:183:MET:HG2	22:BA:404:CLA:HBC1	1.99	0.43
34:AE:101:HEM:HBC2	6:AF:27:ALA:CB	2.39	0.43
3:AC:472:LEU:HD12	3:AC:473:ASP:N	2.28	0.43
22:BB:611:CLA:H92	29:BD:409:SQD:H172	2.00	0.43
2:AB:118:TRP:CH2	11:AL:5:PRO:HD2	2.53	0.43
15:BU:73:PRO:HG2	16:BV:107:THR:HB	2.00	0.43
1:AA:238:LYS:HD3	1:AA:238:LYS:HA	1.86	0.43
5:BE:36:LEU:HA	5:BE:39:SER:OG	2.18	0.43
7:AH:18:TYR:CG	7:AH:19:GLY:N	2.85	0.43
20:BZ:5:PHE:CD2	20:BZ:61:VAL:HG21	2.53	0.43
8:BI:6:ILE:CD1	32:BI:102:LMT:H5'	2.48	0.43
20:AZ:5:PHE:CG	20:AZ:61:VAL:HG21	2.53	0.43
1:BA:324:ALA:O	1:BA:328:MET:HE3	2.18	0.43
2:BB:383:PHE:O	13:BO:192:SER:HA	2.18	0.43
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.18	0.43
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.43
26:AC:514:BCR:HC22	10:AK:18:PHE:HD1	1.83	0.43
3:BC:163:PHE:CG	22:BC:512:CLA:HAB	2.52	0.43
1:AA:217:SER:O	1:AA:220:THR:HG22	2.18	0.43
2:AB:484:PRO:O	2:AB:485:GLU:HG2	2.18	0.43
2:BB:348:ASN:O	2:BB:349:LYS:C	2.56	0.43
3:BC:365:TRP:HB3	3:BC:391:ARG:HG2	1.99	0.43
15:BU:99:GLU:HA	15:BU:102:LYS:HE3	1.99	0.43
18:AX:32:LEU:H	18:AX:32:LEU:HD23	1.83	0.43
3:AC:386:PRO:HB3	16:AV:116:GLU:HG2	2.00	0.43
4:AD:303:ILE:CD1	12:AM:2:GLU:HG2	2.48	0.43
15:BU:64:ALA:O	15:BU:67:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:243:ALA:HB2	2:BB:466:HIS:CE1	2.53	0.43
2:AB:442:ILE:HD11	13:AO:200:LEU:HD23	2.00	0.43
2:BB:343:HIS:O	2:BB:401:PHE:HA	2.18	0.43
12:BM:18:PRO:O	12:BM:21:PHE:HB3	2.18	0.43
4:AD:190:ASN:HB2	4:AD:296:TYR:CD1	2.52	0.43
12:BM:3:VAL:HG11	14:BT:2:GLU:HG2	2.00	0.43
10:AK:17:ILE:HG22	10:AK:17:ILE:O	2.17	0.43
10:BK:16:ALA:O	10:BK:19:ASP:HB2	2.18	0.43
2:BB:113:TRP:CE2	2:BB:117:TYR:CD2	3.06	0.43
15:AU:54:LYS:HD2	15:AU:113:THR:CG2	2.49	0.43
12:AM:33:GLN:HG2	12:AM:34:LYS:N	2.33	0.43
2:BB:474:LEU:HD11	22:BB:611:CLA:HAA1	1.99	0.43
7:BH:9:ASP:O	7:BH:12:ARG:HB3	2.18	0.43
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.43
2:AB:229:LEU:HD11	22:AB:609:CLA:O1A	2.18	0.43
3:AC:362:ARG:H	27:AC:516:DGD:HE4	1.83	0.43
4:AD:152:VAL:HG12	22:AD:402:CLA:H43	2.00	0.43
26:BD:406:BCR:H363	6:BF:33:PHE:HB3	2.01	0.43
26:AB:618:BCR:C38	14:BT:4:ILE:HD13	2.48	0.43
13:BO:86:ARG:O	13:BO:86:ARG:NH1	2.44	0.43
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.83	0.43
2:BB:222:PRO:O	2:BB:223:GLN:C	2.56	0.43
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.18	0.43
13:BO:135:GLN:HE21	13:BO:135:GLN:HB3	1.57	0.43
2:BB:170:ASP:HB2	2:BB:171:PRO:HD2	2.01	0.43
2:AB:164:PRO:HG2	2:AB:165:GLY:H	1.82	0.43
3:BC:456:GLU:N	3:BC:456:GLU:OE1	2.52	0.43
8:AI:6:ILE:CD1	32:AI:102:LMT:H5'	2.48	0.43
15:AU:73:PRO:HG2	16:AV:107:THR:HB	2.01	0.43
22:BC:501:CLA:HMB3	26:BC:515:BCR:C40	2.44	0.43
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.18	0.43
1:BA:10:SER:C	1:BA:12:ASN:N	2.71	0.43
1:BA:329:GLU:O	1:BA:332:HIS:ND1	2.48	0.43
22:AB:602:CLA:H162	22:AB:602:CLA:H122	1.79	0.43
2:AB:86:ILE:HD12	2:AB:86:ILE:C	2.38	0.43
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.34	0.43
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	2.01	0.43
1:AA:60:ILE:HG23	1:AA:61:ASP:N	2.32	0.43
3:AC:318:LEU:HG	3:AC:328:VAL:CG1	2.48	0.43
5:BE:49:THR:HA	5:BE:50:PRO:HD3	1.84	0.43
20:BZ:23:VAL:HB	20:BZ:24:PRO:HD3	2.00	0.43
7:AH:63:LYS:C	7:AH:65:LEU:N	2.70	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:BF:41:GLN:OE1	9:BJ:31:GLY:HA3	2.18	0.43
2:BB:368:VAL:HG21	2:BB:381:ILE:HD12	2.01	0.43
1:BA:212:CYS:HB2	4:BD:211:CYS:HB2	2.01	0.43
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.43
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.53	0.43
26:AT:102:BCR:H271	22:BB:610:CLA:HMD3	2.01	0.43
14:AT:4:ILE:HD13	26:AT:102:BCR:H381	2.00	0.43
22:AB:607:CLA:CAC	26:AB:618:BCR:H393	2.49	0.43
4:BD:244:TYR:HH	4:BD:264:LYS:HE3	1.82	0.43
5:AE:20:TRP:HD1	9:AJ:8:ILE:HD13	1.82	0.43
10:AK:46:ARG:NH1	10:AK:46:ARG:HB2	2.34	0.43
1:AA:39:PRO:HB2	22:AA:406:CLA:CBB	2.48	0.43
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.48	0.43
30:AA:413:LMG:H421	22:AB:611:CLA:H142	2.00	0.43
3:BC:453:ALA:HA	8:BI:34:ARG:O	2.18	0.43
18:BX:42:GLN:O	18:BX:43:ILE:HG13	2.18	0.43
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.18	0.43
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.53	0.43
16:BV:63:CYS:O	16:BV:64:ALA:C	2.56	0.43
10:BK:17:ILE:CD1	10:BK:17:ILE:N	2.80	0.43
19:BY:23:UNK:O	19:BY:24:UNK:C	2.67	0.43
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.53	0.43
1:AA:198:HIS:O	1:AA:202:VAL:HG12	2.18	0.43
20:AZ:36:SER:HA	20:AZ:39:LEU:CD1	2.48	0.43
1:AA:214:MET:HA	1:AA:214:MET:HE2	1.97	0.43
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.38	0.43
3:BC:203:THR:O	3:BC:235:GLY:HA3	2.19	0.43
3:BC:452:ALA:O	3:BC:453:ALA:C	2.57	0.43
13:BO:225:LEU:HD12	13:BO:225:LEU:N	2.34	0.43
20:BZ:17:PHE:HE2	20:BZ:21:ILE:HD11	1.83	0.43
4:AD:253:TRP:HA	4:AD:256:ILE:HG23	2.01	0.43
2:BB:69:LEU:HD21	22:BB:606:CLA:HED3	2.00	0.43
14:BT:29:ILE:O	14:BT:31:LYS:N	2.52	0.43
2:BB:229:LEU:O	2:BB:230:ARG:C	2.56	0.43
3:BC:110:PRO:O	3:BC:114:VAL:HG23	2.19	0.43
3:AC:163:PHE:CG	22:AC:512:CLA:HAB	2.54	0.43
3:AC:162:GLY:O	3:AC:166:ILE:HG13	2.18	0.43
1:AA:153:SER:HB2	22:AA:402:CLA:H43	2.00	0.43
4:AD:126:MET:HE3	4:AD:150:ILE:HG13	2.00	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
26:AD:406:BCR:H363	6:AF:33:PHE:HB3	2.00	0.43
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:220:THR:O	1:BA:223:LEU:HG	2.19	0.43
1:BA:214:MET:HE1	4:BD:142:ASN:HD21	1.84	0.43
5:AE:20:TRP:CD1	9:AJ:8:ILE:HD13	2.53	0.43
16:BV:81:ARG:NH1	16:BV:81:ARG:HG2	2.34	0.43
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.43
1:BA:330:VAL:HG11	4:BD:348:ARG:HG2	1.99	0.43
2:BB:472:ARG:HH11	2:BB:472:ARG:HG2	1.84	0.43
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.19	0.43
4:AD:101:PHE:O	4:AD:104:TRP:HB3	2.18	0.43
15:BU:54:LYS:HD2	15:BU:113:THR:CG2	2.48	0.43
28:BA:412:LHG:HC81	3:BC:36:TRP:CZ3	2.54	0.43
28:BA:412:LHG:HC92	29:BA:413:SQD:O10	2.19	0.43
3:BC:28:GLN:HB2	22:BC:511:CLA:HED3	2.01	0.43
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	2.00	0.43
1:BA:239:PHE:O	14:BT:29:ILE:HA	2.19	0.43
22:BC:505:CLA:H42	26:BC:515:BCR:H342	2.01	0.43
14:AT:21:ILE:HD12	26:AT:102:BCR:H332	2.01	0.43
2:AB:349:LYS:HG2	2:AB:395:GLN:O	2.19	0.43
2:BB:135:LEU:HD23	2:BB:138:MET:HE1	1.98	0.43
2:BB:354:LEU:HD12	2:BB:378:LYS:HB2	2.01	0.43
12:AM:31:SER:HA	30:AM:101:LMG:HC3	2.01	0.43
22:BB:605:CLA:H122	22:BB:605:CLA:H162	1.80	0.43
4:BD:323:GLU:HG2	13:BO:194:TYR:OH	2.19	0.43
16:BV:119:PRO:HG3	16:BV:127:PHE:CD1	2.53	0.43
7:AH:39:LEU:C	7:AH:39:LEU:HD23	2.39	0.43
26:BJ:102:BCR:H371	26:BJ:102:BCR:H24C	1.78	0.43
10:BK:17:ILE:C	10:BK:18:PHE:HD2	2.20	0.43
1:BA:198:HIS:O	1:BA:202:VAL:HG12	2.19	0.43
13:AO:70:CYS:O	13:AO:265:PHE:HB2	2.18	0.43
5:BE:20:TRP:CD1	9:BJ:8:ILE:HD13	2.54	0.43
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.19	0.43
13:BO:168:PHE:O	13:BO:224:SER:HA	2.19	0.43
13:AO:168:PHE:O	13:AO:224:SER:HA	2.19	0.43
4:BD:188:PHE:HE2	4:BD:329:MET:HE2	1.84	0.43
1:BA:131:TRP:CE3	1:BA:132:GLU:CA	3.02	0.43
1:BA:111:PRO:O	1:BA:115:ILE:HG13	2.19	0.43
7:BH:63:LYS:C	7:BH:65:LEU:N	2.71	0.43
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.43
1:BA:288:LEU:O	1:BA:292:THR:HB	2.18	0.43
3:AC:464:GLU:O	3:AC:467:LEU:HB2	2.19	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
19:BY:23:UNK:O	19:BY:25:UNK:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:204:VAL:HG22	4:BD:279:LEU:HD21	2.01	0.43
4:AD:180:ARG:HH11	4:AD:180:ARG:HG3	1.79	0.43
3:BC:165:LEU:HG	22:BC:507:CLA:HED1	2.00	0.43
22:BC:512:CLA:H162	22:BC:512:CLA:HMA2	2.01	0.43
2:BB:280:PHE:O	2:BB:284:ILE:HG13	2.19	0.43
3:BC:415:ASN:O	3:BC:416:SER:CB	2.64	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
13:AO:227:VAL:CG1	13:AO:228:ALA:N	2.82	0.43
13:AO:225:LEU:N	13:AO:225:LEU:HD12	2.33	0.43
2:BB:289:GLN:OE1	2:BB:289:GLN:HA	2.19	0.43
3:BC:386:PRO:HB3	16:BV:116:GLU:HG2	2.00	0.43
2:BB:164:PRO:HG2	2:BB:165:GLY:H	1.83	0.43
2:AB:289:GLN:OE1	2:AB:292:LEU:HD12	2.19	0.43
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.71	0.43
3:AC:28:GLN:HB2	22:AC:511:CLA:HED3	2.00	0.42
10:AK:21:LEU:HD11	26:AK:102:BCR:C3	2.47	0.42
22:BB:615:CLA:H122	22:BB:615:CLA:H162	1.84	0.42
4:AD:217:THR:HG21	24:AD:405:PL9:C1	2.49	0.42
10:BK:46:ARG:HH11	10:BK:46:ARG:CB	2.32	0.42
2:BB:464:PHE:HD2	22:BB:614:CLA:HAC2	1.84	0.42
12:AM:19:SER:O	12:AM:23:ILE:HG13	2.18	0.42
7:AH:41:PHE:O	7:AH:45:ILE:HG23	2.18	0.42
2:AB:222:PRO:CG	7:AH:27:THR:H	2.28	0.42
2:BB:247:PHE:CE1	22:BB:605:CLA:H101	2.48	0.42
15:AU:82:ASN:ND2	15:AU:94:ILE:HG23	2.34	0.42
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.54	0.42
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.54	0.42
4:BD:291:LEU:O	4:BD:292:ASN:HB2	2.19	0.42
3:BC:273:SER:OG	3:BC:274:TYR:N	2.52	0.42
16:BV:68:VAL:O	16:BV:68:VAL:HG13	2.19	0.42
4:BD:193:LEU:HG	4:BD:193:LEU:O	2.19	0.42
9:AJ:15:THR:HG23	26:AK:102:BCR:H392	2.01	0.42
22:BC:511:CLA:HMB2	26:BC:514:BCR:H382	2.01	0.42
19:BY:21:UNK:O	19:BY:22:UNK:C	2.66	0.42
1:BA:317:TRP:HZ3	4:BD:180:ARG:CD	2.20	0.42
12:AM:33:GLN:CG	12:AM:34:LYS:N	2.82	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:HG21	2.01	0.42
6:BF:24:HIS:HA	6:BF:27:ALA:HB3	2.02	0.42
1:AA:73:TYR:CE2	30:AA:416:LMG:HC61	2.53	0.42
22:AC:508:CLA:H172	27:AC:517:DGD:HBW2	2.01	0.42
3:BC:437:PHE:CZ	22:BC:510:CLA:HMB3	2.54	0.42
3:AC:437:PHE:CZ	22:AC:510:CLA:HMB3	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:215:HIS:CD2	4:AD:268:HIS:HD2	2.37	0.42
1:AA:255:PHE:CE2	24:AA:407:PL9:H111	2.54	0.42
32:BT:101:LMT:H3'	32:BT:101:LMT:H1B	1.63	0.42
3:AC:48:LYS:CD	3:AC:138:GLU:HG3	2.49	0.42
2:AB:464:PHE:HD2	22:AB:611:CLA:HAC2	1.84	0.42
18:BX:45:LYS:CD	18:BX:45:LYS:N	2.82	0.42
3:BC:127:PHE:HE1	20:BZ:23:VAL:HG21	1.84	0.42
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.42
15:BU:80:VAL:HG22	15:BU:127:ARG:NH2	2.34	0.42
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.18	0.42
12:AM:5:GLN:NE2	32:AM:102:LMT:O2B	2.52	0.42
15:BU:50:ALA:HB1	15:BU:113:THR:HG21	2.01	0.42
9:AJ:12:ILE:O	9:AJ:16:VAL:HG23	2.19	0.42
26:BJ:102:BCR:H15C	26:BJ:102:BCR:H351	1.91	0.42
30:BD:408:LMG:HC2	30:BD:408:LMG:HC71	1.82	0.42
7:BH:11:LEU:C	7:BH:13:PRO:HD2	2.40	0.42
2:AB:471:ALA:HB2	4:AD:130:PHE:CE2	2.53	0.42
3:BC:170:ILE:HD13	22:BC:513:CLA:H201	2.00	0.42
22:AC:512:CLA:H162	22:AC:512:CLA:HMA2	2.01	0.42
1:AA:42:LEU:HA	1:AA:45:THR:CG2	2.49	0.42
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.54	0.42
13:BO:218:LEU:HD22	15:BU:119:THR:CG2	2.40	0.42
10:BK:46:ARG:NH1	10:BK:46:ARG:CB	2.82	0.42
13:BO:144:LEU:CD1	13:BO:259:VAL:HG11	2.48	0.42
11:BL:12:LEU:HD22	12:BM:25:LEU:HD12	1.99	0.42
4:AD:56:THR:HB	5:AE:49:THR:HG23	2.01	0.42
20:BZ:5:PHE:CG	20:BZ:61:VAL:HG21	2.54	0.42
4:BD:294:ARG:H	4:BD:294:ARG:HG2	1.65	0.42
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.84	0.42
22:BB:617:CLA:HBC2	22:BB:617:CLA:HMC1	2.02	0.42
2:BB:234:ILE:C	2:BB:236:THR:H	2.23	0.42
3:AC:456:GLU:N	3:AC:456:GLU:OE1	2.53	0.42
3:AC:406:SER:HA	3:AC:420:VAL:CG2	2.49	0.42
5:AE:60:GLN:HG2	5:AE:62:SER:H	1.84	0.42
2:BB:393:GLU:HG2	15:BU:44:ASP:O	2.19	0.42
1:AA:160:ILE:HD12	3:AC:431:PHE:CE1	2.54	0.42
9:BJ:15:THR:HG23	26:BK:102:BCR:H392	2.01	0.42
10:BK:18:PHE:O	10:BK:19:ASP:C	2.57	0.42
2:BB:120:LEU:HD13	22:BB:619:CLA:CMD	2.40	0.42
2:AB:145:LEU:CD1	22:AB:615:CLA:HMB2	2.49	0.42
13:AO:69:LEU:HB3	13:AO:107:ILE:CB	2.35	0.42
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.42
3:AC:174:LEU:HD12	22:AC:512:CLA:H71	2.01	0.42
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.48	0.42
4:BD:52:THR:HG22	4:BD:67:TYR:CE2	2.54	0.42
2:AB:327:THR:O	2:AB:444:ARG:NE	2.46	0.42
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.49	0.42
4:AD:160:TYR:CB	4:AD:161:PRO:CD	2.96	0.42
10:BK:28:ILE:O	10:BK:31:LEU:HB2	2.20	0.42
3:BC:33:PHE:CE1	4:BD:229:ALA:HB3	2.54	0.42
27:AB:626:DGD:HA21	32:AB:627:LMT:H121	2.01	0.42
5:AE:34:GLY:O	5:AE:37:PHE:HB3	2.19	0.42
15:BU:42:VAL:HG23	15:BU:43:VAL:N	2.33	0.42
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.19	0.42
5:AE:35:TRP:CD1	5:AE:35:TRP:C	2.93	0.42
26:AA:409:BCR:H342	29:AA:415:SQD:H342	2.02	0.42
1:BA:42:LEU:HA	1:BA:45:THR:CG2	2.50	0.42
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.80	0.42
20:BZ:30:PRO:C	20:BZ:32:ASP:N	2.72	0.42
1:BA:217:SER:O	1:BA:220:THR:HG22	2.18	0.42
4:BD:35:ILE:O	4:BD:39:PRO:HG2	2.20	0.42
1:AA:228:THR:HB	1:AA:231:GLU:HB3	2.01	0.42
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.42
4:BD:161:PRO:HB3	4:BD:170:ALA:HB2	2.02	0.42
13:BO:59:ASP:O	13:BO:61:SER:N	2.53	0.42
20:AZ:5:PHE:CD2	20:AZ:61:VAL:HG21	2.54	0.42
1:BA:136:ARG:NH2	8:BI:27:ASP:OD1	2.49	0.42
2:BB:169:SER:O	7:BH:65:LEU:HG	2.20	0.42
4:AD:89:LEU:HG	7:AH:50:ASN:OD1	2.20	0.42
3:BC:321:ASP:HA	3:BC:324:LEU:HD23	2.01	0.42
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.19	0.42
3:BC:35:TRP:CD2	3:BC:36:TRP:N	2.88	0.42
34:AE:101:HEM:HAD2	34:AE:101:HEM:HHA	1.57	0.42
22:BB:612:CLA:NB	26:BX:101:BCR:H312	2.35	0.42
3:AC:276:LEU:HD21	22:AC:508:CLA:HBB1	2.01	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
2:AB:354:LEU:HD12	2:AB:378:LYS:HB2	2.02	0.42
1:BA:255:PHE:CE2	24:BA:408:PL9:H111	2.55	0.42
9:AJ:7:ARG:HA	9:AJ:7:ARG:HE	1.83	0.42
5:AE:15:THR:CG2	9:AJ:7:ARG:HG3	2.49	0.42
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.19	0.42
16:BV:124:ALA:HB1	16:BV:131:ARG:CG	2.50	0.42
2:AB:472:ARG:HH11	2:AB:472:ARG:HG2	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:192:SER:OG	13:BO:193:GLY:N	2.53	0.42
7:BH:28:THR:N	7:BH:29:PRO:HD2	2.35	0.42
2:AB:215:PHE:CD2	2:AB:215:PHE:C	2.93	0.42
34:BV:201:HEM:HHA	34:BV:201:HEM:HAD2	1.61	0.42
16:BV:59:PHE:CD1	16:BV:63:CYS:SG	3.08	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:CG2	2.50	0.42
5:BE:18:ARG:CD	5:BE:22:ILE:HD11	2.38	0.42
1:AA:73:TYR:CD2	30:AA:416:LMG:HC3	2.55	0.42
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.42
22:AB:612:CLA:H162	22:AB:612:CLA:H122	1.84	0.42
2:AB:237:VAL:HG12	22:AB:612:CLA:HMD1	2.02	0.42
4:AD:125:PHE:O	4:AD:128:ARG:HB3	2.19	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.20	0.42
18:BX:16:LEU:HD11	18:BX:20:PHE:CE2	2.55	0.42
4:AD:204:VAL:HG22	4:AD:279:LEU:HD21	2.01	0.42
4:BD:77:ALA:CB	4:BD:174:GLY:HA3	2.50	0.42
2:AB:59:GLY:HA3	22:AB:607:CLA:CED	2.50	0.42
2:BB:9:HIS:HB2	22:BB:614:CLA:CBA	2.49	0.42
1:AA:22:THR:HG21	8:AI:30:ARG:CD	2.50	0.42
3:BC:48:LYS:HD2	3:BC:138:GLU:HG3	1.99	0.42
6:AF:16:PHE:N	6:AF:16:PHE:CD1	2.88	0.42
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.93	0.42
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.84	0.42
15:AU:91:VAL:HG13	15:AU:92:LEU:N	2.33	0.42
3:AC:321:ASP:HA	3:AC:324:LEU:HD23	2.01	0.42
5:AE:61:ARG:HH22	16:AV:153:GLY:HA3	1.85	0.42
13:BO:215:ARG:NH1	13:BO:252:GLY:O	2.53	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HD13	2.50	0.42
3:BC:429:SER:HA	27:BC:517:DGD:HAT1	2.02	0.42
26:BC:514:BCR:H341	26:BK:102:BCR:H322	2.00	0.42
2:BB:263:THR:HB	2:BB:448:ARG:HH12	1.84	0.42
1:BA:42:LEU:HA	1:BA:45:THR:HG22	2.01	0.42
34:BE:101:HEM:HHA	34:BE:101:HEM:HAD2	1.57	0.42
28:AA:411:LHG:HC92	29:AA:412:SQD:O10	2.20	0.42
26:BC:515:BCR:C33	8:BI:20:VAL:HG13	2.50	0.42
12:BM:31:SER:HA	30:BM:102:LMG:HC3	2.01	0.42
5:AE:30:LEU:HD11	6:AF:28:VAL:HG13	2.02	0.42
6:AF:25:THR:O	6:AF:29:PRO:HG2	2.19	0.42
4:BD:17:ILE:HG21	18:BX:42:GLN:HG3	2.01	0.42
4:AD:17:ILE:HG21	18:AX:42:GLN:HG3	2.02	0.42
4:BD:92:LEU:HA	4:BD:104:TRP:CD1	2.55	0.42
2:BB:442:ILE:HD11	13:BO:200:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:201:HIS:HD2	2:AB:202:HIS:ND1	2.16	0.42
2:BB:463:PHE:CD2	2:BB:463:PHE:C	2.92	0.42
20:AZ:17:PHE:HE2	20:AZ:21:ILE:HD11	1.83	0.42
3:BC:67:MET:HE1	22:BC:504:CLA:ND	2.35	0.42
13:BO:80:GLU:O	13:BO:89:ALA:CB	2.66	0.42
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	2.01	0.42
3:BC:249:ILE:O	3:BC:252:ILE:HB	2.20	0.42
9:BJ:7:ARG:HE	9:BJ:7:ARG:HA	1.85	0.42
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	2.01	0.42
1:BA:306:VAL:CG1	1:BA:316:THR:HG23	2.49	0.42
3:BC:276:LEU:CD1	3:BC:444:HIS:HD2	2.33	0.42
13:BO:227:VAL:CG1	13:BO:228:ALA:N	2.83	0.42
1:AA:279:PRO:HG2	4:AD:212:ALA:HB2	2.00	0.42
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.34	0.42
8:BI:27:ASP:O	8:BI:28:PRO:C	2.56	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.55	0.42
4:BD:203:GLY:O	4:BD:207:GLY:N	2.51	0.42
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	2.02	0.42
16:AV:130:MET:SD	16:AV:133:LEU:HD12	2.60	0.42
2:BB:275:TRP:CH2	2:BB:358:ARG:HD3	2.55	0.42
2:BB:283:GLU:OE1	2:BB:283:GLU:HA	2.19	0.42
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG12	2.55	0.42
30:AI:101:LMG:H132	32:AI:102:LMT:O2'	2.20	0.42
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.85	0.42
3:BC:335:THR:HA	13:BO:178:ARG:CD	2.50	0.42
6:BF:18:VAL:CG1	6:BF:19:ARG:N	2.82	0.42
2:AB:237:VAL:HG22	22:AB:610:CLA:HBC2	2.01	0.42
2:BB:241:SER:HB3	22:BB:615:CLA:HED3	2.01	0.42
2:AB:348:ASN:O	2:AB:349:LYS:C	2.57	0.42
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.20	0.42
1:BA:215:HIS:HA	24:BA:408:PL9:O1	2.20	0.42
22:AB:607:CLA:HMD3	26:AB:618:BCR:H271	2.02	0.42
2:BB:16:PRO:HG3	2:BB:133:LEU:HD11	2.01	0.42
3:BC:142:GLU:C	3:BC:144:SER:H	2.22	0.42
27:AB:626:DGD:HD5	27:AB:626:DGD:HE1	1.66	0.42
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.42
30:AE:102:LMG:HC71	30:AE:102:LMG:O9	2.19	0.42
2:AB:364:GLU:HG3	4:AD:296:TYR:CE2	2.55	0.42
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.20	0.42
5:BE:60:GLN:HG2	5:BE:62:SER:H	1.84	0.42
1:BA:339:PHE:HB3	1:BA:340:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:180:PHE:O	1:BA:184:ILE:HG13	2.20	0.42
1:BA:160:ILE:HD12	3:BC:431:PHE:CE1	2.55	0.42
2:AB:330:MET:SD	2:AB:446:SER:HB3	2.59	0.42
22:AC:511:CLA:HMB2	26:AC:514:BCR:H382	2.02	0.41
3:BC:269:GLU:O	3:BC:272:LEU:HB3	2.20	0.41
9:BJ:11:TRP:CE2	9:BJ:12:ILE:HG12	2.55	0.41
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	2.01	0.41
22:AB:615:CLA:H162	7:AH:7:LEU:HD21	2.02	0.41
1:BA:64:ARG:O	13:BO:178:ARG:NH2	2.53	0.41
18:AX:12:ILE:C	18:AX:12:ILE:HD13	2.40	0.41
22:BC:513:CLA:HBA2	22:BC:513:CLA:H3A	1.81	0.41
1:AA:214:MET:HE1	4:AD:142:ASN:ND2	2.35	0.41
5:BE:15:THR:O	9:BJ:8:ILE:CD1	2.68	0.41
13:AO:92:VAL:HG11	2:BB:84:THR:HG21	2.03	0.41
2:BB:349:LYS:HG2	2:BB:395:GLN:O	2.19	0.41
30:BM:102:LMG:HC72	30:BM:102:LMG:HC2	1.96	0.41
6:BF:15:ILE:HG22	6:BF:16:PHE:N	2.34	0.41
18:BX:42:GLN:HB2	18:BX:42:GLN:HE21	1.63	0.41
1:BA:339:PHE:HB3	1:BA:340:PRO:CD	2.50	0.41
2:BB:153:PHE:O	2:BB:157:HIS:HB3	2.20	0.41
4:BD:190:ASN:HB2	4:BD:296:TYR:CD1	2.55	0.41
2:BB:18:ARG:HD2	2:BB:115:TRP:CE3	2.55	0.41
22:BC:502:CLA:HBD	22:BC:503:CLA:H43	2.02	0.41
2:BB:124:ARG:NH1	2:BB:124:ARG:CG	2.82	0.41
1:AA:214:MET:HE1	4:AD:142:ASN:HD21	1.84	0.41
7:BH:55:LEU:HB2	7:BH:58:VAL:CG1	2.50	0.41
1:BA:333:GLU:HB2	1:BA:337:HIS:HE1	1.85	0.41
20:BZ:22:GLY:O	20:BZ:23:VAL:C	2.58	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
4:BD:185:PHE:HE2	4:BD:289:LEU:HD12	1.85	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HA	2.01	0.41
16:BV:69:GLY:O	16:BV:156:TRP:O	2.38	0.41
16:BV:160:LYS:HA	16:BV:163:TYR:CD2	2.56	0.41
4:BD:19:ASP:O	4:BD:20:ASP:C	2.57	0.41
2:BB:225:LEU:O	2:BB:226:TYR:C	2.59	0.41
4:BD:192:THR:CG2	22:BD:402:CLA:HBC2	2.48	0.41
13:BO:55:ALA:HA	13:BO:230:VAL:HG11	2.03	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
10:BK:43:VAL:CG2	10:BK:46:ARG:HE	2.33	0.41
16:BV:103:LYS:O	16:BV:122:ARG:HG2	2.20	0.41
2:BB:7:ARG:HG2	22:BB:614:CLA:HED1	2.01	0.41
3:AC:188:THR:CG2	3:AC:298:PRO:HB3	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.55	0.41
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.41
15:AU:75:LEU:O	15:AU:79:ILE:HG13	2.21	0.41
30:AD:407:LMG:O4	9:AJ:31:GLY:O	2.39	0.41
1:BA:96:ILE:C	1:BA:98:GLU:H	2.24	0.41
2:BB:239:SER:O	2:BB:466:HIS:ND1	2.49	0.41
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.23	0.41
1:BA:157:VAL:HG13	1:BA:172:MET:HB3	2.01	0.41
19:BY:25:UNK:C	19:BY:27:UNK:N	2.82	0.41
26:AA:409:BCR:H342	29:AA:415:SQD:H311	2.02	0.41
13:AO:80:GLU:O	13:AO:89:ALA:CB	2.66	0.41
13:BO:81:GLU:HA	13:BO:82:PRO:HD3	1.89	0.41
1:AA:317:TRP:O	1:AA:321:ILE:HG13	2.20	0.41
32:AT:101:LMT:H3'	32:AT:101:LMT:H1B	1.64	0.41
2:AB:413:ASP:OD1	2:AB:416:THR:HB	2.20	0.41
19:AY:21:UNK:O	19:AY:22:UNK:C	2.68	0.41
3:BC:114:VAL:CG1	22:BC:503:CLA:HMA3	2.50	0.41
3:BC:250:TRP:HE1	22:BC:506:CLA:HED1	1.84	0.41
22:AC:501:CLA:HMB3	26:AC:515:BCR:C40	2.46	0.41
3:AC:365:TRP:HB3	3:AC:391:ARG:HG2	2.02	0.41
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	2.02	0.41
3:BC:29:GLU:OE2	3:BC:31:SER:N	2.31	0.41
5:BE:30:LEU:HD11	6:BF:28:VAL:HG13	2.03	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
4:BD:209:LEU:O	4:BD:213:ILE:HG22	2.20	0.41
10:BK:28:ILE:HA	10:BK:31:LEU:HD12	2.02	0.41
13:BO:180:ALA:HB2	15:BU:120:ALA:O	2.19	0.41
2:AB:448:ARG:HG3	2:AB:448:ARG:HH11	1.84	0.41
3:AC:199:ILE:N	3:AC:199:ILE:CD1	2.83	0.41
9:BJ:21:VAL:HA	9:BJ:24:ILE:HG22	2.03	0.41
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.54	0.41
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.41
4:BD:79:SER:HA	4:BD:172:SER:HB3	2.02	0.41
3:BC:198:VAL:HG12	3:BC:200:THR:HG23	2.02	0.41
2:BB:105:GLY:O	2:BB:108:PHE:HB3	2.20	0.41
3:BC:42:LEU:HD11	22:BC:511:CLA:C1A	2.50	0.41
30:BC:519:LMG:H221	10:BK:30:VAL:CG1	2.50	0.41
2:BB:18:ARG:HD3	2:BB:118:TRP:HB3	2.01	0.41
18:BX:12:ILE:C	18:BX:12:ILE:HD13	2.40	0.41
1:AA:206:PHE:HA	1:AA:206:PHE:HD2	1.76	0.41
1:AA:45:THR:HB	23:AA:405:PHO:H93	2.02	0.41
13:BO:83:LYS:CG	13:BO:84:ASN:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:64:PRO:HB3	5:BE:84:LYS:CD	2.50	0.41
5:BE:64:PRO:CB	5:BE:84:LYS:HE2	2.50	0.41
7:AH:53:LEU:HD21	7:AH:55:LEU:HD21	2.03	0.41
5:AE:78:THR:HA	5:AE:81:GLU:HG2	2.02	0.41
7:AH:10:ILE:H	7:AH:10:ILE:HG13	1.70	0.41
7:BH:16:SER:C	7:BH:18:TYR:H	2.23	0.41
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.41
4:BD:107:LEU:HD21	5:BE:76:VAL:HG21	2.01	0.41
7:BH:28:THR:O	7:BH:31:MET:HB3	2.20	0.41
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.19	0.41
10:AK:28:ILE:O	10:AK:31:LEU:HB2	2.20	0.41
28:BC:521:LHG:HC41	28:BC:521:LHG:O9	2.20	0.41
2:BB:118:TRP:CH2	11:BL:5:PRO:HD2	2.56	0.41
1:AA:172:MET:SD	22:AA:403:CLA:HMC3	2.61	0.41
4:BD:268:HIS:CE1	33:BD:401:BCT:O3	2.73	0.41
1:AA:215:HIS:HA	24:AA:407:PL9:O1	2.21	0.41
5:AE:15:THR:O	9:AJ:8:ILE:CD1	2.69	0.41
30:AM:101:LMG:HC2	30:AM:101:LMG:HC72	1.96	0.41
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.01	0.41
4:BD:56:THR:HB	5:BE:49:THR:HG23	2.02	0.41
15:AU:89:GLU:N	15:AU:89:GLU:CD	2.73	0.41
11:AL:22:LEU:O	11:AL:26:VAL:HG13	2.21	0.41
2:AB:383:PHE:O	13:AO:192:SER:HA	2.20	0.41
16:AV:83:GLU:H	16:AV:83:GLU:CD	2.23	0.41
5:AE:82:GLN:H	5:AE:82:GLN:HG3	1.54	0.41
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.36	0.41
4:AD:26:ARG:HD3	6:AF:18:VAL:CG1	2.32	0.41
27:AC:518:DGD:HG2	9:AJ:33:TYR:OH	2.21	0.41
3:BC:162:GLY:O	3:BC:166:ILE:HG13	2.21	0.41
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.84	0.41
5:BE:84:LYS:HZ3	5:BE:84:LYS:HB2	1.82	0.41
2:BB:191:ASN:ND2	7:BH:59:ASN:O	2.54	0.41
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.33	0.41
2:AB:191:ASN:OD1	2:AB:193:TYR:N	2.52	0.41
5:BE:27:ILE:CB	5:BE:28:PRO:HD3	2.49	0.41
1:BA:21:VAL:HG11	1:BA:32:TRP:CZ3	2.56	0.41
13:AO:120:THR:HA	13:AO:153:ALA:O	2.21	0.41
3:BC:141:GLU:HA	3:BC:148:GLY:HA3	2.03	0.41
2:BB:377:VAL:HG11	4:BD:342:PRO:HG2	2.02	0.41
1:BA:249:VAL:HG11	2:BB:486:LEU:CD2	2.50	0.41
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:AO:135:GLN:HB3	13:AO:135:GLN:HE21	1.56	0.41
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.56	0.41
13:AO:192:SER:OG	13:AO:193:GLY:N	2.54	0.41
13:BO:229:LYS:HB2	13:BO:238:ALA:HB3	2.02	0.41
16:BV:30:THR:HB	16:BV:31:PRO:HD2	2.02	0.41
2:AB:463:PHE:C	2:AB:463:PHE:CD2	2.94	0.41
26:AC:514:BCR:H341	26:AK:102:BCR:H322	2.02	0.41
1:BA:202:VAL:O	1:BA:206:PHE:HB2	2.20	0.41
22:BA:405:CLA:H202	30:BD:407:LMG:H401	2.03	0.41
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	3.03	0.41
4:BD:128:ARG:O	4:BD:129:GLN:C	2.59	0.41
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.41
2:BB:331:ASN:HB3	2:BB:437:LEU:CD1	2.48	0.41
12:AM:27:VAL:HG12	12:BM:28:GLN:CB	2.47	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
1:BA:105:TRP:CZ3	1:BA:111:PRO:HG3	2.56	0.41
1:BA:296:ASN:HB3	3:BC:401:LEU:HA	2.02	0.41
2:BB:214:LEU:O	2:BB:218:LEU:HG	2.21	0.41
1:AA:277:ALA:O	1:AA:281:VAL:HG23	2.21	0.41
2:AB:479:PHE:O	2:AB:480:SER:CB	2.68	0.41
3:AC:101:PRO:O	3:AC:104:GLU:HB2	2.19	0.41
13:AO:73:PRO:HG2	13:AO:102:THR:HB	2.03	0.41
15:BU:54:LYS:CB	15:BU:113:THR:HG23	2.47	0.41
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.20	0.41
19:BY:21:UNK:HA	19:BY:24:UNK:CB	2.50	0.41
3:BC:85:GLY:CA	27:BC:517:DGD:HE4	2.51	0.41
27:BC:518:DGD:HG2	9:BJ:33:TYR:OH	2.21	0.41
1:BA:45:THR:HB	23:BA:406:PHO:H93	2.02	0.41
2:BB:30:VAL:HG11	22:BB:615:CLA:H112	2.03	0.41
3:AC:307:PRO:HG3	3:AC:358:PHE:CD1	2.56	0.41
3:AC:308:GLU:HG3	3:AC:361:PHE:CZ	2.56	0.41
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.41
26:AJ:102:BCR:H351	26:AJ:102:BCR:H15C	1.91	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
3:BC:160:ILE:HA	3:BC:163:PHE:CD2	2.55	0.41
3:BC:116:VAL:CG2	3:BC:117:VAL:N	2.84	0.41
3:BC:449:ARG:NE	22:BC:505:CLA:HED1	2.21	0.41
3:AC:165:LEU:HG	22:AC:507:CLA:HED1	2.03	0.41
1:AA:183:MET:HB3	22:AA:402:CLA:HBC2	2.02	0.41
1:AA:215:HIS:CD2	4:AD:268:HIS:CD2	3.08	0.41
4:AD:268:HIS:CE1	33:AD:401:BCT:O3	2.74	0.41
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:BM:19:SER:O	12:BM:23:ILE:HG13	2.20	0.41
3:BC:414:ILE:HG22	3:BC:415:ASN:O	2.21	0.41
15:AU:57:LEU:HD22	15:AU:79:ILE:CG2	2.51	0.41
1:BA:22:THR:HG21	8:BI:30:ARG:CD	2.51	0.41
16:AV:124:ALA:HB1	16:AV:131:ARG:CG	2.51	0.41
13:AO:116:ASP:C	13:AO:116:ASP:OD2	2.58	0.41
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.74	0.41
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.24	0.41
3:AC:258:GLY:C	3:AC:262:ARG:NH1	2.74	0.41
13:BO:184:ASP:OD1	13:BO:184:ASP:C	2.59	0.41
2:BB:364:GLU:HG3	4:BD:296:TYR:CE2	2.56	0.41
1:BA:24:THR:OG1	3:BC:469:MET:CE	2.68	0.41
1:AA:288:LEU:O	1:AA:292:THR:HB	2.21	0.41
3:BC:464:GLU:O	3:BC:467:LEU:HB2	2.20	0.41
2:AB:91:TRP:HE1	32:AB:624:LMT:H12	1.86	0.41
3:AC:198:VAL:HG12	3:AC:200:THR:HG23	2.03	0.41
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.20	0.41
2:BB:215:PHE:CD2	2:BB:215:PHE:C	2.95	0.41
22:BC:511:CLA:HBA2	26:BC:514:BCR:H271	2.03	0.41
2:AB:137:LYS:NZ	7:AH:14:LEU:O	2.54	0.41
1:BA:183:MET:HB3	22:BA:403:CLA:HBC2	2.02	0.41
22:BA:404:CLA:H62	22:BA:404:CLA:H41	1.92	0.41
4:BD:126:MET:HE3	4:BD:150:ILE:HG13	2.03	0.41
4:BD:263:ASN:O	4:BD:265:ARG:N	2.54	0.41
4:BD:283:ALA:HA	22:BD:402:CLA:HED2	2.03	0.41
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.41
22:AC:512:CLA:H2A	22:AC:512:CLA:HED2	2.03	0.41
22:AA:403:CLA:H62	22:AA:403:CLA:H41	1.91	0.41
1:AA:10:SER:OG	1:AA:13:LEU:HD12	2.20	0.41
1:BA:215:HIS:CD2	4:BD:268:HIS:CD2	3.09	0.41
4:BD:53:THR:CB	4:BD:67:TYR:HD2	2.34	0.41
2:BB:348:ASN:O	2:BB:350:GLU:N	2.54	0.41
15:BU:38:GLU:CG	15:BU:39:LEU:N	2.81	0.41
1:BA:20:TRP:O	1:BA:23:SER:HB3	2.20	0.41
2:AB:331:ASN:HB3	2:AB:437:LEU:CD1	2.49	0.41
16:AV:81:ARG:CG	16:AV:157:GLY:HA3	2.51	0.41
2:AB:447:PRO:O	2:AB:448:ARG:C	2.59	0.41
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.56	0.41
3:BC:80:PRO:HB3	3:BC:82:TYR:CE1	2.56	0.41
3:BC:261:ARG:HA	3:BC:266:TRP:HZ2	1.86	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41
1:AA:114:LEU:HD23	1:AA:114:LEU:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:334:ARG:NH1	13:AO:183:LEU:O	2.54	0.41
3:BC:455:PHE:C	3:BC:457:LYS:H	2.24	0.41
1:BA:247:ASN:HB3	1:BA:250:ALA:HB3	2.01	0.41
9:BJ:36:LEU:C	9:BJ:38:SER:H	2.22	0.41
8:BI:4:LEU:O	8:BI:8:VAL:HG23	2.20	0.41
16:AV:30:THR:OG1	16:AV:32:GLU:HB3	2.21	0.41
15:AU:55:ILE:HG21	15:AU:65:PHE:CE1	2.56	0.41
2:AB:113:TRP:CE2	2:AB:117:TYR:CD2	3.09	0.41
3:BC:41:ARG:NH1	22:BC:511:CLA:HMD1	2.36	0.40
2:BB:137:LYS:HZ2	7:BH:14:LEU:C	2.23	0.40
2:BB:229:LEU:HD11	22:BB:612:CLA:O1A	2.21	0.40
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.40
22:AA:403:CLA:HAA1	24:AD:405:PL9:C36	2.51	0.40
5:AE:64:PRO:HB3	5:AE:84:LYS:CD	2.50	0.40
2:BB:187:PRO:C	2:BB:189:GLY:H	2.24	0.40
4:BD:14:TRP:CD2	4:BD:15:PHE:N	2.89	0.40
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.20	0.40
1:BA:257:ARG:HG3	1:BA:257:ARG:NH1	2.33	0.40
4:BD:161:PRO:CB	4:BD:170:ALA:HB2	2.51	0.40
2:AB:170:ASP:HB2	2:AB:171:PRO:HD2	2.02	0.40
5:BE:14:ILE:O	5:BE:14:ILE:HG22	2.21	0.40
13:BO:44:LYS:HA	13:BO:72:GLN:OE1	2.21	0.40
30:BD:408:LMG:O6	11:BL:15:THR:HG21	2.21	0.40
3:BC:155:ASN:O	3:BC:158:THR:CG2	2.69	0.40
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	2.03	0.40
3:BC:318:LEU:HG	3:BC:328:VAL:CG1	2.50	0.40
3:AC:461:ARG:NH1	3:AC:461:ARG:HG3	2.33	0.40
15:AU:75:LEU:HD21	15:AU:101:GLN:HB3	2.03	0.40
3:BC:350:ILE:CG2	3:BC:359:TRP:HB2	2.52	0.40
1:AA:105:TRP:CZ3	1:AA:111:PRO:HG3	2.55	0.40
4:BD:205:LEU:HA	4:BD:205:LEU:HD12	1.72	0.40
12:BM:5:GLN:NE2	32:BM:101:LMT:O2B	2.55	0.40
1:BA:126:TYR:O	1:BA:130:GLN:HG3	2.22	0.40
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	2.02	0.40
3:BC:394:GLU:OE2	3:BC:398:HIS:CD2	2.74	0.40
1:AA:339:PHE:HB3	1:AA:340:PRO:HD2	2.03	0.40
4:BD:48:TRP:CE2	23:BD:403:PHO:H161	2.56	0.40
32:AD:411:LMT:O3'	18:AX:21:ILE:HG21	2.21	0.40
3:BC:362:ARG:H	27:BC:516:DGD:HE4	1.87	0.40
5:BE:15:THR:CG2	9:BJ:7:ARG:HG3	2.51	0.40
30:BA:414:LMG:H292	11:BL:20:GLY:HA2	2.04	0.40
1:AA:257:ARG:NH1	1:AA:257:ARG:HG3	2.35	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.20	0.40
7:AH:63:LYS:C	7:AH:65:LEU:H	2.24	0.40
2:AB:289:GLN:OE1	2:AB:289:GLN:HA	2.21	0.40
2:BB:54:PRO:HD2	2:BB:57:ARG:HG3	2.04	0.40
16:BV:83:GLU:CD	16:BV:83:GLU:H	2.25	0.40
3:AC:42:LEU:HD11	22:AC:511:CLA:C1A	2.51	0.40
2:BB:24:LEU:HD13	2:BB:111:ALA:N	2.37	0.40
2:BB:113:TRP:CD1	22:BB:619:CLA:HBA1	2.57	0.40
22:BA:404:CLA:HAA1	24:BD:405:PL9:C36	2.51	0.40
3:BC:109:PHE:CG	30:BC:520:LMG:HC61	2.56	0.40
26:BC:515:BCR:H332	8:BI:20:VAL:HG13	2.02	0.40
22:AC:502:CLA:HBD	22:AC:503:CLA:H43	2.03	0.40
26:AC:515:BCR:C33	8:AI:20:VAL:HG13	2.52	0.40
1:BA:271:LEU:HD21	24:BA:408:PL9:HC71	2.03	0.40
4:AD:43:LEU:HA	4:AD:43:LEU:HD12	1.94	0.40
15:AU:94:ILE:HB	15:AU:97:LEU:HD11	2.03	0.40
4:BD:238:THR:O	4:BD:239:GLN:C	2.59	0.40
3:BC:461:ARG:NH1	3:BC:461:ARG:HG3	2.36	0.40
3:BC:267:SER:O	3:BC:271:TYR:CD2	2.74	0.40
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.70	0.40
3:AC:464:GLU:HA	3:AC:465:PRO:HD2	1.72	0.40
15:AU:90:ASP:HA	15:AU:93:ASN:HD22	1.87	0.40
16:AV:160:LYS:HA	16:AV:163:TYR:CD2	2.56	0.40
15:AU:88:VAL:HG13	15:AU:109:LEU:HD22	2.03	0.40
1:AA:24:THR:OG1	3:AC:469:MET:CE	2.70	0.40
4:AD:302:GLU:OE1	4:AD:302:GLU:HA	2.20	0.40
1:BA:30:VAL:HG22	1:BA:30:VAL:O	2.21	0.40
9:AJ:9:PRO:HB2	9:AJ:12:ILE:HG13	2.03	0.40
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.42	0.40
4:BD:48:TRP:CD2	23:BD:403:PHO:H161	2.56	0.40
2:AB:233:ASN:O	2:AB:236:THR:HG22	2.22	0.40
29:AA:412:SQD:H132	28:AC:521:LHG:H132	2.02	0.40
28:AC:521:LHG:HC41	28:AC:521:LHG:O9	2.21	0.40
3:AC:59:LEU:HD13	22:AC:510:CLA:HMD2	2.04	0.40
26:AT:102:BCR:H393	22:BB:610:CLA:CAC	2.48	0.40
3:AC:414:ILE:CG2	3:AC:415:ASN:N	2.84	0.40
3:BC:416:SER:OG	3:BC:417:VAL:N	2.54	0.40
3:BC:84:GLN:O	3:BC:86:LEU:HD13	2.22	0.40
2:AB:222:PRO:O	2:AB:223:GLN:C	2.59	0.40
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.51	0.40
2:BB:385:ARG:O	2:BB:386:ALA:C	2.60	0.40
6:BF:25:THR:O	6:BF:29:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:205:LEU:HA	4:AD:205:LEU:HD12	1.71	0.40
13:AO:226:ASN:N	13:AO:226:ASN:ND2	2.69	0.40
7:BH:63:LYS:C	7:BH:65:LEU:H	2.23	0.40
3:AC:451:ALA:HA	3:AC:456:GLU:CD	2.41	0.40
1:BA:291:SER:HB3	3:BC:431:PHE:CE2	2.57	0.40
8:BI:7:THR:O	8:BI:8:VAL:C	2.59	0.40
2:BB:254:GLY:O	2:BB:258:TYR:HD2	2.05	0.40
2:BB:475:PHE:HB3	2:BB:478:VAL:CG2	2.52	0.40
1:BA:116:ILE:HG13	1:BA:117:PHE:N	2.37	0.40
2:BB:380:ASP:C	2:BB:380:ASP:OD1	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	39
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	39
2	AB	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	7	28
2	BB	488/510 (96%)	422 (86%)	52 (11%)	14 (3%)	7	28
3	AC	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	5	22
3	BC	445/473 (94%)	372 (84%)	56 (13%)	17 (4%)	5	19
4	AD	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	8	30
4	BD	338/352 (96%)	288 (85%)	42 (12%)	8 (2%)	9	35
5	AE	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	3	11
5	BE	80/84 (95%)	70 (88%)	6 (8%)	4 (5%)	3	11
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	27
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	27
7	AH	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	6
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	7
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	7
9	AJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	6
9	BJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	6
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	8
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	8
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	AM	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	3	11
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	4	14
14	AT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	24
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	24
15	AU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	16
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	16
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	30	72
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	30	72
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	1
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	1	1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	1	1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	11
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	11
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	6	23

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP

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Mol	Chain	Res	Type
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO
3	AC	144	SER
3	AC	257	PHE
3	AC	416	SER
3	AC	452	ALA
4	AD	239	GLN
4	AD	240	ALA
4	AD	262	SER
5	AE	82	GLN
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA
14	AT	30	THR
15	AU	72	TYR
15	AU	83	ALA
16	AV	75	ASN
17	Ay	43	ARG
18	AX	45	LYS
20	AZ	32	ASP
1	BA	12	ASN
1	BA	141	PRO
1	BA	142	TRP
2	BB	176	GLY
2	BB	230	ARG
2	BB	484	PRO
2	BB	488	PRO
3	BC	144	SER
3	BC	257	PHE
3	BC	416	SER
3	BC	452	ALA
4	BD	239	GLN
4	BD	240	ALA
4	BD	262	SER
7	BH	18	TYR
8	BI	25	SER
9	BJ	35	GLY
13	BO	52	ALA
14	BT	30	THR

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Mol	Chain	Res	Type
15	BU	72	TYR
15	BU	83	ALA
17	By	43	ARG
18	BX	45	LYS
20	BZ	32	ASP
2	AB	349	LYS
3	AC	46	SER
3	AC	136	GLY
3	AC	194	GLY
3	AC	209	ILE
3	AC	456	GLU
4	AD	234	ALA
4	AD	264	LYS
7	AH	26	GLY
9	AJ	38	SER
13	AO	231	ASP
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	349	LYS
2	BB	436	THR
3	BC	136	GLY
3	BC	141	GLU
3	BC	194	GLY
4	BD	234	ALA
5	BE	82	GLN
7	BH	26	GLY
9	BJ	38	SER
13	BO	158	ASN
13	BO	231	ASP
15	BU	73	PRO
16	BV	75	ASN
18	BX	43	ILE
2	AB	127	ARG
2	AB	183	PRO
2	AB	414	PRO
2	AB	436	THR
3	AC	32	GLY
3	AC	141	GLU
3	AC	375	LEU
3	AC	453	ALA
4	AD	263	ASN

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Mol	Chain	Res	Type
5	AE	9	PRO
7	AH	16	SER
10	AK	13	GLU
10	AK	45	PHE
13	AO	60	SER
13	AO	158	ASN
13	AO	165	SER
20	AZ	24	PRO
20	AZ	28	ALA
2	BB	13	ILE
2	BB	127	ARG
2	BB	183	PRO
2	BB	414	PRO
3	BC	32	GLY
3	BC	46	SER
3	BC	209	ILE
3	BC	375	LEU
3	BC	411	ALA
3	BC	456	GLU
4	BD	263	ASN
4	BD	264	LYS
5	BE	9	PRO
7	BH	16	SER
10	BK	13	GLU
10	BK	45	PHE
13	BO	165	SER
17	By	25	ILE
20	BZ	24	PRO
20	BZ	28	ALA
2	AB	13	ILE
2	AB	173	GLY
2	AB	231	MET
2	AB	235	GLU
3	AC	154	LYS
4	AD	73	PHE
5	AE	10	PHE
13	AO	51	THR
13	AO	82	PRO
17	Ay	24	MET
18	AX	44	ASP
2	BB	235	GLU
5	BE	10	PHE

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Mol	Chain	Res	Type
13	BO	60	SER
13	BO	82	PRO
1	AA	97	TRP
3	AC	462	GLU
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
18	AX	12	ILE
2	BB	435	GLU
3	BC	453	ALA
3	BC	462	GLU
4	BD	252	PHE
6	BF	41	GLN
7	BH	6	TRP
13	BO	85	LYS
13	BO	88	GLU
15	BU	42	VAL
17	By	24	MET
18	BX	44	ASP
1	AA	334	ARG
4	AD	351	ALA
7	AH	14	LEU
13	AO	88	GLU
1	BA	97	TRP
1	BA	334	ARG
2	BB	173	GLY
3	BC	382	ASN
4	BD	351	ALA
5	BE	52	PRO
13	BO	51	THR
13	BO	159	VAL
18	BX	12	ILE
1	AA	21	VAL
2	AB	16	PRO
13	AO	159	VAL
1	BA	21	VAL
17	By	35	ILE
3	AC	201	ASN
17	Ay	35	ILE
3	BC	201	ASN
5	AE	52	PRO
7	AH	60	VAL

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Mol	Chain	Res	Type
8	AI	32	PRO
13	AO	232	GLY
2	BB	16	PRO
8	BI	32	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	39	PRO
13	AO	152	VAL
13	BO	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	AA	271/280 (97%)	258 (95%)	13 (5%)	35	74
1	BA	271/280 (97%)	259 (96%)	12 (4%)	39	77
2	AB	390/407 (96%)	374 (96%)	16 (4%)	41	80
2	BB	390/407 (96%)	373 (96%)	17 (4%)	39	77
3	AC	347/374 (93%)	329 (95%)	18 (5%)	32	71
3	BC	347/374 (93%)	329 (95%)	18 (5%)	32	71
4	AD	275/283 (97%)	256 (93%)	19 (7%)	22	54
4	BD	275/283 (97%)	256 (93%)	19 (7%)	22	54
5	AE	72/73 (99%)	66 (92%)	6 (8%)	16	43
5	BE	72/73 (99%)	66 (92%)	6 (8%)	16	43
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	29	66
7	BH	53/55 (96%)	50 (94%)	3 (6%)	29	66
8	AI	32/35 (91%)	31 (97%)	1 (3%)	52	88
8	BI	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	40	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	40	79
10	AK	30/30 (100%)	28 (93%)	2 (7%)	23	56
10	BK	30/30 (100%)	28 (93%)	2 (7%)	23	56
11	AL	35/35 (100%)	31 (89%)	4 (11%)	8	24
11	BL	35/35 (100%)	32 (91%)	3 (9%)	15	41
12	AM	31/33 (94%)	31 (100%)	0	100	100
12	BM	31/33 (94%)	31 (100%)	0	100	100
13	AO	202/208 (97%)	195 (96%)	7 (4%)	48	85
13	BO	202/208 (97%)	194 (96%)	8 (4%)	42	81
14	AT	29/29 (100%)	28 (97%)	1 (3%)	49	86
14	BT	29/29 (100%)	28 (97%)	1 (3%)	49	86
15	AU	84/89 (94%)	80 (95%)	4 (5%)	35	74
15	BU	84/89 (94%)	80 (95%)	4 (5%)	35	74
16	AV	116/117 (99%)	111 (96%)	5 (4%)	40	78
16	BV	116/117 (99%)	111 (96%)	5 (4%)	40	78
17	Ay	20/37 (54%)	18 (90%)	2 (10%)	11	32
17	By	20/37 (54%)	18 (90%)	2 (10%)	11	32
18	AX	30/42 (71%)	26 (87%)	4 (13%)	6	16
18	BX	30/42 (71%)	26 (87%)	4 (13%)	6	16
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	12	35
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	12	35
All	All	4244/4492 (94%)	4022 (95%)	222 (5%)	32	71

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	30	VAL
1	AA	32	TRP
1	AA	157	VAL
1	AA	170	ASP
1	AA	202	VAL
1	AA	206	PHE
1	AA	234	ASN
1	AA	243	GLU
1	AA	271	LEU

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Mol	Chain	Res	Type
1	AA	286	THR
1	AA	292	THR
1	AA	298	ASN
1	AA	308	ASP
2	AB	11	VAL
2	AB	18	ARG
2	AB	84	THR
2	AB	223	GLN
2	AB	246	PHE
2	AB	262	THR
2	AB	308	LYS
2	AB	309	LEU
2	AB	362	PHE
2	AB	414	PRO
2	AB	422	ARG
2	AB	433	ASP
2	AB	483	ASP
2	AB	486	LEU
2	AB	488	PRO
2	AB	490	GLN
3	AC	29	GLU
3	AC	78	GLU
3	AC	86	LEU
3	AC	104	GLU
3	AC	165	LEU
3	AC	174	LEU
3	AC	201	ASN
3	AC	207	ARG
3	AC	232	ASP
3	AC	244	CYS
3	AC	289	PHE
3	AC	305	THR
3	AC	355	THR
3	AC	382	ASN
3	AC	391	ARG
3	AC	401	LEU
3	AC	447	ARG
3	AC	472	LEU
4	AD	20	ASP
4	AD	43	LEU
4	AD	53	THR
4	AD	60	THR

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Mol	Chain	Res	Type
4	AD	84	SER
4	AD	91	LEU
4	AD	130	PHE
4	AD	180	ARG
4	AD	201	VAL
4	AD	221	THR
4	AD	236	ASN
4	AD	241	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	279	LEU
4	AD	291	LEU
4	AD	294	ARG
4	AD	323	GLU
4	AD	346	LEU
5	AE	5	THR
5	AE	9	PRO
5	AE	18	ARG
5	AE	77	GLU
5	AE	82	GLN
5	AE	84	LYS
7	AH	27	THR
7	AH	49	TYR
7	AH	60	VAL
8	AI	33	LYS
9	AJ	7	ARG
10	AK	18	PHE
10	AK	19	ASP
11	AL	7	ARG
11	AL	8	GLN
11	AL	11	GLU
11	AL	15	THR
13	AO	31	LEU
13	AO	86	ARG
13	AO	97	VAL
13	AO	106	GLN
13	AO	141	ARG
13	AO	178	ARG
13	AO	219	THR
14	AT	29	ILE
15	AU	61	ASN
15	AU	88	VAL

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Mol	Chain	Res	Type
15	AU	114	VAL
15	AU	132	LEU
16	AV	35	THR
16	AV	63	CYS
16	AV	92	ARG
16	AV	116	GLU
16	AV	122	ARG
17	Ay	28	ILE
17	Ay	46	LEU
18	AX	11	THR
18	AX	12	ILE
18	AX	42	GLN
18	AX	45	LYS
20	AZ	14	ILE
20	AZ	25	VAL
20	AZ	33	TRP
20	AZ	58	ASN
20	AZ	62	VAL
1	BA	30	VAL
1	BA	32	TRP
1	BA	157	VAL
1	BA	170	ASP
1	BA	202	VAL
1	BA	206	PHE
1	BA	243	GLU
1	BA	271	LEU
1	BA	286	THR
1	BA	292	THR
1	BA	298	ASN
1	BA	308	ASP
2	BB	11	VAL
2	BB	18	ARG
2	BB	84	THR
2	BB	223	GLN
2	BB	246	PHE
2	BB	262	THR
2	BB	308	LYS
2	BB	309	LEU
2	BB	362	PHE
2	BB	414	PRO
2	BB	422	ARG
2	BB	433	ASP

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Mol	Chain	Res	Type
2	BB	436	THR
2	BB	483	ASP
2	BB	486	LEU
2	BB	488	PRO
2	BB	490	GLN
3	BC	29	GLU
3	BC	78	GLU
3	BC	86	LEU
3	BC	104	GLU
3	BC	165	LEU
3	BC	174	LEU
3	BC	201	ASN
3	BC	207	ARG
3	BC	232	ASP
3	BC	244	CYS
3	BC	289	PHE
3	BC	305	THR
3	BC	355	THR
3	BC	382	ASN
3	BC	391	ARG
3	BC	401	LEU
3	BC	447	ARG
3	BC	472	LEU
4	BD	20	ASP
4	BD	43	LEU
4	BD	53	THR
4	BD	60	THR
4	BD	84	SER
4	BD	91	LEU
4	BD	130	PHE
4	BD	180	ARG
4	BD	201	VAL
4	BD	221	THR
4	BD	236	ASN
4	BD	241	GLU
4	BD	256	ILE
4	BD	259	ILE
4	BD	279	LEU
4	BD	291	LEU
4	BD	294	ARG
4	BD	323	GLU
4	BD	346	LEU

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Mol	Chain	Res	Type
5	BE	5	THR
5	BE	9	PRO
5	BE	18	ARG
5	BE	77	GLU
5	BE	82	GLN
5	BE	84	LYS
7	BH	27	THR
7	BH	49	TYR
7	BH	60	VAL
8	BI	33	LYS
9	BJ	7	ARG
10	BK	18	PHE
10	BK	19	ASP
11	BL	7	ARG
11	BL	8	GLN
11	BL	11	GLU
13	BO	31	LEU
13	BO	86	ARG
13	BO	97	VAL
13	BO	106	GLN
13	BO	141	ARG
13	BO	178	ARG
13	BO	217	SER
13	BO	219	THR
14	BT	29	ILE
15	BU	61	ASN
15	BU	88	VAL
15	BU	114	VAL
15	BU	132	LEU
16	BV	35	THR
16	BV	63	CYS
16	BV	92	ARG
16	BV	116	GLU
16	BV	122	ARG
17	By	28	ILE
17	By	46	LEU
18	BX	11	THR
18	BX	12	ILE
18	BX	42	GLN
18	BX	45	LYS
20	BZ	14	ILE
20	BZ	25	VAL

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Mol	Chain	Res	Type
20	BZ	33	TRP
20	BZ	58	ASN
20	BZ	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	234	ASN
1	AA	241	GLN
2	AB	201	HIS
2	AB	216	HIS
2	AB	490	GLN
3	AC	155	ASN
3	AC	398	HIS
3	AC	418	ASN
3	AC	444	HIS
4	AD	98	GLN
4	AD	117	HIS
4	AD	129	GLN
4	AD	142	ASN
4	AD	239	GLN
4	AD	250	ASN
7	AH	59	ASN
11	AL	6	ASN
11	AL	8	GLN
12	AM	5	GLN
12	AM	33	GLN
13	AO	87	GLN
13	AO	106	GLN
13	AO	114	ASN
13	AO	135	GLN
13	AO	150	ASN
13	AO	173	ASN
13	AO	222	GLN
13	AO	226	ASN
15	AU	82	ASN
15	AU	93	ASN
17	Ay	21	GLN
18	AX	42	GLN
20	AZ	6	GLN

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Mol	Chain	Res	Type
1	BA	12	ASN
1	BA	19	ASN
1	BA	234	ASN
1	BA	241	GLN
2	BB	201	HIS
2	BB	216	HIS
2	BB	490	GLN
3	BC	155	ASN
3	BC	398	HIS
3	BC	418	ASN
3	BC	444	HIS
4	BD	98	GLN
4	BD	117	HIS
4	BD	129	GLN
4	BD	142	ASN
4	BD	239	GLN
4	BD	250	ASN
7	BH	59	ASN
11	BL	6	ASN
11	BL	8	GLN
12	BM	5	GLN
12	BM	33	GLN
13	BO	87	GLN
13	BO	106	GLN
13	BO	114	ASN
13	BO	135	GLN
13	BO	150	ASN
13	BO	173	ASN
13	BO	222	GLN
13	BO	226	ASN
15	BU	82	ASN
15	BU	93	ASN
18	BX	42	GLN
20	BZ	6	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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$
22	CLA	AA	402	1	73,73,73	1.53	10 (13%)	96,113,113	1.60	19 (19%)
22	CLA	AA	403	-	73,73,73	1.55	10 (13%)	96,113,113	1.72	17 (17%)
22	CLA	AA	404	-	73,73,73	1.45	8 (10%)	96,113,113	1.51	17 (17%)
23	PHO	AA	405	-	69,69,69	1.86	3 (4%)	92,99,99	1.56	17 (18%)
22	CLA	AA	406	1	73,73,73	1.45	8 (10%)	96,113,113	1.52	18 (18%)
24	PL9	AA	407	-	45,45,55	1.00	2 (4%)	55,57,69	1.87	15 (27%)
25	OEC	AA	408	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	AA	409	-	41,41,41	1.61	7 (17%)	56,56,56	2.07	20 (35%)
27	DGD	AA	410	-	57,57,67	2.09	14 (24%)	71,71,81	1.47	9 (12%)
28	LHG	AA	411	-	38,38,48	1.96	6 (15%)	44,44,54	1.31	4 (9%)
29	SQD	AA	412	-	51,51,54	6.74	27 (52%)	62,62,65	3.25	21 (33%)
30	LMG	AA	413	-	51,51,55	1.42	4 (7%)	59,59,63	1.01	4 (6%)
29	SQD	AA	415	-	54,54,54	2.79	29 (53%)	65,65,65	2.96	19 (29%)
30	LMG	AA	416	-	42,42,55	2.22	10 (23%)	50,50,63	1.01	3 (6%)
22	CLA	AB	601	-	73,73,73	1.74	11 (15%)	96,113,113	1.53	19 (19%)
22	CLA	AB	602	2	73,73,73	1.52	11 (15%)	96,113,113	1.52	18 (18%)
22	CLA	AB	603	2	73,73,73	1.52	8 (10%)	96,113,113	1.58	17 (17%)
22	CLA	AB	604	2	73,73,73	1.64	9 (12%)	96,113,113	1.52	19 (19%)
22	CLA	AB	605	-	73,73,73	1.61	11 (15%)	96,113,113	1.53	17 (17%)
22	CLA	AB	606	2	73,73,73	1.54	10 (13%)	96,113,113	1.51	18 (18%)
22	CLA	AB	607	-	73,73,73	1.58	12 (16%)	96,113,113	1.58	17 (17%)
22	CLA	AB	608	2	73,73,73	1.55	9 (12%)	96,113,113	1.58	19 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	AB	609	2	73,73,73	1.70	13 (17%)	96,113,113	1.53	19 (19%)
22	CLA	AB	610	-	73,73,73	1.52	9 (12%)	96,113,113	1.57	23 (23%)
22	CLA	AB	611	2	73,73,73	1.50	7 (9%)	96,113,113	1.53	17 (17%)
22	CLA	AB	612	-	73,73,73	1.55	9 (12%)	96,113,113	1.56	20 (20%)
22	CLA	AB	613	-	73,73,73	1.48	7 (9%)	96,113,113	1.53	20 (20%)
22	CLA	AB	614	2	73,73,73	1.62	11 (15%)	96,113,113	1.61	24 (25%)
22	CLA	AB	615	-	73,73,73	1.66	13 (17%)	96,113,113	1.59	20 (20%)
22	CLA	AB	616	-	73,73,73	1.59	10 (13%)	96,113,113	1.61	21 (21%)
26	BCR	AB	617	-	41,41,41	1.68	7 (17%)	56,56,56	1.96	14 (25%)
26	BCR	AB	618	-	41,41,41	1.68	6 (14%)	56,56,56	2.18	27 (48%)
26	BCR	AB	619	-	41,41,41	1.91	8 (19%)	56,56,56	2.06	15 (26%)
26	BCR	AB	620	-	41,41,41	1.83	7 (17%)	56,56,56	2.03	17 (30%)
30	LMG	AB	621	-	49,49,55	1.53	7 (14%)	57,57,63	1.05	4 (7%)
30	LMG	AB	622	-	49,49,55	1.82	6 (12%)	57,57,63	1.06	4 (7%)
30	LMG	AB	623	-	42,42,55	2.12	9 (21%)	50,50,63	1.03	3 (6%)
32	LMT	AB	624	-	36,36,36	1.42	5 (13%)	47,47,47	1.20	3 (6%)
32	LMT	AB	625	-	36,36,36	1.36	7 (19%)	47,47,47	0.96	3 (6%)
27	DGD	AB	626	-	53,53,67	2.59	18 (33%)	67,67,81	1.66	8 (11%)
32	LMT	AB	627	-	36,36,36	1.44	5 (13%)	47,47,47	1.03	3 (6%)
22	CLA	AC	501	3	73,73,73	1.52	6 (8%)	96,113,113	1.54	19 (19%)
22	CLA	AC	502	3	73,73,73	1.56	11 (15%)	96,113,113	1.51	17 (17%)
22	CLA	AC	503	3	73,73,73	1.70	11 (15%)	96,113,113	1.52	17 (17%)
22	CLA	AC	504	-	73,73,73	1.62	9 (12%)	96,113,113	1.57	17 (17%)
22	CLA	AC	505	3	73,73,73	1.68	10 (13%)	96,113,113	1.60	19 (19%)
22	CLA	AC	506	3	73,73,73	1.54	10 (13%)	96,113,113	1.55	18 (18%)
22	CLA	AC	507	-	73,73,73	1.43	10 (13%)	96,113,113	1.56	21 (21%)
22	CLA	AC	508	3	73,73,73	1.62	12 (16%)	96,113,113	1.58	20 (20%)
22	CLA	AC	509	-	73,73,73	1.61	10 (13%)	96,113,113	1.59	19 (19%)
22	CLA	AC	510	-	73,73,73	1.61	11 (15%)	96,113,113	1.55	19 (19%)
22	CLA	AC	511	3	73,73,73	1.71	10 (13%)	96,113,113	1.55	18 (18%)
22	CLA	AC	512	-	73,73,73	1.73	13 (17%)	96,113,113	1.61	21 (21%)
22	CLA	AC	513	3	73,73,73	1.68	10 (13%)	96,113,113	1.53	19 (19%)
26	BCR	AC	514	-	41,41,41	1.74	6 (14%)	56,56,56	2.11	22 (39%)
26	BCR	AC	515	-	41,41,41	1.66	6 (14%)	56,56,56	2.14	18 (32%)
27	DGD	AC	516	-	54,54,67	1.58	10 (18%)	68,68,81	1.60	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DGD	AC	517	-	63,63,67	1.29	6 (9%)	77,77,81	1.64	8 (10%)
27	DGD	AC	518	-	67,67,67	1.02	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	AC	519	-	48,48,55	1.90	7 (14%)	56,56,63	0.88	3 (5%)
30	LMG	AC	520	-	45,45,55	2.01	10 (22%)	53,53,63	1.04	4 (7%)
28	LHG	AC	521	-	36,36,48	1.73	4 (11%)	42,42,54	1.10	3 (7%)
33	BCT	AD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	AD	402	4	73,73,73	1.65	11 (15%)	96,113,113	1.55	19 (19%)
23	PHO	AD	403	-	69,69,69	1.96	4 (5%)	92,99,99	1.59	16 (17%)
22	CLA	AD	404	-	73,73,73	1.67	10 (13%)	96,113,113	1.54	18 (18%)
24	PL9	AD	405	-	55,55,55	0.54	0	69,69,69	1.87	18 (26%)
26	BCR	AD	406	-	41,41,41	1.82	7 (17%)	56,56,56	2.27	18 (32%)
30	LMG	AD	407	-	46,46,55	2.08	6 (13%)	54,54,63	0.93	2 (3%)
30	LMG	AD	408	-	48,48,55	1.68	5 (10%)	56,56,63	1.04	3 (5%)
29	SQD	AD	409	-	43,43,54	7.74	23 (53%)	54,54,65	3.66	18 (33%)
27	DGD	AD	410	-	64,64,67	1.91	18 (28%)	78,78,81	1.43	7 (8%)
32	LMT	AD	411	-	32,32,36	1.72	5 (15%)	43,43,47	1.01	2 (4%)
34	HEM	AE	101	5,6	50,50,50	2.54	26 (52%)	46,82,82	2.51	11 (23%)
30	LMG	AE	102	-	44,44,55	1.89	7 (15%)	52,52,63	1.12	6 (11%)
29	SQD	AF	101	-	45,45,54	10.21	25 (55%)	56,56,65	3.43	20 (35%)
26	BCR	AH	101	-	41,41,41	1.85	8 (19%)	56,56,56	2.23	21 (37%)
27	DGD	AH	102	-	59,59,67	2.11	10 (16%)	73,73,81	1.47	7 (9%)
30	LMG	AI	101	-	43,43,55	2.18	10 (23%)	51,51,63	1.09	4 (7%)
32	LMT	AI	102	-	36,36,36	1.40	4 (11%)	47,47,47	0.95	1 (2%)
24	PL9	AJ	101	-	35,35,55	1.40	5 (14%)	43,45,69	1.95	13 (30%)
26	BCR	AJ	102	-	41,41,41	2.04	8 (19%)	56,56,56	3.25	22 (39%)
26	BCR	AK	102	-	41,41,41	1.83	7 (17%)	56,56,56	2.50	24 (42%)
30	LMG	AM	101	-	42,42,55	2.34	8 (19%)	50,50,63	1.22	5 (10%)
32	LMT	AM	102	-	36,36,36	1.17	2 (5%)	47,47,47	0.94	2 (4%)
32	LMT	AT	101	-	36,36,36	1.35	5 (13%)	47,47,47	1.09	4 (8%)
26	BCR	AT	102	-	41,41,41	1.60	6 (14%)	56,56,56	2.18	24 (42%)
34	HEM	AV	201	16	50,50,50	2.57	23 (46%)	46,82,82	2.39	13 (28%)
26	BCR	AZ	101	-	41,41,41	1.81	7 (17%)	56,56,56	2.06	18 (32%)
29	SQD	BA	401	-	54,54,54	2.85	30 (55%)	65,65,65	3.00	21 (32%)
22	CLA	BA	403	1	73,73,73	1.54	11 (15%)	96,113,113	1.57	16 (16%)
22	CLA	BA	404	-	73,73,73	1.54	8 (10%)	96,113,113	1.75	20 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	BA	405	-	73,73,73	1.49	9 (12%)	96,113,113	1.52	17 (17%)
23	PHO	BA	406	-	69,69,69	1.97	6 (8%)	92,99,99	1.55	18 (19%)
22	CLA	BA	407	1	73,73,73	1.46	10 (13%)	96,113,113	1.53	18 (18%)
24	PL9	BA	408	-	45,45,55	1.06	3 (6%)	55,57,69	1.80	15 (27%)
25	OEC	BA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	BA	410	-	41,41,41	1.68	7 (17%)	56,56,56	2.06	21 (37%)
27	DGD	BA	411	-	57,57,67	2.18	14 (24%)	71,71,81	1.47	8 (11%)
28	LHG	BA	412	-	38,38,48	1.87	7 (18%)	44,44,54	1.29	4 (9%)
29	SQD	BA	413	-	51,51,54	6.87	26 (50%)	62,62,65	3.19	22 (35%)
30	LMG	BA	414	-	51,51,55	1.32	5 (9%)	59,59,63	1.03	4 (6%)
29	SQD	BB	601	-	47,47,54	3.19	24 (51%)	58,58,65	3.31	16 (27%)
27	DGD	BB	602	-	53,53,67	2.50	19 (35%)	67,67,81	1.64	8 (11%)
32	LMT	BB	603	-	36,36,36	1.42	7 (19%)	47,47,47	1.05	3 (6%)
22	CLA	BB	604	-	73,73,73	1.77	11 (15%)	96,113,113	1.54	19 (19%)
22	CLA	BB	605	2	73,73,73	1.50	11 (15%)	96,113,113	1.54	17 (17%)
22	CLA	BB	606	2	73,73,73	1.49	9 (12%)	96,113,113	1.59	18 (18%)
22	CLA	BB	607	2	73,73,73	1.68	11 (15%)	96,113,113	1.52	18 (18%)
22	CLA	BB	608	2	73,73,73	1.54	9 (12%)	96,113,113	1.52	16 (16%)
22	CLA	BB	609	2	73,73,73	1.58	6 (8%)	96,113,113	1.52	18 (18%)
22	CLA	BB	610	-	73,73,73	1.60	12 (16%)	96,113,113	1.58	18 (18%)
22	CLA	BB	611	2	73,73,73	1.59	12 (16%)	96,113,113	1.57	19 (19%)
22	CLA	BB	612	2	73,73,73	1.65	12 (16%)	96,113,113	1.53	17 (17%)
22	CLA	BB	613	-	73,73,73	1.55	11 (15%)	96,113,113	1.56	23 (23%)
22	CLA	BB	614	2	73,73,73	1.41	8 (10%)	96,113,113	1.52	17 (17%)
22	CLA	BB	615	-	73,73,73	1.57	11 (15%)	96,113,113	1.55	18 (18%)
22	CLA	BB	616	-	73,73,73	1.40	6 (8%)	96,113,113	1.54	20 (20%)
22	CLA	BB	617	2	73,73,73	1.59	10 (13%)	96,113,113	1.60	23 (23%)
22	CLA	BB	618	-	73,73,73	1.61	10 (13%)	96,113,113	1.56	19 (19%)
22	CLA	BB	619	-	73,73,73	1.59	11 (15%)	96,113,113	1.63	21 (21%)
26	BCR	BB	620	-	41,41,41	1.55	8 (19%)	56,56,56	1.97	14 (25%)
26	BCR	BB	621	-	41,41,41	1.84	7 (17%)	56,56,56	2.10	16 (28%)
26	BCR	BB	622	-	41,41,41	1.79	7 (17%)	56,56,56	2.03	18 (32%)
30	LMG	BB	623	-	49,49,55	1.50	7 (14%)	57,57,63	1.07	4 (7%)
30	LMG	BB	624	-	49,49,55	1.80	6 (12%)	57,57,63	1.04	3 (5%)
32	LMT	BB	625	-	36,36,36	1.53	8 (22%)	47,47,47	1.23	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BB	626	-	36,36,36	1.34	5 (13%)	47,47,47	0.94	2 (4%)
22	CLA	BC	501	3	73,73,73	1.55	8 (10%)	96,113,113	1.54	17 (17%)
22	CLA	BC	502	3	73,73,73	1.55	11 (15%)	96,113,113	1.53	16 (16%)
22	CLA	BC	503	3	73,73,73	1.72	11 (15%)	96,113,113	1.51	20 (20%)
22	CLA	BC	504	-	73,73,73	1.66	10 (13%)	96,113,113	1.58	16 (16%)
22	CLA	BC	505	3	73,73,73	1.74	10 (13%)	96,113,113	1.60	19 (19%)
22	CLA	BC	506	3	73,73,73	1.49	8 (10%)	96,113,113	1.52	18 (18%)
22	CLA	BC	507	-	73,73,73	1.45	8 (10%)	96,113,113	1.57	20 (20%)
22	CLA	BC	508	3	73,73,73	1.66	12 (16%)	96,113,113	1.57	20 (20%)
22	CLA	BC	509	-	73,73,73	1.67	13 (17%)	96,113,113	1.60	19 (19%)
22	CLA	BC	510	-	73,73,73	1.54	10 (13%)	96,113,113	1.56	18 (18%)
22	CLA	BC	511	3	73,73,73	1.72	9 (12%)	96,113,113	1.55	20 (20%)
22	CLA	BC	512	-	73,73,73	1.73	11 (15%)	96,113,113	1.60	22 (22%)
22	CLA	BC	513	3	73,73,73	1.65	11 (15%)	96,113,113	1.53	18 (18%)
26	BCR	BC	514	-	41,41,41	1.87	7 (17%)	56,56,56	2.10	20 (35%)
26	BCR	BC	515	-	41,41,41	1.79	7 (17%)	56,56,56	2.12	19 (33%)
27	DGD	BC	516	-	54,54,67	1.63	11 (20%)	68,68,81	1.56	8 (11%)
27	DGD	BC	517	-	63,63,67	1.24	7 (11%)	77,77,81	1.64	8 (10%)
27	DGD	BC	518	-	67,67,67	1.14	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	BC	519	-	48,48,55	2.02	8 (16%)	56,56,63	0.88	3 (5%)
30	LMG	BC	520	-	45,45,55	2.14	12 (26%)	53,53,63	1.06	4 (7%)
28	LHG	BC	521	-	36,36,48	1.71	4 (11%)	42,42,54	1.10	3 (7%)
33	BCT	BD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	BD	402	4	73,73,73	1.66	9 (12%)	96,113,113	1.54	20 (20%)
23	PHO	BD	403	-	69,69,69	1.94	4 (5%)	92,99,99	1.60	18 (19%)
22	CLA	BD	404	-	73,73,73	1.71	12 (16%)	96,113,113	1.50	15 (15%)
24	PL9	BD	405	-	55,55,55	0.51	0	69,69,69	1.89	18 (26%)
26	BCR	BD	406	-	41,41,41	1.90	8 (19%)	56,56,56	2.26	20 (35%)
30	LMG	BD	407	-	46,46,55	1.65	6 (13%)	54,54,63	0.95	2 (3%)
30	LMG	BD	408	-	48,48,55	1.61	4 (8%)	56,56,63	1.03	3 (5%)
29	SQD	BD	409	-	43,43,54	7.63	23 (53%)	54,54,65	3.63	19 (35%)
27	DGD	BD	410	-	64,64,67	1.82	18 (28%)	78,78,81	1.43	7 (8%)
32	LMT	BD	411	-	32,32,36	1.62	5 (15%)	43,43,47	0.96	2 (4%)
34	HEM	BE	101	5,6	50,50,50	2.60	26 (52%)	46,82,82	2.56	14 (30%)
30	LMG	BE	102	-	44,44,55	1.97	8 (18%)	52,52,63	1.12	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	BF	101	-	45,45,54	10.47	25 (55%)	56,56,65	3.41	19 (33%)
27	DGD	BH	101	-	59,59,67	1.89	11 (18%)	73,73,81	1.47	7 (9%)
30	LMG	BI	101	-	43,43,55	2.18	10 (23%)	51,51,63	1.12	4 (7%)
32	LMT	BI	102	-	36,36,36	1.49	4 (11%)	47,47,47	0.97	2 (4%)
24	PL9	BJ	101	-	35,35,55	1.44	6 (17%)	43,45,69	1.88	13 (30%)
26	BCR	BJ	102	-	41,41,41	2.15	8 (19%)	56,56,56	3.25	24 (42%)
26	BCR	BK	102	-	41,41,41	1.84	7 (17%)	56,56,56	2.50	26 (46%)
29	SQD	BL	101	-	47,47,54	3.30	23 (48%)	58,58,65	3.33	16 (27%)
32	LMT	BM	101	-	36,36,36	1.17	3 (8%)	47,47,47	0.96	2 (4%)
30	LMG	BM	102	-	42,42,55	2.45	10 (23%)	50,50,63	1.16	5 (10%)
32	LMT	BT	101	-	36,36,36	1.29	4 (11%)	47,47,47	1.05	4 (8%)
34	HEM	BV	201	16	50,50,50	2.55	23 (46%)	46,82,82	2.39	13 (28%)
26	BCR	BX	101	-	41,41,41	1.83	8 (19%)	56,56,56	2.24	22 (39%)
26	BCR	BZ	101	-	41,41,41	1.92	9 (21%)	56,56,56	2.05	19 (33%)

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
22	CLA	AA	402	1	-	0/37/135/135	0/0/9/9
22	CLA	AA	403	-	-	1/37/135/135	0/0/9/9
22	CLA	AA	404	-	-	0/37/135/135	0/0/9/9
23	PHO	AA	405	-	3/3/17/22	1/49/103/103	0/1/6/6
22	CLA	AA	406	1	-	0/37/135/135	0/0/9/9
24	PL9	AA	407	-	-	0/41/61/73	0/1/1/1
25	OEC	AA	408	1,3	-	0/0/0/54	0/0/0/5
26	BCR	AA	409	-	-	0/29/63/63	0/2/2/2
27	DGD	AA	410	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	AA	411	-	-	0/43/43/53	0/0/0/0
29	SQD	AA	412	-	-	0/46/66/69	0/1/1/1
30	LMG	AA	413	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	AA	415	-	-	0/49/69/69	0/1/1/1
30	LMG	AA	416	-	2/2/8/8	0/37/57/70	0/1/1/1
22	CLA	AB	601	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	602	2	-	1/37/135/135	0/0/9/9
22	CLA	AB	603	2	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	AB	604	2	-	0/37/135/135	0/0/9/9
22	CLA	AB	605	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	606	2	-	1/37/135/135	0/0/9/9
22	CLA	AB	607	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	608	2	-	0/37/135/135	0/0/9/9
22	CLA	AB	609	2	-	0/37/135/135	0/0/9/9
22	CLA	AB	610	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	611	2	-	1/37/135/135	0/0/9/9
22	CLA	AB	612	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	613	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	614	2	-	0/37/135/135	0/0/9/9
22	CLA	AB	615	-	-	0/37/135/135	0/0/9/9
22	CLA	AB	616	-	-	0/37/135/135	0/0/9/9
26	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	620	-	-	0/29/63/63	0/2/2/2
30	LMG	AB	621	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	622	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	623	-	2/2/8/8	0/37/57/70	0/1/1/1
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	625	-	-	0/21/61/61	0/2/2/2
27	DGD	AB	626	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	AB	627	-	-	0/21/61/61	0/2/2/2
22	CLA	AC	501	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	502	3	-	1/37/135/135	0/0/9/9
22	CLA	AC	503	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	504	-	-	0/37/135/135	0/0/9/9
22	CLA	AC	505	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	506	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	507	-	-	0/37/135/135	0/0/9/9
22	CLA	AC	508	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	509	-	-	1/37/135/135	0/0/9/9
22	CLA	AC	510	-	-	1/37/135/135	0/0/9/9
22	CLA	AC	511	3	-	0/37/135/135	0/0/9/9
22	CLA	AC	512	-	-	0/37/135/135	0/0/9/9
22	CLA	AC	513	3	-	1/37/135/135	0/0/9/9
26	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	AC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	AC	517	-	3/3/13/13	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	AC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	AC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	AC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	AC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	AD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	AD	402	4	-	0/37/135/135	0/0/9/9
23	PHO	AD	403	-	3/3/17/22	0/49/103/103	0/1/6/6
22	CLA	AD	404	-	-	0/37/135/135	0/0/9/9
24	PL9	AD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	AD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	AD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	AD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	AD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	AE	101	5,6	-	0/14/114/114	0/0/8/8
30	LMG	AE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	AF	101	-	-	0/40/60/69	0/1/1/1
26	BCR	AH	101	-	-	0/29/63/63	0/2/2/2
27	DGD	AH	102	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	AI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	AJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	AJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
30	LMG	AM	101	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AT	101	-	-	0/21/61/61	0/2/2/2
26	BCR	AT	102	-	-	0/29/63/63	0/2/2/2
34	HEM	AV	201	16	-	0/14/114/114	0/0/8/8
26	BCR	AZ	101	-	-	0/29/63/63	0/2/2/2
29	SQD	BA	401	-	-	0/49/69/69	0/1/1/1
22	CLA	BA	403	1	-	0/37/135/135	0/0/9/9
22	CLA	BA	404	-	-	1/37/135/135	0/0/9/9
22	CLA	BA	405	-	-	0/37/135/135	0/0/9/9
23	PHO	BA	406	-	3/3/17/22	1/49/103/103	0/1/6/6
22	CLA	BA	407	1	-	0/37/135/135	0/0/9/9
24	PL9	BA	408	-	-	0/41/61/73	0/1/1/1
25	OEC	BA	409	1,3	-	0/0/0/54	0/0/0/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	BA	410	-	-	0/29/63/63	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	BA	412	-	-	0/43/43/53	0/0/0/0
29	SQD	BA	413	-	-	0/46/66/69	0/1/1/1
30	LMG	BA	414	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	BB	601	-	-	0/42/62/69	0/1/1/1
27	DGD	BB	602	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	BB	603	-	-	0/21/61/61	0/2/2/2
22	CLA	BB	604	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	605	2	-	1/37/135/135	0/0/9/9
22	CLA	BB	606	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	607	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	608	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	609	2	-	1/37/135/135	0/0/9/9
22	CLA	BB	610	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	611	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	612	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	613	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	614	2	-	1/37/135/135	0/0/9/9
22	CLA	BB	615	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	616	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	617	2	-	0/37/135/135	0/0/9/9
22	CLA	BB	618	-	-	0/37/135/135	0/0/9/9
22	CLA	BB	619	-	-	0/37/135/135	0/0/9/9
26	BCR	BB	620	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	622	-	-	0/29/63/63	0/2/2/2
30	LMG	BB	623	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	BB	624	-	2/2/8/8	0/44/64/70	0/1/1/1
32	LMT	BB	625	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	626	-	-	0/21/61/61	0/2/2/2
22	CLA	BC	501	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	502	3	-	1/37/135/135	0/0/9/9
22	CLA	BC	503	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	504	-	-	0/37/135/135	0/0/9/9
22	CLA	BC	505	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	506	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	507	-	-	0/37/135/135	0/0/9/9
22	CLA	BC	508	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	509	-	-	1/37/135/135	0/0/9/9
22	CLA	BC	510	-	-	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BC	511	3	-	0/37/135/135	0/0/9/9
22	CLA	BC	512	-	-	0/37/135/135	0/0/9/9
22	CLA	BC	513	3	-	1/37/135/135	0/0/9/9
26	BCR	BC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	BC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	BC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	BC	517	-	3/3/13/13	0/51/91/95	0/2/2/2
27	DGD	BC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	BC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	BC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	BD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	BD	402	4	-	0/37/135/135	0/0/9/9
23	PHO	BD	403	-	3/3/17/22	0/49/103/103	0/1/6/6
22	CLA	BD	404	-	-	0/37/135/135	0/0/9/9
24	PL9	BD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	BD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	BD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	BD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	BD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	BE	101	5,6	-	0/14/114/114	0/0/8/8
30	LMG	BE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	BF	101	-	-	0/40/60/69	0/1/1/1
27	DGD	BH	101	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	BI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	BJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	BJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	0/29/63/63	0/2/2/2
29	SQD	BL	101	-	-	0/42/62/69	0/1/1/1
32	LMT	BM	101	-	-	0/21/61/61	0/2/2/2
30	LMG	BM	102	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	BT	101	-	-	0/21/61/61	0/2/2/2
34	HEM	BV	201	16	-	0/14/114/114	0/0/8/8
26	BCR	BX	101	-	-	0/29/63/63	0/2/2/2
26	BCR	BZ	101	-	-	0/29/63/63	0/2/2/2

All (1683) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BF	101	SQD	C19-C18	-47.81	1.36	1.55
29	BF	101	SQD	C32-C31	-47.75	1.36	1.55
29	AF	101	SQD	C19-C18	-47.49	1.36	1.55
29	AF	101	SQD	C32-C31	-45.64	1.37	1.55
29	AD	409	SQD	C18-C17	-45.22	1.37	1.55
29	BA	413	SQD	C35-C34	-44.89	1.37	1.55
29	BD	409	SQD	C18-C17	-44.60	1.37	1.55
29	AA	412	SQD	C35-C34	-43.95	1.37	1.55
30	AD	407	LMG	C22-C21	-11.81	1.50	1.55
23	BA	406	PHO	CHC-C1C	11.72	1.43	1.35
29	AD	409	SQD	C31-C30	11.62	1.59	1.55
29	BL	101	SQD	C31-C30	11.53	1.59	1.55
29	BD	409	SQD	C31-C30	11.45	1.59	1.55
23	BD	403	PHO	CHC-C1C	11.19	1.43	1.35
29	BB	601	SQD	C31-C30	11.15	1.59	1.55
27	AH	102	DGD	CDB-CCB	-11.07	1.50	1.55
27	AA	410	DGD	CDB-CCB	-11.07	1.50	1.55
27	BA	411	DGD	CDB-CCB	-10.94	1.50	1.55
23	AD	403	PHO	CHC-C1C	10.84	1.42	1.35
23	AA	405	PHO	CHC-C1C	10.36	1.42	1.35
30	AB	622	LMG	C23-C22	-10.30	1.51	1.55
29	BA	401	SQD	C6-C5	-10.29	1.39	1.52
29	AA	415	SQD	C6-C5	-10.23	1.39	1.52
30	BB	624	LMG	C23-C22	-10.23	1.51	1.55
29	BA	413	SQD	C6-C5	-10.14	1.40	1.52
27	AB	626	DGD	CDB-CCB	-9.89	1.51	1.55
29	AA	412	SQD	C6-C5	-9.89	1.40	1.52
30	AA	416	LMG	C22-C21	-9.66	1.51	1.55
30	BC	520	LMG	C22-C21	-9.63	1.51	1.55
30	BM	102	LMG	C37-C36	-9.54	1.51	1.55
27	BH	101	DGD	CDB-CCB	-9.36	1.51	1.55
30	BC	519	LMG	C23-C22	-9.34	1.51	1.55
29	AD	409	SQD	C6-C5	-9.08	1.41	1.52
27	AB	626	DGD	C9A-C8A	-9.07	1.51	1.55
27	BB	602	DGD	C9A-C8A	-9.06	1.51	1.55
30	AM	101	LMG	C37-C36	-8.92	1.51	1.55
29	AF	101	SQD	C6-C5	-8.87	1.41	1.52
29	BD	409	SQD	C6-C5	-8.86	1.41	1.52
30	AC	519	LMG	C23-C22	-8.86	1.51	1.55
30	BI	101	LMG	C23-C22	-8.86	1.51	1.55
30	AI	101	LMG	C23-C22	-8.72	1.51	1.55
30	AD	408	LMG	C25-C24	-8.70	1.51	1.55
30	AC	520	LMG	C22-C21	-8.69	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	602	DGD	CDB-CCB	-8.64	1.51	1.55
29	BF	101	SQD	C6-C5	-8.49	1.42	1.52
30	AE	102	LMG	C22-C21	-8.27	1.51	1.55
30	BE	102	LMG	C22-C21	-8.26	1.51	1.55
30	BD	407	LMG	C22-C21	-8.26	1.51	1.55
29	BL	101	SQD	C4-C3	8.21	1.74	1.52
30	AB	623	LMG	C22-C21	-8.03	1.52	1.55
30	BD	408	LMG	C25-C24	-7.84	1.52	1.55
22	AB	601	CLA	CHB-C4A	7.83	1.43	1.33
22	BB	604	CLA	CHB-C4A	7.72	1.43	1.33
22	BB	618	CLA	CHB-C4A	7.69	1.43	1.33
29	BB	601	SQD	C4-C3	7.69	1.72	1.52
28	AA	411	LHG	P-O5	7.67	1.79	1.51
29	AA	412	SQD	C4-C3	7.64	1.72	1.52
29	BA	413	SQD	C4-C3	7.61	1.72	1.52
29	BA	401	SQD	C4-C3	7.58	1.72	1.52
22	AB	615	CLA	CHB-C4A	7.51	1.43	1.33
22	BC	511	CLA	CHB-C4A	7.51	1.43	1.33
29	AA	415	SQD	C4-C3	7.50	1.72	1.52
30	AA	413	LMG	C25-C24	-7.49	1.52	1.55
22	AC	512	CLA	CHB-C4A	7.48	1.43	1.33
30	AB	621	LMG	C25-C24	-7.47	1.52	1.55
22	AB	609	CLA	CHB-C4A	7.44	1.43	1.33
22	BC	512	CLA	CHB-C4A	7.44	1.43	1.33
22	AC	511	CLA	CHB-C4A	7.42	1.43	1.33
22	AD	404	CLA	CHB-C4A	7.42	1.43	1.33
29	AD	409	SQD	C4-C3	7.41	1.72	1.52
28	BA	412	LHG	P-O5	7.37	1.78	1.51
30	BM	102	LMG	C22-C21	-7.29	1.52	1.55
22	AC	503	CLA	CHB-C4A	7.26	1.43	1.33
22	BD	404	CLA	CHB-C4A	7.21	1.43	1.33
22	AB	604	CLA	CHB-C4A	7.18	1.43	1.33
29	BD	409	SQD	C4-C3	7.16	1.71	1.52
22	BB	615	CLA	CHB-C4A	7.15	1.43	1.33
22	BC	504	CLA	C3B-C4B	7.14	1.49	1.41
22	AC	505	CLA	CHB-C4A	7.14	1.43	1.33
22	BC	503	CLA	CHB-C4A	7.12	1.43	1.33
22	AC	504	CLA	C3B-C4B	7.10	1.49	1.41
22	BC	510	CLA	CHB-C4A	7.10	1.42	1.33
22	AD	402	CLA	CHB-C4A	7.04	1.42	1.33
22	BC	505	CLA	CHB-C4A	7.02	1.42	1.33
22	AA	403	CLA	CHB-C4A	6.98	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AH	102	DGD	CFA-CEA	-6.98	1.52	1.55
23	BA	406	PHO	C1D-CHD	6.97	1.43	1.35
22	AC	509	CLA	CHB-C4A	6.96	1.42	1.33
22	AB	612	CLA	CHB-C4A	6.95	1.42	1.33
29	BB	601	SQD	C6-C5	-6.91	1.43	1.52
22	AB	605	CLA	CHB-C4A	6.91	1.42	1.33
29	BF	101	SQD	C4-C3	6.89	1.70	1.52
22	AB	607	CLA	CHB-C4A	6.89	1.42	1.33
22	BB	612	CLA	CHB-C4A	6.89	1.42	1.33
23	AD	403	PHO	C3B-C4B	6.87	1.49	1.41
22	AC	510	CLA	C3B-C4B	6.86	1.49	1.41
27	AC	516	DGD	CEA-CDA	-6.86	1.52	1.55
22	BB	613	CLA	CHB-C4A	6.85	1.42	1.33
30	BA	414	LMG	C25-C24	-6.82	1.52	1.55
22	BC	509	CLA	CHB-C4A	6.80	1.42	1.33
22	BB	609	CLA	CHB-C4A	6.79	1.42	1.33
30	AM	101	LMG	C22-C21	-6.78	1.52	1.55
29	BL	101	SQD	C6-C5	-6.76	1.44	1.52
29	AF	101	SQD	C4-C3	6.75	1.70	1.52
22	BD	402	CLA	CHB-C4A	6.73	1.42	1.33
22	BC	504	CLA	CHB-C4A	6.68	1.42	1.33
22	AC	501	CLA	CHB-C4A	6.67	1.42	1.33
22	BB	607	CLA	CHB-C4A	6.66	1.42	1.33
22	BC	513	CLA	CHB-C4A	6.65	1.42	1.33
22	AB	611	CLA	CHB-C4A	6.64	1.42	1.33
22	BB	619	CLA	CHB-C4A	6.63	1.42	1.33
23	AD	403	PHO	C1D-CHD	6.59	1.42	1.35
30	BB	623	LMG	C25-C24	-6.58	1.52	1.55
23	BD	403	PHO	C1D-CHD	6.58	1.42	1.35
22	AB	616	CLA	CHB-C4A	6.55	1.42	1.33
22	BB	608	CLA	CHB-C4A	6.53	1.42	1.33
22	AC	508	CLA	CHB-C4A	6.53	1.42	1.33
22	AB	613	CLA	CHB-C4A	6.52	1.42	1.33
22	AB	615	CLA	C3B-C4B	6.51	1.49	1.41
22	AB	606	CLA	CHB-C4A	6.50	1.42	1.33
22	BC	505	CLA	MG-NA	6.49	2.26	2.07
22	BC	501	CLA	CHB-C4A	6.49	1.42	1.33
22	AB	610	CLA	CHB-C4A	6.49	1.42	1.33
23	AA	405	PHO	C1D-CHD	6.47	1.42	1.35
22	AB	614	CLA	CHB-C4A	6.47	1.42	1.33
22	BC	508	CLA	CHB-C4A	6.44	1.42	1.33
22	BD	404	CLA	C3B-C4B	6.43	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	506	CLA	CHB-C4A	6.41	1.42	1.33
22	AB	608	CLA	CHB-C4A	6.41	1.42	1.33
22	BC	508	CLA	C3B-C4B	6.39	1.48	1.41
27	BC	516	DGD	CEA-CDA	-6.36	1.52	1.55
22	BC	512	CLA	C3B-C4B	6.36	1.48	1.41
22	AC	513	CLA	CHB-C4A	6.32	1.41	1.33
22	BC	509	CLA	C3B-C4B	6.32	1.48	1.41
23	BD	403	PHO	C3B-C4B	6.30	1.48	1.41
22	BA	404	CLA	C3B-C4B	6.28	1.48	1.41
27	BH	101	DGD	CFA-CEA	-6.28	1.52	1.55
22	BB	616	CLA	CHB-C4A	6.26	1.41	1.33
22	BA	405	CLA	CHB-C4A	6.24	1.41	1.33
22	BC	502	CLA	CHB-C4A	6.23	1.41	1.33
22	BB	610	CLA	CHB-C4A	6.22	1.41	1.33
26	BX	101	BCR	C26-C25	6.22	1.44	1.34
22	AB	602	CLA	C3B-C4B	6.17	1.48	1.41
22	AB	609	CLA	C3B-C4B	6.17	1.48	1.41
22	BB	611	CLA	CHB-C4A	6.16	1.41	1.33
23	AA	405	PHO	C3B-C4B	6.16	1.48	1.41
22	BB	618	CLA	C3B-C4B	6.14	1.48	1.41
26	BC	514	BCR	C1-C6	6.14	1.62	1.53
22	BC	511	CLA	MG-NA	6.07	2.25	2.07
22	AC	504	CLA	CHB-C4A	6.07	1.41	1.33
22	AC	511	CLA	MG-NA	6.04	2.25	2.07
30	AI	101	LMG	C37-C36	-6.01	1.52	1.55
26	AJ	102	BCR	C5-C6	6.01	1.43	1.34
22	AA	402	CLA	C3B-C4B	6.00	1.48	1.41
27	AC	517	DGD	CEA-CDA	-5.99	1.52	1.55
22	BB	617	CLA	C3B-C4B	5.92	1.48	1.41
28	AC	521	LHG	C30-C29	-5.92	1.52	1.55
22	BC	507	CLA	CHB-C4A	5.91	1.41	1.33
22	BC	503	CLA	C3B-C4B	5.90	1.48	1.41
30	AB	623	LMG	C37-C36	-5.89	1.52	1.55
26	AH	101	BCR	C26-C25	5.89	1.43	1.34
22	AC	510	CLA	CHB-C4A	5.88	1.41	1.33
22	AC	512	CLA	C3B-C4B	5.87	1.48	1.41
22	BB	617	CLA	CHB-C4A	5.87	1.41	1.33
22	BB	608	CLA	C3B-C4B	5.86	1.48	1.41
28	BC	521	LHG	C30-C29	-5.86	1.52	1.55
22	AC	507	CLA	CHB-C4A	5.85	1.41	1.33
22	BC	506	CLA	CHB-C4A	5.85	1.41	1.33
22	AC	508	CLA	C3B-C4B	5.85	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	502	CLA	C3B-C4B	5.84	1.48	1.41
22	BB	605	CLA	C3B-C4B	5.84	1.48	1.41
27	BD	410	DGD	O3G-C1D	5.83	1.50	1.40
26	BZ	101	BCR	C1-C6	5.83	1.62	1.53
22	AB	605	CLA	C3B-C4B	5.82	1.48	1.41
28	AC	521	LHG	C18-C17	-5.82	1.52	1.55
22	AA	404	CLA	CHB-C4A	5.82	1.41	1.33
28	BC	521	LHG	C18-C17	-5.79	1.52	1.55
30	BC	519	LMG	C42-C41	-5.78	1.52	1.55
29	BL	101	SQD	C6-S	5.78	1.86	1.77
22	BC	511	CLA	C3B-C4B	5.78	1.48	1.41
22	AB	603	CLA	C3B-C4B	5.75	1.48	1.41
26	BJ	102	BCR	C5-C6	5.74	1.43	1.34
22	BC	505	CLA	C3B-C4B	5.74	1.48	1.41
22	AA	406	CLA	CHB-C4A	5.73	1.41	1.33
34	BV	201	HEM	C2D-C1D	-5.71	1.41	1.45
22	BB	606	CLA	C3B-C4B	5.69	1.48	1.41
22	BB	605	CLA	CHB-C4A	5.68	1.41	1.33
22	BB	611	CLA	C3B-C4B	5.67	1.48	1.41
22	AC	511	CLA	C3B-C4B	5.65	1.48	1.41
34	AV	201	HEM	CHA-C4D	5.64	1.43	1.35
22	BA	407	CLA	CHB-C4A	5.64	1.41	1.33
27	AD	410	DGD	CFA-CEA	-5.63	1.52	1.55
26	BD	406	BCR	C26-C25	5.62	1.43	1.34
26	BJ	102	BCR	C30-C25	5.61	1.61	1.53
22	AC	503	CLA	MG-NA	5.61	2.23	2.07
22	BB	612	CLA	C3B-C4B	5.60	1.47	1.41
22	BC	510	CLA	C3B-C4B	5.59	1.47	1.41
22	AC	513	CLA	MG-NA	5.59	2.23	2.07
22	AC	509	CLA	C3B-C4B	5.57	1.47	1.41
26	BJ	102	BCR	C26-C25	5.57	1.43	1.34
22	BA	404	CLA	CHB-C4A	5.55	1.40	1.33
22	BB	614	CLA	CHB-C4A	5.55	1.40	1.33
22	AA	402	CLA	CHB-C4A	5.54	1.40	1.33
22	BD	402	CLA	MG-NA	5.54	2.23	2.07
26	BC	514	BCR	C30-C25	5.53	1.61	1.53
22	BB	609	CLA	MG-NA	5.53	2.23	2.07
22	AD	402	CLA	MG-NA	5.53	2.23	2.07
22	AC	502	CLA	CHB-C4A	5.52	1.40	1.33
26	BB	622	BCR	C30-C25	5.52	1.61	1.53
22	BB	607	CLA	C3B-C4B	5.51	1.47	1.41
22	AB	602	CLA	CHB-C4A	5.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	606	CLA	CHB-C4A	5.50	1.40	1.33
22	AC	503	CLA	C3B-C4B	5.50	1.47	1.41
22	BC	503	CLA	MG-NA	5.50	2.23	2.07
22	AB	614	CLA	C3B-C4B	5.49	1.47	1.41
26	AB	619	BCR	C30-C25	5.47	1.61	1.53
29	BL	101	SQD	O8-S	5.46	1.60	1.46
26	AK	102	BCR	C5-C6	5.46	1.43	1.34
27	AD	410	DGD	O3G-C1D	5.45	1.50	1.40
22	AC	505	CLA	MG-NA	5.44	2.23	2.07
22	AD	404	CLA	C3B-C4B	5.44	1.47	1.41
34	BE	101	HEM	C3B-C2B	-5.41	1.38	1.45
22	AC	505	CLA	C3B-C4B	5.40	1.47	1.41
22	BD	402	CLA	C3B-C4B	5.40	1.47	1.41
34	BV	201	HEM	CHA-C4D	5.39	1.43	1.35
22	BB	607	CLA	MG-NA	5.38	2.23	2.07
22	BA	403	CLA	C3B-C4B	5.38	1.47	1.41
22	AB	616	CLA	C3B-C4B	5.37	1.47	1.41
22	BC	502	CLA	C3B-C4B	5.34	1.47	1.41
22	BC	513	CLA	MG-NA	5.32	2.23	2.07
26	BZ	101	BCR	C30-C25	5.31	1.61	1.53
22	BA	405	CLA	C3B-C4B	5.30	1.47	1.41
22	BB	604	CLA	MG-NA	5.29	2.22	2.07
26	BK	102	BCR	C5-C6	5.29	1.42	1.34
26	AC	514	BCR	C1-C6	5.29	1.61	1.53
22	AC	513	CLA	C3B-C4B	5.29	1.47	1.41
26	AK	102	BCR	C30-C25	5.26	1.61	1.53
22	AB	612	CLA	C3B-C4B	5.26	1.47	1.41
26	BK	102	BCR	C30-C25	5.25	1.61	1.53
34	AV	201	HEM	C3B-C2B	-5.23	1.38	1.45
26	BB	621	BCR	C30-C25	5.22	1.61	1.53
22	AB	603	CLA	CHB-C4A	5.22	1.40	1.33
22	BA	407	CLA	C3B-C4B	5.21	1.47	1.41
29	BB	601	SQD	O8-S	5.20	1.59	1.46
26	AZ	101	BCR	C1-C6	5.18	1.61	1.53
22	AA	404	CLA	C3B-C4B	5.18	1.47	1.41
34	BV	201	HEM	C1A-NA	5.17	1.45	1.36
29	AD	409	SQD	O8-S	5.17	1.59	1.46
34	AV	201	HEM	C1A-NA	5.15	1.45	1.36
30	BE	102	LMG	C39-C38	-5.13	1.53	1.55
22	AC	506	CLA	C3B-C4B	5.12	1.47	1.41
29	BD	409	SQD	O8-S	5.11	1.59	1.46
29	BA	401	SQD	O8-S	5.11	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AV	201	HEM	C2D-C1D	-5.10	1.41	1.45
22	BB	615	CLA	C3B-C4B	5.09	1.47	1.41
22	AB	604	CLA	MG-NA	5.09	2.22	2.07
22	AB	608	CLA	C3B-C4B	5.09	1.47	1.41
26	AB	620	BCR	C30-C25	5.09	1.61	1.53
22	AB	601	CLA	C3B-C4B	5.08	1.47	1.41
22	AC	508	CLA	MG-NA	5.07	2.22	2.07
22	BC	513	CLA	C3B-C4B	5.06	1.47	1.41
26	AD	406	BCR	C26-C25	5.06	1.42	1.34
26	BC	515	BCR	C1-C6	5.04	1.61	1.53
22	BC	512	CLA	MG-NA	5.03	2.22	2.07
22	AB	611	CLA	C3B-C4B	5.02	1.47	1.41
22	AB	613	CLA	C3B-C4B	5.02	1.47	1.41
22	BB	614	CLA	C3B-C4B	5.02	1.47	1.41
29	AA	415	SQD	O8-S	5.02	1.59	1.46
26	AC	514	BCR	C30-C25	5.00	1.60	1.53
34	AV	201	HEM	C3C-C2C	-5.00	1.38	1.45
22	BA	403	CLA	CHB-C4A	4.99	1.40	1.33
26	AB	619	BCR	C1-C6	4.99	1.60	1.53
30	BI	101	LMG	C37-C36	-4.99	1.53	1.55
22	BB	619	CLA	C3B-C4B	4.99	1.47	1.41
22	BB	604	CLA	C3B-C4B	4.98	1.47	1.41
26	AB	620	BCR	C1-C6	4.97	1.60	1.53
22	BB	610	CLA	C3B-C4B	4.97	1.47	1.41
22	BC	506	CLA	C3B-C4B	4.95	1.47	1.41
34	AE	101	HEM	C3C-C2C	-4.94	1.39	1.45
34	AE	101	HEM	C3B-C2B	-4.94	1.39	1.45
27	BC	517	DGD	CEA-CDA	-4.90	1.53	1.55
26	AZ	101	BCR	C30-C25	4.90	1.60	1.53
22	AA	406	CLA	C3B-C4B	4.89	1.47	1.41
32	AD	411	LMT	C8-C7	-4.89	1.53	1.55
22	BB	612	CLA	MG-NA	4.89	2.21	2.07
29	AD	409	SQD	C1-C2	4.85	1.66	1.52
26	AJ	102	BCR	C26-C25	4.84	1.42	1.34
22	AB	606	CLA	MG-NA	4.82	2.21	2.07
26	AJ	102	BCR	C30-C25	4.81	1.60	1.53
22	BB	613	CLA	C3B-C4B	4.81	1.46	1.41
22	AB	606	CLA	C3B-C4B	4.81	1.46	1.41
23	BA	406	PHO	C3B-C4B	4.80	1.46	1.41
22	AB	610	CLA	C3B-C4B	4.80	1.46	1.41
30	AC	519	LMG	C42-C41	-4.80	1.53	1.55
29	BD	409	SQD	O5-C5	4.79	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BE	101	HEM	C1A-NA	4.79	1.44	1.36
22	AB	604	CLA	C3B-C4B	4.78	1.46	1.41
29	BF	101	SQD	O8-S	4.78	1.58	1.46
26	AB	619	BCR	C26-C25	4.77	1.41	1.34
26	BD	406	BCR	C1-C6	4.76	1.60	1.53
22	BC	501	CLA	C3B-C4B	4.73	1.46	1.41
32	BD	411	LMT	C8-C7	-4.70	1.53	1.55
22	AC	512	CLA	MG-NA	4.69	2.21	2.07
26	AA	409	BCR	C1-C6	4.69	1.60	1.53
26	BB	621	BCR	C26-C25	4.68	1.41	1.34
22	AB	601	CLA	MG-NA	4.68	2.21	2.07
27	BD	410	DGD	CFA-CEA	-4.68	1.53	1.55
26	AD	406	BCR	C30-C25	4.67	1.60	1.53
34	BV	201	HEM	C3C-C2C	-4.67	1.39	1.45
27	BA	411	DGD	O5D-C1E	4.66	1.48	1.40
26	BX	101	BCR	C30-C25	4.65	1.60	1.53
22	BC	508	CLA	MG-NA	4.65	2.21	2.07
30	AA	416	LMG	C37-C36	-4.63	1.53	1.55
29	AD	409	SQD	O5-C5	4.63	1.56	1.44
29	BD	409	SQD	O7-S	4.62	1.59	1.45
22	BC	501	CLA	MG-NA	4.61	2.20	2.07
22	AA	403	CLA	C3B-C4B	4.61	1.46	1.41
26	BA	410	BCR	C1-C6	4.60	1.60	1.53
26	BA	410	BCR	C30-C25	4.58	1.60	1.53
26	BB	622	BCR	C1-C6	4.58	1.60	1.53
26	AJ	102	BCR	C1-C6	4.57	1.60	1.53
22	BB	609	CLA	C3B-C4B	4.54	1.46	1.41
26	AB	618	BCR	C5-C6	4.54	1.41	1.34
26	BJ	102	BCR	C1-C6	4.53	1.60	1.53
22	AC	501	CLA	C3B-C4B	4.53	1.46	1.41
30	AM	101	LMG	O1-C1	4.52	1.48	1.40
34	AE	101	HEM	C1A-NA	4.52	1.44	1.36
29	BB	601	SQD	O7-S	4.51	1.59	1.45
29	BF	101	SQD	O5-C5	4.51	1.55	1.44
29	AD	409	SQD	O48-C23	4.50	1.47	1.33
22	AD	404	CLA	MG-NA	4.49	2.20	2.07
30	BM	102	LMG	O1-C1	4.49	1.48	1.40
34	BE	101	HEM	C3C-C2C	-4.48	1.39	1.45
29	BA	413	SQD	O8-S	4.48	1.58	1.46
26	BB	621	BCR	C1-C6	4.47	1.60	1.53
26	AB	618	BCR	C30-C25	4.47	1.60	1.53
26	AH	101	BCR	C30-C25	4.46	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BC	515	BCR	C30-C25	4.45	1.60	1.53
29	BL	101	SQD	O5-C5	4.44	1.55	1.44
22	AB	609	CLA	MG-NA	4.44	2.20	2.07
28	BA	412	LHG	P-O3	4.44	1.79	1.59
22	AD	402	CLA	C3B-C4B	4.43	1.46	1.41
26	AB	617	BCR	C26-C25	4.43	1.41	1.34
29	BD	409	SQD	C16-C17	-4.41	1.35	1.52
26	AC	515	BCR	C30-C25	4.41	1.60	1.53
22	BA	404	CLA	CAA-C2A	4.40	1.62	1.54
29	BF	101	SQD	O48-C23	4.39	1.46	1.33
22	BC	507	CLA	C3B-C4B	4.39	1.46	1.41
26	AH	101	BCR	C1-C6	4.39	1.60	1.53
34	BV	201	HEM	CBC-CAC	4.39	1.54	1.29
34	AV	201	HEM	CBC-CAC	4.38	1.54	1.29
22	AC	501	CLA	MG-NA	4.37	2.20	2.07
26	AC	515	BCR	C1-C6	4.37	1.60	1.53
29	BL	101	SQD	O7-S	4.37	1.58	1.45
26	AZ	101	BCR	C26-C25	4.36	1.41	1.34
29	BA	413	SQD	O7-S	4.36	1.58	1.45
34	BE	101	HEM	C2D-C1D	-4.36	1.42	1.45
26	BC	515	BCR	C5-C6	4.35	1.41	1.34
26	AT	102	BCR	C1-C6	4.35	1.60	1.53
29	BD	409	SQD	C1-C2	4.34	1.65	1.52
29	BB	601	SQD	O5-C5	4.33	1.55	1.44
26	BD	406	BCR	C30-C25	4.33	1.60	1.53
29	AD	409	SQD	O7-S	4.30	1.58	1.45
22	AB	614	CLA	MG-NA	4.30	2.20	2.07
26	AD	406	BCR	C5-C6	4.30	1.41	1.34
29	BA	401	SQD	O47-C7	4.29	1.47	1.34
29	AF	101	SQD	O8-S	4.28	1.57	1.46
28	AA	411	LHG	P-O3	4.28	1.78	1.59
34	BE	101	HEM	CBC-CAC	4.27	1.53	1.29
29	BF	101	SQD	O47-C7	4.26	1.47	1.34
29	AF	101	SQD	O47-C7	4.26	1.47	1.34
22	AA	402	CLA	MG-NA	4.24	2.19	2.07
22	AC	506	CLA	MG-NA	4.23	2.19	2.07
26	BZ	101	BCR	C26-C25	4.23	1.41	1.34
29	BA	401	SQD	C1-C2	4.22	1.65	1.52
22	AB	607	CLA	C3B-C4B	4.22	1.46	1.41
34	BV	201	HEM	C3D-C2D	-4.21	1.40	1.44
29	AF	101	SQD	O48-C23	4.21	1.46	1.33
34	AE	101	HEM	CHC-C1C	4.20	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BD	409	SQD	O47-C7	4.20	1.47	1.34
30	AD	407	LMG	C41-C40	-4.19	1.53	1.55
26	BB	620	BCR	C30-C25	4.19	1.59	1.53
29	BL	101	SQD	C1-C2	4.19	1.65	1.52
29	AD	409	SQD	C16-C17	-4.19	1.36	1.52
29	BB	601	SQD	C6-S	4.19	1.84	1.77
22	BB	616	CLA	C3B-C4B	4.18	1.46	1.41
29	BA	401	SQD	O5-C5	4.18	1.54	1.44
34	BE	101	HEM	CAA-C2A	4.14	1.59	1.52
22	BD	404	CLA	MG-NA	4.14	2.19	2.07
29	BA	413	SQD	O47-C7	4.14	1.46	1.34
26	AK	102	BCR	C1-C6	4.13	1.59	1.53
22	BC	509	CLA	MG-NA	4.13	2.19	2.07
27	AB	626	DGD	C4E-C3E	4.13	1.63	1.52
26	AB	620	BCR	C5-C6	4.13	1.40	1.34
22	AC	503	CLA	CAA-C2A	4.12	1.61	1.54
34	AE	101	HEM	CBC-CAC	4.12	1.52	1.29
26	AA	409	BCR	C30-C25	4.12	1.59	1.53
28	AC	521	LHG	O8-C23	4.11	1.45	1.33
26	AB	617	BCR	C30-C25	4.11	1.59	1.53
26	AT	102	BCR	C5-C6	4.11	1.40	1.34
26	AB	618	BCR	C1-C6	4.10	1.59	1.53
22	BC	502	CLA	MG-NA	4.10	2.19	2.07
22	AB	605	CLA	MG-NA	4.09	2.19	2.07
28	BC	521	LHG	O8-C23	4.09	1.45	1.33
22	AC	507	CLA	C3B-C4B	4.08	1.46	1.41
26	BX	101	BCR	C1-C6	4.08	1.59	1.53
26	BK	102	BCR	C1-C6	4.07	1.59	1.53
29	AA	412	SQD	O8-S	4.07	1.56	1.46
27	AD	410	DGD	O5D-C1E	4.06	1.47	1.40
22	BB	615	CLA	MG-NA	4.06	2.19	2.07
34	BE	101	HEM	CAD-CBD	4.04	1.63	1.52
34	AE	101	HEM	C3D-C2D	-4.04	1.40	1.44
29	BA	401	SQD	O7-S	4.04	1.57	1.45
26	AB	619	BCR	C5-C6	4.03	1.40	1.34
22	BC	503	CLA	CAA-C2A	4.02	1.61	1.54
22	BA	403	CLA	MG-NA	4.02	2.19	2.07
29	AA	412	SQD	O47-C7	4.01	1.46	1.34
22	BB	610	CLA	CAA-C2A	4.00	1.61	1.54
34	BE	101	HEM	CHC-C1C	4.00	1.42	1.36
29	AF	101	SQD	O5-C5	4.00	1.54	1.44
29	AF	101	SQD	O7-S	4.00	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BI	101	LMG	O6-C1	3.99	1.52	1.41
29	AD	409	SQD	O6-C1	3.99	1.47	1.40
34	BE	101	HEM	C3D-C2D	-3.98	1.40	1.44
29	BB	601	SQD	C1-C2	3.99	1.64	1.52
22	AC	502	CLA	MG-NA	3.97	2.19	2.07
34	BV	201	HEM	C3B-C2B	-3.96	1.40	1.45
34	AV	201	HEM	C3C-CAC	3.95	1.53	1.40
26	BD	406	BCR	C5-C6	3.94	1.40	1.34
22	AB	608	CLA	CAA-C2A	3.94	1.61	1.54
29	BF	101	SQD	O7-S	3.94	1.57	1.45
22	BB	617	CLA	MG-NA	3.94	2.18	2.07
27	AA	410	DGD	O5D-C1E	3.94	1.47	1.40
29	BA	401	SQD	O48-C23	3.93	1.45	1.33
29	BD	409	SQD	O48-C23	3.93	1.45	1.33
27	BB	602	DGD	C4E-C3E	3.93	1.62	1.52
22	AB	607	CLA	MG-NA	3.93	2.18	2.07
22	AC	510	CLA	C1A-NA	3.92	1.40	1.32
22	AB	603	CLA	MG-NA	3.92	2.18	2.07
29	AA	412	SQD	C33-C34	-3.92	1.37	1.52
29	AA	415	SQD	O7-S	3.92	1.57	1.45
22	AC	513	CLA	CAA-C2A	3.91	1.61	1.54
29	AA	415	SQD	O5-C5	3.91	1.54	1.44
34	AE	101	HEM	C2D-C1D	-3.90	1.42	1.45
26	AC	515	BCR	C5-C6	3.90	1.40	1.34
34	AE	101	HEM	CAA-C2A	3.90	1.58	1.52
26	BC	514	BCR	C26-C25	3.89	1.40	1.34
29	AD	409	SQD	O47-C7	3.89	1.46	1.34
26	BB	621	BCR	C5-C6	3.88	1.40	1.34
26	AB	617	BCR	C5-C6	3.87	1.40	1.34
29	AA	415	SQD	O47-C7	3.86	1.46	1.34
26	AD	406	BCR	C1-C6	3.86	1.59	1.53
28	AC	521	LHG	O7-C7	3.85	1.45	1.34
28	BC	521	LHG	O7-C7	3.83	1.45	1.34
26	BB	622	BCR	C5-C6	3.83	1.40	1.34
29	BA	413	SQD	C1-C2	3.83	1.63	1.52
32	AI	102	LMT	O1'-C1'	3.83	1.47	1.40
32	BB	625	LMT	O5'-C1'	3.83	1.51	1.41
24	BA	408	PL9	C7-C3	3.82	1.54	1.51
27	AD	410	DGD	O6D-C5D	3.82	1.53	1.44
30	AC	520	LMG	C4-C3	3.81	1.62	1.52
30	BD	408	LMG	O1-C1	3.81	1.47	1.40
34	BE	101	HEM	CHA-C4D	3.80	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BI	102	LMT	O1'-C1'	3.79	1.47	1.40
22	BB	611	CLA	CAA-C2A	3.79	1.61	1.54
29	AA	415	SQD	C1-C2	3.78	1.63	1.52
30	AB	623	LMG	O6-C1	3.78	1.51	1.41
26	AC	514	BCR	C26-C25	3.78	1.40	1.34
22	BB	610	CLA	MG-NA	3.77	2.18	2.07
30	BI	101	LMG	C4-C3	3.76	1.62	1.52
29	BF	101	SQD	C1-C2	3.75	1.63	1.52
26	AB	617	BCR	C1-C6	3.75	1.59	1.53
22	BB	608	CLA	MG-NA	3.74	2.18	2.07
27	BB	602	DGD	C4E-C5E	3.74	1.61	1.53
29	BA	413	SQD	C33-C34	-3.74	1.37	1.52
28	AA	411	LHG	C12-C11	-3.73	1.53	1.55
29	BL	101	SQD	O47-C7	3.73	1.45	1.34
29	AA	412	SQD	C1-C2	3.73	1.63	1.52
22	AC	501	CLA	CAA-C2A	3.72	1.60	1.54
26	BJ	102	BCR	C29-C30	3.72	1.63	1.54
22	BC	501	CLA	CAA-C2A	3.72	1.60	1.54
26	BA	410	BCR	C5-C6	3.71	1.40	1.34
30	AM	101	LMG	O7-C10	3.71	1.45	1.34
27	AD	410	DGD	O6D-C1D	3.71	1.51	1.41
34	AE	101	HEM	CHA-C4D	3.70	1.41	1.35
27	AD	410	DGD	O6E-C1E	3.69	1.51	1.41
34	BV	201	HEM	C3C-CAC	3.69	1.52	1.40
26	BC	515	BCR	C26-C25	3.69	1.40	1.34
27	AH	102	DGD	O5D-C1E	3.69	1.46	1.40
29	AF	101	SQD	C17-C18	-3.69	1.38	1.52
30	AI	101	LMG	O6-C1	3.69	1.51	1.41
29	BL	101	SQD	O48-C23	3.69	1.44	1.33
29	BF	101	SQD	C17-C18	-3.68	1.38	1.52
32	AB	624	LMT	O5'-C1'	3.67	1.51	1.41
22	BC	513	CLA	CAA-C2A	3.66	1.60	1.54
26	AJ	102	BCR	C29-C30	3.66	1.63	1.54
30	BM	102	LMG	O6-C1	3.66	1.51	1.41
22	BC	502	CLA	CAA-C2A	3.65	1.60	1.54
27	BC	516	DGD	O5D-C1E	3.65	1.46	1.40
34	BE	101	HEM	C1A-C2A	3.64	1.49	1.43
27	AC	516	DGD	O5D-C1E	3.64	1.46	1.40
22	AB	610	CLA	MG-NA	3.63	2.18	2.07
26	AH	101	BCR	C29-C30	3.63	1.63	1.54
32	AM	102	LMT	O1'-C1'	3.63	1.46	1.40
22	AA	403	CLA	CAA-C2A	3.62	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AE	102	LMG	O6-C1	3.62	1.51	1.41
22	AC	507	CLA	C1A-NA	3.61	1.40	1.32
22	AD	404	CLA	CAA-C2A	3.61	1.60	1.54
22	BB	614	CLA	C1A-NA	3.61	1.40	1.32
29	BA	413	SQD	O5-C5	3.60	1.53	1.44
22	BC	507	CLA	MG-NA	3.60	2.17	2.07
22	BC	511	CLA	CAA-C2A	3.60	1.60	1.54
27	BA	411	DGD	C4D-C5D	3.59	1.60	1.53
22	BB	607	CLA	C1A-NA	3.59	1.40	1.32
30	AA	416	LMG	O6-C1	3.59	1.51	1.41
29	BB	601	SQD	O48-C23	3.59	1.44	1.33
32	AD	411	LMT	O1'-C1'	3.58	1.46	1.40
26	BD	406	BCR	C29-C30	3.58	1.63	1.54
26	AB	620	BCR	C26-C25	3.58	1.40	1.34
27	BD	410	DGD	O6D-C1D	3.57	1.50	1.41
27	BB	602	DGD	O6E-C1E	3.56	1.50	1.41
22	AC	509	CLA	MG-NA	3.56	2.17	2.07
22	AA	404	CLA	CAA-C2A	3.56	1.60	1.54
29	BB	601	SQD	O47-C7	3.55	1.45	1.34
30	BM	102	LMG	O7-C10	3.56	1.45	1.34
22	BA	405	CLA	MG-NA	3.55	2.17	2.07
27	AB	626	DGD	C4D-C5D	3.54	1.60	1.53
26	AT	102	BCR	C30-C25	3.54	1.58	1.53
26	BA	410	BCR	C26-C25	3.54	1.39	1.34
30	AC	520	LMG	O6-C1	3.52	1.50	1.41
26	BB	620	BCR	C1-C6	3.51	1.58	1.53
22	BB	606	CLA	MG-NA	3.52	2.17	2.07
30	AM	101	LMG	O6-C1	3.51	1.50	1.41
29	BD	409	SQD	O6-C1	3.51	1.46	1.40
29	AA	412	SQD	O7-S	3.51	1.56	1.45
34	AV	201	HEM	C3D-C2D	-3.51	1.41	1.44
22	AB	614	CLA	CAA-C2A	3.51	1.60	1.54
32	BD	411	LMT	O1'-C1'	3.51	1.46	1.40
30	BC	520	LMG	O6-C1	3.50	1.50	1.41
22	AC	509	CLA	C1A-NA	3.50	1.39	1.32
30	AD	408	LMG	O1-C1	3.50	1.46	1.40
22	AC	504	CLA	C1A-NA	3.49	1.39	1.32
22	BC	504	CLA	C1A-NA	3.49	1.39	1.32
29	AA	412	SQD	O48-C23	3.49	1.44	1.33
30	BB	623	LMG	C41-C40	-3.48	1.53	1.55
27	AB	626	DGD	O5D-C1E	3.48	1.46	1.40
28	AA	411	LHG	P-O6	3.48	1.74	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AD	406	BCR	C29-C30	3.48	1.62	1.54
30	BD	408	LMG	O6-C1	3.47	1.50	1.41
28	AA	411	LHG	O7-C7	3.47	1.44	1.34
27	AB	626	DGD	O6D-C5D	3.47	1.53	1.44
30	BC	520	LMG	C4-C3	3.47	1.61	1.52
22	AA	406	CLA	MG-NA	3.47	2.17	2.07
34	BE	101	HEM	C3C-CAC	3.46	1.51	1.40
22	AC	502	CLA	C1A-NA	3.46	1.39	1.32
22	AC	507	CLA	MG-NA	3.46	2.17	2.07
22	AB	615	CLA	MG-NA	3.46	2.17	2.07
22	AB	615	CLA	C1A-NA	3.46	1.39	1.32
30	BC	520	LMG	C4-C5	3.45	1.60	1.53
27	BH	101	DGD	O5D-C1E	3.45	1.46	1.40
29	AD	409	SQD	O3-C3	3.45	1.51	1.43
22	BB	607	CLA	CAA-C2A	3.44	1.60	1.54
26	BZ	101	BCR	C2-C1	3.44	1.62	1.54
26	AA	409	BCR	C26-C25	3.43	1.39	1.34
30	AE	102	LMG	C39-C38	-3.42	1.53	1.55
30	AI	101	LMG	C4-C3	3.42	1.61	1.52
22	AB	601	CLA	C4B-NB	3.42	1.40	1.34
22	AC	504	CLA	CAA-C2A	3.42	1.60	1.54
27	BC	517	DGD	O6D-C1D	3.42	1.50	1.41
29	AA	415	SQD	O6-C1	3.41	1.46	1.40
22	BC	505	CLA	CAA-C2A	3.41	1.60	1.54
26	BB	620	BCR	C26-C25	3.40	1.39	1.34
22	AB	604	CLA	CAA-C2A	3.40	1.60	1.54
29	BF	101	SQD	O6-C1	3.39	1.46	1.40
34	BE	101	HEM	FE-NB	3.39	2.09	1.96
22	BB	619	CLA	C1A-NA	3.39	1.39	1.32
22	AB	612	CLA	C1A-NA	3.38	1.39	1.32
26	AB	619	BCR	C29-C30	3.38	1.62	1.54
22	AB	612	CLA	MG-NA	3.38	2.17	2.07
27	BD	410	DGD	O6D-C5D	3.38	1.52	1.44
22	BC	503	CLA	C1A-NA	3.38	1.39	1.32
32	BM	101	LMT	O1'-C1'	3.37	1.46	1.40
29	AA	415	SQD	O48-C23	3.37	1.43	1.33
22	BB	618	CLA	C1A-NA	3.37	1.39	1.32
34	AV	201	HEM	CHC-C1C	3.37	1.41	1.36
22	AB	616	CLA	MG-NA	3.37	2.17	2.07
22	AB	601	CLA	C1A-NA	3.37	1.39	1.32
29	AF	101	SQD	O6-C1	3.37	1.46	1.40
22	BB	611	CLA	MG-NA	3.37	2.17	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	506	CLA	CAA-C2A	3.36	1.60	1.54
22	BA	405	CLA	CAA-C2A	3.35	1.60	1.54
22	AD	402	CLA	CAA-C2A	3.35	1.60	1.54
30	AB	623	LMG	C4-C5	3.35	1.60	1.53
22	BB	613	CLA	MG-NA	3.35	2.17	2.07
26	BX	101	BCR	C29-C30	3.35	1.62	1.54
30	BM	102	LMG	O6-C5	3.34	1.52	1.44
26	AZ	101	BCR	C29-C30	3.34	1.62	1.54
22	BB	608	CLA	CAA-C2A	3.34	1.60	1.54
27	BA	411	DGD	O6D-C1D	3.34	1.50	1.41
26	BZ	101	BCR	C29-C30	3.34	1.62	1.54
34	BV	201	HEM	C1A-C2A	3.33	1.49	1.43
22	AB	609	CLA	CAA-C2A	3.33	1.60	1.54
27	BC	518	DGD	O5D-C1E	3.33	1.46	1.40
32	AB	627	LMT	O1B-C1B	3.33	1.50	1.41
34	AE	101	HEM	CAD-CBD	3.33	1.61	1.52
27	BB	602	DGD	O3G-C1D	3.33	1.46	1.40
27	BC	518	DGD	O3G-C1D	3.32	1.46	1.40
22	BC	507	CLA	C1A-NA	3.32	1.39	1.32
22	BA	403	CLA	CAA-C2A	3.32	1.60	1.54
27	BC	518	DGD	O6D-C1D	3.32	1.50	1.41
22	AB	605	CLA	CAA-C2A	3.31	1.60	1.54
30	AA	413	LMG	O6-C1	3.31	1.50	1.41
22	AA	404	CLA	MG-NA	3.31	2.17	2.07
29	AF	101	SQD	C1-C2	3.31	1.62	1.52
22	BB	604	CLA	C4B-NB	3.31	1.39	1.34
22	BD	402	CLA	CAA-C2A	3.30	1.60	1.54
30	BI	101	LMG	O6-C5	3.30	1.52	1.44
22	BD	404	CLA	C1A-NA	3.28	1.39	1.32
26	BB	621	BCR	C29-C30	3.28	1.62	1.54
22	BB	612	CLA	CAA-C2A	3.28	1.60	1.54
26	AB	620	BCR	C29-C30	3.28	1.62	1.54
27	AB	626	DGD	O6E-C1E	3.28	1.50	1.41
34	AE	101	HEM	FE-NB	3.28	2.09	1.96
22	AC	512	CLA	C4B-NB	3.28	1.39	1.34
30	AD	408	LMG	O6-C1	3.28	1.50	1.41
29	BD	409	SQD	O3-C3	3.28	1.50	1.43
34	AV	201	HEM	C3D-C4D	3.27	1.47	1.45
30	BA	414	LMG	O6-C1	3.27	1.50	1.41
27	BB	602	DGD	C4D-C5D	3.27	1.60	1.53
34	BV	201	HEM	FE-NC	3.27	2.08	1.95
22	BB	619	CLA	CAA-C2A	3.27	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	622	BCR	C29-C30	3.26	1.62	1.54
30	BC	519	LMG	O6-C1	3.26	1.50	1.41
26	BC	515	BCR	C2-C1	3.26	1.62	1.54
22	BB	619	CLA	MG-NA	3.26	2.16	2.07
22	AC	511	CLA	C1A-NA	3.26	1.39	1.32
27	BD	410	DGD	O6E-C1E	3.25	1.50	1.41
22	AB	602	CLA	C1A-NA	3.25	1.39	1.32
30	AC	519	LMG	O1-C1	3.25	1.46	1.40
26	BX	101	BCR	C2-C1	3.25	1.62	1.54
22	AB	611	CLA	C1A-NA	3.25	1.39	1.32
22	BC	504	CLA	CAA-C2A	3.24	1.60	1.54
22	BA	404	CLA	MG-NA	3.24	2.16	2.07
22	BD	404	CLA	CAA-C2A	3.24	1.60	1.54
22	AB	616	CLA	CAA-C2A	3.24	1.60	1.54
26	AA	409	BCR	C2-C1	3.24	1.62	1.54
22	BC	509	CLA	C1A-NA	3.23	1.39	1.32
34	AE	101	HEM	C3C-CAC	3.23	1.50	1.40
26	AA	409	BCR	C5-C6	3.23	1.39	1.34
22	AB	607	CLA	CAA-C2A	3.23	1.60	1.54
34	BV	201	HEM	CAD-CBD	3.23	1.61	1.52
22	BB	610	CLA	C1A-NA	3.23	1.39	1.32
22	BC	502	CLA	C1A-NA	3.23	1.39	1.32
22	AC	505	CLA	C1A-NA	3.23	1.39	1.32
27	BD	410	DGD	O5D-C1E	3.22	1.46	1.40
22	AB	604	CLA	C1A-NA	3.23	1.39	1.32
22	AC	513	CLA	C1A-NA	3.23	1.39	1.32
29	BA	413	SQD	O48-C23	3.22	1.43	1.33
22	AC	505	CLA	CAA-C2A	3.22	1.60	1.54
28	BA	412	LHG	P-O6	3.22	1.73	1.59
22	BB	617	CLA	CAA-C2A	3.22	1.60	1.54
30	AC	520	LMG	O6-C5	3.22	1.52	1.44
22	BC	513	CLA	C1A-NA	3.22	1.39	1.32
22	BC	511	CLA	C1A-NA	3.22	1.39	1.32
27	AB	626	DGD	O3G-C1D	3.21	1.46	1.40
34	BV	201	HEM	CHC-C1C	3.21	1.41	1.36
29	AA	412	SQD	O5-C5	3.21	1.52	1.44
22	AB	616	CLA	C1A-NA	3.20	1.39	1.32
34	AV	201	HEM	FE-NB	3.20	2.09	1.96
26	AB	618	BCR	C2-C1	3.20	1.62	1.54
22	BB	611	CLA	C1A-NA	3.19	1.39	1.32
26	AB	620	BCR	C2-C1	3.19	1.62	1.54
29	BL	101	SQD	O3-C3	3.19	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BD	407	LMG	C41-C40	-3.19	1.53	1.55
27	BB	602	DGD	O5D-C1E	3.19	1.45	1.40
22	BB	604	CLA	C1A-NA	3.18	1.39	1.32
34	AV	201	HEM	FE-NC	3.19	2.08	1.95
27	BC	516	DGD	O6D-C1D	3.18	1.50	1.41
32	BB	603	LMT	O1B-C1B	3.18	1.50	1.41
30	BC	519	LMG	O1-C1	3.18	1.45	1.40
22	AC	512	CLA	C1A-NA	3.18	1.39	1.32
26	AK	102	BCR	C29-C30	3.17	1.62	1.54
28	BA	412	LHG	O7-C7	3.17	1.43	1.34
22	AA	404	CLA	C1A-NA	3.17	1.39	1.32
32	AT	101	LMT	O5B-C1B	3.17	1.49	1.41
22	BB	617	CLA	C1A-NA	3.17	1.39	1.32
34	BV	201	HEM	CAA-C2A	3.17	1.57	1.52
34	AE	101	HEM	C1A-C2A	3.17	1.48	1.43
22	BB	604	CLA	C1B-C2B	3.17	1.48	1.43
22	AC	508	CLA	C1A-NA	3.16	1.39	1.32
30	AA	416	LMG	C4-C5	3.16	1.59	1.53
22	BC	508	CLA	C1A-NA	3.16	1.39	1.32
26	BC	514	BCR	C29-C30	3.16	1.62	1.54
22	BC	506	CLA	MG-NA	3.16	2.16	2.07
26	AT	102	BCR	C2-C1	3.16	1.62	1.54
22	BB	615	CLA	C1A-NA	3.15	1.39	1.32
26	BC	514	BCR	C2-C1	3.15	1.62	1.54
27	AA	410	DGD	O3G-C1D	3.15	1.45	1.40
22	AB	601	CLA	C1B-C2B	3.15	1.48	1.43
26	BB	622	BCR	C2-C1	3.15	1.62	1.54
29	BD	409	SQD	C6-S	3.15	1.82	1.77
27	BA	411	DGD	O3G-C1D	3.15	1.45	1.40
22	BD	402	CLA	C1A-NA	3.15	1.39	1.32
22	AB	603	CLA	C1A-NA	3.14	1.39	1.32
30	AB	623	LMG	O1-C1	3.14	1.45	1.40
34	AE	101	HEM	FE-NC	3.14	2.08	1.95
22	BB	616	CLA	C1A-NA	3.14	1.39	1.32
22	AB	613	CLA	MG-NA	3.14	2.16	2.07
29	AD	409	SQD	O5-C1	3.14	1.49	1.41
22	AB	608	CLA	C1A-NA	3.14	1.39	1.32
22	AC	506	CLA	CAA-C2A	3.13	1.59	1.54
26	BZ	101	BCR	C5-C6	3.14	1.39	1.34
27	AB	626	DGD	C4E-C5E	3.13	1.59	1.53
27	AD	410	DGD	C4E-C5E	3.13	1.59	1.53
30	BE	102	LMG	O1-C1	3.13	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	401	SQD	C6-S	3.12	1.82	1.77
30	AC	519	LMG	O6-C1	3.12	1.49	1.41
29	BB	601	SQD	O5-C1	3.12	1.49	1.41
22	BC	501	CLA	C1A-NA	3.12	1.39	1.32
26	BB	620	BCR	C5-C6	3.12	1.39	1.34
34	BE	101	HEM	C4D-ND	-3.12	1.33	1.39
30	AB	621	LMG	C41-C40	-3.12	1.53	1.55
22	AC	511	CLA	CAA-C2A	3.12	1.59	1.54
27	BB	602	DGD	O6D-C5D	3.11	1.52	1.44
30	AC	520	LMG	C4-C5	3.11	1.59	1.53
34	AV	201	HEM	CAA-C2A	3.10	1.57	1.52
22	BA	403	CLA	C4A-NA	-3.10	1.33	1.38
26	BK	102	BCR	C29-C30	3.09	1.61	1.54
22	AA	402	CLA	CAA-C2A	3.09	1.59	1.54
26	BD	406	BCR	C2-C1	3.09	1.61	1.54
26	AB	617	BCR	C29-C30	3.09	1.61	1.54
27	AA	410	DGD	O6D-C1D	3.09	1.49	1.41
24	AA	407	PL9	C7-C3	3.09	1.54	1.51
22	BC	512	CLA	C1A-NA	3.08	1.39	1.32
29	AA	415	SQD	O3-C3	3.08	1.50	1.43
29	BA	401	SQD	O3-C3	3.08	1.50	1.43
26	AZ	101	BCR	C5-C6	3.08	1.39	1.34
22	AB	607	CLA	C1A-NA	3.08	1.39	1.32
27	AA	410	DGD	C4D-C5D	3.07	1.59	1.53
30	AM	101	LMG	O6-C5	3.07	1.52	1.44
22	BC	506	CLA	C1A-NA	3.07	1.39	1.32
22	BC	505	CLA	C1A-NA	3.07	1.39	1.32
26	BC	514	BCR	C5-C6	3.07	1.39	1.34
30	BI	101	LMG	C4-C5	3.06	1.59	1.53
22	BB	606	CLA	C1A-NA	3.06	1.39	1.32
22	BB	609	CLA	CAA-C2A	3.06	1.59	1.54
26	AC	515	BCR	C26-C25	3.06	1.39	1.34
27	AC	516	DGD	C9B-C8B	-3.06	1.53	1.55
22	BA	403	CLA	C1A-NA	3.05	1.39	1.32
22	AA	402	CLA	C1A-NA	3.05	1.39	1.32
26	AC	514	BCR	C29-C30	3.05	1.61	1.54
27	BC	516	DGD	C9B-C8B	-3.05	1.53	1.55
30	AI	101	LMG	O6-C5	3.04	1.52	1.44
27	BB	602	DGD	O2G-C1B	3.04	1.43	1.34
22	AB	613	CLA	C1A-NA	3.04	1.38	1.32
30	BC	520	LMG	O6-C5	3.04	1.52	1.44
26	BJ	102	BCR	C2-C1	3.04	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BK	102	BCR	C26-C25	3.04	1.39	1.34
29	BF	101	SQD	C6-S	3.04	1.82	1.77
22	AB	610	CLA	C1A-NA	3.04	1.38	1.32
27	BA	411	DGD	C4E-C3E	3.03	1.60	1.52
34	AE	101	HEM	C4D-ND	-3.03	1.33	1.39
22	AA	403	CLA	C1A-NA	3.03	1.38	1.32
26	AB	618	BCR	C29-C30	3.03	1.61	1.54
29	AD	409	SQD	C6-S	3.03	1.82	1.77
26	AB	618	BCR	C26-C25	3.03	1.39	1.34
32	BB	603	LMT	O5B-C1B	3.03	1.49	1.41
30	AI	101	LMG	C4-C5	3.03	1.59	1.53
22	AB	611	CLA	CAA-C2A	3.03	1.59	1.54
22	BB	613	CLA	C1A-NA	3.03	1.38	1.32
32	BB	626	LMT	O1'-C1'	3.02	1.45	1.40
27	BA	411	DGD	C4E-C5E	3.02	1.59	1.53
22	AC	502	CLA	CAA-C2A	3.02	1.59	1.54
32	BT	101	LMT	O5B-C1B	3.02	1.49	1.41
22	AC	501	CLA	C1A-NA	3.02	1.38	1.32
26	BA	410	BCR	C2-C1	3.02	1.61	1.54
22	AB	603	CLA	CAA-C2A	3.02	1.59	1.54
29	AA	412	SQD	O3-C3	3.02	1.50	1.43
22	BC	504	CLA	MG-NB	3.01	2.11	2.05
22	BC	510	CLA	C1A-NA	3.01	1.38	1.32
24	AJ	101	PL9	C6-C1	3.01	1.54	1.48
30	AB	622	LMG	O6-C1	3.01	1.49	1.41
30	AE	102	LMG	O1-C1	3.01	1.45	1.40
22	AB	606	CLA	CAA-C2A	3.01	1.59	1.54
22	BA	407	CLA	MG-NA	3.01	2.16	2.07
22	AB	608	CLA	MG-NA	3.01	2.16	2.07
32	BB	625	LMT	O5B-C1B	3.00	1.49	1.41
26	BC	515	BCR	C29-C30	3.00	1.61	1.54
24	BJ	101	PL9	C6-C1	3.00	1.54	1.48
22	AB	614	CLA	C1A-NA	3.00	1.38	1.32
32	AB	625	LMT	O1'-C1'	3.00	1.45	1.40
26	AB	617	BCR	C2-C1	3.00	1.61	1.54
26	AC	515	BCR	C2-C1	3.00	1.61	1.54
26	AZ	101	BCR	C2-C1	2.99	1.61	1.54
30	AD	408	LMG	C40-C39	-2.99	1.54	1.55
22	BA	405	CLA	C1A-NA	2.99	1.38	1.32
29	BF	101	SQD	C8-C7	2.99	1.59	1.50
27	AC	517	DGD	O6D-C1D	2.98	1.49	1.41
29	BL	101	SQD	O5-C1	2.98	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	620	BCR	C29-C30	2.97	1.61	1.54
30	BC	520	LMG	C40-C39	-2.97	1.54	1.55
22	AC	503	CLA	C1A-NA	2.97	1.38	1.32
32	BD	411	LMT	O5'-C1'	2.97	1.49	1.41
34	BE	101	HEM	FE-NC	2.97	2.07	1.95
24	BJ	101	PL9	C7-C3	2.97	1.53	1.51
34	BE	101	HEM	C3B-CAB	2.97	1.50	1.40
22	BB	618	CLA	MG-NA	2.96	2.16	2.07
29	BF	101	SQD	O3-C3	2.96	1.50	1.43
27	AA	410	DGD	C4E-C3E	2.96	1.60	1.52
30	BB	623	LMG	O6-C1	2.95	1.49	1.41
30	BE	102	LMG	O6-C1	2.95	1.49	1.41
22	BB	616	CLA	C4A-NA	-2.95	1.33	1.38
29	BF	101	SQD	O5-C1	2.94	1.49	1.41
22	BC	512	CLA	C4B-NB	2.94	1.39	1.34
26	BB	621	BCR	C2-C1	2.94	1.61	1.54
22	AC	510	CLA	C4A-NA	-2.94	1.33	1.38
27	AB	626	DGD	O6D-C1D	2.94	1.49	1.41
26	BB	620	BCR	C2-C1	2.94	1.61	1.54
26	AB	619	BCR	C2-C1	2.94	1.61	1.54
34	AV	201	HEM	CAD-CBD	2.93	1.60	1.52
22	AD	402	CLA	C1A-NA	2.93	1.38	1.32
26	AC	514	BCR	C5-C6	2.93	1.39	1.34
30	BB	624	LMG	O6-C1	2.93	1.49	1.41
24	AJ	101	PL9	C7-C3	2.93	1.53	1.51
22	BB	612	CLA	C1A-NA	2.93	1.38	1.32
30	AA	416	LMG	O1-C1	2.92	1.45	1.40
26	AK	102	BCR	C2-C1	2.92	1.61	1.54
26	AH	101	BCR	C2-C1	2.92	1.61	1.54
27	BD	410	DGD	C4E-C3E	2.91	1.60	1.52
22	AA	406	CLA	C1A-NA	2.92	1.38	1.32
34	AE	101	HEM	C3B-CAB	2.92	1.49	1.40
26	AA	409	BCR	C29-C30	2.91	1.61	1.54
29	BA	401	SQD	O6-C1	2.91	1.45	1.40
32	AB	627	LMT	O5B-C1B	2.91	1.49	1.41
22	AC	504	CLA	MG-NB	2.91	2.11	2.05
27	BA	411	DGD	CDA-CCA	-2.91	1.54	1.55
27	AA	410	DGD	O6E-C1E	2.90	1.49	1.41
22	AC	506	CLA	C1A-NA	2.90	1.38	1.32
26	BK	102	BCR	C14-C13	2.90	1.39	1.35
22	AB	609	CLA	C1A-NA	2.89	1.38	1.32
28	BA	412	LHG	O8-C23	2.89	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BV	201	HEM	C3D-C4D	2.89	1.47	1.45
32	BI	102	LMT	O5'-C1'	2.89	1.49	1.41
26	AD	406	BCR	C2-C1	2.89	1.61	1.54
29	AA	415	SQD	O5-C1	2.89	1.49	1.41
29	AF	101	SQD	C8-C7	2.88	1.59	1.50
22	BC	509	CLA	CAA-C2A	2.88	1.59	1.54
22	BC	510	CLA	MG-NA	2.88	2.15	2.07
22	AC	509	CLA	CAA-C2A	2.88	1.59	1.54
27	BD	410	DGD	C4E-C5E	2.88	1.59	1.53
29	AF	101	SQD	C44-C45	2.88	1.58	1.50
30	AA	416	LMG	O6-C5	2.88	1.51	1.44
32	BD	411	LMT	O5B-C1B	2.88	1.49	1.41
27	AC	518	DGD	O6D-C1D	2.87	1.49	1.41
26	BK	102	BCR	C2-C1	2.87	1.61	1.54
32	AD	411	LMT	O5'-C1'	2.87	1.49	1.41
27	AD	410	DGD	C1D-C2D	2.87	1.61	1.52
30	AI	101	LMG	C3-C2	2.87	1.60	1.52
22	AB	613	CLA	C4A-NA	-2.86	1.33	1.38
32	AB	624	LMT	O5B-C1B	2.86	1.49	1.41
22	BB	605	CLA	C1A-NA	2.86	1.38	1.32
28	AA	411	LHG	O8-C23	2.86	1.42	1.33
29	BB	601	SQD	O3-C3	2.85	1.49	1.43
27	BB	602	DGD	C4D-C3D	2.85	1.59	1.52
29	AA	412	SQD	C6-S	2.85	1.82	1.77
30	AM	101	LMG	C3-C2	2.85	1.59	1.52
22	BB	619	CLA	C2-C3	2.85	1.38	1.32
26	AT	102	BCR	C26-C25	2.84	1.38	1.34
22	BC	503	CLA	C4B-NB	2.84	1.39	1.34
22	AB	610	CLA	C4A-NA	-2.84	1.33	1.38
22	BC	505	CLA	C4A-NA	-2.84	1.33	1.38
29	AF	101	SQD	O3-C3	2.84	1.49	1.43
22	AA	406	CLA	C1B-CHB	-2.84	1.32	1.39
22	AC	504	CLA	C4B-NB	2.83	1.39	1.34
32	AD	411	LMT	O5B-C1B	2.83	1.49	1.41
30	BB	624	LMG	O1-C1	2.83	1.45	1.40
22	AD	404	CLA	C1A-NA	2.83	1.38	1.32
22	BC	508	CLA	C4B-NB	2.82	1.39	1.34
22	AB	605	CLA	C1A-NA	2.82	1.38	1.32
22	BB	605	CLA	C1B-CHB	-2.82	1.32	1.39
34	AE	101	HEM	C2A-C3A	2.82	1.46	1.37
29	BF	101	SQD	C44-C45	2.82	1.58	1.50
27	AD	410	DGD	C4E-C3E	2.81	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AB	602	CLA	MG-NA	2.81	2.15	2.07
27	AD	410	DGD	C3D-C2D	2.80	1.59	1.52
26	AK	102	BCR	C26-C25	2.80	1.38	1.34
30	BD	407	LMG	O6-C1	2.80	1.49	1.41
27	BC	517	DGD	O3G-C1D	2.80	1.45	1.40
34	AV	201	HEM	CMA-C3A	2.79	1.57	1.51
22	AB	603	CLA	C4A-NA	-2.79	1.33	1.38
32	BB	603	LMT	O5'-C1'	2.79	1.48	1.41
22	AB	606	CLA	C1A-NA	2.78	1.38	1.32
26	AH	101	BCR	C14-C13	2.78	1.39	1.35
22	AC	510	CLA	C1B-C2B	2.78	1.48	1.43
22	BA	407	CLA	C1A-NA	2.78	1.38	1.32
22	AB	606	CLA	C4A-NA	-2.78	1.33	1.38
32	BI	102	LMT	O5B-C1B	2.78	1.48	1.41
32	AI	102	LMT	O5B-C1B	2.78	1.48	1.41
30	BM	102	LMG	C3-C2	2.78	1.59	1.52
28	BA	412	LHG	C12-C11	-2.78	1.54	1.55
26	BB	622	BCR	C26-C25	2.77	1.38	1.34
27	BC	516	DGD	O3G-C1D	2.77	1.45	1.40
30	BI	101	LMG	C3-C2	2.77	1.59	1.52
30	BD	407	LMG	C4-C3	2.77	1.59	1.52
30	AC	519	LMG	O6-C5	2.77	1.51	1.44
32	AT	101	LMT	O1B-C1B	2.76	1.49	1.41
22	BB	617	CLA	MG-NB	2.76	2.11	2.05
22	AB	615	CLA	C4B-NB	2.76	1.39	1.34
22	BB	606	CLA	CAA-C2A	2.76	1.59	1.54
29	BA	401	SQD	O5-C1	2.75	1.48	1.41
22	AB	602	CLA	C1B-CHB	-2.75	1.32	1.39
26	AT	102	BCR	C29-C30	2.75	1.61	1.54
32	AB	625	LMT	O5'-C1'	2.75	1.48	1.41
34	AV	201	HEM	C1A-C2A	2.75	1.48	1.43
26	AC	515	BCR	C29-C30	2.75	1.61	1.54
22	AB	614	CLA	MG-NB	2.75	2.11	2.05
34	BV	201	HEM	CHB-C1B	-2.74	1.32	1.35
22	BC	510	CLA	C4A-NA	-2.74	1.33	1.38
29	BD	409	SQD	C12-C11	-2.74	1.35	1.51
27	AH	102	DGD	C1E-C2E	2.73	1.60	1.52
29	BD	409	SQD	C16-C15	-2.73	1.35	1.51
30	BC	519	LMG	O6-C5	2.73	1.51	1.44
26	AK	102	BCR	C14-C13	2.73	1.39	1.35
27	AB	626	DGD	O2G-C1B	2.73	1.42	1.34
22	BA	404	CLA	C1A-NA	2.73	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AE	101	HEM	CMA-C3A	2.73	1.57	1.51
29	AA	412	SQD	C32-C31	-2.72	1.35	1.51
32	AD	411	LMT	C4B-C5B	2.72	1.59	1.53
32	AB	627	LMT	O5'-C1'	2.72	1.48	1.41
27	AA	410	DGD	C4E-C5E	2.72	1.59	1.53
22	BA	404	CLA	C4A-NA	-2.72	1.33	1.38
27	AC	518	DGD	O3G-C1D	2.72	1.45	1.40
22	BB	614	CLA	C1B-CHB	-2.71	1.32	1.39
26	BA	410	BCR	C29-C30	2.71	1.60	1.54
34	AE	101	HEM	C2C-C1C	2.71	1.50	1.45
22	AB	611	CLA	C1B-CHB	-2.71	1.32	1.39
30	BB	623	LMG	O7-C10	2.71	1.42	1.34
30	BC	520	LMG	O7-C10	2.71	1.42	1.34
22	AC	511	CLA	C4B-NB	2.71	1.38	1.34
32	BT	101	LMT	O1'-C1'	2.71	1.45	1.40
29	BD	409	SQD	C15-C14	-2.70	1.35	1.51
22	BB	604	CLA	C1B-NB	2.70	1.38	1.34
29	BA	413	SQD	O3-C3	2.70	1.49	1.43
30	AA	416	LMG	C3-C2	2.70	1.59	1.52
29	AA	415	SQD	C17-C16	-2.70	1.35	1.51
29	BB	601	SQD	C17-C16	-2.70	1.35	1.51
29	BA	401	SQD	C15-C14	-2.70	1.35	1.51
22	BB	605	CLA	C4A-NA	-2.69	1.33	1.38
22	AA	403	CLA	MG-NA	2.69	2.15	2.07
26	AJ	102	BCR	C14-C13	2.69	1.39	1.35
29	AA	412	SQD	O6-C44	-2.69	1.38	1.43
22	AC	510	CLA	C4B-NB	2.68	1.38	1.34
29	AF	101	SQD	O5-C1	2.68	1.48	1.41
22	BB	609	CLA	C1A-NA	2.68	1.38	1.32
29	AA	415	SQD	C15-C14	-2.68	1.35	1.51
22	AA	406	CLA	C4A-NA	-2.67	1.33	1.38
29	AA	415	SQD	C11-C10	-2.67	1.35	1.51
22	AA	403	CLA	C4A-NA	-2.67	1.33	1.38
30	AB	622	LMG	O1-C1	2.67	1.45	1.40
22	AB	605	CLA	C4B-NB	2.67	1.38	1.34
30	AB	621	LMG	O6-C1	2.67	1.48	1.41
22	BB	613	CLA	CAA-C2A	2.67	1.59	1.54
32	AI	102	LMT	O5'-C1'	2.66	1.48	1.41
30	BB	623	LMG	C4-C3	2.66	1.59	1.52
27	BC	516	DGD	C4E-C3E	2.66	1.59	1.52
30	AM	101	LMG	C4-C5	2.66	1.58	1.53
34	BE	101	HEM	CHB-C1B	-2.66	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	626	DGD	C3D-C2D	2.65	1.59	1.52
29	BA	401	SQD	C11-C10	-2.65	1.35	1.51
27	AC	518	DGD	O6D-C5D	2.65	1.51	1.44
29	BB	601	SQD	O6-C1	2.65	1.44	1.40
22	BA	407	CLA	C1B-CHB	-2.65	1.32	1.39
29	AD	409	SQD	C11-C10	-2.65	1.35	1.51
22	AC	505	CLA	CHC-C1C	2.65	1.44	1.35
29	BB	601	SQD	C19-C18	-2.65	1.35	1.51
22	BC	509	CLA	C4A-NA	-2.65	1.33	1.38
30	AB	622	LMG	C4-C5	2.65	1.58	1.53
26	BJ	102	BCR	C14-C13	2.65	1.39	1.35
22	BB	606	CLA	C1B-CHB	-2.64	1.32	1.39
34	BE	101	HEM	C4A-C3A	2.64	1.47	1.43
22	AC	504	CLA	C1B-CHB	-2.64	1.32	1.39
22	AD	404	CLA	C4A-NA	-2.64	1.33	1.38
29	BA	401	SQD	C17-C16	-2.64	1.35	1.51
29	BL	101	SQD	C19-C18	-2.64	1.35	1.51
34	BE	101	HEM	CMA-C3A	2.63	1.57	1.51
22	BB	618	CLA	MG-NB	2.63	2.10	2.05
22	BA	404	CLA	C1B-CHB	-2.63	1.32	1.39
22	AC	510	CLA	MG-NA	2.63	2.15	2.07
29	AA	412	SQD	C33-C32	-2.63	1.35	1.51
22	AC	502	CLA	C4B-NB	2.62	1.38	1.34
27	BD	410	DGD	O2G-C1B	2.62	1.42	1.34
22	AA	403	CLA	MG-NB	2.62	2.10	2.05
22	AB	603	CLA	C1B-CHB	-2.62	1.32	1.39
27	AA	410	DGD	C3E-C2E	2.62	1.59	1.52
29	AA	415	SQD	C12-C11	-2.62	1.35	1.51
22	AC	508	CLA	MG-NB	2.62	2.10	2.05
26	AB	619	BCR	C14-C13	2.62	1.39	1.35
34	AV	201	HEM	CHB-C1B	-2.61	1.32	1.35
26	AJ	102	BCR	C2-C1	2.62	1.60	1.54
29	BD	409	SQD	O5-C1	2.61	1.48	1.41
29	AD	409	SQD	C12-C11	-2.61	1.35	1.51
22	AA	404	CLA	C4A-NA	-2.61	1.33	1.38
30	AC	519	LMG	C4-C5	2.61	1.58	1.53
27	AH	102	DGD	C4E-C5E	2.60	1.58	1.53
34	BE	101	HEM	C2A-C3A	2.60	1.45	1.37
30	BB	624	LMG	C4-C5	2.60	1.58	1.53
30	BD	408	LMG	O6-C5	2.60	1.50	1.44
22	BB	609	CLA	C4A-NA	-2.60	1.33	1.38
22	AC	505	CLA	C1C-C2C	2.60	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	411	DGD	O6E-C1E	2.59	1.48	1.41
22	AC	507	CLA	C1B-CHB	-2.59	1.32	1.39
29	AD	409	SQD	C15-C14	-2.59	1.35	1.51
29	AF	101	SQD	C6-S	2.59	1.81	1.77
26	AH	101	BCR	C5-C6	2.58	1.38	1.34
30	AB	623	LMG	C3-C2	2.59	1.59	1.52
29	BL	101	SQD	C11-C10	-2.59	1.36	1.51
29	BL	101	SQD	C17-C16	-2.59	1.36	1.51
26	BB	622	BCR	C14-C13	2.59	1.39	1.35
30	BI	101	LMG	C1-C2	2.59	1.60	1.52
30	BI	101	LMG	O7-C10	2.59	1.42	1.34
22	AC	508	CLA	CHC-C1C	2.58	1.43	1.35
27	AC	516	DGD	O6D-C5D	2.58	1.50	1.44
30	AB	622	LMG	O6-C5	2.58	1.50	1.44
22	AB	612	CLA	C4B-NB	2.58	1.38	1.34
27	AC	517	DGD	O6D-C5D	2.58	1.50	1.44
22	BB	606	CLA	C4A-NA	-2.58	1.34	1.38
22	BB	610	CLA	C1B-CHB	-2.58	1.32	1.39
22	BB	617	CLA	CHC-C1C	2.58	1.43	1.35
26	AH	101	BCR	C38-C26	2.58	1.55	1.51
29	BB	601	SQD	C16-C15	-2.58	1.36	1.51
27	BC	516	DGD	O6D-C5D	2.57	1.50	1.44
29	AD	409	SQD	C16-C15	-2.57	1.36	1.51
22	AB	609	CLA	C4B-NB	2.57	1.38	1.34
26	AC	514	BCR	C2-C1	2.57	1.60	1.54
22	AA	406	CLA	C4-C3	2.57	1.57	1.50
29	BA	413	SQD	C12-C11	-2.57	1.36	1.51
29	BB	601	SQD	C20-C19	-2.57	1.36	1.51
26	BX	101	BCR	C38-C26	2.57	1.55	1.51
30	AC	520	LMG	C9-C8	2.57	1.57	1.50
32	AT	101	LMT	O1'-C1'	2.57	1.44	1.40
29	BD	409	SQD	C11-C10	-2.56	1.36	1.51
22	BB	618	CLA	CAA-C2A	2.57	1.58	1.54
22	BC	509	CLA	C4B-NB	2.56	1.38	1.34
29	AA	415	SQD	C16-C15	-2.56	1.36	1.51
27	AC	516	DGD	O6D-C1D	2.56	1.48	1.41
27	AD	410	DGD	O2G-C1B	2.56	1.42	1.34
29	BA	413	SQD	C32-C31	-2.56	1.36	1.51
30	AI	101	LMG	O7-C10	2.56	1.42	1.34
27	BD	410	DGD	C1D-C2D	2.56	1.60	1.52
26	BD	406	BCR	C38-C26	2.56	1.55	1.51
22	AC	513	CLA	C4B-NB	2.55	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BB	601	SQD	C15-C14	-2.55	1.36	1.51
27	AD	410	DGD	C4D-C3D	2.55	1.59	1.52
34	BV	201	HEM	FE-NB	2.55	2.06	1.96
29	BD	409	SQD	C14-C13	-2.55	1.36	1.51
29	BL	101	SQD	C12-C11	-2.54	1.36	1.51
22	BA	405	CLA	C4A-NA	-2.54	1.34	1.38
23	BA	406	PHO	C4-C3	2.54	1.57	1.50
29	AA	412	SQD	C12-C11	-2.54	1.36	1.51
24	BJ	101	PL9	C2-C1	2.54	1.52	1.44
29	BL	101	SQD	C15-C14	-2.54	1.36	1.51
29	BD	409	SQD	C13-C12	-2.53	1.36	1.51
29	AA	412	SQD	C17-C16	-2.53	1.36	1.51
30	BC	520	LMG	C9-C8	2.53	1.57	1.50
29	BA	413	SQD	O5-C1	2.53	1.48	1.41
29	BB	601	SQD	C12-C11	-2.53	1.36	1.51
30	AB	623	LMG	O6-C5	2.53	1.50	1.44
32	BB	625	LMT	C4B-C5B	2.53	1.58	1.53
27	AC	518	DGD	C4E-C3E	2.53	1.59	1.52
22	BC	503	CLA	C1B-C2B	2.53	1.47	1.43
22	BB	605	CLA	MG-NA	2.52	2.14	2.07
22	BB	611	CLA	C4B-NB	2.52	1.38	1.34
30	AD	408	LMG	O6-C5	2.52	1.50	1.44
29	AA	415	SQD	C19-C18	-2.52	1.36	1.51
29	BB	601	SQD	C11-C10	-2.52	1.36	1.51
22	AB	616	CLA	C2-C3	2.52	1.38	1.32
22	AB	615	CLA	CAA-C2A	2.52	1.58	1.54
29	BF	101	SQD	C17-C16	-2.52	1.36	1.51
22	BB	616	CLA	C1B-CHB	-2.51	1.32	1.39
22	BC	508	CLA	MG-NB	2.51	2.10	2.05
27	BB	602	DGD	O6D-C1D	2.51	1.48	1.41
22	BC	505	CLA	CHC-C1C	2.51	1.43	1.35
22	AB	604	CLA	MG-NB	2.51	2.10	2.05
30	AC	520	LMG	O7-C10	2.51	1.41	1.34
34	AE	101	HEM	CHB-C1B	-2.51	1.32	1.35
29	AA	412	SQD	C15-C14	-2.51	1.36	1.51
29	AA	412	SQD	C16-C15	-2.51	1.36	1.51
30	AB	621	LMG	O1-C1	2.51	1.44	1.40
27	BD	410	DGD	C4D-C3D	2.51	1.59	1.52
22	BB	619	CLA	C4A-NA	-2.51	1.34	1.38
27	BH	101	DGD	O3G-C1D	2.50	1.44	1.40
22	BC	508	CLA	CAA-C2A	2.50	1.58	1.54
27	AC	517	DGD	C4D-C5D	2.50	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BL	101	SQD	C20-C19	-2.50	1.36	1.51
22	BB	613	CLA	C4A-NA	-2.50	1.34	1.38
27	BH	101	DGD	O6E-C1E	2.50	1.48	1.41
22	AA	402	CLA	C4A-NA	-2.50	1.34	1.38
22	BB	615	CLA	CAA-C2A	2.49	1.58	1.54
29	BL	101	SQD	C14-C13	-2.49	1.36	1.51
22	AB	616	CLA	C4A-NA	-2.49	1.34	1.38
27	AB	626	DGD	O6E-C5E	2.49	1.50	1.44
29	BL	101	SQD	O6-C1	2.49	1.44	1.40
22	AC	513	CLA	C4A-NA	-2.49	1.34	1.38
30	AE	102	LMG	O6-C5	2.49	1.50	1.44
29	BL	101	SQD	C16-C15	-2.49	1.36	1.51
29	BA	413	SQD	C33-C32	-2.49	1.36	1.51
22	AB	607	CLA	C1B-CHB	-2.49	1.33	1.39
30	AD	407	LMG	O6-C1	2.49	1.48	1.41
30	AB	623	LMG	C4-C3	2.49	1.59	1.52
29	AD	409	SQD	C14-C13	-2.48	1.36	1.51
30	BB	623	LMG	O6-C5	2.48	1.50	1.44
29	AF	101	SQD	C17-C16	-2.48	1.36	1.51
27	AC	516	DGD	C4E-C3E	2.48	1.59	1.52
29	BA	413	SQD	C16-C15	-2.48	1.36	1.51
22	AB	602	CLA	C4A-NA	-2.48	1.34	1.38
22	BC	507	CLA	C1B-CHB	-2.48	1.33	1.39
34	AV	201	HEM	C3B-CAB	2.48	1.48	1.40
27	BC	517	DGD	O6D-C5D	2.48	1.50	1.44
32	AB	627	LMT	O1'-C1'	2.48	1.44	1.40
27	BA	411	DGD	C1E-C2E	2.48	1.59	1.52
29	BA	413	SQD	C11-C10	-2.48	1.36	1.51
27	AD	410	DGD	C3E-C2E	2.48	1.59	1.52
27	BB	602	DGD	O6E-C5E	2.48	1.50	1.44
22	BA	403	CLA	CHC-C1C	2.48	1.43	1.35
27	BC	518	DGD	O6D-C5D	2.48	1.50	1.44
22	BC	504	CLA	MG-NA	2.48	2.14	2.07
22	AB	615	CLA	C1B-C2B	2.48	1.47	1.43
34	AV	201	HEM	C2A-C3A	2.47	1.45	1.37
29	BA	413	SQD	C15-C14	-2.47	1.36	1.51
22	AB	605	CLA	MG-NB	2.47	2.10	2.05
27	BA	411	DGD	O2G-C1B	2.47	1.41	1.34
22	BB	612	CLA	C4B-NB	2.47	1.38	1.34
32	BB	626	LMT	O5B-C1B	2.47	1.48	1.41
34	BV	201	HEM	CMB-C2B	2.47	1.55	1.47
29	BA	401	SQD	C12-C11	-2.47	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AF	101	SQD	C15-C14	-2.47	1.36	1.51
22	BB	617	CLA	C1B-CHB	-2.46	1.33	1.39
29	BA	401	SQD	C19-C18	-2.46	1.36	1.51
30	BE	102	LMG	O6-C5	2.46	1.50	1.44
29	AA	412	SQD	C14-C13	-2.46	1.36	1.51
27	AH	102	DGD	O3G-C1D	2.46	1.44	1.40
29	AA	412	SQD	C11-C10	-2.46	1.36	1.51
27	BB	602	DGD	C3E-C2E	2.46	1.58	1.52
22	BD	402	CLA	C4A-NA	-2.46	1.34	1.38
27	AB	626	DGD	C1D-C2D	2.45	1.59	1.52
27	AD	410	DGD	C4D-C5D	2.45	1.58	1.53
29	AD	409	SQD	C44-C45	2.45	1.57	1.50
22	AD	402	CLA	MG-NB	2.45	2.10	2.05
29	BA	413	SQD	C17-C16	-2.45	1.36	1.51
22	BB	607	CLA	C4B-NB	2.45	1.38	1.34
22	AB	609	CLA	C1B-C2B	2.45	1.47	1.43
30	AD	407	LMG	C4-C3	2.45	1.58	1.52
22	AB	613	CLA	C1B-CHB	-2.45	1.33	1.39
22	BC	510	CLA	CAA-C2A	2.45	1.58	1.54
27	BC	516	DGD	C4D-C3D	2.45	1.58	1.52
30	BC	519	LMG	C4-C5	2.45	1.58	1.53
22	AB	614	CLA	CHC-C1C	2.44	1.43	1.35
22	AC	510	CLA	CAA-C2A	2.44	1.58	1.54
27	BH	101	DGD	C1E-C2E	2.44	1.59	1.52
22	BA	403	CLA	C1B-CHB	-2.44	1.33	1.39
30	AA	413	LMG	O1-C1	2.44	1.44	1.40
27	BH	101	DGD	C4E-C3E	2.44	1.58	1.52
22	AA	404	CLA	C1B-CHB	-2.44	1.33	1.39
26	AB	620	BCR	C14-C13	2.44	1.39	1.35
22	AC	512	CLA	MG-NB	2.44	2.10	2.05
22	BC	512	CLA	C1B-NB	2.44	1.38	1.34
22	BC	512	CLA	C1B-C2B	2.44	1.47	1.43
22	BC	504	CLA	CHC-C1C	2.44	1.43	1.35
22	AC	512	CLA	C1B-NB	2.44	1.38	1.34
30	AC	520	LMG	O8-C28	2.43	1.40	1.33
22	BB	611	CLA	C4A-NA	-2.43	1.34	1.38
32	BB	626	LMT	O5'-C1'	2.43	1.48	1.41
22	BA	407	CLA	C4A-NA	-2.43	1.34	1.38
22	AC	509	CLA	C4B-NB	2.43	1.38	1.34
22	AC	513	CLA	C4-C3	2.43	1.56	1.50
22	BA	407	CLA	C4-C3	2.43	1.56	1.50
24	BJ	101	PL9	C7-C8	2.43	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AD	409	SQD	C13-C12	-2.43	1.36	1.51
27	AC	518	DGD	O5D-C1E	2.43	1.44	1.40
22	AC	505	CLA	C4A-NA	-2.43	1.34	1.38
29	BB	601	SQD	C18-C17	-2.43	1.36	1.51
22	AA	402	CLA	C1B-CHB	-2.43	1.33	1.39
27	BD	410	DGD	C1E-C2E	2.43	1.59	1.52
22	BB	618	CLA	C4B-NB	2.42	1.38	1.34
29	BA	401	SQD	C16-C15	-2.42	1.36	1.51
24	AJ	101	PL9	C31-C29	2.42	1.51	1.39
29	BB	601	SQD	C14-C13	-2.42	1.36	1.51
34	AE	101	HEM	CHD-C4C	2.42	1.39	1.36
32	AB	625	LMT	O5B-C1B	2.42	1.48	1.41
22	AC	512	CLA	C1B-C2B	2.42	1.47	1.43
34	BV	201	HEM	C2C-C1C	2.42	1.49	1.45
22	AB	607	CLA	C2-C3	2.42	1.37	1.32
22	BC	504	CLA	C4B-NB	2.42	1.38	1.34
22	AB	615	CLA	MG-NB	2.42	2.10	2.05
22	AB	612	CLA	CAA-C2A	2.42	1.58	1.54
22	BB	608	CLA	C4B-NB	2.41	1.38	1.34
29	AF	101	SQD	C16-C15	-2.41	1.37	1.51
30	BM	102	LMG	C4-C5	2.41	1.58	1.53
29	BA	401	SQD	C14-C13	-2.41	1.37	1.51
22	BB	616	CLA	CAA-C2A	2.41	1.58	1.54
22	BB	615	CLA	C1B-CHB	-2.40	1.33	1.39
30	AC	520	LMG	C3-C2	2.40	1.58	1.52
27	AD	410	DGD	O1G-C1A	2.40	1.40	1.33
22	AB	614	CLA	C1B-CHB	-2.40	1.33	1.39
22	AA	403	CLA	C1B-CHB	-2.40	1.33	1.39
30	BE	102	LMG	O7-C10	2.40	1.41	1.34
23	BA	406	PHO	C3D-CAD	-2.40	1.42	1.47
22	AC	509	CLA	C4A-NA	-2.40	1.34	1.38
22	BC	505	CLA	C4B-NB	2.40	1.38	1.34
30	AA	413	LMG	C43-C42	-2.40	1.54	1.55
22	AD	402	CLA	C1C-C2C	2.40	1.49	1.44
22	BB	615	CLA	C4A-NA	-2.40	1.34	1.38
22	AB	603	CLA	C4-C3	2.40	1.56	1.50
30	BB	624	LMG	O6-C5	2.40	1.50	1.44
30	AA	416	LMG	O8-C28	2.40	1.40	1.33
24	BJ	101	PL9	C31-C29	2.40	1.51	1.39
30	BD	407	LMG	O1-C1	2.40	1.44	1.40
22	BB	619	CLA	C4-C3	2.40	1.56	1.50
22	AA	403	CLA	C4B-NB	2.39	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BD	409	SQD	C8-C7	2.39	1.57	1.50
30	BA	414	LMG	O1-C1	2.39	1.44	1.40
32	AB	627	LMT	O1B-C4'	2.39	1.49	1.43
22	BB	612	CLA	MG-NB	2.39	2.10	2.05
30	AA	416	LMG	C4-C3	2.39	1.58	1.52
29	BD	409	SQD	C44-C45	2.39	1.57	1.50
22	BC	504	CLA	C1B-CHB	-2.39	1.33	1.39
27	BC	517	DGD	C4D-C5D	2.39	1.58	1.53
22	AB	604	CLA	CHC-C1C	2.39	1.43	1.35
27	BD	410	DGD	C3D-C2D	2.39	1.58	1.52
22	BC	506	CLA	C1B-CHB	-2.39	1.33	1.39
22	BB	607	CLA	CHC-C1C	2.38	1.43	1.35
22	BB	612	CLA	C4A-NA	-2.38	1.34	1.38
34	AV	201	HEM	C2C-C1C	2.38	1.49	1.45
29	BA	413	SQD	C19-C18	-2.38	1.37	1.51
24	AA	407	PL9	C41-C39	2.38	1.51	1.39
22	AB	604	CLA	C4B-NB	2.38	1.38	1.34
30	AB	621	LMG	O7-C10	2.38	1.41	1.34
22	AC	504	CLA	CHC-C1C	2.38	1.43	1.35
29	BA	401	SQD	C18-C17	-2.38	1.37	1.51
30	BE	102	LMG	C4-C5	2.38	1.58	1.53
30	AD	407	LMG	O1-C1	2.38	1.44	1.40
30	AB	621	LMG	C4-C3	2.38	1.58	1.52
29	AA	415	SQD	C20-C19	-2.38	1.37	1.51
29	AA	412	SQD	C20-C19	-2.37	1.37	1.51
29	AA	415	SQD	C33-C32	-2.37	1.37	1.51
26	BX	101	BCR	C5-C6	2.37	1.38	1.34
29	AA	412	SQD	C19-C18	-2.37	1.37	1.51
22	AD	402	CLA	C4C-C3C	2.37	1.49	1.45
29	BF	101	SQD	C15-C14	-2.37	1.37	1.51
22	AC	512	CLA	CHC-C1C	2.37	1.43	1.35
22	BC	508	CLA	C4-C3	2.37	1.56	1.50
32	AB	624	LMT	O1'-C1'	2.37	1.44	1.40
22	BB	605	CLA	CHC-C1C	2.37	1.43	1.35
22	AC	513	CLA	CHC-C1C	2.37	1.43	1.35
29	BF	101	SQD	C12-C11	-2.37	1.37	1.51
22	BB	608	CLA	MG-NB	2.37	2.10	2.05
22	BC	508	CLA	CHC-C1C	2.37	1.43	1.35
30	BC	519	LMG	C4-C3	2.37	1.58	1.52
30	BC	520	LMG	O1-C1	2.36	1.44	1.40
22	AB	608	CLA	C4A-NA	-2.36	1.34	1.38
26	AA	409	BCR	C19-C18	-2.36	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AB	602	CLA	CHC-C1C	2.36	1.43	1.35
22	AB	610	CLA	C4-C3	2.36	1.56	1.50
22	BB	619	CLA	C1B-CHB	-2.36	1.33	1.39
22	AB	613	CLA	CAA-C2A	2.36	1.58	1.54
30	BD	407	LMG	O6-C5	2.36	1.50	1.44
27	AH	102	DGD	C4E-C3E	2.36	1.58	1.52
29	BL	101	SQD	C18-C17	-2.36	1.37	1.51
22	BC	512	CLA	CHC-C1C	2.36	1.43	1.35
29	BA	401	SQD	C24-C23	2.36	1.57	1.50
30	AC	519	LMG	C4-C3	2.36	1.58	1.52
22	AB	616	CLA	C1B-CHB	-2.36	1.33	1.39
27	BD	410	DGD	O6E-C5E	2.35	1.50	1.44
29	AA	415	SQD	C18-C17	-2.35	1.37	1.51
22	BB	608	CLA	C1A-NA	2.35	1.37	1.32
22	BB	605	CLA	C4B-NB	2.35	1.38	1.34
23	AD	403	PHO	C4-C3	2.35	1.56	1.50
27	BA	411	DGD	O6E-C5E	2.35	1.50	1.44
22	AC	503	CLA	C4B-NB	2.35	1.38	1.34
22	BC	504	CLA	C4-C3	2.35	1.56	1.50
26	BZ	101	BCR	C23-C22	-2.35	1.40	1.45
22	AA	403	CLA	C5-C3	2.35	1.56	1.51
27	BC	518	DGD	O6E-C1E	2.35	1.47	1.41
29	AA	412	SQD	O5-C1	2.35	1.47	1.41
22	AD	402	CLA	CHC-C1C	2.35	1.43	1.35
27	AH	102	DGD	O6D-C1D	2.34	1.47	1.41
29	BF	101	SQD	C11-C10	-2.34	1.37	1.51
32	BB	625	LMT	C1B-C2B	2.34	1.59	1.52
29	BA	413	SQD	C14-C13	-2.34	1.37	1.51
22	BB	611	CLA	C4-C3	2.34	1.56	1.50
29	AA	415	SQD	C32-C31	-2.34	1.37	1.51
22	AC	508	CLA	C4-C3	2.34	1.56	1.50
30	BC	520	LMG	C3-C2	2.34	1.58	1.52
29	BB	601	SQD	C13-C12	-2.34	1.37	1.51
29	BF	101	SQD	C16-C15	-2.34	1.37	1.51
30	BC	520	LMG	O8-C28	2.34	1.40	1.33
29	BA	413	SQD	C20-C19	-2.34	1.37	1.51
22	AC	508	CLA	CAA-C2A	2.34	1.58	1.54
22	BA	407	CLA	MG-NB	2.34	2.10	2.05
27	BD	410	DGD	C4D-C5D	2.34	1.58	1.53
24	AJ	101	PL9	C3-C4	2.34	1.53	1.49
32	BB	625	LMT	O5B-C5B	2.33	1.50	1.44
22	BB	606	CLA	C4-C3	2.33	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BB	623	LMG	O1-C1	2.33	1.44	1.40
22	BC	510	CLA	C4B-NB	2.33	1.38	1.34
32	BB	625	LMT	O1'-C1'	2.33	1.44	1.40
22	BC	513	CLA	C4B-NB	2.33	1.38	1.34
22	BB	615	CLA	C4B-NB	2.33	1.38	1.34
32	BB	625	LMT	C4B-C3B	2.33	1.58	1.52
22	AB	602	CLA	C4B-NB	2.33	1.38	1.34
34	BE	101	HEM	CHD-C4C	2.33	1.39	1.36
22	AB	616	CLA	C4B-NB	2.32	1.38	1.34
22	AB	611	CLA	MG-NB	2.32	2.10	2.05
22	BB	607	CLA	MG-NB	2.32	2.10	2.05
27	AD	410	DGD	C1E-C2E	2.32	1.59	1.52
22	BD	404	CLA	C4A-NA	-2.32	1.34	1.38
24	BA	408	PL9	C41-C39	2.32	1.51	1.39
27	AB	626	DGD	C4D-C3D	2.31	1.58	1.52
24	AJ	101	PL9	C2-C1	2.31	1.51	1.44
22	AB	602	CLA	MG-NB	2.31	2.10	2.05
29	BA	413	SQD	C13-C12	-2.31	1.37	1.51
22	AD	402	CLA	C4B-NB	2.31	1.38	1.34
34	BE	101	HEM	CMB-C2B	2.31	1.54	1.47
27	BC	516	DGD	O6E-C1E	2.31	1.47	1.41
22	AB	612	CLA	CHC-C1C	2.31	1.43	1.35
29	AA	415	SQD	C14-C13	-2.31	1.37	1.51
29	BA	401	SQD	C32-C31	-2.30	1.37	1.51
22	BD	404	CLA	C4B-NB	2.30	1.38	1.34
32	AT	101	LMT	O1B-C4'	2.30	1.49	1.43
32	AB	625	LMT	C4B-C5B	2.30	1.58	1.53
26	AB	619	BCR	C24-C23	2.30	1.39	1.32
27	AH	102	DGD	O6E-C1E	2.30	1.47	1.41
22	AB	606	CLA	C4B-NB	2.30	1.38	1.34
29	BA	401	SQD	C33-C32	-2.30	1.37	1.51
22	AC	505	CLA	C4B-NB	2.30	1.38	1.34
22	BD	404	CLA	CHC-C1C	2.30	1.43	1.35
34	BV	201	HEM	CMD-C2D	2.29	1.54	1.47
22	BB	614	CLA	CAA-C2A	2.29	1.58	1.54
22	BC	513	CLA	C1C-C2C	2.29	1.49	1.44
22	AC	505	CLA	C4C-C3C	2.29	1.49	1.45
29	BL	101	SQD	C13-C12	-2.29	1.37	1.51
27	AC	516	DGD	O6E-C1E	2.29	1.47	1.41
22	BC	512	CLA	MG-NB	2.29	2.10	2.05
34	BV	201	HEM	C4D-ND	-2.29	1.35	1.39
22	BB	618	CLA	CHC-C1C	2.29	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	508	CLA	C4B-NB	2.29	1.38	1.34
22	BC	507	CLA	MG-NC	2.29	2.14	2.07
34	AE	101	HEM	CMD-C2D	2.29	1.54	1.47
29	AF	101	SQD	C11-C10	-2.28	1.37	1.51
22	AB	607	CLA	CHC-C1C	2.28	1.42	1.35
34	AE	101	HEM	CMB-C2B	2.28	1.54	1.47
22	BB	612	CLA	CHC-C1C	2.28	1.42	1.35
22	AC	502	CLA	C4A-NA	-2.28	1.34	1.38
27	AC	518	DGD	O6E-C1E	2.28	1.47	1.41
22	BB	613	CLA	C4B-NB	2.28	1.38	1.34
22	AB	614	CLA	C4B-NB	2.28	1.38	1.34
22	BB	607	CLA	C4A-NA	-2.28	1.34	1.38
26	BA	410	BCR	C19-C18	-2.28	1.40	1.45
22	AB	609	CLA	C4A-NA	-2.28	1.34	1.38
22	AB	607	CLA	MG-NB	2.27	2.10	2.05
22	BB	610	CLA	CHC-C1C	2.27	1.42	1.35
22	AB	609	CLA	MG-NC	2.27	2.13	2.07
22	BB	614	CLA	C4B-NB	2.27	1.38	1.34
22	AC	511	CLA	C1B-C2B	2.27	1.47	1.43
32	BT	101	LMT	O1B-C1B	2.27	1.47	1.41
22	BC	502	CLA	CHC-C1C	2.27	1.42	1.35
26	BB	620	BCR	C19-C18	-2.27	1.40	1.45
34	AV	201	HEM	CMB-C2B	2.27	1.54	1.47
22	BB	614	CLA	MG-NC	2.26	2.13	2.07
29	AA	412	SQD	C13-C12	-2.26	1.37	1.51
27	AD	410	DGD	O6E-C5E	2.26	1.50	1.44
22	BB	617	CLA	C4B-NB	2.26	1.38	1.34
34	BV	201	HEM	C3B-CAB	2.26	1.47	1.40
22	AB	601	CLA	C4-C3	2.26	1.56	1.50
22	BB	615	CLA	CHC-C1C	2.25	1.42	1.35
22	AB	609	CLA	C1B-NB	2.25	1.38	1.34
22	AC	507	CLA	MG-NC	2.26	2.13	2.07
22	AB	601	CLA	C1B-NB	2.25	1.38	1.34
27	AB	626	DGD	O5D-C6D	2.25	1.47	1.43
22	BC	510	CLA	C1B-C2B	2.25	1.47	1.43
22	BD	404	CLA	C1B-CHB	-2.25	1.33	1.39
32	BD	411	LMT	C4B-C5B	2.25	1.57	1.53
29	BA	401	SQD	C13-C12	-2.25	1.38	1.51
27	AA	410	DGD	CDA-CCA	-2.25	1.54	1.55
29	AA	415	SQD	C13-C12	-2.25	1.38	1.51
29	AF	101	SQD	C12-C11	-2.25	1.38	1.51
22	AB	610	CLA	CAA-C2A	2.25	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	502	CLA	MG-NB	2.24	2.10	2.05
27	BA	411	DGD	C3E-C2E	2.24	1.58	1.52
27	AA	410	DGD	C1E-C2E	2.24	1.59	1.52
22	BB	608	CLA	C4A-NA	-2.24	1.34	1.38
30	AE	102	LMG	O7-C10	2.24	1.41	1.34
30	BB	624	LMG	C4-C3	2.24	1.58	1.52
26	BJ	102	BCR	C3-C4	2.24	1.59	1.52
34	BV	201	HEM	FE-ND	2.23	2.05	1.96
22	BB	612	CLA	C1B-C2B	2.23	1.47	1.43
29	BA	401	SQD	C20-C19	-2.23	1.38	1.51
27	BH	101	DGD	C3D-C2D	2.23	1.58	1.52
22	BD	402	CLA	CHC-C1C	2.23	1.42	1.35
29	BA	401	SQD	C36-C35	-2.23	1.38	1.51
22	BB	617	CLA	C4A-NA	-2.23	1.34	1.38
22	BA	403	CLA	C4B-NB	2.23	1.38	1.34
22	AC	506	CLA	MG-NB	2.23	2.10	2.05
22	AC	512	CLA	C4A-NA	-2.23	1.34	1.38
29	BA	413	SQD	C6-S	2.23	1.81	1.77
34	AE	101	HEM	C4A-C3A	2.23	1.47	1.43
22	BB	613	CLA	C1B-CHB	-2.22	1.33	1.39
22	BB	610	CLA	C4B-NB	2.22	1.38	1.34
22	BC	501	CLA	C4B-NB	2.22	1.38	1.34
22	AB	607	CLA	C1C-C2C	2.22	1.49	1.44
30	AD	407	LMG	O6-C5	2.22	1.49	1.44
32	BT	101	LMT	O1B-C4'	2.22	1.49	1.43
22	BC	511	CLA	C1B-NB	2.22	1.38	1.34
22	AB	605	CLA	C1B-NB	2.21	1.38	1.34
29	BA	401	SQD	C44-C45	2.21	1.56	1.50
22	AB	601	CLA	CAA-C2A	2.21	1.58	1.54
22	BC	506	CLA	C4B-NB	2.21	1.38	1.34
22	BB	611	CLA	C5-C3	2.21	1.56	1.51
30	AB	621	LMG	O6-C5	2.21	1.49	1.44
26	AD	406	BCR	C38-C26	2.21	1.54	1.51
22	AC	509	CLA	C1B-CHB	-2.20	1.33	1.39
27	BC	516	DGD	C4D-C5D	2.20	1.57	1.53
22	AB	610	CLA	C4C-C3C	2.20	1.49	1.45
22	AC	502	CLA	C1B-CHB	-2.20	1.33	1.39
22	AB	607	CLA	C4B-NB	2.20	1.38	1.34
22	BB	606	CLA	MG-NC	2.20	2.13	2.07
22	BC	502	CLA	C4B-NB	2.20	1.38	1.34
30	BA	414	LMG	O6-C5	2.20	1.49	1.44
29	BF	101	SQD	C14-C13	-2.20	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AD	404	CLA	CHC-C1C	2.20	1.42	1.35
26	BB	620	BCR	C23-C22	-2.20	1.41	1.45
22	BB	605	CLA	MG-NC	2.20	2.13	2.07
27	BD	410	DGD	C3E-C2E	2.20	1.58	1.52
22	AA	402	CLA	CHC-C1C	2.20	1.42	1.35
30	AI	101	LMG	C1-C2	2.20	1.59	1.52
22	AC	503	CLA	C4A-NA	-2.19	1.34	1.38
22	AD	402	CLA	C4A-NA	-2.19	1.34	1.38
27	AB	626	DGD	C1E-C2E	2.19	1.59	1.52
32	AM	102	LMT	O5'-C1'	2.19	1.47	1.41
22	BB	610	CLA	MG-NB	2.19	2.09	2.05
27	AC	517	DGD	C6D-C5D	2.19	1.58	1.51
22	BB	615	CLA	MG-NB	2.19	2.09	2.05
29	AF	101	SQD	C30-C31	2.19	1.60	1.52
22	BC	513	CLA	C1B-NB	2.19	1.38	1.34
22	AB	607	CLA	C4A-NA	-2.19	1.34	1.38
22	BB	619	CLA	C4B-NB	2.19	1.38	1.34
32	BM	101	LMT	O5'-C1'	2.19	1.47	1.41
22	AC	502	CLA	CHC-C1C	2.19	1.42	1.35
32	BB	625	LMT	C3B-C2B	2.18	1.58	1.52
24	BA	408	PL9	C2-C1	2.18	1.51	1.44
22	AC	502	CLA	C1B-C2B	2.18	1.47	1.43
22	BC	513	CLA	C4-C3	2.18	1.56	1.50
22	BC	510	CLA	CHC-C1C	2.18	1.42	1.35
24	BJ	101	PL9	C3-C4	2.18	1.53	1.49
27	AB	626	DGD	C3E-C2E	2.18	1.58	1.52
22	BA	405	CLA	MG-NB	2.18	2.09	2.05
29	AF	101	SQD	C14-C13	-2.18	1.38	1.51
22	AA	402	CLA	MG-NB	2.18	2.09	2.05
29	BF	101	SQD	C30-C31	2.18	1.60	1.52
22	AC	508	CLA	C4A-NA	-2.18	1.34	1.38
22	BC	513	CLA	CHC-C1C	2.17	1.42	1.35
30	AA	416	LMG	C9-C8	2.17	1.56	1.50
22	BA	407	CLA	C4B-NB	2.17	1.38	1.34
29	BA	413	SQD	O6-C44	-2.17	1.39	1.43
22	BC	507	CLA	MG-NB	2.17	2.09	2.05
22	BC	508	CLA	C1B-NB	2.17	1.38	1.34
22	BB	613	CLA	C4C-C3C	2.17	1.49	1.45
22	BC	503	CLA	C4A-NA	-2.17	1.34	1.38
27	AC	516	DGD	O3G-C1D	2.17	1.44	1.40
32	BB	626	LMT	C4B-C5B	2.17	1.57	1.53
29	AD	409	SQD	C8-C7	2.17	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AC	509	CLA	CHC-C1C	2.17	1.42	1.35
27	BB	602	DGD	O5D-C6D	2.17	1.47	1.43
34	BE	101	HEM	C2C-C1C	2.17	1.49	1.45
30	AB	622	LMG	C4-C3	2.17	1.58	1.52
22	BC	509	CLA	C4C-C3C	2.17	1.49	1.45
27	BB	602	DGD	O1G-C1A	2.17	1.39	1.33
22	BA	405	CLA	C1B-CHB	-2.16	1.33	1.39
22	AA	402	CLA	CAA-CBA	-2.16	1.45	1.52
22	BD	404	CLA	MG-NB	2.16	2.09	2.05
22	AC	510	CLA	C1B-CHB	-2.16	1.33	1.39
30	AI	101	LMG	O1-C1	2.16	1.44	1.40
22	BB	607	CLA	C4-C3	2.16	1.56	1.50
32	BB	603	LMT	O1B-C4'	2.16	1.49	1.43
22	BA	403	CLA	CAA-CBA	-2.16	1.45	1.52
30	BE	102	LMG	C1-C2	2.16	1.58	1.52
32	AB	624	LMT	C4B-C5B	2.16	1.57	1.53
32	BB	603	LMT	C4B-C5B	2.16	1.57	1.53
34	BV	201	HEM	C2A-C3A	2.16	1.44	1.37
22	BA	405	CLA	C4B-NB	2.16	1.38	1.34
22	BB	610	CLA	C2-C3	2.16	1.37	1.32
22	AC	513	CLA	C1C-C2C	2.16	1.48	1.44
29	AA	415	SQD	C6-S	2.16	1.81	1.77
22	BC	510	CLA	C4-C3	2.16	1.56	1.50
27	AC	516	DGD	C4D-C5D	2.16	1.57	1.53
29	AA	415	SQD	C36-C35	-2.15	1.38	1.51
22	AB	606	CLA	MG-NC	2.15	2.13	2.07
34	BE	101	HEM	CMD-C2D	2.15	1.54	1.47
27	AC	517	DGD	O3G-C1D	2.15	1.44	1.40
27	BD	410	DGD	O1G-C1A	2.15	1.39	1.33
22	AB	605	CLA	C1B-CHB	-2.15	1.33	1.39
22	AB	615	CLA	CHC-C1C	2.15	1.42	1.35
29	AA	415	SQD	C34-C33	-2.15	1.38	1.51
22	AC	512	CLA	MG-NC	2.15	2.13	2.07
30	AE	102	LMG	C7-C8	2.15	1.56	1.50
30	BA	414	LMG	C4-C3	2.14	1.58	1.52
27	BC	517	DGD	C6D-C5D	2.14	1.58	1.51
27	BH	101	DGD	O6D-C5D	2.14	1.49	1.44
22	BC	502	CLA	C1B-CHB	-2.14	1.33	1.39
22	BB	604	CLA	C4-C3	2.14	1.56	1.50
22	BA	407	CLA	CAA-C2A	2.14	1.58	1.54
27	BD	410	DGD	C1G-C2G	2.14	1.56	1.50
26	BZ	101	BCR	C38-C26	2.14	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	617	BCR	C23-C22	-2.14	1.41	1.45
32	AB	625	LMT	O1B-C1B	2.14	1.47	1.41
22	AD	404	CLA	MG-NB	2.13	2.09	2.05
26	BC	514	BCR	C38-C26	2.13	1.54	1.51
22	BB	610	CLA	C1C-C2C	2.13	1.48	1.44
29	AA	415	SQD	C35-C34	-2.13	1.38	1.51
22	AB	602	CLA	CAA-CBA	-2.13	1.45	1.52
27	BB	602	DGD	C1D-C2D	2.13	1.58	1.52
22	BC	505	CLA	C4C-C3C	2.13	1.48	1.45
27	AC	516	DGD	C4D-C3D	2.13	1.58	1.52
23	BA	406	PHO	CAA-CBA	-2.13	1.45	1.52
22	AB	616	CLA	C4-C3	2.13	1.56	1.50
22	AC	507	CLA	C4-C3	2.13	1.56	1.50
22	AB	611	CLA	MG-NC	2.12	2.13	2.07
26	BX	101	BCR	C14-C13	2.12	1.38	1.35
22	BC	512	CLA	C4-C3	2.12	1.56	1.50
22	BC	508	CLA	C1B-CHB	-2.12	1.34	1.39
22	BB	604	CLA	C3C-C2C	2.12	1.41	1.36
23	BD	403	PHO	C4-C3	2.12	1.56	1.50
30	AC	520	LMG	C40-C39	-2.12	1.54	1.55
26	BZ	101	BCR	C35-C13	2.12	1.55	1.50
32	BB	626	LMT	O1B-C1B	2.12	1.47	1.41
22	AB	610	CLA	C1B-CHB	-2.12	1.34	1.39
22	BC	501	CLA	C1B-C2B	2.12	1.47	1.43
22	AC	508	CLA	C1B-CHB	-2.12	1.34	1.39
22	AC	503	CLA	MG-NB	2.11	2.09	2.05
22	AA	406	CLA	CHC-C1C	2.11	1.42	1.35
22	BC	509	CLA	C1B-C2B	2.11	1.47	1.43
22	AD	404	CLA	C4B-NB	2.11	1.38	1.34
29	AA	415	SQD	C44-C45	2.11	1.56	1.50
30	AB	623	LMG	C1-C2	2.11	1.58	1.52
29	BA	401	SQD	C8-C7	2.11	1.57	1.50
22	AC	510	CLA	C1C-C2C	2.10	1.48	1.44
22	AD	404	CLA	C4C-C3C	2.10	1.48	1.45
22	AB	601	CLA	MG-NC	2.10	2.13	2.07
27	BH	101	DGD	O6D-C1D	2.10	1.47	1.41
22	AB	609	CLA	C1C-C2C	2.10	1.48	1.44
22	AB	608	CLA	C1B-CHB	-2.11	1.34	1.39
22	BC	509	CLA	C1B-CHB	-2.10	1.34	1.39
30	BM	102	LMG	C4-C3	2.10	1.58	1.52
32	AB	625	LMT	O5B-C5B	2.10	1.49	1.44
22	BC	512	CLA	C4A-NA	-2.10	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	401	SQD	C35-C34	-2.10	1.38	1.51
34	AV	201	HEM	CMD-C2D	2.10	1.54	1.47
22	BC	503	CLA	C1B-NB	2.10	1.38	1.34
22	BC	509	CLA	C4-C3	2.10	1.56	1.50
27	BC	518	DGD	C4E-C3E	2.10	1.58	1.52
26	AZ	101	BCR	C38-C26	2.10	1.54	1.51
22	AB	608	CLA	C4B-NB	2.10	1.38	1.34
29	BF	101	SQD	C13-C12	-2.10	1.38	1.51
22	BD	404	CLA	C1B-C2B	2.10	1.47	1.43
32	BI	102	LMT	C4B-C5B	2.09	1.57	1.53
22	AC	503	CLA	CHC-C1C	2.09	1.42	1.35
22	BB	614	CLA	MG-NB	2.09	2.09	2.05
22	AB	605	CLA	CHC-C1C	2.09	1.42	1.35
22	AC	503	CLA	C1B-C2B	2.09	1.47	1.43
30	BI	101	LMG	O1-C1	2.09	1.43	1.40
22	AB	609	CLA	MG-NB	2.09	2.09	2.05
22	BB	615	CLA	C4-C3	2.08	1.55	1.50
22	BC	501	CLA	C1B-CHB	-2.08	1.34	1.39
22	BB	608	CLA	C1B-CHB	-2.08	1.34	1.39
22	BC	502	CLA	C4A-NA	-2.08	1.34	1.38
28	BA	412	LHG	O8-C6	-2.08	1.40	1.45
32	AI	102	LMT	C4B-C5B	2.08	1.57	1.53
32	AT	101	LMT	C3'-C4'	2.08	1.58	1.52
22	BC	511	CLA	C1C-C2C	2.08	1.48	1.44
22	AC	501	CLA	C1B-CHB	-2.08	1.34	1.39
26	BB	621	BCR	C24-C23	2.08	1.39	1.32
22	BB	607	CLA	C1B-NB	2.08	1.37	1.34
29	BA	413	SQD	C18-C17	-2.08	1.39	1.51
22	BC	502	CLA	C1B-NB	2.08	1.37	1.34
22	AC	506	CLA	C4A-NA	-2.07	1.34	1.38
26	BC	515	BCR	C19-C18	-2.08	1.41	1.45
22	BB	613	CLA	C4-C3	2.07	1.55	1.50
22	AC	510	CLA	CHC-C1C	2.07	1.42	1.35
32	BB	603	LMT	C1B-C2B	2.07	1.58	1.52
22	AB	614	CLA	C4A-NA	-2.07	1.34	1.38
27	AA	410	DGD	O6E-C5E	2.07	1.49	1.44
22	AC	511	CLA	C1B-NB	2.07	1.37	1.34
22	BC	513	CLA	C4A-NA	-2.07	1.34	1.38
22	BD	402	CLA	C4B-NB	2.07	1.37	1.34
22	AC	511	CLA	C4-C3	2.07	1.55	1.50
22	BB	605	CLA	MG-NB	2.06	2.09	2.05
22	BC	506	CLA	C4-C3	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	503	CLA	MG-NC	2.06	2.13	2.07
32	AB	625	LMT	C4'-C5'	2.06	1.58	1.52
22	BC	507	CLA	CHC-C1C	2.06	1.42	1.35
27	BC	516	DGD	C4E-C5E	2.06	1.57	1.53
27	AA	410	DGD	O2G-C1B	2.06	1.40	1.34
27	AA	410	DGD	C1G-C2G	2.06	1.56	1.50
22	AB	601	CLA	C3C-C2C	2.06	1.41	1.36
27	BH	101	DGD	C4E-C5E	2.06	1.57	1.53
22	BC	509	CLA	CHC-C1C	2.06	1.42	1.35
22	AC	511	CLA	CHC-C1C	2.06	1.42	1.35
22	BB	604	CLA	MG-NB	2.05	2.09	2.05
29	AF	101	SQD	C24-C23	2.05	1.56	1.50
22	BC	503	CLA	CHC-C1C	2.05	1.42	1.35
22	BD	404	CLA	MG-NC	2.05	2.13	2.07
22	AC	504	CLA	C4-C3	2.05	1.55	1.50
22	BC	508	CLA	C1B-C2B	2.05	1.47	1.43
22	BB	618	CLA	MG-NC	2.05	2.13	2.07
22	AC	507	CLA	MG-NB	2.05	2.09	2.05
22	AC	506	CLA	C1B-CHB	-2.05	1.34	1.39
22	AB	609	CLA	CHC-C1C	2.05	1.42	1.35
22	AC	512	CLA	CAA-C2A	2.05	1.57	1.54
22	BA	403	CLA	MG-NB	2.05	2.09	2.05
22	BB	612	CLA	C1B-NB	2.04	1.37	1.34
22	BB	604	CLA	CAA-C2A	2.04	1.57	1.54
22	BC	505	CLA	C1C-C2C	2.05	1.48	1.44
29	BB	601	SQD	C8-C7	2.04	1.56	1.50
22	AB	614	CLA	C1C-C2C	2.04	1.48	1.44
22	AB	605	CLA	C4A-NA	-2.04	1.34	1.38
22	AC	507	CLA	CHC-C1C	2.04	1.42	1.35
22	AC	503	CLA	C1C-C2C	2.04	1.48	1.44
32	BM	101	LMT	O5B-C1B	2.04	1.47	1.41
22	AA	404	CLA	C4-C3	2.04	1.55	1.50
22	BC	509	CLA	C5-C3	2.04	1.56	1.51
22	BD	402	CLA	C1C-C2C	2.04	1.48	1.44
22	BB	611	CLA	C1B-C2B	2.04	1.47	1.43
22	BB	612	CLA	MG-NC	2.04	2.13	2.07
22	BB	611	CLA	C1B-NB	2.04	1.37	1.34
22	AB	606	CLA	C1B-CHB	-2.04	1.34	1.39
22	AB	615	CLA	C4A-NA	-2.04	1.34	1.38
34	AE	101	HEM	C4A-NA	2.04	1.39	1.36
22	AC	509	CLA	C4-C3	2.03	1.55	1.50
22	AC	502	CLA	OBD-CAD	2.03	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	605	CLA	CAA-CBA	-2.03	1.45	1.52
22	AB	608	CLA	C5-C3	2.03	1.56	1.51
26	BD	406	BCR	C19-C18	-2.03	1.41	1.45
22	AC	506	CLA	C4B-NB	2.03	1.37	1.34
29	AA	415	SQD	C24-C23	2.03	1.56	1.50
34	AE	101	HEM	C3B-C4B	2.03	1.49	1.43
22	BC	511	CLA	C4-C3	2.03	1.55	1.50
22	AC	507	CLA	C4A-NA	-2.03	1.34	1.38
22	BB	619	CLA	CHC-C1C	2.03	1.42	1.35
22	AB	612	CLA	MG-NC	2.03	2.13	2.07
29	AA	412	SQD	C18-C17	-2.02	1.39	1.51
22	BB	613	CLA	CHC-C1C	2.02	1.42	1.35
27	BB	602	DGD	C3D-C2D	2.02	1.57	1.52
34	BE	101	HEM	C4A-NA	2.02	1.39	1.36
29	BA	401	SQD	C34-C33	-2.02	1.39	1.51
22	AB	615	CLA	C4-C3	2.02	1.55	1.50
34	AV	201	HEM	CMC-C2C	2.02	1.53	1.47
22	BA	404	CLA	C4B-NB	2.02	1.37	1.34
22	AC	512	CLA	C1C-C2C	2.02	1.48	1.44
27	BA	411	DGD	O1G-C1A	2.02	1.39	1.33
29	AA	412	SQD	C8-C7	2.02	1.56	1.50
22	AB	604	CLA	C4-C3	2.02	1.55	1.50
30	BM	102	LMG	C11-C10	2.02	1.56	1.50
27	BB	602	DGD	C1E-C2E	2.02	1.58	1.52
22	AB	615	CLA	MG-NC	2.02	2.13	2.07
22	AB	606	CLA	CHC-C1C	2.01	1.42	1.35
32	BB	603	LMT	C3'-C4'	2.01	1.58	1.52
26	AJ	102	BCR	C3-C4	2.01	1.58	1.52
22	AB	612	CLA	C4A-NA	-2.01	1.34	1.38
30	BC	519	LMG	O7-C10	2.01	1.40	1.34
22	AC	506	CLA	CHC-C1C	2.01	1.42	1.35
32	AB	624	LMT	C3B-C2B	2.01	1.57	1.52
22	AB	615	CLA	C1B-CHB	-2.01	1.34	1.39
30	BC	520	LMG	C29-C28	2.01	1.56	1.50
27	AD	410	DGD	C1G-C2G	2.01	1.56	1.50
22	AC	508	CLA	C1B-NB	2.01	1.37	1.34
27	BC	517	DGD	C4E-C3E	2.01	1.57	1.52
22	AB	602	CLA	MG-NC	2.01	2.13	2.07
22	BB	611	CLA	C1B-CHB	-2.01	1.34	1.39
27	AH	102	DGD	C3D-C2D	2.00	1.57	1.52
22	BB	618	CLA	C1B-CHB	-2.00	1.34	1.39
34	BE	101	HEM	C3B-C4B	2.00	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	610	CLA	C1-C2	2.00	1.55	1.49
22	BC	511	CLA	CHC-C1C	2.00	1.42	1.35

All (2425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AD	409	SQD	O7-S-C6	12.40	117.79	106.83
29	BD	409	SQD	O7-S-C6	12.22	117.63	106.83
29	AA	412	SQD	O7-S-C6	11.43	116.93	106.83
29	BA	413	SQD	O7-S-C6	10.83	116.40	106.83
29	BL	101	SQD	O7-S-C6	10.80	116.37	106.83
29	BB	601	SQD	O7-S-C6	10.38	116.00	106.83
29	AF	101	SQD	O7-S-C6	10.27	115.91	106.83
29	BA	401	SQD	O7-S-C6	10.01	115.68	106.83
29	BL	101	SQD	C5-C6-S	9.93	128.29	114.40
29	BF	101	SQD	O7-S-C6	9.92	115.60	106.83
26	AJ	102	BCR	C32-C1-C6	-9.82	94.07	110.33
29	BB	601	SQD	C5-C6-S	9.76	128.05	114.40
29	AA	415	SQD	O7-S-C6	9.68	115.38	106.83
26	BJ	102	BCR	C32-C1-C6	-9.66	94.32	110.33
29	AD	409	SQD	O6-C1-C2	9.57	120.42	108.15
29	BD	409	SQD	O6-C1-C2	9.43	120.24	108.15
29	BB	601	SQD	O6-C1-C2	9.41	120.21	108.15
29	AF	101	SQD	O5-C1-O6	9.19	131.79	109.93
29	BF	101	SQD	O5-C1-O6	9.11	131.61	109.93
29	BL	101	SQD	O6-C1-C2	9.09	119.80	108.15
29	AD	409	SQD	C5-C6-S	8.81	126.72	114.40
29	AA	412	SQD	C5-C6-S	8.81	126.71	114.40
29	BD	409	SQD	C5-C6-S	8.77	126.66	114.40
29	BA	401	SQD	O6-C1-C2	8.77	119.39	108.15
26	BJ	102	BCR	C32-C1-C31	-8.74	78.96	108.47
29	BF	101	SQD	C5-C6-S	8.63	126.46	114.40
29	AA	415	SQD	O6-C1-C2	8.56	119.12	108.15
29	AA	415	SQD	O5-C1-O6	8.54	130.25	109.93
29	BA	413	SQD	O6-C1-C2	8.53	119.08	108.15
29	AA	412	SQD	O6-C1-C2	8.52	119.08	108.15
29	AD	409	SQD	O5-C1-O6	8.51	130.18	109.93
29	BA	413	SQD	C5-C6-S	8.45	126.22	114.40
26	AJ	102	BCR	C32-C1-C31	-8.45	79.94	108.47
29	AF	101	SQD	C5-C6-S	8.44	126.21	114.40
29	BD	409	SQD	O5-C1-O6	8.42	129.98	109.93
29	AA	412	SQD	O5-C1-O6	8.41	129.94	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BA	413	SQD	O5-C1-O6	8.35	129.80	109.93
29	AD	409	SQD	O8-S-C6	-8.34	95.95	105.89
29	BA	401	SQD	O5-C1-O6	8.34	129.78	109.93
29	AF	101	SQD	O6-C1-C2	8.12	118.56	108.15
29	BF	101	SQD	O6-C1-C2	8.02	118.42	108.15
29	BB	601	SQD	O5-C1-O6	7.93	128.79	109.93
29	BL	101	SQD	O5-C1-O6	7.88	128.68	109.93
29	BD	409	SQD	O8-S-C6	-7.78	96.62	105.89
29	AA	412	SQD	O8-S-C6	-7.63	96.80	105.89
34	BE	101	HEM	CAD-C3D-C4D	-7.61	110.97	124.92
34	AE	101	HEM	CAD-C3D-C4D	-7.48	111.20	124.92
34	BE	101	HEM	C3B-C4B-NB	-7.46	108.66	114.00
27	BC	517	DGD	O6E-C5E-C4E	7.32	123.34	109.73
27	AC	517	DGD	O6E-C5E-C4E	7.32	123.33	109.73
34	AE	101	HEM	C3B-C4B-NB	-7.29	108.78	114.00
27	BA	411	DGD	O6E-C5E-C4E	7.27	123.25	109.73
27	AA	410	DGD	O6E-C5E-C4E	7.26	123.23	109.73
27	AH	102	DGD	O6E-C5E-C4E	7.23	123.17	109.73
27	BH	101	DGD	O6E-C5E-C4E	7.07	122.88	109.73
26	AJ	102	BCR	C32-C1-C2	-7.07	80.67	108.78
29	BA	413	SQD	O8-S-C6	-7.06	97.48	105.89
29	AD	409	SQD	C31-C30-C29	7.01	132.96	112.94
26	BJ	102	BCR	C32-C1-C2	-7.00	80.97	108.78
27	BC	516	DGD	O6E-C5E-C4E	6.96	122.67	109.73
27	BD	410	DGD	O6E-C5E-C4E	6.95	122.66	109.73
27	BC	518	DGD	O6E-C5E-C4E	6.95	122.65	109.73
27	AB	626	DGD	O6E-C5E-C4E	6.93	122.61	109.73
26	BX	101	BCR	C38-C26-C25	6.93	132.32	124.50
27	AD	410	DGD	O6E-C5E-C4E	6.92	122.59	109.73
29	BD	409	SQD	C31-C30-C29	6.89	132.63	112.94
29	BB	601	SQD	C31-C30-C29	6.88	132.62	112.94
26	AJ	102	BCR	C2-C1-C6	6.87	121.32	110.37
27	BB	602	DGD	O6E-C5E-C4E	6.84	122.44	109.73
29	BL	101	SQD	C31-C30-C29	6.83	132.47	112.94
34	BV	201	HEM	C3B-C4B-NB	-6.80	109.13	114.00
27	AC	518	DGD	O6E-C5E-C4E	6.79	122.36	109.73
26	AJ	102	BCR	C38-C26-C25	6.78	132.16	124.50
26	BJ	102	BCR	C38-C26-C25	6.76	132.13	124.50
29	AA	415	SQD	C5-C6-S	6.75	123.85	114.40
26	BJ	102	BCR	C33-C5-C6	6.74	132.11	124.50
26	AH	101	BCR	C38-C26-C25	6.69	132.05	124.50
27	AC	516	DGD	O6E-C5E-C4E	6.66	122.12	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BJ	102	BCR	C2-C1-C6	6.66	120.99	110.37
29	AF	101	SQD	O8-S-C6	-6.66	97.96	105.89
26	BD	406	BCR	C38-C26-C25	6.64	132.00	124.50
34	AV	201	HEM	C3B-C4B-NB	-6.64	109.25	114.00
26	AJ	102	BCR	C33-C5-C6	6.62	131.97	124.50
26	AK	102	BCR	C33-C5-C6	6.59	131.94	124.50
34	BE	101	HEM	CAD-C3D-C2D	6.58	143.98	127.19
29	BF	101	SQD	O8-S-C6	-6.54	98.09	105.89
26	AD	406	BCR	C38-C26-C25	6.54	131.88	124.50
34	AE	101	HEM	CAD-C3D-C2D	6.51	143.81	127.19
29	BA	401	SQD	O8-S-C6	-6.50	98.14	105.89
34	AV	201	HEM	CAD-C3D-C4D	-6.48	113.05	124.92
29	BA	401	SQD	C5-C6-S	6.46	123.43	114.40
29	AA	415	SQD	O8-S-C6	-6.44	98.21	105.89
34	BV	201	HEM	CAD-C3D-C4D	-6.43	113.13	124.92
26	BB	621	BCR	C38-C26-C25	6.38	131.69	124.50
27	AC	517	DGD	O5D-C6D-C5D	6.30	119.90	108.96
29	BB	601	SQD	O8-S-C6	-6.30	98.38	105.89
26	AD	406	BCR	C33-C5-C6	6.29	131.60	124.50
26	BK	102	BCR	C33-C5-C6	6.25	131.55	124.50
29	BL	101	SQD	O8-S-C6	-6.22	98.48	105.89
29	BF	101	SQD	C10-C9-C8	6.22	136.31	113.28
29	AF	101	SQD	C10-C9-C8	6.20	136.26	113.28
27	BC	517	DGD	O5D-C6D-C5D	6.20	119.71	108.96
29	AA	412	SQD	C10-C9-C8	6.19	136.20	113.28
29	BA	413	SQD	C10-C9-C8	6.15	136.06	113.28
26	AB	619	BCR	C38-C26-C25	6.08	131.36	124.50
29	BB	601	SQD	C10-C9-C8	6.03	135.62	113.28
26	AZ	101	BCR	C38-C26-C25	5.92	131.18	124.50
29	AF	101	SQD	C32-C31-C30	5.92	129.86	112.94
34	BE	101	HEM	CBD-CAD-C3D	-5.90	101.50	114.37
29	AD	409	SQD	C10-C9-C8	5.90	135.12	113.28
29	BL	101	SQD	C10-C9-C8	5.89	135.09	113.28
28	BA	412	LHG	C25-C24-C23	5.89	136.36	113.51
28	AA	411	LHG	C25-C24-C23	5.88	136.33	113.51
27	BD	410	DGD	O3G-C1D-C2D	5.88	115.68	108.15
27	AD	410	DGD	O3G-C1D-C2D	5.88	115.68	108.15
26	AT	102	BCR	C38-C26-C25	5.87	131.13	124.50
27	AB	626	DGD	O5D-C1E-C2E	5.87	115.68	108.15
26	BD	406	BCR	C33-C5-C6	5.87	131.13	124.50
29	BF	101	SQD	C32-C31-C30	5.87	129.71	112.94
29	AA	415	SQD	C10-C9-C8	5.86	134.98	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	617	BCR	C38-C26-C25	5.85	131.10	124.50
29	BD	409	SQD	C10-C9-C8	5.85	134.96	113.28
26	BC	515	BCR	C33-C5-C6	5.82	131.06	124.50
24	BD	405	PL9	C7-C3-C2	-5.79	118.48	123.75
26	BZ	101	BCR	C38-C26-C25	5.77	131.01	124.50
26	AT	102	BCR	C33-C5-C6	5.76	131.00	124.50
29	BA	401	SQD	C10-C9-C8	5.75	134.57	113.28
34	AV	201	HEM	CAD-C3D-C2D	5.74	141.84	127.19
34	AE	101	HEM	CBD-CAD-C3D	-5.74	101.85	114.37
24	BD	405	PL9	C7-C3-C4	5.72	121.50	116.92
26	AB	620	BCR	C38-C26-C25	5.71	130.95	124.50
23	AD	403	PHO	C4D-CHA-C1A	-5.69	122.80	129.57
34	BV	201	HEM	CAD-C3D-C2D	5.68	141.69	127.19
26	AC	515	BCR	C33-C5-C6	5.68	130.91	124.50
24	AD	405	PL9	C7-C3-C2	-5.67	118.59	123.75
26	AB	618	BCR	C33-C5-C6	5.65	130.87	124.50
26	AC	515	BCR	C38-C26-C25	5.63	130.86	124.50
24	AD	405	PL9	C7-C3-C4	5.62	121.41	116.92
26	AB	618	BCR	C38-C26-C25	5.60	130.82	124.50
26	BB	620	BCR	C33-C5-C6	5.57	130.78	124.50
23	BD	403	PHO	C4D-CHA-C1A	-5.57	122.94	129.57
26	BC	515	BCR	C38-C26-C25	5.56	130.77	124.50
29	BA	401	SQD	C25-C24-C23	5.54	135.03	113.51
23	AA	405	PHO	C4D-CHA-C1A	-5.54	122.97	129.57
26	BB	620	BCR	C38-C26-C25	5.53	130.74	124.50
32	BB	625	LMT	C1-O1'-C1'	-5.52	104.17	113.91
26	AK	102	BCR	C7-C8-C9	5.51	134.46	126.22
29	AA	415	SQD	C25-C24-C23	5.50	134.88	113.51
26	BC	514	BCR	C38-C26-C25	5.50	130.71	124.50
27	AC	516	DGD	O5D-C1E-C2E	5.50	115.20	108.15
23	BA	406	PHO	C4D-CHA-C1A	-5.49	123.03	129.57
26	BK	102	BCR	C7-C8-C9	5.48	134.41	126.22
29	BF	101	SQD	C25-C24-C23	5.47	134.74	113.51
29	BA	413	SQD	C25-C24-C23	5.46	134.72	113.51
26	AB	617	BCR	C33-C5-C6	5.46	130.66	124.50
29	BL	101	SQD	O9-S-C6	-5.44	102.02	106.83
26	AC	514	BCR	C38-C26-C25	5.41	130.61	124.50
32	AB	624	LMT	C1-O1'-C1'	-5.40	104.38	113.91
29	AA	412	SQD	C25-C24-C23	5.40	134.46	113.51
26	AB	619	BCR	C33-C5-C6	5.38	130.57	124.50
26	AB	620	BCR	C33-C5-C6	5.37	130.56	124.50
26	BB	622	BCR	C33-C5-C6	5.35	130.54	124.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	622	BCR	C38-C26-C25	5.33	130.51	124.50
34	BV	201	HEM	CBD-CAD-C3D	-5.32	102.76	114.37
29	BL	101	SQD	C25-C24-C23	5.32	134.16	113.51
27	BB	602	DGD	O5D-C1E-C2E	5.31	114.95	108.15
29	BD	409	SQD	O9-S-C6	-5.29	102.15	106.83
26	BB	621	BCR	C33-C5-C6	5.29	130.47	124.50
29	BB	601	SQD	C25-C24-C23	5.29	134.05	113.51
29	AF	101	SQD	C25-C24-C23	5.29	134.03	113.51
26	AC	514	BCR	C33-C5-C6	5.26	130.44	124.50
29	BA	413	SQD	O9-S-C6	-5.26	102.18	106.83
26	AA	409	BCR	C33-C5-C6	5.26	130.43	124.50
29	AD	409	SQD	C25-C24-C23	5.22	133.76	113.51
26	BA	410	BCR	C33-C5-C6	5.17	130.34	124.50
26	BA	410	BCR	C38-C26-C25	5.17	130.34	124.50
29	BD	409	SQD	C25-C24-C23	5.17	133.58	113.51
34	AV	201	HEM	CBD-CAD-C3D	-5.13	103.18	114.37
26	AK	102	BCR	C11-C10-C9	5.10	134.66	127.29
24	AJ	101	PL9	C7-C3-C2	-5.10	119.11	123.75
29	BA	401	SQD	O9-S-C6	-5.08	102.34	106.83
29	BF	101	SQD	C44-O6-C1	5.08	124.00	113.80
26	BK	102	BCR	C11-C10-C9	5.08	134.63	127.29
26	AA	409	BCR	C38-C26-C25	5.08	130.23	124.50
26	AZ	101	BCR	C33-C5-C6	5.07	130.22	124.50
26	AJ	102	BCR	C23-C24-C25	5.06	142.16	127.23
26	BC	514	BCR	C33-C5-C6	5.05	130.20	124.50
22	AA	403	CLA	CAA-C2A-C3A	-5.02	100.76	113.32
29	AF	101	SQD	C44-O6-C1	5.00	123.83	113.80
22	AA	402	CLA	C2B-C3B-CAB	-4.99	117.11	127.33
26	BJ	102	BCR	C23-C24-C25	4.97	141.90	127.23
26	BK	102	BCR	C38-C26-C25	4.93	130.06	124.50
29	BF	101	SQD	O9-S-C6	-4.92	102.48	106.83
22	AA	403	CLA	C2B-C3B-CAB	-4.87	117.37	127.33
24	AJ	101	PL9	C7-C3-C4	4.87	120.81	116.92
27	BC	516	DGD	O5D-C1E-C2E	4.85	114.37	108.15
22	BA	404	CLA	CAA-C2A-C3A	-4.83	101.22	113.32
26	BZ	101	BCR	C33-C5-C6	4.83	129.95	124.50
29	BB	601	SQD	O9-S-C6	-4.81	102.58	106.83
26	BJ	102	BCR	C31-C1-C6	4.81	118.29	110.33
22	BC	507	CLA	C3D-C4D-CHA	4.80	115.87	108.16
29	BF	101	SQD	C29-C30-C31	4.77	132.93	113.73
22	BC	504	CLA	C2B-C3B-CAB	-4.76	117.59	127.33
29	AF	101	SQD	C29-C30-C31	4.76	132.88	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	507	CLA	C3D-C4D-CHA	4.75	115.79	108.16
22	BA	403	CLA	C2B-C3B-CAB	-4.75	117.62	127.33
22	AC	504	CLA	C2B-C3B-CAB	-4.74	117.64	127.33
22	BA	404	CLA	C2B-C3B-CAB	-4.72	117.67	127.33
26	AJ	102	BCR	C31-C1-C6	4.72	118.14	110.33
22	BA	403	CLA	C3D-C4D-CHA	4.70	115.71	108.16
22	AB	601	CLA	C3D-C4D-CHA	4.69	115.69	108.16
22	BB	605	CLA	C3D-C4D-CHA	4.68	115.68	108.16
22	BB	618	CLA	C3D-C4D-CHA	4.68	115.67	108.16
26	AJ	102	BCR	C8-C7-C6	4.67	141.01	127.23
22	BB	616	CLA	C3D-C4D-CHA	4.67	115.65	108.16
27	BC	517	DGD	C3G-O3G-C1D	-4.67	104.44	113.80
24	BJ	101	PL9	C7-C3-C2	-4.66	119.51	123.75
27	AH	102	DGD	O5D-C1E-C2E	4.65	114.11	108.15
29	AD	409	SQD	O9-S-C6	-4.65	102.72	106.83
22	BC	511	CLA	C3D-C4D-CHA	4.65	115.63	108.16
27	AC	517	DGD	C3G-O3G-C1D	-4.65	104.47	113.80
22	BC	502	CLA	C3D-C4D-CHA	4.65	115.62	108.16
22	AC	512	CLA	C3D-C4D-CHA	4.65	115.62	108.16
22	BC	506	CLA	C3D-C4D-CHA	4.64	115.60	108.16
22	BB	604	CLA	C3D-C4D-CHA	4.63	115.60	108.16
27	BA	411	DGD	O5D-C6D-C5D	4.63	117.00	108.96
22	AB	604	CLA	C3D-C4D-CHA	4.63	115.59	108.16
26	AK	102	BCR	C38-C26-C25	4.63	129.72	124.50
22	AB	602	CLA	C3D-C4D-CHA	4.62	115.58	108.16
22	AC	509	CLA	C2B-C3B-CAB	-4.62	117.87	127.33
22	AB	616	CLA	C3D-C4D-CHA	4.62	115.57	108.16
22	AC	511	CLA	C3D-C4D-CHA	4.62	115.57	108.16
22	BB	608	CLA	C3D-C4D-CHA	4.62	115.56	108.16
22	AC	508	CLA	C3D-C4D-CHA	4.61	115.56	108.16
22	AC	510	CLA	C2B-C3B-CAB	-4.61	117.90	127.33
34	BE	101	HEM	CHA-C4D-ND	4.61	130.76	124.28
22	AB	615	CLA	C3D-C4D-CHA	4.61	115.55	108.16
26	BX	101	BCR	C33-C5-C6	4.61	129.70	124.50
22	AB	613	CLA	C3D-C4D-CHA	4.60	115.55	108.16
26	AH	101	BCR	C33-C5-C6	4.60	129.69	124.50
22	BB	606	CLA	C3D-C4D-CHA	4.60	115.55	108.16
22	AA	402	CLA	C3D-C4D-CHA	4.60	115.54	108.16
22	BC	504	CLA	C3D-C4D-CHA	4.60	115.54	108.16
22	BB	607	CLA	C3D-C4D-CHA	4.59	115.53	108.16
22	AC	506	CLA	C3D-C4D-CHA	4.59	115.53	108.16
22	AB	611	CLA	C3D-C4D-CHA	4.59	115.53	108.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	610	CLA	C3D-C4D-CHA	4.58	115.51	108.16
26	BJ	102	BCR	C8-C7-C6	4.58	140.74	127.23
22	BB	619	CLA	C3D-C4D-CHA	4.58	115.50	108.16
22	BC	512	CLA	C3D-C4D-CHA	4.57	115.50	108.16
22	AB	603	CLA	C3D-C4D-CHA	4.57	115.50	108.16
22	AC	504	CLA	C3D-C4D-CHA	4.57	115.49	108.16
26	AJ	102	BCR	C38-C26-C27	-4.57	104.74	113.39
22	AC	502	CLA	C3D-C4D-CHA	4.56	115.48	108.16
29	AF	101	SQD	O9-S-C6	-4.56	102.80	106.83
22	AB	606	CLA	C3D-C4D-CHA	4.56	115.48	108.16
26	BJ	102	BCR	C38-C26-C27	-4.56	104.75	113.39
22	AB	608	CLA	C3D-C4D-CHA	4.55	115.47	108.16
24	BJ	101	PL9	C7-C3-C4	4.55	120.56	116.92
22	BC	509	CLA	C2B-C3B-CAB	-4.55	118.02	127.33
22	AB	609	CLA	C3D-C4D-CHA	4.55	115.45	108.16
22	BB	611	CLA	C3D-C4D-CHA	4.54	115.45	108.16
29	BD	409	SQD	C44-O6-C1	4.54	122.92	113.80
22	BA	404	CLA	C4B-C3B-CAB	4.54	136.38	127.18
22	AB	610	CLA	C3D-C4D-CHA	4.54	115.45	108.16
22	AA	403	CLA	CBA-CAA-C2A	4.54	125.05	113.95
22	BA	407	CLA	C3D-C4D-CHA	4.54	115.45	108.16
22	BB	617	CLA	C3D-C4D-CHA	4.54	115.44	108.16
22	BB	613	CLA	C3D-C4D-CHA	4.53	115.43	108.16
27	BH	101	DGD	O5D-C1E-C2E	4.53	113.96	108.15
22	AB	612	CLA	C3D-C4D-CHA	4.52	115.41	108.16
22	AD	404	CLA	C3D-C4D-CHA	4.52	115.41	108.16
22	BC	508	CLA	C3D-C4D-CHA	4.52	115.41	108.16
22	AA	402	CLA	C4B-C3B-CAB	4.51	136.31	127.18
22	BB	612	CLA	C3D-C4D-CHA	4.51	115.39	108.16
22	BA	404	CLA	C3D-C4D-CHA	4.50	115.39	108.16
22	BD	402	CLA	C3D-C4D-CHA	4.50	115.39	108.16
22	AA	403	CLA	C4B-C3B-CAB	4.50	136.29	127.18
22	AA	406	CLA	C3D-C4D-CHA	4.49	115.37	108.16
22	BB	614	CLA	C3D-C4D-CHA	4.49	115.36	108.16
34	AE	101	HEM	CHA-C4D-ND	4.49	130.60	124.28
22	BC	501	CLA	C3D-C4D-CHA	4.49	115.36	108.16
22	BC	510	CLA	C2B-C3B-CAB	-4.49	118.14	127.33
22	AC	504	CLA	C4B-C3B-CAB	4.49	136.26	127.18
22	BC	513	CLA	C3D-C4D-CHA	4.48	115.36	108.16
22	AA	403	CLA	C3D-C4D-CHA	4.48	115.35	108.16
22	AB	614	CLA	C3D-C4D-CHA	4.48	115.35	108.16
29	AA	412	SQD	O9-S-C6	-4.48	102.87	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	508	CLA	C2B-C3B-CAB	-4.48	118.16	127.33
22	AB	605	CLA	C3D-C4D-CHA	4.47	115.34	108.16
22	BC	504	CLA	C4B-C3B-CAB	4.47	136.23	127.18
22	AC	501	CLA	C3D-C4D-CHA	4.47	115.33	108.16
22	BB	609	CLA	C3D-C4D-CHA	4.47	115.33	108.16
22	BB	614	CLA	C2B-C3B-CAB	-4.46	118.19	127.33
22	AC	510	CLA	C3D-C4D-CHA	4.46	115.32	108.16
22	AB	604	CLA	C4A-NA-C1A	4.46	112.67	106.38
22	AC	513	CLA	C3D-C4D-CHA	4.46	115.32	108.16
27	AA	410	DGD	O5D-C6D-C5D	4.45	116.69	108.96
22	BD	404	CLA	C3D-C4D-CHA	4.44	115.28	108.16
22	AC	509	CLA	C3D-C4D-CHA	4.44	115.28	108.16
22	BB	615	CLA	C3D-C4D-CHA	4.43	115.27	108.16
22	BC	509	CLA	C3D-C4D-CHA	4.43	115.27	108.16
22	AB	612	CLA	C2B-C3B-CAB	-4.43	118.26	127.33
22	AB	607	CLA	C2B-C3B-CAB	-4.43	118.26	127.33
34	AV	201	HEM	CHA-C4D-ND	4.43	130.51	124.28
22	BC	503	CLA	C3D-C4D-CHA	4.43	115.26	108.16
22	BB	615	CLA	C2B-C3B-CAB	-4.42	118.28	127.33
22	AB	607	CLA	C3D-C4D-CHA	4.42	115.25	108.16
22	BB	607	CLA	C4A-NA-C1A	4.41	112.61	106.38
22	BC	510	CLA	C3D-C4D-CHA	4.41	115.23	108.16
26	AK	102	BCR	C2-C1-C6	4.39	117.38	110.37
22	AD	402	CLA	C3D-C4D-CHA	4.39	115.21	108.16
22	AC	503	CLA	C3D-C4D-CHA	4.39	115.21	108.16
22	BB	607	CLA	C2B-C3B-CAB	-4.39	118.35	127.33
22	AC	508	CLA	C2B-C3B-CAB	-4.39	118.35	127.33
22	AC	508	CLA	C4A-NA-C1A	4.38	112.56	106.38
22	AB	611	CLA	C2B-C3B-CAB	-4.35	118.42	127.33
22	BA	404	CLA	CBA-CAA-C2A	4.35	124.57	113.95
23	AA	405	PHO	C2B-C3B-CAB	-4.34	118.44	127.33
22	AC	505	CLA	C3D-C4D-CHA	4.34	115.12	108.16
22	BC	511	CLA	C4A-NA-C1A	4.34	112.50	106.38
22	BA	405	CLA	C3D-C4D-CHA	4.33	115.10	108.16
22	AC	503	CLA	C4A-NA-C1A	4.32	112.47	106.38
22	BA	403	CLA	C4B-C3B-CAB	4.32	135.92	127.18
22	AB	609	CLA	C2B-C3B-CAB	-4.31	118.50	127.33
22	AB	605	CLA	C2B-C3B-CAB	-4.29	118.54	127.33
22	AC	511	CLA	C4A-NA-C1A	4.29	112.43	106.38
34	BV	201	HEM	CHA-C4D-ND	4.28	130.31	124.28
22	AA	404	CLA	C3D-C4D-CHA	4.28	115.03	108.16
22	AC	506	CLA	C2B-C3B-CAB	-4.28	118.57	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AK	102	BCR	C33-C5-C4	-4.28	105.28	113.39
22	AB	603	CLA	C2B-C3B-CAB	-4.28	118.57	127.33
22	BB	618	CLA	C2B-C3B-CAB	-4.28	118.57	127.33
22	AC	509	CLA	C4B-C3B-CAB	4.27	135.83	127.18
22	BC	505	CLA	C3D-C4D-CHA	4.27	115.02	108.16
22	AC	512	CLA	C2B-C3B-CAB	-4.27	118.58	127.33
22	BC	505	CLA	C2B-C3B-CAB	-4.27	118.59	127.33
22	BB	612	CLA	C2B-C3B-CAB	-4.27	118.60	127.33
22	BD	404	CLA	C2B-C3B-CAB	-4.26	118.61	127.33
26	AD	406	BCR	C38-C26-C27	-4.26	105.32	113.39
22	BC	512	CLA	C2B-C3B-CAB	-4.26	118.61	127.33
22	AC	501	CLA	C2B-C3B-CAB	-4.23	118.67	127.33
22	BB	608	CLA	C2B-C3B-CAB	-4.23	118.68	127.33
26	BD	406	BCR	C38-C26-C27	-4.23	105.38	113.39
22	BC	513	CLA	C2B-C3B-CAB	-4.22	118.68	127.33
22	AB	615	CLA	C2B-C3B-CAB	-4.22	118.70	127.33
22	BB	610	CLA	C2B-C3B-CAB	-4.21	118.70	127.33
29	BA	401	SQD	C44-O6-C1	4.21	122.25	113.80
22	BC	502	CLA	C2B-C3B-CAB	-4.21	118.71	127.33
29	AD	409	SQD	C44-O6-C1	4.21	122.25	113.80
22	BB	606	CLA	C2B-C3B-CAB	-4.21	118.72	127.33
22	AC	505	CLA	C2B-C3B-CAB	-4.21	118.72	127.33
22	AB	615	CLA	C4A-NA-C1A	4.20	112.30	106.38
22	AB	601	CLA	C4A-NA-C1A	4.19	112.30	106.38
22	BC	501	CLA	C2B-C3B-CAB	-4.19	118.75	127.33
22	BB	604	CLA	C4A-NA-C1A	4.19	112.29	106.38
22	BB	618	CLA	C4A-NA-C1A	4.19	112.29	106.38
34	AV	201	HEM	C1A-CHA-C4D	-4.19	121.96	127.47
27	BC	517	DGD	O2G-C1B-C2B	4.19	120.46	111.54
22	BC	505	CLA	C4A-NA-C1A	4.18	112.28	106.38
22	BA	405	CLA	C2B-C3B-CAB	-4.18	118.77	127.33
26	BK	102	BCR	C33-C5-C4	-4.18	105.48	113.39
22	BC	508	CLA	C4A-NA-C1A	4.17	112.26	106.38
22	AB	604	CLA	C2B-C3B-CAB	-4.17	118.79	127.33
24	AA	407	PL9	C7-C8-C9	-4.17	119.71	126.76
29	AA	415	SQD	C44-O6-C1	4.17	122.17	113.80
22	BC	503	CLA	C4A-NA-C1A	4.17	112.26	106.38
23	BA	406	PHO	C2B-C3B-CAB	-4.17	118.80	127.33
22	AB	608	CLA	C2B-C3B-CAB	-4.17	118.80	127.33
26	BK	102	BCR	C2-C1-C6	4.16	117.01	110.37
22	AD	404	CLA	C2B-C3B-CAB	-4.16	118.82	127.33
22	AB	606	CLA	C2B-C3B-CAB	-4.16	118.82	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	509	CLA	C4B-C3B-CAB	4.16	135.59	127.18
22	AB	616	CLA	C2B-C3B-CAB	-4.15	118.83	127.33
22	BC	511	CLA	C2B-C3B-CAB	-4.15	118.84	127.33
26	BB	621	BCR	C38-C26-C27	-4.14	105.54	113.39
22	AC	502	CLA	C2B-C3B-CAB	-4.14	118.85	127.33
22	AC	510	CLA	C4B-C3B-CAB	4.12	135.52	127.18
22	AC	503	CLA	C2B-C3B-CAB	-4.12	118.90	127.33
22	BC	512	CLA	C4A-NA-C1A	4.11	112.18	106.38
30	AM	101	LMG	O7-C10-C11	4.10	120.28	111.54
26	BX	101	BCR	C38-C26-C27	-4.10	105.61	113.39
22	BB	619	CLA	CAA-C2A-C3A	-4.10	103.04	113.32
22	BC	506	CLA	C2B-C3B-CAB	-4.10	118.94	127.33
26	AD	406	BCR	C33-C5-C4	-4.10	105.62	113.39
22	AA	406	CLA	C2B-C3B-CAB	-4.10	118.94	127.33
26	AH	101	BCR	C38-C26-C27	-4.10	105.63	113.39
22	BB	611	CLA	C2B-C3B-CAB	-4.10	118.94	127.33
29	AA	415	SQD	O9-S-C6	-4.09	103.21	106.83
22	BC	503	CLA	C2B-C3B-CAB	-4.09	118.95	127.33
26	AB	619	BCR	C38-C26-C27	-4.09	105.63	113.39
22	AA	404	CLA	C2B-C3B-CAB	-4.09	118.95	127.33
22	BC	502	CLA	C4A-NA-C1A	4.09	112.15	106.38
22	BB	619	CLA	C2B-C3B-CAB	-4.09	118.95	127.33
26	BD	406	BCR	C24-C23-C22	4.09	132.34	126.22
22	BB	609	CLA	C2B-C3B-CAB	-4.08	118.98	127.33
22	BC	513	CLA	C4A-NA-C1A	4.08	112.14	106.38
22	AD	402	CLA	C4A-NA-C1A	4.08	112.13	106.38
22	BB	610	CLA	C4A-NA-C1A	4.08	112.13	106.38
26	AT	102	BCR	C38-C26-C27	-4.07	105.68	113.39
28	BC	521	LHG	O7-C7-C8	4.07	120.21	111.54
26	AJ	102	BCR	C1-C6-C5	-4.06	116.71	122.59
22	BD	402	CLA	C4A-NA-C1A	4.06	112.11	106.38
22	AC	513	CLA	C2B-C3B-CAB	-4.06	119.03	127.33
26	BK	102	BCR	C8-C9-C10	-4.05	112.74	118.98
22	AB	616	CLA	CAA-C2A-C3A	-4.05	103.18	113.32
28	AC	521	LHG	O7-C7-C8	4.05	120.17	111.54
22	BA	407	CLA	C2B-C3B-CAB	-4.04	119.05	127.33
23	AD	403	PHO	C2B-C3B-CAB	-4.04	119.05	127.33
22	AC	513	CLA	C4A-NA-C1A	4.05	112.09	106.38
22	AC	506	CLA	C4A-NA-C1A	4.04	112.08	106.38
30	BM	102	LMG	O7-C10-C11	4.04	120.15	111.54
27	AC	517	DGD	O2G-C1B-C2B	4.04	120.15	111.54
22	AC	511	CLA	C2B-C3B-CAB	-4.04	119.06	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	614	CLA	C4A-NA-C1A	4.03	112.06	106.38
22	BB	617	CLA	C2B-C3B-CAB	-4.02	119.09	127.33
22	AC	512	CLA	C4A-NA-C1A	4.02	112.05	106.38
29	BA	401	SQD	O48-C23-C24	4.00	124.16	111.90
22	BB	619	CLA	C4A-NA-C1A	4.00	112.03	106.38
22	AC	507	CLA	C4A-NA-C1A	4.00	112.02	106.38
22	BC	501	CLA	C4A-NA-C1A	4.00	112.02	106.38
26	BX	101	BCR	C24-C23-C22	4.00	132.19	126.22
22	AB	603	CLA	C4B-C3B-CAB	3.99	135.26	127.18
22	BB	609	CLA	C4A-NA-C1A	3.99	112.00	106.38
26	AT	102	BCR	C29-C30-C25	3.99	116.73	110.37
29	BB	601	SQD	O48-C23-C24	3.99	124.10	111.90
22	AC	505	CLA	C4A-NA-C1A	3.99	112.00	106.38
22	BD	404	CLA	C4A-NA-C1A	3.99	112.00	106.38
27	AB	626	DGD	O2G-C1B-C2B	3.98	120.02	111.54
22	AC	507	CLA	C2B-C3B-CAB	-3.98	119.19	127.33
22	AD	404	CLA	C4A-NA-C1A	3.97	111.98	106.38
27	AC	518	DGD	O6D-C5D-C6D	3.97	114.57	106.62
22	AB	607	CLA	C4A-NA-C1A	3.97	111.97	106.38
22	BC	506	CLA	C4A-NA-C1A	3.96	111.97	106.38
22	BC	507	CLA	C4A-NA-C1A	3.96	111.96	106.38
22	BB	615	CLA	C4B-C3B-CAB	3.96	135.19	127.18
34	BV	201	HEM	C1A-CHA-C4D	-3.96	122.26	127.47
29	AA	415	SQD	O48-C23-C24	3.95	124.00	111.90
26	BC	515	BCR	C29-C30-C25	3.95	116.67	110.37
22	AB	612	CLA	C4B-C3B-CAB	3.95	135.17	127.18
22	BB	614	CLA	C4B-C3B-CAB	3.94	135.16	127.18
26	AK	102	BCR	C8-C9-C10	-3.93	112.93	118.98
22	BB	617	CLA	C4A-NA-C1A	3.93	111.92	106.38
22	AC	501	CLA	C4A-NA-C1A	3.93	111.92	106.38
22	BC	510	CLA	C4B-C3B-CAB	3.92	135.12	127.18
22	BB	605	CLA	C2B-C3B-CAB	-3.92	119.31	127.33
22	BC	508	CLA	C4B-C3B-CAB	3.92	135.12	127.18
26	AB	618	BCR	C33-C5-C4	-3.92	105.97	113.39
26	AC	515	BCR	C38-C26-C27	-3.92	105.97	113.39
22	BD	404	CLA	C4B-C3B-CAB	3.92	135.11	127.18
22	AB	610	CLA	C4A-NA-C1A	3.91	111.90	106.38
22	BA	405	CLA	C4A-NA-C1A	3.91	111.89	106.38
26	BJ	102	BCR	C33-C5-C4	-3.91	105.99	113.39
22	AB	602	CLA	C2B-C3B-CAB	-3.91	119.33	127.33
22	AC	502	CLA	C4A-NA-C1A	3.90	111.89	106.38
22	BC	507	CLA	C2B-C3B-CAB	-3.91	119.33	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	406	BCR	C29-C30-C25	3.90	116.60	110.37
29	BL	101	SQD	O48-C23-C24	3.90	123.84	111.90
26	AC	514	BCR	C33-C5-C4	-3.90	106.00	113.39
26	AH	101	BCR	C24-C23-C22	3.90	132.04	126.22
22	BB	615	CLA	C4A-NA-C1A	3.89	111.87	106.38
24	AJ	101	PL9	C10-C9-C11	3.89	121.30	115.39
22	BC	509	CLA	C4A-NA-C1A	3.89	111.87	106.38
22	AB	603	CLA	CAA-C2A-C3A	-3.89	103.58	113.32
22	AB	613	CLA	C4A-NA-C1A	3.89	111.86	106.38
22	BB	613	CLA	C2B-C3B-CAB	-3.88	119.38	127.33
26	AC	515	BCR	C29-C30-C25	3.88	116.56	110.37
23	BD	403	PHO	C2B-C3B-CAB	-3.88	119.38	127.33
22	AB	606	CLA	C4A-NA-C1A	3.88	111.85	106.38
22	BB	607	CLA	C4B-C3B-CAB	3.88	135.03	127.18
26	AB	620	BCR	C38-C26-C27	-3.87	106.05	113.39
22	AD	402	CLA	CBA-CAA-C2A	3.87	123.42	113.95
22	BB	613	CLA	C4A-NA-C1A	3.87	111.83	106.38
26	AB	618	BCR	C29-C30-C25	3.87	116.53	110.37
26	AB	618	BCR	C38-C26-C27	-3.85	106.09	113.39
22	BB	618	CLA	C4B-C3B-CAB	3.85	134.97	127.18
34	BV	201	HEM	C4A-NA-C1A	3.85	110.82	107.12
26	AD	406	BCR	C29-C30-C25	3.85	116.50	110.37
24	BA	408	PL9	C7-C8-C9	-3.85	120.26	126.76
22	BB	606	CLA	CAA-C2A-C3A	-3.84	103.71	113.32
27	BB	602	DGD	O2G-C1B-C2B	3.84	119.71	111.54
26	BC	515	BCR	C38-C26-C27	-3.84	106.12	113.39
22	BB	612	CLA	C4A-NA-C1A	3.83	111.78	106.38
26	AT	102	BCR	C33-C5-C4	-3.83	106.14	113.39
26	BB	622	BCR	C29-C30-C25	3.83	116.47	110.37
26	AJ	102	BCR	C29-C30-C25	3.82	116.47	110.37
22	AB	610	CLA	C2B-C3B-CAB	-3.82	119.51	127.33
22	BC	504	CLA	C4A-NA-C1A	3.82	111.76	106.38
26	BJ	102	BCR	C1-C6-C5	-3.81	117.07	122.59
22	BB	606	CLA	C4B-C3B-CAB	3.81	134.89	127.18
22	AB	616	CLA	C4A-NA-C1A	3.81	111.75	106.38
26	BD	406	BCR	C33-C5-C4	-3.81	106.18	113.39
22	AA	402	CLA	C4A-NA-C1A	3.80	111.74	106.38
22	AC	508	CLA	C4B-C3B-CAB	3.80	134.88	127.18
27	BC	518	DGD	O6D-C5D-C6D	3.80	114.23	106.62
22	BB	608	CLA	C4A-NA-C1A	3.79	111.73	106.38
22	BA	405	CLA	C4B-C3B-CAB	3.79	134.86	127.18
26	BB	620	BCR	C38-C26-C27	-3.79	106.21	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	612	CLA	C4A-NA-C1A	3.78	111.72	106.38
22	BA	403	CLA	C4A-NA-C1A	3.78	111.71	106.38
34	AE	101	HEM	C4A-NA-C1A	3.78	110.76	107.12
22	AB	615	CLA	C4B-C3B-CAB	3.78	134.83	127.18
22	BC	503	CLA	C1-C2-C3	3.78	132.78	126.23
22	AA	404	CLA	C4A-NA-C1A	3.78	111.71	106.38
22	BB	610	CLA	CBD-CHA-C1A	3.77	133.70	128.77
22	AB	611	CLA	C4B-C3B-CAB	3.77	134.81	127.18
22	AC	509	CLA	C4A-NA-C1A	3.77	111.69	106.38
26	AZ	101	BCR	C23-C24-C25	3.76	138.34	127.23
22	BB	616	CLA	C4A-NA-C1A	3.76	111.69	106.38
34	AV	201	HEM	C4A-NA-C1A	3.76	110.74	107.12
26	AD	406	BCR	C24-C23-C22	3.76	131.84	126.22
26	AB	619	BCR	C33-C5-C4	-3.76	106.27	113.39
22	AB	605	CLA	C4A-NA-C1A	3.76	111.68	106.38
22	BC	512	CLA	C4B-C3B-CAB	3.76	134.78	127.18
22	AB	616	CLA	C4B-C3B-CAB	3.76	134.78	127.18
27	BB	602	DGD	C1E-O6E-C5E	3.75	120.99	113.73
22	AD	404	CLA	C4B-C3B-CAB	3.75	134.77	127.18
27	AB	626	DGD	C1E-O6E-C5E	3.75	120.98	113.73
22	AB	605	CLA	C4B-C3B-CAB	3.75	134.76	127.18
22	AB	611	CLA	C4A-NA-C1A	3.75	111.66	106.38
26	BC	515	BCR	C33-C5-C4	-3.75	106.29	113.39
22	AB	614	CLA	C2B-C3B-CAB	-3.74	119.67	127.33
26	BB	620	BCR	C33-C5-C4	-3.74	106.30	113.39
26	AC	515	BCR	C2-C1-C6	3.74	116.34	110.37
22	AC	504	CLA	C4A-NA-C1A	3.74	111.66	106.38
26	BB	621	BCR	C33-C5-C4	-3.74	106.31	113.39
22	AA	404	CLA	C4B-C3B-CAB	3.74	134.74	127.18
22	AB	603	CLA	C4A-NA-C1A	3.74	111.65	106.38
22	BC	510	CLA	C4A-NA-C1A	3.73	111.64	106.38
22	AC	505	CLA	CAA-C2A-C3A	-3.73	103.98	113.32
22	AC	505	CLA	C4B-C3B-CAB	3.73	134.73	127.18
22	AB	609	CLA	C4B-C3B-CAB	3.73	134.73	127.18
22	AB	608	CLA	C4A-NA-C1A	3.73	111.64	106.38
26	AB	620	BCR	C33-C5-C4	-3.73	106.33	113.39
22	AB	607	CLA	CBD-CHA-C1A	3.72	133.63	128.77
22	AC	503	CLA	C1-C2-C3	3.72	132.67	126.23
22	BB	619	CLA	C4B-C3B-CAB	3.71	134.70	127.18
22	AB	601	CLA	C2B-C3B-CAB	-3.71	119.73	127.33
26	AC	515	BCR	C33-C5-C4	-3.71	106.36	113.39
22	BB	612	CLA	C4B-C3B-CAB	3.71	134.69	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BC	514	BCR	C38-C26-C27	-3.71	106.36	113.39
22	AB	608	CLA	C4B-C3B-CAB	3.71	134.69	127.18
24	BJ	101	PL9	C10-C9-C11	3.71	121.02	115.39
27	AC	516	DGD	C1E-O6E-C5E	3.71	120.91	113.73
26	BC	514	BCR	C33-C5-C4	-3.69	106.39	113.39
29	AF	101	SQD	C19-C18-C17	3.69	123.49	112.94
22	AB	609	CLA	C4A-NA-C1A	3.69	111.58	106.38
22	BC	505	CLA	C4B-C3B-CAB	3.69	134.64	127.18
26	AZ	101	BCR	C38-C26-C27	-3.68	106.41	113.39
22	AC	506	CLA	C4B-C3B-CAB	3.68	134.63	127.18
26	AC	514	BCR	C38-C26-C27	-3.68	106.41	113.39
22	AC	512	CLA	C4B-C3B-CAB	3.68	134.63	127.18
22	AA	404	CLA	CAA-C2A-C3A	-3.67	104.12	113.32
26	AA	409	BCR	C38-C26-C27	-3.67	106.43	113.39
22	BB	604	CLA	C2B-C3B-CAB	-3.67	119.81	127.33
22	AA	406	CLA	C4A-NA-C1A	3.67	111.55	106.38
22	AB	604	CLA	C4B-C3B-CAB	3.67	134.60	127.18
22	BB	606	CLA	C4A-NA-C1A	3.67	111.55	106.38
22	AC	502	CLA	C4B-C3B-CAB	3.67	134.60	127.18
30	AD	408	LMG	O6-C5-C6	3.67	115.47	106.34
22	BA	404	CLA	C4A-NA-C1A	3.66	111.54	106.38
32	AT	101	LMT	C1-O1'-C1'	-3.66	107.45	113.91
22	BB	608	CLA	C4B-C3B-CAB	3.66	134.58	127.18
26	BZ	101	BCR	C23-C24-C25	3.66	138.02	127.23
22	AB	607	CLA	C4B-C3B-CAB	3.66	134.58	127.18
22	BB	611	CLA	C4A-NA-C1A	3.65	111.53	106.38
22	AC	503	CLA	C4B-C3B-CAB	3.65	134.57	127.18
29	AD	409	SQD	O48-C23-C24	3.65	123.07	111.90
22	BC	505	CLA	CAA-C2A-C3A	-3.65	104.18	113.32
26	BK	102	BCR	C29-C30-C25	3.65	116.19	110.37
22	BB	606	CLA	CBD-CHA-C1A	3.65	133.54	128.77
22	BC	506	CLA	C4B-C3B-CAB	3.65	134.56	127.18
26	AB	619	BCR	C30-C25-C26	-3.64	117.31	122.59
32	AI	102	LMT	C1-O1'-C1'	-3.64	107.49	113.91
26	AB	617	BCR	C38-C26-C27	-3.64	106.49	113.39
26	BJ	102	BCR	C16-C15-C14	3.64	131.46	123.45
22	BB	611	CLA	C4B-C3B-CAB	3.64	134.54	127.18
22	BB	610	CLA	C4B-C3B-CAB	3.63	134.54	127.18
22	BA	404	CLA	O2A-CGA-CBA	3.63	123.02	111.90
26	BJ	102	BCR	C29-C30-C25	3.63	116.16	110.37
26	AH	101	BCR	C29-C30-C25	3.63	116.16	110.37
26	BX	101	BCR	C29-C30-C25	3.63	116.16	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AJ	101	PL9	C7-C8-C9	-3.63	120.63	126.76
26	AA	409	BCR	C33-C5-C4	-3.63	106.52	113.39
24	AA	407	PL9	C27-C28-C29	-3.62	119.97	127.81
22	AB	613	CLA	C2B-C3B-CAB	-3.62	119.92	127.33
27	BH	101	DGD	O6D-C5D-C6D	3.62	113.87	106.62
26	AA	409	BCR	C24-C23-C22	3.62	131.63	126.22
26	AJ	102	BCR	C33-C5-C4	-3.62	106.53	113.39
22	BD	402	CLA	CBA-CAA-C2A	3.62	122.79	113.95
29	AA	412	SQD	C11-C10-C9	3.61	133.75	114.56
26	BK	102	BCR	C38-C26-C27	-3.61	106.54	113.39
34	BE	101	HEM	C4A-NA-C1A	3.61	110.60	107.12
22	AB	606	CLA	C4B-C3B-CAB	3.61	134.49	127.18
22	AB	602	CLA	C4B-C3B-CAB	3.61	134.49	127.18
24	BA	408	PL9	C27-C28-C29	-3.60	120.01	127.81
22	BC	503	CLA	C4B-C3B-CAB	3.60	134.47	127.18
22	BC	502	CLA	C4B-C3B-CAB	3.60	134.47	127.18
29	BF	101	SQD	C19-C18-C17	3.60	123.24	112.94
22	AA	406	CLA	C4B-C3B-CAB	3.60	134.47	127.18
26	BB	622	BCR	C33-C5-C4	-3.60	106.57	113.39
22	AC	510	CLA	C4A-NA-C1A	3.60	111.45	106.38
22	BB	618	CLA	CBD-CHA-C1A	3.60	133.47	128.77
24	AA	407	PL9	C17-C18-C19	-3.60	120.03	127.81
22	AC	501	CLA	C4B-C3B-CAB	3.60	134.46	127.18
22	BB	611	CLA	O2A-CGA-CBA	3.59	122.90	111.90
22	BA	405	CLA	CAA-C2A-C3A	-3.59	104.33	113.32
27	AC	518	DGD	C1E-O6E-C5E	3.59	120.68	113.73
26	AK	102	BCR	C29-C30-C25	3.59	116.09	110.37
26	BZ	101	BCR	C38-C26-C27	-3.59	106.59	113.39
26	AB	619	BCR	C24-C23-C22	3.59	131.58	126.22
22	BB	617	CLA	C4B-C3B-CAB	3.59	134.44	127.18
26	AB	617	BCR	C33-C5-C4	-3.59	106.60	113.39
29	BA	413	SQD	C11-C10-C9	3.59	133.61	114.56
32	BI	102	LMT	C1-O1'-C1'	-3.58	107.59	113.91
26	BZ	101	BCR	C29-C30-C25	3.58	116.08	110.37
22	BB	605	CLA	C4B-C3B-CAB	3.58	134.43	127.18
26	BB	622	BCR	C38-C26-C27	-3.58	106.61	113.39
22	BA	407	CLA	C4A-NA-C1A	3.57	111.41	106.38
27	BH	101	DGD	O2G-C1B-C2B	3.56	119.14	111.54
22	BC	511	CLA	C4B-C3B-CAB	3.56	134.39	127.18
22	AC	511	CLA	C4B-C3B-CAB	3.56	134.39	127.18
22	BB	614	CLA	C4A-NA-C1A	3.56	111.40	106.38
29	BD	409	SQD	O48-C23-C24	3.56	122.80	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AJ	102	BCR	C16-C15-C14	3.56	131.28	123.45
26	AB	620	BCR	C29-C30-C25	3.55	116.04	110.37
26	AZ	101	BCR	C29-C30-C25	3.55	116.03	110.37
26	BB	621	BCR	C30-C25-C26	-3.55	117.45	122.59
27	AC	516	DGD	O5D-C6D-C5D	3.55	115.11	108.96
22	AD	402	CLA	OBD-CAD-CBD	-3.54	120.59	125.94
26	BA	410	BCR	C38-C26-C27	-3.54	106.68	113.39
22	AA	403	CLA	O2A-CGA-CBA	3.54	122.73	111.90
29	BA	413	SQD	C31-C30-C29	3.53	133.32	114.56
29	AA	412	SQD	C31-C30-C29	3.52	133.27	114.56
26	AK	102	BCR	C1-C6-C5	-3.52	117.49	122.59
30	BA	414	LMG	O6-C5-C6	3.52	115.10	106.34
26	BB	622	BCR	C2-C1-C6	3.51	115.97	110.37
30	AD	408	LMG	O7-C10-C11	3.51	119.03	111.54
22	BC	501	CLA	C4B-C3B-CAB	3.51	134.28	127.18
22	BB	612	CLA	CED-O2D-CGD	3.51	124.36	116.00
22	BB	609	CLA	C4B-C3B-CAB	3.51	134.28	127.18
24	AA	407	PL9	C22-C23-C24	-3.51	120.22	127.81
26	BB	621	BCR	C29-C30-C25	3.51	115.96	110.37
29	AA	415	SQD	C31-C30-C29	3.51	133.18	114.56
22	AC	505	CLA	CBD-CHA-C1A	3.51	133.35	128.77
29	BD	409	SQD	C11-C10-C9	3.50	133.17	114.56
22	BC	504	CLA	CBD-CHA-C1A	3.50	133.35	128.77
26	AA	409	BCR	C7-C8-C9	3.50	131.46	126.22
22	AC	501	CLA	CAA-C2A-C3A	-3.50	104.55	113.32
22	AA	406	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
22	BB	605	CLA	CAA-C2A-C3A	-3.50	104.56	113.32
26	BK	102	BCR	C1-C6-C5	-3.50	117.53	122.59
26	BK	102	BCR	C16-C17-C18	3.50	132.34	127.29
22	BC	510	CLA	CBD-CHA-C1A	3.50	133.34	128.77
22	AC	512	CLA	O2A-CGA-CBA	3.50	122.60	111.90
22	AC	510	CLA	CBD-CHA-C1A	3.49	133.34	128.77
22	BA	407	CLA	C4B-C3B-CAB	3.49	134.25	127.18
24	AA	407	PL9	C35-C34-C36	3.49	120.69	115.39
22	BB	616	CLA	C2B-C3B-CAB	-3.49	120.18	127.33
22	AC	513	CLA	C4B-C3B-CAB	3.49	134.24	127.18
22	AC	507	CLA	CBD-CHA-C1A	3.49	133.33	128.77
23	BD	403	PHO	CBD-CHA-C1A	3.49	132.72	126.67
22	AB	608	CLA	O2A-CGA-CBA	3.48	122.56	111.90
30	BB	623	LMG	O6-C5-C6	3.48	115.01	106.34
26	BB	621	BCR	C24-C23-C22	3.48	131.42	126.22
22	AC	504	CLA	CBD-CHA-C1A	3.48	133.31	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AH	102	DGD	O6D-C5D-C6D	3.47	113.58	106.62
30	BD	408	LMG	O6-C5-C6	3.47	114.99	106.34
26	AK	102	BCR	C38-C26-C27	-3.47	106.81	113.39
26	BD	406	BCR	C30-C25-C26	-3.47	117.56	122.59
22	BC	512	CLA	O2A-CGA-CBA	3.47	122.51	111.90
22	AC	508	CLA	CBD-CHA-C1A	3.47	133.30	128.77
26	BC	515	BCR	C2-C1-C6	3.47	115.90	110.37
26	BA	410	BCR	C33-C5-C4	-3.46	106.83	113.39
24	BD	405	PL9	C20-C19-C21	3.46	120.65	115.39
22	BC	507	CLA	O2A-CGA-CBA	3.46	122.50	111.90
27	AH	102	DGD	O2G-C1B-C2B	3.46	118.91	111.54
30	BD	408	LMG	O7-C10-C11	3.46	118.91	111.54
23	AD	403	PHO	CBD-CHA-C1A	3.46	132.67	126.67
23	BA	406	PHO	CBD-CHA-C1A	3.46	132.66	126.67
22	AD	404	CLA	CAA-C2A-C3A	-3.45	104.68	113.32
22	AB	602	CLA	CAA-C2A-C3A	-3.45	104.67	113.32
30	AC	520	LMG	O7-C10-C11	3.45	118.89	111.54
22	BC	505	CLA	CBA-CAA-C2A	3.45	122.38	113.95
26	AH	101	BCR	C30-C25-C26	-3.45	117.60	122.59
29	AD	409	SQD	C11-C10-C9	3.45	132.86	114.56
26	AD	406	BCR	C30-C25-C26	-3.45	117.60	122.59
29	BA	401	SQD	C11-C10-C9	3.44	132.86	114.56
29	AF	101	SQD	C11-C10-C9	3.44	132.85	114.56
22	BC	511	CLA	CBD-CHA-C1A	3.44	133.27	128.77
26	BA	410	BCR	C24-C23-C22	3.44	131.36	126.22
29	BB	601	SQD	C11-C10-C9	3.44	132.81	114.56
23	AD	403	PHO	CAA-C2A-C3A	-3.43	104.72	113.32
26	BB	620	BCR	C2-C1-C6	3.43	115.84	110.37
22	AB	615	CLA	CBD-CHA-C1A	3.43	133.25	128.77
30	BC	520	LMG	O7-C10-C11	3.43	118.85	111.54
26	BC	515	BCR	C30-C25-C26	-3.43	117.62	122.59
27	AC	516	DGD	O6D-C5D-C6D	3.43	113.49	106.62
27	BD	410	DGD	C1E-O6E-C5E	3.43	120.36	113.73
30	AB	621	LMG	O6-C5-C6	3.42	114.86	106.34
26	BX	101	BCR	C30-C25-C26	-3.42	117.64	122.59
24	BJ	101	PL9	C25-C24-C26	3.42	120.58	115.39
24	BA	408	PL9	C22-C23-C24	-3.42	120.42	127.81
22	AC	507	CLA	O2A-CGA-CBA	3.42	122.36	111.90
30	AA	413	LMG	O6-C5-C6	3.41	114.84	106.34
29	AA	415	SQD	C11-C10-C9	3.41	132.69	114.56
24	AA	407	PL9	C12-C13-C14	-3.41	120.42	127.81
27	BC	518	DGD	C1E-O6E-C5E	3.41	120.33	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AZ	101	BCR	C16-C17-C18	3.41	132.22	127.29
22	BC	513	CLA	C4B-C3B-CAB	3.41	134.08	127.18
23	BD	403	PHO	CAA-C2A-C3A	-3.41	104.78	113.32
24	BA	408	PL9	C17-C18-C19	-3.41	120.44	127.81
29	BL	101	SQD	C11-C10-C9	3.41	132.66	114.56
22	BC	512	CLA	CBD-CHA-C1A	3.40	133.22	128.77
22	AB	614	CLA	C4B-C3B-CAB	3.40	134.07	127.18
22	AC	505	CLA	OBD-CAD-CBD	-3.40	120.80	125.94
29	AF	101	SQD	O48-C23-C24	3.40	122.31	111.90
26	AH	101	BCR	C33-C5-C4	-3.40	106.96	113.39
22	AB	613	CLA	CBD-CHA-C1A	3.39	133.21	128.77
29	BA	401	SQD	C31-C30-C29	3.39	132.58	114.56
28	AA	411	LHG	O8-C23-C24	3.39	122.28	111.90
22	BB	613	CLA	C1-C2-C3	3.39	132.11	126.23
27	BC	516	DGD	O6D-C5D-C6D	3.39	113.41	106.62
26	BC	514	BCR	C2-C1-C6	3.39	115.78	110.37
22	AB	602	CLA	C4A-NA-C1A	3.39	111.16	106.38
26	AZ	101	BCR	C2-C1-C6	3.38	115.76	110.37
22	BB	616	CLA	C1D-CHD-C4C	3.38	127.84	122.60
22	AA	403	CLA	C4A-NA-C1A	3.38	111.14	106.38
22	BC	508	CLA	CBD-CHA-C1A	3.38	133.19	128.77
32	BT	101	LMT	C1-O1'-C1'	-3.38	107.95	113.91
22	BB	617	CLA	CBD-CHA-C1A	3.38	133.18	128.77
29	BF	101	SQD	C11-C10-C9	3.38	132.49	114.56
22	BA	403	CLA	O2A-CGA-CBA	3.37	122.22	111.90
22	BB	605	CLA	CBD-CHA-C1A	3.37	133.17	128.77
26	BX	101	BCR	C33-C5-C4	-3.37	107.01	113.39
24	AA	407	PL9	C30-C29-C31	3.37	120.50	115.39
22	AB	612	CLA	C6-C5-C3	3.36	120.29	112.62
27	BH	101	DGD	C1E-O6E-C5E	3.36	120.23	113.73
22	AB	607	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
30	BE	102	LMG	O1-C1-C2	3.36	112.45	108.15
22	BB	616	CLA	CBD-CHA-C1A	3.36	133.16	128.77
26	AC	515	BCR	C30-C25-C26	-3.36	117.73	122.59
23	BA	406	PHO	C4D-CHA-CBD	-3.36	104.22	107.88
26	BZ	101	BCR	C33-C5-C4	-3.35	107.03	113.39
22	AB	609	CLA	CED-O2D-CGD	3.35	123.99	116.00
22	BC	507	CLA	CBD-CHA-C1A	3.35	133.15	128.77
22	AC	511	CLA	CBD-CHA-C1A	3.35	133.15	128.77
23	AD	403	PHO	C7-C6-C5	-3.35	103.19	112.97
26	BB	622	BCR	C30-C25-C26	-3.35	117.74	122.59
26	AK	102	BCR	C30-C25-C26	-3.35	117.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	505	CLA	OBD-CAD-CBD	-3.35	120.89	125.94
22	AA	406	CLA	CAA-C2A-C3A	-3.34	104.96	113.32
26	AC	515	BCR	C23-C24-C25	3.34	137.08	127.23
30	BI	101	LMG	O7-C10-C11	3.34	118.65	111.54
24	BD	405	PL9	C17-C18-C19	-3.33	120.60	127.81
27	BC	516	DGD	C1E-O6E-C5E	3.33	120.18	113.73
22	AB	613	CLA	C4B-C3B-CAB	3.33	133.92	127.18
22	BB	613	CLA	C4B-C3B-CAB	3.33	133.92	127.18
22	AB	601	CLA	C4B-C3B-CAB	3.33	133.92	127.18
27	AD	410	DGD	C1E-O6E-C5E	3.33	120.17	113.73
29	BF	101	SQD	O48-C23-C24	3.33	122.09	111.90
22	BD	402	CLA	O2A-CGA-CBA	3.33	122.09	111.90
22	BB	605	CLA	C4A-NA-C1A	3.33	111.07	106.38
24	BA	408	PL9	C37-C38-C39	-3.33	120.58	128.69
26	AA	409	BCR	C29-C30-C25	3.33	115.68	110.37
24	BA	408	PL9	C12-C13-C14	-3.33	120.62	127.81
22	AC	505	CLA	CBA-CAA-C2A	3.32	122.08	113.95
22	BA	407	CLA	CAA-C2A-C3A	-3.32	105.00	113.32
26	BA	410	BCR	C29-C30-C25	3.32	115.67	110.37
22	BB	604	CLA	C1-C2-C3	3.32	131.99	126.23
26	AD	406	BCR	C1-C6-C5	-3.32	117.78	122.59
24	AA	407	PL9	C37-C38-C39	-3.32	120.60	128.69
26	BA	410	BCR	C7-C8-C9	3.32	131.18	126.22
22	AB	611	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
30	BI	101	LMG	C7-O1-C1	-3.32	107.14	113.80
22	BC	505	CLA	CBD-CHA-C1A	3.32	133.11	128.77
22	BB	614	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
26	AD	406	BCR	C2-C1-C6	3.32	115.66	110.37
27	AA	410	DGD	C1E-O6E-C5E	3.32	120.15	113.73
29	BA	413	SQD	O48-C23-C24	3.32	122.05	111.90
22	AC	510	CLA	C1D-CHD-C4C	3.31	127.74	122.60
23	AA	405	PHO	CBD-CHA-C1A	3.31	132.41	126.67
24	AJ	101	PL9	C25-C24-C26	3.31	120.42	115.39
22	AC	512	CLA	CBD-CHA-C1A	3.31	133.10	128.77
24	BA	408	PL9	C30-C29-C31	3.31	120.41	115.39
26	BC	514	BCR	C24-C23-C22	3.31	131.16	126.22
22	BC	501	CLA	CAA-C2A-C3A	-3.30	105.05	113.32
23	BD	403	PHO	C3D-C4D-CHA	3.30	115.45	109.88
30	AB	623	LMG	O7-C10-C11	3.30	118.58	111.54
22	AB	604	CLA	CBD-CHA-C1A	3.30	133.09	128.77
26	BB	622	BCR	C24-C23-C22	3.30	131.16	126.22
22	BC	506	CLA	CED-O2D-CGD	3.30	123.85	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	614	CLA	CBD-CHA-C1A	3.29	133.08	128.77
22	AB	608	CLA	CAA-C2A-C3A	-3.29	105.07	113.32
26	AC	515	BCR	C8-C7-C6	3.29	136.95	127.23
22	BB	615	CLA	C6-C5-C3	3.29	120.13	112.62
26	AB	618	BCR	C30-C25-C26	-3.29	117.82	122.59
22	AA	402	CLA	O2A-CGA-CBA	3.29	121.97	111.90
22	AB	603	CLA	O2A-CGA-CBA	3.29	121.97	111.90
26	AB	619	BCR	C29-C30-C25	3.29	115.61	110.37
26	BD	406	BCR	C2-C1-C6	3.29	115.61	110.37
26	AA	409	BCR	C30-C25-C26	-3.29	117.83	122.59
23	BD	403	PHO	C4D-CHA-CBD	-3.29	104.30	107.88
26	AB	617	BCR	C29-C30-C25	3.29	115.61	110.37
22	BB	606	CLA	O2A-CGA-CBA	3.28	121.95	111.90
22	AB	610	CLA	C4B-C3B-CAB	3.29	133.83	127.18
29	AA	412	SQD	O48-C23-C24	3.28	121.95	111.90
27	BC	516	DGD	O5D-C6D-C5D	3.28	114.66	108.96
26	BK	102	BCR	C23-C24-C25	3.28	136.92	127.23
22	BB	604	CLA	C4B-C3B-CAB	3.28	133.82	127.18
23	BA	406	PHO	C3D-C4D-CHA	3.28	115.41	109.88
26	AH	101	BCR	C12-C13-C14	-3.28	113.94	118.98
26	AZ	101	BCR	C33-C5-C4	-3.28	107.18	113.39
30	AI	101	LMG	O7-C10-C11	3.28	118.52	111.54
22	AB	615	CLA	C1D-CHD-C4C	3.27	127.68	122.60
26	AB	620	BCR	C30-C25-C26	-3.27	117.85	122.59
26	AK	102	BCR	C23-C24-C25	3.27	136.88	127.23
22	BB	611	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
26	BC	515	BCR	C23-C24-C25	3.27	136.88	127.23
26	AB	618	BCR	C8-C7-C6	3.27	136.87	127.23
26	AC	514	BCR	C24-C23-C22	3.27	131.11	126.22
26	BX	101	BCR	C2-C1-C6	3.26	115.58	110.37
26	BD	406	BCR	C1-C6-C5	-3.26	117.86	122.59
30	BD	407	LMG	O7-C10-C11	3.26	118.49	111.54
22	AB	614	CLA	C1-C2-C3	3.26	131.88	126.23
26	AT	102	BCR	C30-C25-C26	-3.26	117.87	122.59
27	BB	602	DGD	O5D-C6D-C5D	3.26	114.62	108.96
22	AC	506	CLA	CED-O2D-CGD	3.26	123.75	116.00
22	AD	402	CLA	O2A-CGA-CBA	3.26	121.87	111.90
22	BA	405	CLA	CBD-CHA-C1A	3.25	133.02	128.77
26	AD	406	BCR	C8-C7-C6	3.25	136.83	127.23
26	AK	102	BCR	C24-C23-C22	3.25	131.08	126.22
27	AH	102	DGD	C1E-O6E-C5E	3.25	120.02	113.73
23	AD	403	PHO	C3D-C4D-CHA	3.25	115.36	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BX	101	BCR	C12-C13-C14	-3.25	113.97	118.98
27	BA	411	DGD	C1E-O6E-C5E	3.25	120.01	113.73
30	AB	621	LMG	O7-C10-C11	3.25	118.46	111.54
22	BC	513	CLA	CBD-CHA-C1A	3.25	133.01	128.77
26	AH	101	BCR	C2-C1-C6	3.24	115.54	110.37
22	AB	601	CLA	C1-C2-C3	3.24	131.86	126.23
24	AD	405	PL9	C17-C18-C19	-3.24	120.79	127.81
26	BZ	101	BCR	C16-C17-C18	3.24	131.98	127.29
30	AB	622	LMG	C7-O1-C1	-3.24	107.29	113.80
26	AT	102	BCR	C8-C7-C6	3.24	136.80	127.23
22	AB	601	CLA	CBD-CHA-C1A	3.24	133.01	128.77
22	AC	505	CLA	O2A-CGA-CBA	3.24	121.81	111.90
22	BB	608	CLA	CAA-C2A-C3A	-3.24	105.22	113.32
22	BB	617	CLA	C1-C2-C3	3.23	131.84	126.23
26	BC	515	BCR	C8-C7-C6	3.23	136.78	127.23
26	BD	406	BCR	C8-C7-C6	3.23	136.77	127.23
22	AB	612	CLA	CBD-CHA-C1A	3.23	132.99	128.77
22	AC	509	CLA	C1D-CHD-C4C	3.23	127.61	122.60
22	BC	509	CLA	C1-C2-C3	3.23	131.83	126.23
22	BB	607	CLA	CBD-CHA-C1A	3.22	132.98	128.77
26	AC	514	BCR	C2-C1-C6	3.22	115.51	110.37
26	AB	620	BCR	C24-C23-C22	3.22	131.03	126.22
26	BK	102	BCR	C24-C23-C22	3.22	131.03	126.22
26	AJ	102	BCR	C30-C25-C26	-3.22	117.93	122.59
22	BB	616	CLA	C4B-C3B-CAB	3.21	133.69	127.18
34	BE	101	HEM	C4C-NC-C1C	3.21	108.78	105.51
24	BA	408	PL9	C35-C34-C36	3.21	120.27	115.39
29	AA	415	SQD	C3-C4-C5	-3.21	104.41	110.17
24	BJ	101	PL9	C27-C28-C29	-3.21	120.87	128.69
22	BC	501	CLA	O2A-CGA-CBA	3.21	121.72	111.90
22	AA	404	CLA	OBD-CAD-CBD	-3.21	121.10	125.94
30	BB	623	LMG	C7-O1-C1	-3.21	107.36	113.80
22	AA	404	CLA	CBD-CHA-C1A	3.20	132.96	128.77
24	AD	405	PL9	C20-C19-C21	3.20	120.25	115.39
22	AB	603	CLA	CBD-CHA-C1A	3.20	132.95	128.77
27	AC	518	DGD	O2G-C1B-C2B	3.20	118.36	111.54
22	AB	610	CLA	OBD-CAD-CBD	-3.20	121.11	125.94
26	BZ	101	BCR	C2-C1-C6	3.20	115.47	110.37
22	AC	513	CLA	CBD-CHA-C1A	3.20	132.95	128.77
23	AA	405	PHO	C3D-C4D-CHA	3.19	115.26	109.88
26	AH	101	BCR	C15-C14-C13	3.19	131.90	127.29
27	AA	410	DGD	O2G-C1B-C2B	3.19	118.34	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	507	CLA	C4B-C3B-CAB	3.19	133.64	127.18
22	AB	605	CLA	CAA-C2A-C3A	-3.19	105.34	113.32
22	BB	615	CLA	C1D-CHD-C4C	3.19	127.54	122.60
22	AC	509	CLA	OBD-CAD-CBD	-3.19	121.13	125.94
26	BK	102	BCR	C30-C25-C26	-3.18	117.98	122.59
30	BB	624	LMG	C7-O1-C1	-3.18	107.41	113.80
27	BC	518	DGD	O2G-C1B-C2B	3.18	118.32	111.54
22	AB	616	CLA	CED-O2D-CGD	3.18	123.58	116.00
22	BB	619	CLA	OBD-CAD-CBD	-3.18	121.14	125.94
22	BC	508	CLA	CAA-C2A-C3A	-3.18	105.37	113.32
22	BC	509	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
22	BC	511	CLA	CED-O2D-CGD	3.17	123.56	116.00
28	BA	412	LHG	O8-C23-C24	3.17	121.61	111.90
22	AB	602	CLA	CBD-CHA-C1A	3.17	132.91	128.77
26	AK	102	BCR	C16-C17-C18	3.17	131.87	127.29
24	BJ	101	PL9	C7-C8-C9	-3.17	121.40	126.76
22	BD	402	CLA	C1D-CHD-C4C	3.17	127.52	122.60
30	BB	623	LMG	O7-C10-C11	3.17	118.29	111.54
23	BD	403	PHO	C7-C6-C5	-3.16	103.74	112.97
29	BA	401	SQD	C3-C4-C5	-3.16	104.50	110.17
22	AC	511	CLA	C1D-CHD-C4C	3.16	127.49	122.60
22	AD	402	CLA	C1D-CHD-C4C	3.15	127.49	122.60
22	AC	507	CLA	C7-C6-C5	-3.15	103.76	112.97
24	AJ	101	PL9	C22-C23-C24	-3.15	120.99	127.81
22	BB	610	CLA	CAA-C2A-C3A	-3.15	105.44	113.32
22	AB	607	CLA	CAA-C2A-C3A	-3.15	105.44	113.32
22	AC	501	CLA	O2A-CGA-CBA	3.15	121.53	111.90
24	AJ	101	PL9	C27-C28-C29	-3.14	121.03	128.69
22	BD	404	CLA	CAA-C2A-C3A	-3.14	105.45	113.32
22	BC	511	CLA	C1D-CHD-C4C	3.14	127.48	122.60
22	AB	616	CLA	CBD-CHA-C1A	3.14	132.88	128.77
22	AB	613	CLA	C1D-CHD-C4C	3.14	127.47	122.60
22	AC	506	CLA	CAA-C2A-C3A	-3.14	105.45	113.32
26	BJ	102	BCR	C30-C25-C26	-3.14	118.04	122.59
22	AB	610	CLA	CBD-CHA-C1A	3.14	132.87	128.77
30	AB	622	LMG	O7-C10-C11	3.14	118.22	111.54
22	BB	605	CLA	C7-C6-C5	-3.13	103.82	112.97
26	BB	620	BCR	C29-C30-C25	3.13	115.36	110.37
22	BC	505	CLA	C1D-CHD-C4C	3.13	127.46	122.60
30	AD	407	LMG	O7-C10-C11	3.13	118.22	111.54
22	AB	611	CLA	CBD-CHA-C1A	3.13	132.86	128.77
24	AA	407	PL9	C25-C24-C26	3.13	120.14	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	507	CLA	C4B-C3B-CAB	3.13	133.52	127.18
24	AD	405	PL9	C37-C38-C39	-3.13	121.04	127.81
30	AE	102	LMG	O7-C10-C11	3.13	118.21	111.54
22	AB	611	CLA	C7-C6-C5	-3.12	103.86	112.97
26	AC	514	BCR	C29-C30-C25	3.12	115.34	110.37
22	BC	502	CLA	CBD-CHA-C1A	3.12	132.84	128.77
22	AC	501	CLA	CBD-CHA-C1A	3.11	132.84	128.77
23	AD	403	PHO	C4D-CHA-CBD	-3.11	104.49	107.88
24	AD	405	PL9	C25-C24-C26	3.11	120.11	115.39
23	AD	403	PHO	CED-O2D-CGD	3.11	123.40	116.00
27	BA	411	DGD	O2G-C1B-C2B	3.11	118.16	111.54
24	AD	405	PL9	C42-C43-C44	-3.11	121.09	127.81
26	BA	410	BCR	C30-C25-C26	-3.10	118.10	122.59
26	AB	618	BCR	C2-C1-C6	3.10	115.31	110.37
27	BC	516	DGD	O2G-C1B-C2B	3.10	118.15	111.54
22	BB	610	CLA	OBD-CAD-CBD	-3.10	121.26	125.94
22	BC	510	CLA	C1D-CHD-C4C	3.10	127.41	122.60
22	BB	619	CLA	CBD-CHA-C1A	3.10	132.82	128.77
22	BC	513	CLA	CED-O2D-CGD	3.10	123.37	116.00
34	BE	101	HEM	C1A-CHA-C4D	-3.09	123.40	127.47
22	BB	607	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
26	BX	101	BCR	C8-C7-C6	3.09	136.36	127.23
22	AC	508	CLA	C1D-CHD-C4C	3.09	127.39	122.60
26	AC	514	BCR	C1-C6-C5	-3.09	118.11	122.59
32	AM	102	LMT	C1B-O1B-C4'	-3.09	110.15	118.00
24	BJ	101	PL9	C22-C23-C24	-3.09	121.13	127.81
22	BB	614	CLA	CBD-CHA-C1A	3.09	132.81	128.77
22	BC	509	CLA	CED-O2D-CGD	3.09	123.35	116.00
26	AH	101	BCR	C8-C7-C6	3.08	136.33	127.23
22	AC	508	CLA	CAA-C2A-C3A	-3.08	105.60	113.32
22	AB	610	CLA	C1-C2-C3	3.08	131.57	126.23
22	AB	616	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
22	BB	618	CLA	C1D-CHD-C4C	3.08	127.37	122.60
22	BA	407	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
22	BA	407	CLA	CED-O2D-CGD	3.07	123.32	116.00
22	BB	614	CLA	C7-C6-C5	-3.07	104.00	112.97
22	AB	614	CLA	OBD-CAD-CBD	-3.07	121.30	125.94
22	AC	513	CLA	CED-O2D-CGD	3.07	123.31	116.00
22	BB	616	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
24	BA	408	PL9	C25-C24-C26	3.07	120.05	115.39
22	AD	402	CLA	C2B-C3B-CAB	-3.07	121.05	127.33
22	BC	509	CLA	O2A-CGA-CBA	3.07	121.29	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AA	412	SQD	C44-O6-C1	3.07	119.95	113.80
22	BB	610	CLA	O2A-CGA-CBA	3.07	121.28	111.90
24	BD	405	PL9	C15-C14-C16	3.07	120.04	115.39
22	BC	505	CLA	O2A-CGA-CBA	3.07	121.28	111.90
26	BB	621	BCR	C2-C1-C6	3.06	115.25	110.37
24	BA	408	PL9	C15-C14-C16	3.06	120.04	115.39
23	AA	405	PHO	C4D-CHA-CBD	-3.06	104.54	107.88
22	BC	502	CLA	CED-O2D-CGD	3.06	123.30	116.00
23	AD	403	PHO	OBD-CAD-CBD	-3.06	121.32	125.94
22	AC	509	CLA	O2A-CGA-CBA	3.06	121.26	111.90
26	AB	617	BCR	C2-C1-C6	3.05	115.24	110.37
26	BC	514	BCR	C1-C6-C5	-3.05	118.17	122.59
26	AB	617	BCR	C8-C7-C6	3.05	136.23	127.23
22	BB	604	CLA	CBD-CHA-C1A	3.05	132.75	128.77
22	BB	619	CLA	C1-C2-C3	3.05	131.52	126.23
22	AB	612	CLA	C1D-CHD-C4C	3.05	127.32	122.60
22	AB	607	CLA	O2A-CGA-CBA	3.05	121.22	111.90
22	BB	618	CLA	C1-C2-C3	3.04	131.51	126.23
22	AB	602	CLA	CED-O2D-CGD	3.05	123.25	116.00
30	AA	416	LMG	O7-C10-C11	3.04	118.02	111.54
22	BC	504	CLA	CAA-C2A-C3A	-3.04	105.71	113.32
22	BC	504	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
22	AC	512	CLA	C1-C2-C3	3.04	131.50	126.23
24	AD	405	PL9	C15-C14-C16	3.04	120.01	115.39
22	BC	507	CLA	C1-C2-C3	3.04	131.50	126.23
22	BD	402	CLA	C2B-C3B-CAB	-3.04	121.11	127.33
24	AD	405	PL9	C7-C8-C9	-3.04	121.62	126.76
23	BD	403	PHO	OBD-CAD-CBD	-3.04	121.35	125.94
26	BB	620	BCR	C8-C7-C6	3.04	136.19	127.23
22	BB	613	CLA	CBD-CHA-C1A	3.03	132.74	128.77
24	BD	405	PL9	C37-C38-C39	-3.03	121.25	127.81
30	AB	621	LMG	C7-O1-C1	-3.03	107.71	113.80
26	AH	101	BCR	C11-C10-C9	3.03	131.67	127.29
22	AC	509	CLA	C1-C2-C3	3.03	131.49	126.23
24	BD	405	PL9	C42-C43-C44	-3.03	121.25	127.81
22	BA	403	CLA	C6-C5-C3	3.03	119.53	112.62
26	BC	514	BCR	C29-C30-C25	3.03	115.20	110.37
22	BB	615	CLA	CBD-CHA-C1A	3.03	132.73	128.77
30	AI	101	LMG	C7-O1-C1	-3.03	107.72	113.80
30	BB	624	LMG	O7-C10-C11	3.02	117.98	111.54
30	AE	102	LMG	O6-C5-C6	3.02	113.87	106.34
26	AB	617	BCR	C23-C24-C25	3.02	136.14	127.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	612	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
22	AB	609	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
26	AT	102	BCR	C2-C1-C6	3.02	115.19	110.37
22	AB	610	CLA	C1D-CHD-C4C	3.02	127.28	122.60
22	BB	617	CLA	OBD-CAD-CBD	-3.02	121.39	125.94
22	AC	505	CLA	C1D-CHD-C4C	3.02	127.28	122.60
32	BD	411	LMT	C1-O1'-C1'	-3.01	108.59	113.91
23	AA	405	PHO	C1-C2-C3	3.01	131.46	126.23
24	AA	407	PL9	C10-C9-C11	3.01	119.97	115.39
22	BD	404	CLA	CBD-CHA-C1A	3.01	132.71	128.77
22	BC	507	CLA	CED-O2D-CGD	3.01	123.18	116.00
26	AB	620	BCR	C2-C1-C6	3.01	115.17	110.37
22	BA	407	CLA	CBD-CHA-C1A	3.01	132.70	128.77
22	BC	512	CLA	CAA-C2A-C3A	-3.01	105.79	113.32
22	BB	613	CLA	C1D-CHD-C4C	3.01	127.27	122.60
22	AC	510	CLA	O2A-CGA-CBA	3.01	121.10	111.90
22	BB	605	CLA	O2A-CGA-CBA	3.01	121.11	111.90
22	AB	608	CLA	C1D-CHD-C4C	3.01	127.26	122.60
22	AB	608	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
27	AD	410	DGD	O2G-C1B-C2B	3.01	117.95	111.54
22	BC	512	CLA	C1-C2-C3	3.01	131.44	126.23
22	AA	402	CLA	C6-C5-C3	3.01	119.48	112.62
22	BB	611	CLA	C1D-CHD-C4C	3.00	127.26	122.60
22	BB	608	CLA	CED-O2D-CGD	3.00	123.15	116.00
27	BD	410	DGD	O2G-C1B-C2B	3.00	117.94	111.54
22	BB	609	CLA	OBD-CAD-CBD	-3.00	121.40	125.94
22	BB	609	CLA	O2A-CGA-CBA	3.00	121.09	111.90
32	BM	101	LMT	C1B-O1B-C4'	-3.00	110.38	118.00
22	BA	405	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
32	AD	411	LMT	C1-O1'-C1'	-3.00	108.61	113.91
26	BB	620	BCR	C23-C24-C25	3.00	136.08	127.23
26	BK	102	BCR	C34-C9-C8	3.00	122.94	118.09
22	BC	509	CLA	C1D-CHD-C4C	3.00	127.25	122.60
22	AC	502	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
22	AC	512	CLA	C1D-CHD-C4C	3.00	127.25	122.60
26	BB	621	BCR	C1-C6-C5	-3.00	118.25	122.59
22	BB	611	CLA	CAA-C2A-C3A	-3.00	105.82	113.32
22	BC	513	CLA	C1D-CHD-C4C	3.00	127.25	122.60
26	AT	102	BCR	C24-C23-C22	3.00	130.70	126.22
30	BM	102	LMG	O6-C5-C6	3.00	113.81	106.34
22	BC	507	CLA	C7-C6-C5	-3.00	104.22	112.97
26	BB	621	BCR	C23-C24-C25	2.99	136.07	127.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BA	414	LMG	O7-C10-C11	2.99	117.91	111.54
26	AA	409	BCR	C2-C1-C6	2.99	115.14	110.37
24	AD	405	PL9	C45-C44-C46	2.99	119.93	115.39
30	BE	102	LMG	O6-C5-C6	2.99	113.78	106.34
22	BD	402	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
22	AB	605	CLA	C1-C2-C3	2.99	131.41	126.23
26	AB	618	BCR	C24-C23-C22	2.99	130.68	126.22
23	BA	406	PHO	C3D-C4D-ND	2.99	110.57	106.81
26	BC	514	BCR	C35-C13-C12	2.98	122.91	118.09
22	AA	406	CLA	C7-C6-C5	-2.98	104.27	112.97
26	AB	617	BCR	C30-C25-C26	-2.98	118.28	122.59
22	AC	513	CLA	C1D-CHD-C4C	2.98	127.22	122.60
22	BB	606	CLA	C1D-CHD-C4C	2.98	127.22	122.60
22	AB	603	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	BC	508	CLA	C1D-CHD-C4C	2.98	127.22	122.60
22	AB	615	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	AB	608	CLA	C6-C5-C3	2.98	119.42	112.62
22	AB	602	CLA	O2A-CGA-CBA	2.98	121.01	111.90
26	BX	101	BCR	C15-C14-C13	2.98	131.59	127.29
30	BE	102	LMG	O7-C10-C11	2.98	117.88	111.54
22	AC	508	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	AD	404	CLA	C1D-CHD-C4C	2.98	127.21	122.60
22	AB	601	CLA	O2A-CGA-CBA	2.98	121.01	111.90
26	AB	619	BCR	C2-C1-C6	2.98	115.11	110.37
34	AE	101	HEM	C1A-CHA-C4D	-2.98	123.56	127.47
22	BC	506	CLA	CAA-C2A-C3A	-2.97	105.88	113.32
22	AB	615	CLA	C1-C2-C3	2.97	131.38	126.23
22	AC	502	CLA	CED-O2D-CGD	2.97	123.08	116.00
22	BC	501	CLA	CBD-CHA-C1A	2.97	132.65	128.77
26	BK	102	BCR	C12-C13-C14	-2.97	114.41	118.98
22	AC	502	CLA	C1D-CHD-C4C	2.97	127.21	122.60
22	BB	619	CLA	CED-O2D-CGD	2.97	123.08	116.00
22	AB	602	CLA	C7-C6-C5	-2.97	104.30	112.97
22	BC	512	CLA	C1D-CHD-C4C	2.97	127.20	122.60
22	BB	615	CLA	CED-O2D-CGD	2.97	123.06	116.00
22	AB	606	CLA	CBD-CHA-C1A	2.97	132.65	128.77
22	AB	606	CLA	O2A-CGA-CBA	2.97	120.98	111.90
24	BD	405	PL9	C7-C8-C9	-2.97	121.74	126.76
22	AC	513	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
27	BB	602	DGD	O3G-C1D-C2D	2.97	111.95	108.15
23	AA	405	PHO	OBD-CAD-CBD	-2.97	121.46	125.94
27	AB	626	DGD	O3G-C1D-C2D	2.96	111.95	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AC	515	BCR	C1-C6-C5	-2.96	118.31	122.59
22	AB	609	CLA	CAA-C2A-C3A	-2.96	105.92	113.32
30	AM	101	LMG	O6-C5-C6	2.95	113.70	106.34
34	AE	101	HEM	C3A-C4A-NA	-2.95	107.52	109.50
29	BA	413	SQD	C32-C31-C30	2.95	130.25	114.56
26	AC	514	BCR	C35-C13-C12	2.95	122.86	118.09
22	AB	610	CLA	CAA-C2A-C3A	-2.95	105.93	113.32
22	AC	504	CLA	CAA-C2A-C3A	-2.95	105.93	113.32
26	AH	101	BCR	C16-C17-C18	2.95	131.55	127.29
22	BB	604	CLA	O2A-CGA-CBA	2.95	120.93	111.90
22	BA	403	CLA	CBD-CHA-C1A	2.95	132.62	128.77
22	BB	615	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
26	BB	621	BCR	C8-C7-C6	2.94	135.92	127.23
26	AT	102	BCR	C23-C24-C25	2.95	135.92	127.23
26	BB	620	BCR	C30-C25-C26	-2.94	118.33	122.59
22	AC	504	CLA	C1D-CHD-C4C	2.94	127.16	122.60
22	AC	503	CLA	C1D-CHD-C4C	2.94	127.15	122.60
26	AC	514	BCR	C32-C1-C6	2.94	115.19	110.33
22	BC	505	CLA	CED-O2D-CGD	2.94	122.99	116.00
22	BB	609	CLA	C1-C2-C3	2.94	131.32	126.23
22	BC	509	CLA	C6-C5-C3	2.94	119.32	112.62
26	AJ	102	BCR	C21-C20-C19	2.93	133.08	123.23
30	AC	520	LMG	O6-C5-C6	2.93	113.64	106.34
34	BV	201	HEM	C2A-C1A-NA	-2.93	105.66	109.73
22	AC	506	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
29	AA	412	SQD	C32-C31-C30	2.93	130.13	114.56
29	AF	101	SQD	C3-C4-C5	-2.93	104.91	110.17
22	BB	611	CLA	C6-C5-C3	2.93	119.31	112.62
22	AA	402	CLA	CBD-CHA-C1A	2.93	132.60	128.77
22	AC	509	CLA	C6-C5-C3	2.93	119.30	112.62
30	AM	101	LMG	O1-C1-C2	2.93	111.90	108.15
24	BD	405	PL9	C25-C24-C26	2.93	119.83	115.39
22	AB	611	CLA	CED-O2D-CGD	2.92	122.96	116.00
24	AA	407	PL9	C15-C14-C16	2.92	119.83	115.39
30	AE	102	LMG	O1-C1-C2	2.92	111.89	108.15
24	AA	407	PL9	C20-C19-C21	2.92	119.83	115.39
22	BD	402	CLA	CBD-CHA-C1A	2.92	132.59	128.77
22	AC	503	CLA	CBD-CHA-C1A	2.92	132.59	128.77
24	AJ	101	PL9	C20-C19-C21	2.92	119.82	115.39
27	AC	516	DGD	O2G-C1B-C2B	2.92	117.75	111.54
30	AA	416	LMG	C7-O1-C1	-2.92	107.94	113.80
22	BB	611	CLA	C2D-C3D-CAD	2.92	146.83	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AD	404	CLA	CBD-CHA-C1A	2.91	132.58	128.77
22	BB	612	CLA	CAA-C2A-C3A	-2.92	106.02	113.32
22	AC	509	CLA	CED-O2D-CGD	2.92	122.94	116.00
32	BB	626	LMT	C1B-O1B-C4'	-2.91	110.60	118.00
27	AB	626	DGD	O5D-C6D-C5D	2.91	114.01	108.96
22	BA	404	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
22	AC	507	CLA	C1-C2-C3	2.91	131.28	126.23
26	AK	102	BCR	C34-C9-C8	2.91	122.79	118.09
32	BM	101	LMT	C1-O1'-C1'	-2.91	108.78	113.91
22	BA	405	CLA	C1D-CHD-C4C	2.91	127.11	122.60
22	BD	402	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
22	AB	614	CLA	C1D-CHD-C4C	2.91	127.11	122.60
24	BJ	101	PL9	C17-C18-C19	-2.90	121.53	127.81
26	BD	406	BCR	C12-C13-C14	-2.90	114.51	118.98
23	AA	405	PHO	C6-C5-C3	2.90	119.24	112.62
22	BB	613	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
22	AC	504	CLA	C1-C2-C3	2.90	131.26	126.23
22	BB	608	CLA	CBD-CHA-C1A	2.90	132.56	128.77
22	AB	615	CLA	O2A-CGA-CBA	2.90	120.77	111.90
22	BC	503	CLA	CBD-CHA-C1A	2.90	132.56	128.77
30	AC	519	LMG	O7-C10-C11	2.90	117.71	111.54
22	BC	508	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
22	AC	505	CLA	CED-O2D-CGD	2.89	122.89	116.00
22	BC	507	CLA	C1D-CHD-C4C	2.89	127.09	122.60
24	AD	405	PL9	C12-C13-C14	-2.89	121.55	127.81
22	AC	501	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
22	BB	607	CLA	C1D-CHD-C4C	2.89	127.08	122.60
27	BC	517	DGD	C1E-O6E-C5E	2.89	119.32	113.73
22	AB	608	CLA	C2D-C3D-CAD	2.89	146.71	134.94
26	BD	406	BCR	C23-C22-C21	-2.89	114.54	118.98
29	AD	409	SQD	C18-C17-C16	2.88	121.18	112.94
26	AB	618	BCR	C23-C24-C25	2.88	135.74	127.23
22	BC	509	CLA	CBD-CHA-C1A	2.88	132.54	128.77
22	AB	605	CLA	O2A-CGA-CBA	2.88	120.71	111.90
22	AB	601	CLA	CED-O2D-CGD	2.88	122.86	116.00
22	AC	509	CLA	CBD-CHA-C1A	2.88	132.53	128.77
26	BJ	102	BCR	C21-C20-C19	2.88	132.89	123.23
26	BJ	102	BCR	C16-C17-C18	2.88	131.45	127.29
22	AB	603	CLA	CED-O2D-CGD	2.88	122.85	116.00
22	AB	605	CLA	CED-O2D-CGD	2.87	122.84	116.00
26	AB	619	BCR	C8-C7-C6	2.87	135.71	127.23
26	AB	619	BCR	C23-C24-C25	2.87	135.71	127.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BD	403	PHO	CED-O2D-CGD	2.87	122.84	116.00
22	BB	606	CLA	OBD-CAD-CBD	-2.87	121.60	125.94
24	AD	405	PL9	C40-C39-C41	2.87	119.75	115.39
22	AB	606	CLA	C1-C2-C3	2.87	131.21	126.23
22	BB	605	CLA	CED-O2D-CGD	2.87	122.83	116.00
26	AC	514	BCR	C30-C25-C26	-2.87	118.43	122.59
23	AA	405	PHO	CED-O2D-CGD	2.87	122.83	116.00
29	AD	409	SQD	C15-C16-C17	2.87	125.28	113.73
22	BC	506	CLA	CBD-CHA-C1A	2.87	132.52	128.77
22	AB	604	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
29	AA	415	SQD	C32-C31-C30	2.87	129.80	114.56
22	BD	404	CLA	C1D-CHD-C4C	2.87	127.05	122.60
22	BB	619	CLA	O2A-CGA-CBA	2.87	120.68	111.90
29	AD	409	SQD	O47-C7-C8	2.87	117.65	111.54
24	BD	405	PL9	C45-C44-C46	2.87	119.74	115.39
22	AD	402	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
22	AC	504	CLA	OBD-CAD-CBD	-2.86	121.61	125.94
22	AB	609	CLA	C1D-CHD-C4C	2.86	127.04	122.60
22	AC	511	CLA	O2A-CGA-CBA	2.86	120.66	111.90
22	BA	403	CLA	CBA-CAA-C2A	2.86	120.95	113.95
22	AC	510	CLA	C1-C2-C3	2.86	131.19	126.23
24	BD	405	PL9	C30-C29-C31	2.86	119.73	115.39
22	AA	402	CLA	CED-O2D-CGD	2.86	122.81	116.00
22	AB	611	CLA	C6-C5-C3	2.86	119.14	112.62
22	AC	512	CLA	CAA-C2A-C3A	-2.86	106.17	113.32
26	BA	410	BCR	C2-C1-C6	2.85	114.92	110.37
22	BB	618	CLA	O2A-CGA-CBA	2.86	120.64	111.90
23	AA	405	PHO	C3D-C4D-ND	2.86	110.41	106.81
22	BC	510	CLA	O2A-CGA-CBA	2.85	120.64	111.90
22	AA	403	CLA	CBD-CHA-C1A	2.85	132.50	128.77
30	AD	407	LMG	O6-C5-C6	2.85	113.45	106.34
22	AB	605	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
22	AB	615	CLA	CED-O2D-CGD	2.85	122.79	116.00
22	BB	613	CLA	C6-C5-C3	2.85	119.12	112.62
26	BX	101	BCR	C16-C17-C18	2.85	131.41	127.29
22	AC	508	CLA	O2A-CGA-CBA	2.85	120.62	111.90
29	BD	409	SQD	C3-C4-C5	-2.85	105.06	110.17
22	BC	504	CLA	C1-C2-C3	2.85	131.17	126.23
24	BD	405	PL9	C35-C34-C36	2.85	119.71	115.39
22	BC	501	CLA	OBD-CAD-CBD	-2.85	121.64	125.94
22	BC	502	CLA	C1D-CHD-C4C	2.85	127.01	122.60
34	AE	101	HEM	C4C-NC-C1C	2.85	108.41	105.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	404	CLA	C6-C5-C3	2.84	119.11	112.62
22	BC	508	CLA	O2A-CGA-CBA	2.85	120.61	111.90
22	AB	604	CLA	O2A-CGA-CBA	2.84	120.61	111.90
26	BB	622	BCR	C1-C6-C5	-2.84	118.47	122.59
26	BD	406	BCR	C37-C22-C23	2.85	122.69	118.09
22	AA	404	CLA	CED-O2D-CGD	2.84	122.77	116.00
22	AA	402	CLA	CBA-CAA-C2A	2.84	120.90	113.95
22	BA	403	CLA	CED-O2D-CGD	2.84	122.77	116.00
29	BA	401	SQD	C32-C31-C30	2.84	129.66	114.56
30	BC	519	LMG	O6-C5-C6	2.84	113.42	106.34
22	AC	511	CLA	CED-O2D-CGD	2.84	122.77	116.00
22	AB	614	CLA	CED-O2D-CGD	2.84	122.76	116.00
29	BD	409	SQD	O47-C7-C8	2.84	117.59	111.54
22	BA	407	CLA	C7-C6-C5	-2.84	104.68	112.97
26	BC	514	BCR	C30-C25-C26	-2.84	118.48	122.59
22	BB	617	CLA	C1D-CHD-C4C	2.84	127.00	122.60
22	BC	501	CLA	C1D-CHD-C4C	2.84	127.00	122.60
23	BA	406	PHO	C1-C2-C3	2.84	131.15	126.23
22	BD	402	CLA	C4B-C3B-CAB	2.83	132.92	127.18
22	AC	507	CLA	C1D-CHD-C4C	2.83	127.00	122.60
22	BB	615	CLA	O2A-CGA-CBA	2.83	120.57	111.90
32	BB	603	LMT	C1B-O1B-C4'	-2.83	110.80	118.00
22	BB	614	CLA	O2A-CGA-CBA	2.83	120.57	111.90
22	AA	406	CLA	C1D-CHD-C4C	2.83	126.99	122.60
22	AA	404	CLA	C1D-CHD-C4C	2.83	126.99	122.60
22	BB	616	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
32	AB	625	LMT	C1B-O1B-C4'	-2.83	110.81	118.00
22	BB	613	CLA	O2A-CGA-CBA	2.83	120.56	111.90
22	AB	605	CLA	CBD-CHA-C1A	2.83	132.47	128.77
22	AB	604	CLA	C1D-CHD-C4C	2.83	126.99	122.60
23	BA	406	PHO	C7-C6-C5	-2.83	104.71	112.97
26	BC	515	BCR	C1-C6-C5	-2.83	118.50	122.59
27	BC	517	DGD	C3G-C2G-C1G	-2.83	105.37	111.86
26	BB	620	BCR	C1-C6-C5	-2.82	118.50	122.59
24	BA	408	PL9	C10-C9-C11	2.82	119.68	115.39
22	BC	502	CLA	CAA-C2A-C3A	-2.82	106.25	113.32
22	AB	612	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
22	BB	617	CLA	CED-O2D-CGD	2.82	122.72	116.00
23	AD	403	PHO	C3D-C4D-ND	2.82	110.36	106.81
26	BZ	101	BCR	C35-C13-C12	2.82	122.65	118.09
22	BC	503	CLA	C1D-CHD-C4C	2.82	126.97	122.60
22	AD	404	CLA	O2A-CGA-CBA	2.82	120.52	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	603	CLA	C1D-CHD-C4C	2.82	126.97	122.60
22	BA	405	CLA	C7-C6-C5	-2.82	104.75	112.97
22	AC	506	CLA	CBD-CHA-C1A	2.82	132.45	128.77
22	AD	402	CLA	C4B-C3B-CAB	2.82	132.88	127.18
26	BA	410	BCR	C37-C22-C23	2.82	122.64	118.09
22	BB	607	CLA	O2A-CGA-CBA	2.81	120.51	111.90
26	AK	102	BCR	C12-C13-C14	-2.81	114.65	118.98
22	AB	615	CLA	C7-C6-C5	-2.81	104.76	112.97
26	AA	409	BCR	C1-C6-C5	-2.81	118.52	122.59
22	AC	502	CLA	C1-C2-C3	2.81	131.10	126.23
22	AB	616	CLA	O2A-CGA-CBA	2.81	120.50	111.90
22	BB	609	CLA	CBD-CHA-C1A	2.81	132.44	128.77
22	BB	609	CLA	C1D-CHD-C4C	2.81	126.96	122.60
27	AC	517	DGD	C3G-C2G-C1G	-2.81	105.41	111.86
22	BD	404	CLA	O2A-CGA-CBA	2.81	120.49	111.90
22	AD	404	CLA	CED-O2D-CGD	2.81	122.68	116.00
22	BB	612	CLA	C1D-CHD-C4C	2.81	126.95	122.60
22	AB	616	CLA	C1-C2-C3	2.81	131.10	126.23
22	BA	407	CLA	C1D-CHD-C4C	2.80	126.95	122.60
32	AB	627	LMT	C1B-O1B-C4'	-2.80	110.88	118.00
22	BA	407	CLA	O2A-CGA-CBA	2.80	120.47	111.90
22	BC	506	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
22	AB	616	CLA	C7-C6-C5	-2.80	104.80	112.97
22	AC	501	CLA	C1D-CHD-C4C	2.80	126.94	122.60
22	BB	608	CLA	C1D-CHD-C4C	2.80	126.94	122.60
22	BC	504	CLA	C1D-CHD-C4C	2.79	126.93	122.60
24	BD	405	PL9	C27-C28-C29	-2.80	121.76	127.81
26	AD	406	BCR	C37-C22-C23	2.79	122.61	118.09
22	AB	612	CLA	O2A-CGA-CBA	2.79	120.45	111.90
27	AC	517	DGD	C1E-O6E-C5E	2.79	119.14	113.73
22	BA	404	CLA	CBD-CHA-C1A	2.79	132.42	128.77
22	AA	406	CLA	O2A-CGA-CBA	2.79	120.44	111.90
32	AT	101	LMT	O1B-C1B-C2B	2.79	114.79	108.11
29	BD	409	SQD	C18-C17-C16	2.79	120.91	112.94
34	BV	201	HEM	C4A-C3A-C2A	2.79	108.94	107.00
22	AB	614	CLA	O2A-CGA-CBA	2.79	120.42	111.90
22	BB	604	CLA	CAA-C2A-C3A	-2.79	106.35	113.32
22	AA	406	CLA	CED-O2D-CGD	2.78	122.63	116.00
26	AB	619	BCR	C1-C6-C5	-2.78	118.56	122.59
22	AB	612	CLA	C1-C2-C3	2.78	131.05	126.23
22	BB	617	CLA	O2A-CGA-CBA	2.78	120.41	111.90
22	BB	614	CLA	CAA-C2A-C3A	-2.78	106.37	113.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	512	CLA	OBD-CAD-CBD	-2.78	121.75	125.94
26	AD	406	BCR	C23-C22-C21	-2.77	114.71	118.98
22	BC	510	CLA	C1-C2-C3	2.78	131.04	126.23
22	AC	503	CLA	OBD-CAD-CBD	-2.77	121.76	125.94
22	BB	618	CLA	C7-C6-C5	-2.77	104.89	112.97
22	BB	611	CLA	CBA-CAA-C2A	2.77	120.71	113.95
22	BB	604	CLA	CED-O2D-CGD	2.77	122.59	116.00
26	AD	406	BCR	C12-C13-C14	-2.77	114.72	118.98
22	BC	503	CLA	OBD-CAD-CBD	-2.77	121.76	125.94
26	BA	410	BCR	C23-C24-C25	2.76	135.38	127.23
22	BB	614	CLA	CED-O2D-CGD	2.76	122.58	116.00
22	BB	606	CLA	CED-O2D-CGD	2.76	122.58	116.00
22	BB	617	CLA	O2D-CGD-CBD	2.76	116.92	111.34
22	AD	402	CLA	CBD-CHA-C1A	2.76	132.38	128.77
22	BB	619	CLA	C7-C6-C5	-2.76	104.91	112.97
22	BA	404	CLA	C1D-CHD-C4C	2.76	126.88	122.60
22	BB	613	CLA	CAA-C2A-C3A	-2.76	106.41	113.32
22	BB	614	CLA	C1D-CHD-C4C	2.76	126.88	122.60
22	AB	608	CLA	CED-O2D-CGD	2.76	122.56	116.00
22	AB	614	CLA	C6-C5-C3	2.75	118.91	112.62
22	AC	513	CLA	O2A-CGA-CBA	2.75	120.33	111.90
22	AC	507	CLA	CED-O2D-CGD	2.76	122.56	116.00
22	AA	403	CLA	C6-C5-C3	2.75	118.91	112.62
22	BC	501	CLA	CED-O2D-CGD	2.75	122.56	116.00
22	AC	503	CLA	O2A-CGA-CBA	2.75	120.33	111.90
22	BC	508	CLA	CED-O2D-CGD	2.75	122.56	116.00
22	AC	506	CLA	C1D-CHD-C4C	2.75	126.87	122.60
26	BX	101	BCR	C35-C13-C12	2.75	122.54	118.09
22	AB	616	CLA	C6-C5-C3	2.75	118.91	112.62
24	AD	405	PL9	C30-C29-C31	2.75	119.57	115.39
22	BB	619	CLA	C2A-C3A-C4A	2.75	106.34	101.89
26	AK	102	BCR	C30-C25-C24	2.75	123.31	115.69
30	AB	623	LMG	C7-O1-C1	-2.75	108.28	113.80
22	AA	403	CLA	C2A-C3A-C4A	2.75	106.33	101.89
22	BC	502	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
22	AA	402	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
22	AB	606	CLA	OBD-CAD-CBD	-2.75	121.80	125.94
22	AC	502	CLA	CBD-CHA-C1A	2.75	132.36	128.77
22	BB	605	CLA	C1D-CHD-C4C	2.74	126.86	122.60
22	AC	506	CLA	C1-C2-C3	2.74	130.99	126.23
22	BC	512	CLA	C7-C6-C5	-2.74	104.96	112.97
22	AC	513	CLA	C1-C2-C3	2.74	130.99	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BC	520	LMG	O6-C5-C6	2.74	113.17	106.34
22	BC	506	CLA	C7-C6-C5	-2.74	104.96	112.97
26	BB	622	BCR	C7-C8-C9	2.74	130.32	126.22
22	AB	608	CLA	CBD-CHA-C1A	2.74	132.35	128.77
34	BE	101	HEM	C3A-C4A-NA	-2.74	107.67	109.50
24	BA	408	PL9	C20-C19-C21	2.74	119.55	115.39
29	BF	101	SQD	C3-C4-C5	-2.74	105.25	110.17
24	BD	405	PL9	C12-C13-C14	-2.74	121.88	127.81
22	AB	611	CLA	C1D-CHD-C4C	2.74	126.85	122.60
22	BB	611	CLA	CED-O2D-CGD	2.74	122.52	116.00
22	BB	618	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
23	BD	403	PHO	C4A-NA-C1A	2.74	112.02	108.42
26	AA	409	BCR	C23-C24-C25	2.73	135.30	127.23
23	BD	403	PHO	C2D-C3D-CAD	2.74	146.10	134.94
22	AB	614	CLA	CAA-C2A-C3A	-2.73	106.48	113.32
22	AB	609	CLA	C7-C6-C5	-2.73	104.99	112.97
22	BB	615	CLA	C2D-C3D-CAD	2.73	146.07	134.94
22	BB	610	CLA	C1-C2-C3	2.73	130.96	126.23
22	AB	612	CLA	C2D-C3D-CAD	2.73	146.07	134.94
29	BD	409	SQD	C15-C16-C17	2.73	124.71	113.73
22	BB	614	CLA	C2D-C3D-CAD	2.73	146.05	134.94
26	BK	102	BCR	C35-C13-C12	2.73	122.50	118.09
22	AB	606	CLA	C1D-CHD-C4C	2.72	126.82	122.60
22	BB	617	CLA	C6-C5-C3	2.72	118.83	112.62
29	AA	412	SQD	C3-C4-C5	-2.72	105.28	110.17
22	BB	610	CLA	C1D-CHD-C4C	2.72	126.82	122.60
22	BC	510	CLA	C7-C6-C5	-2.72	105.03	112.97
22	AB	602	CLA	C1D-CHD-C4C	2.72	126.82	122.60
24	BJ	101	PL9	C20-C19-C21	2.72	119.52	115.39
22	AB	610	CLA	C6-C5-C3	2.72	118.83	112.62
22	BB	605	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
22	AC	511	CLA	C1-C2-C3	2.72	130.94	126.23
22	AC	510	CLA	C2A-C3A-C4A	2.72	106.29	101.89
22	BC	501	CLA	C7-C6-C5	-2.72	105.04	112.97
29	BA	401	SQD	C45-O47-C7	2.72	124.24	117.86
26	AD	406	BCR	C23-C24-C25	2.71	135.24	127.23
22	BD	402	CLA	CED-O2D-CGD	2.72	122.47	116.00
22	AA	406	CLA	C2D-C3D-CAD	2.71	146.01	134.94
24	AD	405	PL9	C27-C28-C29	-2.71	121.94	127.81
22	AC	510	CLA	CED-O2D-CGD	2.71	122.46	116.00
24	BD	405	PL9	C40-C39-C41	2.71	119.51	115.39
32	AD	411	LMT	C1B-O1B-C4'	-2.71	111.11	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	618	BCR	C1-C6-C5	-2.71	118.66	122.59
29	AA	412	SQD	O8-S-O9	-2.71	105.66	111.69
22	AB	607	CLA	C1-C2-C3	2.71	130.93	126.23
22	AB	609	CLA	C6-C5-C3	2.71	118.80	112.62
22	BC	513	CLA	O2A-CGA-CBA	2.71	120.19	111.90
22	BB	608	CLA	O2A-CGA-CBA	2.71	120.19	111.90
22	BC	506	CLA	C1D-CHD-C4C	2.71	126.80	122.60
22	AB	606	CLA	CBA-CAA-C2A	2.71	120.56	113.95
22	BB	618	CLA	CED-O2D-CGD	2.71	122.45	116.00
22	BC	511	CLA	C7-C6-C5	-2.71	105.07	112.97
22	BC	510	CLA	CAA-C2A-C3A	-2.71	106.55	113.32
30	AC	519	LMG	O6-C5-C6	2.70	113.08	106.34
26	AT	102	BCR	C1-C6-C5	-2.70	118.67	122.59
22	AB	613	CLA	C7-C6-C5	-2.70	105.08	112.97
26	BX	101	BCR	C1-C6-C5	-2.70	118.67	122.59
22	AB	611	CLA	C2D-C3D-CAD	2.70	145.95	134.94
26	AC	514	BCR	C23-C24-C25	2.70	135.20	127.23
22	AB	601	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
30	BD	407	LMG	O6-C5-C6	2.70	113.07	106.34
28	AC	521	LHG	O8-C23-C24	2.70	120.17	111.90
28	BC	521	LHG	O8-C23-C24	2.70	120.16	111.90
22	AA	404	CLA	C7-C6-C5	-2.70	105.09	112.97
23	BD	403	PHO	O2A-CGA-CBA	2.70	120.16	111.90
26	AB	617	BCR	C1-C6-C5	-2.70	118.69	122.59
30	BI	101	LMG	O6-C5-C6	2.70	113.06	106.34
22	BB	609	CLA	CBA-CAA-C2A	2.70	120.54	113.95
29	BA	413	SQD	C32-C33-C34	2.70	124.59	113.73
22	AD	402	CLA	C2D-C3D-CAD	2.70	145.94	134.94
22	AB	614	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
22	AA	406	CLA	CBD-CHA-C1A	2.69	132.29	128.77
22	AB	605	CLA	C1D-CHD-C4C	2.69	126.78	122.60
22	AB	609	CLA	CBD-CHA-C1A	2.69	132.29	128.77
26	BX	101	BCR	C11-C10-C9	2.69	131.18	127.29
26	BC	514	BCR	C23-C24-C25	2.69	135.17	127.23
22	BC	502	CLA	C1-C2-C3	2.69	130.90	126.23
30	BC	519	LMG	O7-C10-C11	2.69	117.28	111.54
22	AC	512	CLA	C7-C6-C5	-2.69	105.12	112.97
22	BC	511	CLA	O2A-CGA-CBA	2.69	120.13	111.90
29	BL	101	SQD	C44-O6-C1	2.69	119.20	113.80
22	BB	604	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
22	BB	612	CLA	CBD-CHA-C1A	2.69	132.28	128.77
22	BA	404	CLA	C1-C2-C3	2.69	130.89	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	510	CLA	C7-C6-C5	-2.68	105.14	112.97
30	AA	413	LMG	O7-C10-C11	2.68	117.26	111.54
22	BB	616	CLA	C2D-C3D-CAD	2.68	145.89	134.94
22	BC	503	CLA	O2A-CGA-CBA	2.68	120.11	111.90
22	AC	502	CLA	CAA-C2A-C3A	-2.68	106.60	113.32
23	AD	403	PHO	O2A-CGA-CBA	2.68	120.11	111.90
22	AA	402	CLA	C1D-CHD-C4C	2.68	126.76	122.60
22	AD	404	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
22	AB	613	CLA	O2A-CGA-CBA	2.68	120.09	111.90
22	BB	612	CLA	C7-C6-C5	-2.68	105.16	112.97
22	AB	610	CLA	C2D-C3D-CAD	2.68	145.85	134.94
22	AC	501	CLA	CED-O2D-CGD	2.68	122.37	116.00
22	AC	503	CLA	CED-O2D-CGD	2.67	122.37	116.00
27	AA	410	DGD	O6D-C5D-C6D	2.67	111.98	106.62
22	BC	509	CLA	C2D-C3D-CAD	2.67	145.85	134.94
22	AB	602	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
22	AC	502	CLA	C2D-C3D-CAD	2.67	145.83	134.94
22	BD	404	CLA	CED-O2D-CGD	2.67	122.35	116.00
22	AB	611	CLA	O2A-CGA-CBA	2.67	120.06	111.90
22	AB	608	CLA	CBA-CAA-C2A	2.67	120.47	113.95
22	AB	610	CLA	O2A-CGA-CBA	2.66	120.06	111.90
26	BA	410	BCR	C1-C6-C5	-2.66	118.73	122.59
22	BA	405	CLA	CED-O2D-CGD	2.66	122.34	116.00
32	BB	603	LMT	C1-O1'-C1'	-2.66	109.22	113.91
32	AM	102	LMT	C1-O1'-C1'	-2.66	109.21	113.91
26	BC	515	BCR	C40-C30-C29	-2.66	98.20	108.78
26	AB	620	BCR	C1-C6-C5	-2.66	118.74	122.59
26	BX	101	BCR	C23-C24-C25	2.66	135.07	127.23
23	AD	403	PHO	C2D-C3D-CAD	2.65	145.76	134.94
22	AA	402	CLA	C2D-C3D-CAD	2.65	145.76	134.94
22	AB	601	CLA	CAA-C2A-C3A	-2.65	106.68	113.32
26	BZ	101	BCR	C8-C7-C6	2.65	135.05	127.23
22	BB	606	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
22	BB	612	CLA	C2D-C3D-CAD	2.65	145.73	134.94
22	AA	403	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
26	BC	514	BCR	C32-C1-C6	2.64	114.71	110.33
22	BB	614	CLA	C6-C5-C3	2.64	118.66	112.62
22	BC	502	CLA	C7-C6-C5	-2.64	105.25	112.97
22	BC	506	CLA	C1-C2-C3	2.64	130.81	126.23
22	BB	606	CLA	C2D-C3D-CAD	2.64	145.72	134.94
26	AC	515	BCR	C40-C30-C29	-2.64	98.28	108.78
22	BC	513	CLA	C7-C6-C5	-2.64	105.26	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BC	515	BCR	C16-C17-C18	2.64	131.11	127.29
22	AB	614	CLA	O2D-CGD-CBD	2.64	116.68	111.34
26	AC	515	BCR	C16-C17-C18	2.64	131.10	127.29
22	BC	513	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
23	BA	406	PHO	OBD-CAD-CBD	-2.64	121.95	125.94
22	BB	616	CLA	O2A-CGA-CBA	2.64	119.98	111.90
22	BC	504	CLA	C2D-C3D-CAD	2.64	145.70	134.94
22	BB	612	CLA	C6-C5-C3	2.64	118.64	112.62
27	BB	602	DGD	O6D-C5D-C6D	2.64	111.90	106.62
26	AK	102	BCR	C35-C13-C12	2.64	122.35	118.09
29	AA	412	SQD	O47-C7-C8	2.64	117.16	111.54
22	AC	506	CLA	C7-C6-C5	-2.64	105.28	112.97
22	BC	510	CLA	OBD-CAD-CBD	-2.64	121.96	125.94
22	BC	513	CLA	C1-C2-C3	2.64	130.80	126.23
22	AB	614	CLA	C2D-C3D-CAD	2.63	145.67	134.94
22	AC	509	CLA	C2D-C3D-CAD	2.63	145.67	134.94
22	AC	504	CLA	O2A-CGA-CBA	2.63	119.95	111.90
23	BD	403	PHO	C1-C2-C3	2.63	130.79	126.23
22	BB	611	CLA	CBD-CHA-C1A	2.63	132.21	128.77
22	AB	612	CLA	CED-O2D-CGD	2.63	122.26	116.00
22	BB	617	CLA	C2D-C3D-CAD	2.63	145.66	134.94
29	BA	413	SQD	C3-C4-C5	-2.63	105.45	110.17
23	AA	405	PHO	C2D-C3D-CAD	2.63	145.65	134.94
22	BC	502	CLA	C2D-C3D-CAD	2.63	145.65	134.94
22	AB	613	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
22	AC	502	CLA	O2A-CGA-CBA	2.63	119.94	111.90
22	AC	512	CLA	CED-O2D-CGD	2.63	122.25	116.00
22	AC	510	CLA	C2D-C3D-CAD	2.62	145.64	134.94
34	AV	201	HEM	C2A-C1A-NA	-2.62	106.09	109.73
22	AC	505	CLA	C2D-C3D-CAD	2.62	145.63	134.94
26	AH	101	BCR	C23-C24-C25	2.62	134.96	127.23
27	BA	411	DGD	O6D-C5D-C6D	2.62	111.87	106.62
22	BA	403	CLA	C1D-CHD-C4C	2.62	126.66	122.60
23	BD	403	PHO	C3D-C4D-ND	2.62	110.11	106.81
22	BA	407	CLA	C2D-C3D-CAD	2.62	145.61	134.94
22	BB	608	CLA	C1-C2-C3	2.62	130.77	126.23
22	AB	607	CLA	C1D-CHD-C4C	2.62	126.66	122.60
22	BB	613	CLA	CMB-C2B-C1B	-2.61	124.44	128.46
22	AD	402	CLA	CED-O2D-CGD	2.61	122.23	116.00
26	BC	515	BCR	C30-C25-C24	2.62	122.94	115.69
22	AB	613	CLA	C2D-C3D-CAD	2.61	145.59	134.94
22	BD	402	CLA	C2D-C3D-CAD	2.61	145.60	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	603	CLA	C2D-C3D-CAD	2.61	145.59	134.94
26	AZ	101	BCR	C8-C7-C6	2.61	134.94	127.23
22	AB	601	CLA	C7-C6-C5	-2.61	105.34	112.97
24	BD	405	PL9	C10-C9-C11	2.61	119.36	115.39
22	AB	613	CLA	CAA-C2A-C3A	-2.61	106.78	113.32
22	BC	504	CLA	O2A-CGA-CBA	2.61	119.89	111.90
26	AZ	101	BCR	C1-C6-C5	-2.61	118.81	122.59
22	AC	511	CLA	C7-C6-C5	-2.61	105.35	112.97
22	BC	510	CLA	C2D-C3D-CAD	2.61	145.58	134.94
22	AB	610	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
22	AC	506	CLA	O2A-CGA-CBA	2.61	119.88	111.90
26	BK	102	BCR	C30-C25-C24	2.61	122.92	115.69
29	AA	412	SQD	C32-C33-C34	2.61	124.22	113.73
22	BB	613	CLA	C2D-C3D-CAD	2.61	145.57	134.94
22	AB	605	CLA	C2D-C3D-CAD	2.60	145.56	134.94
22	BB	609	CLA	C2D-C3D-CAD	2.60	145.56	134.94
22	AB	604	CLA	CAA-C2A-C3A	-2.60	106.80	113.32
22	BD	404	CLA	OBD-CAD-CBD	-2.60	122.01	125.94
30	BM	102	LMG	O1-C1-C2	2.60	111.49	108.15
24	AD	405	PL9	C35-C34-C36	2.60	119.34	115.39
22	BB	616	CLA	C7-C6-C5	-2.60	105.37	112.97
22	AC	507	CLA	C2A-C1A-NA	-2.60	108.01	111.33
27	AH	102	DGD	O3G-C1D-C2D	2.60	111.48	108.15
22	AC	506	CLA	C2D-C3D-CAD	2.60	145.54	134.94
22	BC	503	CLA	CED-O2D-CGD	2.60	122.19	116.00
22	AC	505	CLA	C7-C6-C5	-2.60	105.38	112.97
22	BC	507	CLA	CAA-C2A-C3A	-2.60	106.81	113.32
22	AC	504	CLA	C2D-C3D-CAD	2.60	145.54	134.94
22	BB	608	CLA	C2D-C3D-CAD	2.60	145.53	134.94
26	BC	514	BCR	C40-C30-C25	2.60	114.63	110.33
22	AB	609	CLA	C2D-C3D-CAD	2.60	145.53	134.94
22	BB	605	CLA	C2D-C3D-CAD	2.59	145.52	134.94
29	BA	413	SQD	C35-C34-C33	2.59	120.36	112.94
23	BA	406	PHO	CED-O2D-CGD	2.59	122.18	116.00
22	AC	512	CLA	C2D-C3D-CAD	2.59	145.52	134.94
23	AA	405	PHO	C7-C6-C5	-2.59	105.40	112.97
27	BB	602	DGD	C3G-O3G-C1D	-2.59	108.60	113.80
22	BB	619	CLA	CBA-CAA-C2A	2.59	120.29	113.95
29	AA	412	SQD	O8-S-O7	2.59	117.45	111.69
26	AC	515	BCR	C24-C23-C22	2.59	130.09	126.22
23	BA	406	PHO	C2D-C3D-CAD	2.59	145.51	134.94
26	AB	620	BCR	C7-C8-C9	2.59	130.09	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	613	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
26	AH	101	BCR	C1-C6-C5	-2.59	118.84	122.59
23	AA	405	PHO	C4A-NA-C1A	2.59	111.83	108.42
22	BC	510	CLA	CED-O2D-CGD	2.59	122.17	116.00
26	BD	406	BCR	C23-C24-C25	2.59	134.88	127.23
22	AB	611	CLA	CAA-C2A-C3A	-2.59	106.84	113.32
22	BC	505	CLA	C2D-C3D-CAD	2.59	145.49	134.94
22	AA	404	CLA	C2D-C3D-CAD	2.59	145.49	134.94
30	AI	101	LMG	O6-C5-C6	2.59	112.79	106.34
22	BA	404	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
22	BA	404	CLA	CED-O2D-CGD	2.59	122.16	116.00
22	BC	506	CLA	C2D-C3D-CAD	2.59	145.49	134.94
32	BT	101	LMT	O1B-C1B-C2B	2.59	114.31	108.11
22	AB	616	CLA	C2D-C3D-CAD	2.59	145.49	134.94
28	BC	521	LHG	C5-O7-C7	-2.58	111.79	117.86
30	BA	414	LMG	C7-O1-C1	-2.58	108.61	113.80
26	AA	409	BCR	C37-C22-C23	2.58	122.27	118.09
22	AB	607	CLA	C2D-C3D-CAD	2.58	145.47	134.94
22	BB	605	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
28	AC	521	LHG	C5-O7-C7	-2.58	111.79	117.86
29	BF	101	SQD	C45-O47-C7	2.58	123.92	117.86
26	AB	620	BCR	C23-C24-C25	2.58	134.84	127.23
22	AC	501	CLA	C2D-C3D-CAD	2.58	145.46	134.94
26	AH	101	BCR	C35-C13-C12	2.58	122.25	118.09
22	BB	607	CLA	C2D-C3D-CAD	2.58	145.45	134.94
24	AJ	101	PL9	C17-C18-C19	-2.58	122.24	127.81
22	BB	604	CLA	C2D-C3D-CAD	2.58	145.44	134.94
22	AB	605	CLA	C7-C6-C5	-2.57	105.46	112.97
22	AC	502	CLA	C7-C6-C5	-2.57	105.46	112.97
22	AB	615	CLA	C2D-C3D-CAD	2.57	145.42	134.94
22	AC	508	CLA	CED-O2D-CGD	2.57	122.12	116.00
22	BB	619	CLA	C2D-C3D-CAD	2.57	145.42	134.94
22	BA	403	CLA	C2D-C3D-CAD	2.57	145.42	134.94
23	BA	406	PHO	C4A-NA-C1A	2.57	111.80	108.42
26	BA	410	BCR	C30-C25-C24	2.57	122.80	115.69
22	BB	604	CLA	C7-C6-C5	-2.57	105.48	112.97
29	AF	101	SQD	C45-O47-C7	2.57	123.88	117.86
26	AB	617	BCR	C35-C13-C12	2.56	122.23	118.09
22	BC	502	CLA	O2A-CGA-CBA	2.56	119.75	111.90
22	BC	509	CLA	C2A-C3A-C4A	2.56	106.04	101.89
22	BB	613	CLA	O2D-CGD-CBD	2.56	116.52	111.34
23	BA	406	PHO	C6-C5-C3	2.56	118.46	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	508	CLA	C7-C6-C5	-2.56	105.50	112.97
26	AC	515	BCR	C30-C25-C24	2.56	122.78	115.69
22	AB	616	CLA	C2A-C3A-C4A	2.56	106.03	101.89
26	BZ	101	BCR	C1-C6-C5	-2.56	118.89	122.59
22	BB	611	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
22	BD	402	CLA	C7-C6-C5	-2.56	105.51	112.97
24	AD	405	PL9	C10-C9-C11	2.56	119.27	115.39
22	AB	606	CLA	C2D-C3D-CAD	2.56	145.36	134.94
28	BA	412	LHG	O7-C7-C8	2.55	116.98	111.54
22	BA	405	CLA	CAA-CBA-CGA	2.55	120.77	113.24
26	AJ	102	BCR	C20-C21-C22	-2.55	123.60	127.29
24	BJ	101	PL9	C12-C13-C14	-2.55	122.29	127.81
22	BC	506	CLA	O2A-CGA-CBA	2.55	119.70	111.90
29	BA	413	SQD	O8-S-O9	-2.55	106.02	111.69
30	AB	622	LMG	O6-C5-C6	2.55	112.69	106.34
22	BA	404	CLA	C2A-C3A-C4A	2.55	106.01	101.89
26	AT	102	BCR	C23-C22-C21	-2.55	115.06	118.98
22	BB	619	CLA	C1D-CHD-C4C	2.55	126.55	122.60
22	BB	617	CLA	CAA-C2A-C3A	-2.54	106.95	113.32
22	AB	603	CLA	C6-C5-C3	2.54	118.43	112.62
22	AC	508	CLA	C2D-C3D-CAD	2.55	145.32	134.94
26	BZ	101	BCR	C30-C25-C26	-2.54	118.91	122.59
22	BC	512	CLA	OBD-CAD-CBD	-2.54	122.10	125.94
22	BC	504	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
22	BC	501	CLA	C2D-C3D-CAD	2.54	145.30	134.94
26	AZ	101	BCR	C35-C13-C12	2.54	122.19	118.09
26	AZ	101	BCR	C19-C18-C17	-2.54	115.07	118.98
22	AB	603	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
34	AV	201	HEM	O2A-CGA-CBA	2.54	122.97	114.19
22	AC	510	CLA	OBD-CAD-CBD	-2.54	122.11	125.94
22	AC	501	CLA	C7-C6-C5	-2.54	105.56	112.97
26	AC	514	BCR	C7-C8-C9	2.53	130.01	126.22
22	AC	513	CLA	C2D-C3D-CAD	2.54	145.28	134.94
24	BD	405	PL9	C22-C23-C24	-2.53	122.33	127.81
26	AJ	102	BCR	C15-C16-C17	-2.53	117.87	123.45
22	BC	512	CLA	C2D-C3D-CAD	2.53	145.27	134.94
22	BA	404	CLA	C2D-C3D-CAD	2.53	145.27	134.94
22	BB	610	CLA	C2D-C3D-CAD	2.53	145.27	134.94
28	AA	411	LHG	O7-C7-C8	2.53	116.93	111.54
24	AD	405	PL9	C22-C23-C24	-2.53	122.33	127.81
22	BC	508	CLA	C2D-C3D-CAD	2.53	145.25	134.94
22	AB	601	CLA	C2D-C3D-CAD	2.53	145.25	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AD	404	CLA	C2D-C3D-CAD	2.53	145.25	134.94
26	AB	618	BCR	C23-C22-C21	-2.53	115.08	118.98
26	AK	102	BCR	C32-C1-C2	-2.53	98.74	108.78
26	AC	514	BCR	C12-C13-C14	-2.53	115.09	118.98
22	AC	511	CLA	C2D-C3D-CAD	2.53	145.25	134.94
22	AB	608	CLA	C6-C7-C8	2.52	123.29	115.44
22	AD	402	CLA	C1-C2-C3	2.52	130.61	126.23
22	AB	604	CLA	C2D-C3D-CAD	2.52	145.22	134.94
29	BB	601	SQD	O47-C7-C8	2.52	116.92	111.54
22	BC	505	CLA	C7-C6-C5	-2.52	105.61	112.97
29	BB	601	SQD	C44-O6-C1	2.52	118.86	113.80
22	AB	602	CLA	OBD-CAD-CBD	-2.52	122.14	125.94
22	BB	617	CLA	CMB-C2B-C1B	-2.52	124.60	128.46
26	AZ	101	BCR	C30-C25-C26	-2.52	118.94	122.59
22	BC	507	CLA	C2A-C1A-NA	-2.52	108.11	111.33
22	BB	616	CLA	C2A-C3A-C4A	2.52	105.96	101.89
22	BB	619	CLA	C6-C5-C3	2.52	118.36	112.62
22	AB	601	CLA	C1D-CHD-C4C	2.51	126.50	122.60
26	BZ	101	BCR	C12-C13-C14	-2.51	115.11	118.98
22	BB	608	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
22	BA	405	CLA	C2D-C3D-CAD	2.51	145.18	134.94
22	AC	513	CLA	C7-C6-C5	-2.51	105.64	112.97
22	AB	602	CLA	C2D-C3D-CAD	2.51	145.18	134.94
22	BC	503	CLA	C2D-C3D-CAD	2.51	145.18	134.94
22	BD	404	CLA	C2D-C3D-CAD	2.51	145.18	134.94
29	BA	413	SQD	O8-S-O7	2.51	117.27	111.69
29	BA	413	SQD	C44-O6-C1	2.51	118.84	113.80
26	AJ	102	BCR	C16-C17-C18	2.51	130.91	127.29
26	BB	622	BCR	C23-C24-C25	2.51	134.64	127.23
22	BC	501	CLA	CBA-CAA-C2A	2.51	120.08	113.95
22	AC	513	CLA	CBA-CAA-C2A	2.51	120.08	113.95
30	BB	624	LMG	O6-C5-C6	2.51	112.58	106.34
22	AA	404	CLA	CAA-CBA-CGA	2.50	120.62	113.24
22	AC	512	CLA	C4D-CHA-CBD	-2.50	103.57	109.45
22	AB	612	CLA	CAA-C2A-C3A	-2.50	107.05	113.32
27	BD	410	DGD	O6D-C5D-C6D	2.50	111.63	106.62
22	AB	616	CLA	C1D-CHD-C4C	2.50	126.48	122.60
22	AC	511	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
22	AA	403	CLA	C1D-CHD-C4C	2.50	126.47	122.60
22	AB	606	CLA	CED-O2D-CGD	2.50	121.95	116.00
22	BC	508	CLA	C7-C6-C5	-2.50	105.68	112.97
26	AB	618	BCR	C8-C9-C10	-2.50	115.13	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	503	CLA	C2D-C3D-CAD	2.50	145.12	134.94
26	AC	514	BCR	C23-C22-C21	-2.50	115.14	118.98
30	AA	413	LMG	C7-O1-C1	-2.50	108.79	113.80
26	AD	406	BCR	C15-C14-C13	2.50	130.90	127.29
22	BC	511	CLA	C2D-C3D-CAD	2.50	145.12	134.94
22	BB	606	CLA	C6-C5-C3	2.49	118.31	112.62
26	BA	410	BCR	C8-C9-C10	-2.49	115.14	118.98
30	BC	520	LMG	O8-C28-C29	2.49	119.53	111.90
22	AC	507	CLA	C2D-C3D-CAD	2.49	145.11	134.94
26	AJ	102	BCR	C3-C4-C5	2.49	117.91	113.81
22	AA	403	CLA	C2D-C3D-CAD	2.49	145.10	134.94
32	AB	627	LMT	C1-O1'-C1'	-2.49	109.52	113.91
26	AA	409	BCR	C16-C17-C18	2.49	130.89	127.29
26	BC	515	BCR	C24-C23-C22	2.49	129.94	126.22
22	AA	403	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
22	AB	606	CLA	C7-C6-C5	-2.49	105.71	112.97
34	BV	201	HEM	O2A-CGA-CBA	2.49	122.78	114.19
22	BB	607	CLA	CAA-C2A-C3A	-2.49	107.09	113.32
29	AD	409	SQD	C3-C4-C5	-2.48	105.71	110.17
26	AB	618	BCR	C7-C8-C9	2.48	129.93	126.22
22	BC	513	CLA	C2D-C3D-CAD	2.48	145.06	134.94
22	AC	505	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
22	AC	508	CLA	C4D-CHA-CBD	-2.48	103.62	109.45
22	BB	604	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
22	AA	403	CLA	CED-O2D-CGD	2.48	121.90	116.00
29	AA	412	SQD	C35-C34-C33	2.48	120.02	112.94
22	BC	507	CLA	C2D-C3D-CAD	2.48	145.04	134.94
22	AC	503	CLA	C7-C6-C5	-2.47	105.75	112.97
26	BC	514	BCR	C12-C13-C14	-2.47	115.17	118.98
22	BB	609	CLA	C1D-C2D-C3D	-2.47	104.55	106.97
32	BD	411	LMT	C1B-O1B-C4'	-2.47	111.73	118.00
32	BB	603	LMT	O1B-C1B-C2B	2.47	114.02	108.11
26	BJ	102	BCR	C20-C21-C22	-2.47	123.72	127.29
22	AC	507	CLA	C2A-C1A-CHA	2.47	128.37	123.87
26	BD	406	BCR	C15-C14-C13	2.47	130.85	127.29
22	AA	403	CLA	O2D-CGD-CBD	2.46	116.32	111.34
22	BC	503	CLA	C7-C6-C5	-2.47	105.77	112.97
22	AC	513	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
29	BA	413	SQD	O47-C7-C8	2.46	116.79	111.54
26	AH	101	BCR	C1-C6-C7	2.46	122.52	115.69
22	BC	512	CLA	C4D-CHA-CBD	-2.46	103.67	109.45
22	AC	509	CLA	C2A-C3A-C4A	2.46	105.88	101.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AV	201	HEM	C4A-C3A-C2A	2.46	108.71	107.00
22	BC	507	CLA	C2A-C1A-CHA	2.46	128.36	123.87
26	AC	515	BCR	C35-C13-C12	2.46	122.07	118.09
29	AA	415	SQD	C45-O47-C7	2.46	123.64	117.86
22	BC	511	CLA	C1-C2-C3	2.46	130.50	126.23
22	BB	618	CLA	C2D-C3D-CAD	2.46	144.96	134.94
34	AE	101	HEM	O2A-CGA-CBA	2.46	122.69	114.19
27	AD	410	DGD	O6D-C5D-C4D	2.46	114.30	109.73
26	BC	514	BCR	C1-C6-C7	2.46	122.50	115.69
22	AB	616	CLA	CBA-CAA-C2A	2.46	119.95	113.95
30	AA	416	LMG	O6-C5-C6	2.46	112.46	106.34
22	BB	615	CLA	CAA-C2A-C3A	-2.45	107.18	113.32
30	BB	623	LMG	C9-C8-C7	-2.45	106.23	111.86
26	AD	406	BCR	C35-C13-C12	2.45	122.05	118.09
22	BB	607	CLA	C4D-CHA-CBD	-2.45	103.70	109.45
22	AB	612	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
22	AC	504	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
26	BJ	102	BCR	C8-C9-C10	-2.45	115.21	118.98
27	AD	410	DGD	C2G-O2G-C1B	2.45	123.60	117.86
27	AD	410	DGD	O6D-C5D-C6D	2.45	111.52	106.62
26	AJ	102	BCR	C28-C27-C26	2.45	117.83	113.81
22	BB	608	CLA	C7-C6-C5	-2.44	105.84	112.97
30	AC	519	LMG	O1-C1-C2	2.44	111.28	108.15
22	BC	510	CLA	C2A-C3A-C4A	2.44	105.85	101.89
24	AJ	101	PL9	C12-C13-C14	-2.44	122.52	127.81
22	BB	607	CLA	C2A-C3A-C4A	2.44	105.84	101.89
22	AB	604	CLA	C7-C6-C5	-2.44	105.85	112.97
22	AC	507	CLA	CAA-C2A-C3A	-2.44	107.21	113.32
34	BE	101	HEM	O2A-CGA-CBA	2.44	122.61	114.19
22	BB	609	CLA	C7-C6-C5	-2.44	105.86	112.97
22	AD	404	CLA	C2A-C3A-C4A	2.43	105.83	101.89
22	BB	613	CLA	C2A-C3A-C4A	2.43	105.83	101.89
30	BC	520	LMG	C7-O1-C1	-2.43	108.92	113.80
26	AB	617	BCR	C12-C13-C14	-2.43	115.23	118.98
22	BC	511	CLA	C4D-CHA-CBD	-2.43	103.74	109.45
22	BB	619	CLA	C1D-C2D-C3D	-2.43	104.59	106.97
26	AZ	101	BCR	C12-C13-C14	-2.43	115.24	118.98
22	BB	612	CLA	C1-C2-C3	2.43	130.44	126.23
22	BB	604	CLA	C1D-CHD-C4C	2.43	126.36	122.60
34	AV	201	HEM	C3A-C4A-NA	-2.42	107.88	109.50
32	AT	101	LMT	O1B-C4'-C3'	2.42	113.31	107.17
22	AD	404	CLA	O2D-CGD-CBD	2.42	116.23	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	505	CLA	C6-C5-C3	2.42	118.14	112.62
30	AM	101	LMG	O8-C9-C8	-2.42	102.44	108.80
22	AC	506	CLA	C6-C5-C3	2.42	118.14	112.62
26	AA	409	BCR	C30-C25-C24	2.42	122.39	115.69
22	AA	404	CLA	O2A-CGA-CBA	2.42	119.29	111.90
22	BA	403	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
22	BA	407	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
24	BD	405	PL9	C32-C33-C34	-2.41	122.59	127.81
22	AA	402	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
22	AC	508	CLA	O2D-CGD-CBD	2.41	116.22	111.34
26	BC	514	BCR	C23-C22-C21	-2.41	115.26	118.98
22	AB	604	CLA	C4D-CHA-CBD	-2.41	103.78	109.45
22	BB	609	CLA	CED-O2D-CGD	2.41	121.74	116.00
22	AB	604	CLA	C1-C2-C3	2.41	130.41	126.23
22	BC	512	CLA	CED-O2D-CGD	2.41	121.74	116.00
26	BZ	101	BCR	C36-C18-C19	2.41	121.98	118.09
26	BK	102	BCR	C32-C1-C2	-2.41	99.20	108.78
22	BC	511	CLA	C2A-C1A-CHA	2.41	128.26	123.87
26	BB	621	BCR	C32-C1-C6	2.41	114.31	110.33
30	AE	102	LMG	O7-C8-C7	2.41	117.42	108.50
26	AB	618	BCR	C30-C25-C24	2.41	122.36	115.69
22	BB	612	CLA	O2A-CGA-CBA	2.40	119.25	111.90
22	AC	501	CLA	CBA-CAA-C2A	2.40	119.83	113.95
22	BC	508	CLA	C4D-CHA-CBD	-2.40	103.81	109.45
22	BC	513	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
30	AC	520	LMG	O8-C28-C29	2.40	119.24	111.90
27	AB	626	DGD	C3G-O3G-C1D	-2.40	108.98	113.80
29	BA	413	SQD	C15-C14-C13	2.40	127.30	114.56
22	AB	608	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
22	AB	608	CLA	C7-C6-C5	-2.40	105.97	112.97
29	BB	601	SQD	C3-C4-C5	-2.40	105.86	110.17
26	BB	620	BCR	C35-C13-C12	2.40	121.96	118.09
26	BC	514	BCR	C37-C22-C23	2.40	121.96	118.09
22	AC	511	CLA	C4D-CHA-CBD	-2.40	103.82	109.45
22	BA	405	CLA	O2A-CGA-CBA	2.40	119.23	111.90
22	AB	601	CLA	CMB-C2B-C1B	-2.40	124.78	128.46
22	BB	616	CLA	CAA-C2A-C3A	-2.40	107.32	113.32
22	BA	403	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
24	AJ	101	PL9	C15-C14-C16	2.39	119.02	115.39
22	BA	403	CLA	C7-C6-C5	-2.39	105.98	112.97
22	AB	609	CLA	O2A-CGA-CBA	2.39	119.22	111.90
26	AC	514	BCR	C1-C6-C7	2.39	122.31	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	507	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
22	BB	616	CLA	CED-O2D-CGD	2.39	121.69	116.00
22	BB	615	CLA	CBA-CAA-C2A	2.38	119.78	113.95
26	AT	102	BCR	C7-C8-C9	2.38	129.78	126.22
22	BB	616	CLA	C6-C5-C3	2.39	118.06	112.62
22	AC	511	CLA	C2A-C1A-CHA	2.38	128.22	123.87
22	BB	608	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
26	BB	620	BCR	C12-C13-C14	-2.38	115.31	118.98
29	BL	101	SQD	O47-C7-C8	2.38	116.62	111.54
22	AC	509	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
22	AA	404	CLA	C2A-C3A-C4A	2.38	105.75	101.89
22	AB	614	CLA	CBA-CAA-C2A	2.38	119.76	113.95
27	AB	626	DGD	O6D-C5D-C6D	2.38	111.38	106.62
27	AC	517	DGD	O6D-C5D-C6D	2.38	111.38	106.62
26	BJ	102	BCR	C31-C1-C2	2.38	118.23	108.78
22	BD	404	CLA	C2A-C3A-C4A	2.38	105.74	101.89
26	AB	618	BCR	C11-C10-C9	2.38	130.72	127.29
22	AB	614	CLA	C16-C15-C13	2.38	122.83	115.44
22	BB	611	CLA	C6-C7-C8	2.38	122.83	115.44
29	AA	415	SQD	C36-C35-C34	2.38	127.18	114.56
22	AD	402	CLA	C7-C6-C5	-2.37	106.04	112.97
22	AB	615	CLA	C2A-C3A-C4A	2.37	105.73	101.89
24	AA	407	PL9	C32-C33-C34	-2.37	122.68	127.81
22	AA	402	CLA	C7-C6-C5	-2.37	106.04	112.97
26	BX	101	BCR	C1-C6-C7	2.37	122.26	115.69
23	AD	403	PHO	C4A-NA-C1A	2.37	111.54	108.42
29	AA	412	SQD	C15-C14-C13	2.37	127.14	114.56
24	BA	408	PL9	C32-C33-C34	-2.37	122.69	127.81
26	BC	514	BCR	C30-C25-C24	2.37	122.25	115.69
26	AJ	102	BCR	C31-C1-C2	2.37	118.20	108.78
26	AB	618	BCR	C36-C18-C19	2.37	121.91	118.09
22	BB	619	CLA	C4D-CHA-CBD	-2.37	103.89	109.45
29	AD	409	SQD	O8-S-O7	2.36	116.95	111.69
22	BB	610	CLA	C4D-CHA-CBD	-2.36	103.90	109.45
22	BB	619	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
22	AB	601	CLA	C4D-CHA-CBD	-2.36	103.90	109.45
22	AB	612	CLA	O2D-CGD-CBD	2.36	116.11	111.34
22	AB	613	CLA	C2A-C3A-C4A	2.36	105.71	101.89
26	BJ	102	BCR	C15-C16-C17	-2.36	118.25	123.45
26	AB	619	BCR	C32-C1-C6	2.36	114.24	110.33
30	BM	102	LMG	O8-C9-C8	-2.36	102.59	108.80
26	AB	618	BCR	C32-C1-C6	2.36	114.23	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	609	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
26	BC	515	BCR	C37-C22-C23	2.36	121.90	118.09
22	BC	512	CLA	O2D-CGD-CBD	2.35	116.10	111.34
22	BB	618	CLA	C4D-CHA-CBD	-2.35	103.92	109.45
27	BD	410	DGD	C2G-O2G-C1B	2.35	123.38	117.86
22	AC	508	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
22	BC	505	CLA	C2A-C1A-CHA	2.35	128.16	123.87
22	AC	507	CLA	C6-C5-C3	2.35	117.99	112.62
22	AC	511	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
26	BD	406	BCR	C35-C13-C12	2.35	121.89	118.09
22	AB	613	CLA	CED-O2D-CGD	2.35	121.59	116.00
22	BC	512	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
22	BA	404	CLA	O2D-CGD-CBD	2.35	116.08	111.34
22	BC	505	CLA	C6-C5-C3	2.35	117.98	112.62
27	BH	101	DGD	O3G-C1D-C2D	2.35	111.16	108.15
22	BC	507	CLA	C4D-CHA-CBD	-2.35	103.93	109.45
22	AB	616	CLA	C4D-CHA-CBD	-2.35	103.93	109.45
22	AB	616	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
24	AD	405	PL9	C32-C33-C34	-2.35	122.73	127.81
26	BZ	101	BCR	C19-C18-C17	-2.35	115.36	118.98
26	BB	620	BCR	C16-C17-C18	2.35	130.68	127.29
26	BK	102	BCR	C37-C22-C23	2.35	121.88	118.09
22	AC	505	CLA	C2A-C3A-C4A	2.35	105.69	101.89
22	BC	511	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
22	AC	507	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
26	AZ	101	BCR	C36-C18-C19	2.34	121.88	118.09
22	BC	505	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
22	AB	609	CLA	C1D-C2D-C3D	-2.34	104.68	106.97
23	BA	406	PHO	C1D-C2D-C3D	-2.34	104.84	107.12
26	AT	102	BCR	C40-C30-C29	-2.34	99.47	108.78
22	AB	610	CLA	CED-O2D-CGD	2.34	121.58	116.00
22	BD	402	CLA	C2A-C1A-CHA	2.34	128.14	123.87
26	BC	514	BCR	C7-C8-C9	2.34	129.72	126.22
26	AH	101	BCR	C23-C22-C21	-2.34	115.38	118.98
26	BJ	102	BCR	C28-C27-C26	2.34	117.66	113.81
22	AB	613	CLA	C6-C5-C3	2.34	117.95	112.62
22	AB	615	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
29	BD	409	SQD	O8-S-O7	2.34	116.88	111.69
23	AA	405	PHO	O2A-CGA-CBA	2.34	119.05	111.90
22	AC	504	CLA	C1D-C2D-C3D	-2.34	104.68	106.97
22	BC	502	CLA	C4D-CHA-CBD	-2.34	103.97	109.45
30	AM	101	LMG	C7-O1-C1	-2.33	109.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	405	PHO	O2D-CGD-CBD	2.33	116.06	111.34
22	BA	405	CLA	C2A-C3A-C4A	2.33	105.67	101.89
22	AC	507	CLA	C4D-CHA-CBD	-2.33	103.97	109.45
22	AD	404	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
30	AB	621	LMG	C9-C8-C7	-2.33	106.51	111.86
22	BC	511	CLA	CMB-C2B-C1B	-2.33	124.88	128.46
22	AC	509	CLA	C7-C6-C5	-2.33	106.17	112.97
22	BA	405	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
29	AA	415	SQD	C34-C33-C32	2.33	126.93	114.56
26	AA	409	BCR	C35-C13-C12	2.33	121.85	118.09
22	AC	504	CLA	C7-C6-C5	-2.33	106.17	112.97
26	AB	620	BCR	C8-C7-C6	2.33	134.10	127.23
26	AK	102	BCR	C37-C22-C23	2.32	121.84	118.09
29	BL	101	SQD	C3-C4-C5	-2.32	106.00	110.17
22	BC	511	CLA	CAA-C2A-C3A	-2.32	107.50	113.32
22	BC	512	CLA	C2A-C1A-CHA	2.32	128.10	123.87
29	BA	401	SQD	C36-C35-C34	2.32	126.90	114.56
26	BA	410	BCR	C16-C17-C18	2.32	130.64	127.29
22	AC	506	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
22	AC	513	CLA	C6-C5-C3	2.32	117.92	112.62
22	BD	402	CLA	CMB-C2B-C3B	2.32	129.54	125.16
22	AC	510	CLA	CAA-C2A-C3A	-2.32	107.51	113.32
22	BC	504	CLA	C7-C6-C5	-2.32	106.20	112.97
26	AT	102	BCR	C36-C18-C19	2.32	121.84	118.09
34	AV	201	HEM	C4C-NC-C1C	2.32	107.87	105.51
22	BC	509	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
26	AB	618	BCR	C12-C13-C14	-2.31	115.42	118.98
26	AZ	101	BCR	C1-C6-C7	2.31	122.09	115.69
22	BB	616	CLA	C1D-C2D-C3D	-2.31	104.71	106.97
22	BB	617	CLA	C16-C15-C13	2.31	122.62	115.44
22	BB	613	CLA	C7-C6-C5	-2.31	106.23	112.97
26	AT	102	BCR	C11-C10-C9	2.31	130.62	127.29
22	BB	616	CLA	C1-C2-C3	2.31	130.23	126.23
22	AB	614	CLA	C1D-C2D-C3D	-2.30	104.71	106.97
22	AB	602	CLA	C1-C2-C3	2.30	130.23	126.23
22	AB	607	CLA	C4D-CHA-CBD	-2.31	104.04	109.45
30	BC	519	LMG	O1-C1-C2	2.30	111.10	108.15
26	BX	101	BCR	C23-C22-C21	-2.30	115.44	118.98
22	BB	604	CLA	C4D-CHA-CBD	-2.30	104.06	109.45
26	AC	514	BCR	C37-C22-C23	2.30	121.80	118.09
22	BB	613	CLA	CED-O2D-CGD	2.30	121.47	116.00
22	BB	615	CLA	C1-C2-C3	2.29	130.21	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	506	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
26	BA	410	BCR	C34-C9-C8	2.29	121.79	118.09
22	BB	607	CLA	C7-C6-C5	-2.29	106.29	112.97
22	BB	611	CLA	C7-C6-C5	-2.29	106.29	112.97
22	AA	404	CLA	C1-C2-C3	2.28	130.19	126.23
26	AT	102	BCR	C8-C9-C10	-2.28	115.46	118.98
22	AB	606	CLA	C4D-CHA-CBD	-2.28	104.09	109.45
32	BT	101	LMT	O1B-C4'-C3'	2.28	112.96	107.17
27	AC	516	DGD	O3G-C1D-C2D	2.28	111.08	108.15
22	AD	402	CLA	C2A-C1A-CHA	2.28	128.03	123.87
22	AC	502	CLA	CMB-C2B-C1B	-2.28	124.95	128.46
22	AA	404	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
26	BX	101	BCR	C36-C18-C19	2.28	121.78	118.09
26	BB	622	BCR	C30-C25-C24	2.28	122.01	115.69
22	BC	501	CLA	O2D-CGD-CBD	2.28	115.95	111.34
26	AC	515	BCR	C12-C13-C14	-2.28	115.47	118.98
30	AE	102	LMG	C9-C8-C7	-2.28	106.63	111.86
22	BB	604	CLA	C6-C5-C3	2.28	117.82	112.62
27	BC	517	DGD	O6D-C5D-C6D	2.28	111.18	106.62
22	AB	610	CLA	O2D-CGD-CBD	2.28	115.94	111.34
22	BC	507	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
22	BC	506	CLA	C1D-C2D-C3D	-2.28	104.74	106.97
22	AB	611	CLA	C2A-C3A-C4A	2.27	105.57	101.89
22	AB	606	CLA	C1D-C2D-C3D	-2.27	104.75	106.97
27	AA	410	DGD	C3G-C2G-C1G	-2.27	106.64	111.86
22	AC	505	CLA	C4D-CHA-CBD	-2.27	104.11	109.45
24	BJ	101	PL9	C15-C14-C16	2.27	118.84	115.39
22	BC	502	CLA	C2A-C3A-C4A	2.27	105.57	101.89
26	AT	102	BCR	C35-C13-C12	2.27	121.76	118.09
22	BB	618	CLA	C2A-C3A-C4A	2.27	105.57	101.89
22	AC	509	CLA	CAA-C2A-C3A	-2.27	107.64	113.32
22	AA	402	CLA	C16-C15-C13	2.27	122.50	115.44
22	BA	405	CLA	C1-C2-C3	2.27	130.16	126.23
22	AB	610	CLA	C7-C6-C5	-2.27	106.34	112.97
29	AA	415	SQD	O8-S-O7	2.27	116.73	111.69
30	BE	102	LMG	C8-O7-C10	2.27	123.18	117.86
26	BX	101	BCR	C37-C22-C23	2.27	121.75	118.09
22	AB	612	CLA	C2A-C3A-C4A	2.26	105.56	101.89
32	AB	627	LMT	O1B-C1B-C2B	2.26	113.53	108.11
26	BK	102	BCR	C23-C22-C21	-2.26	115.49	118.98
22	AB	609	CLA	C1-C2-C3	2.26	130.15	126.23
22	AB	608	CLA	C2A-C3A-C4A	2.26	105.55	101.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AT	102	BCR	C30-C25-C24	2.26	121.96	115.69
22	BC	512	CLA	C1D-C2D-C3D	-2.26	104.76	106.97
22	AB	605	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
26	AC	514	BCR	C30-C25-C24	2.26	121.95	115.69
23	AA	405	PHO	C1D-C2D-C3D	-2.26	104.92	107.12
22	AC	505	CLA	C2A-C1A-CHA	2.26	127.99	123.87
29	BA	401	SQD	C15-C14-C13	2.26	126.55	114.56
27	BD	410	DGD	O6D-C5D-C4D	2.26	113.93	109.73
26	AB	618	BCR	C20-C21-C22	2.26	130.55	127.29
22	AC	506	CLA	C4D-CHA-CBD	-2.26	104.15	109.45
22	BC	506	CLA	C4D-CHA-CBD	-2.25	104.16	109.45
22	AB	615	CLA	C4D-CHA-CBD	-2.26	104.15	109.45
22	BC	513	CLA	C6-C5-C3	2.25	117.77	112.62
22	BB	617	CLA	CBA-CAA-C2A	2.25	119.46	113.95
22	BC	502	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
22	BB	618	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
22	AB	604	CLA	C2A-C3A-C4A	2.25	105.53	101.89
29	BB	601	SQD	C15-C14-C13	2.25	126.52	114.56
22	BC	507	CLA	C6-C5-C3	2.25	117.76	112.62
26	AB	618	BCR	C40-C30-C29	-2.25	99.85	108.78
22	AB	610	CLA	C2A-C3A-C4A	2.25	105.53	101.89
22	BB	617	CLA	C4D-CHA-CBD	-2.25	104.17	109.45
34	BV	201	HEM	C1B-NB-C4B	2.25	107.44	105.11
26	AB	618	BCR	C37-C22-C23	2.25	121.72	118.09
26	AT	102	BCR	C12-C13-C14	-2.25	115.52	118.98
26	BB	622	BCR	C8-C7-C6	2.25	133.86	127.23
22	AB	610	CLA	C4D-CHA-CBD	-2.25	104.18	109.45
22	BB	616	CLA	C4D-CHA-CBD	-2.24	104.18	109.45
22	AB	609	CLA	C2A-C3A-C4A	2.24	105.52	101.89
23	BA	406	PHO	O2A-CGA-CBA	2.24	118.76	111.90
23	BD	403	PHO	C2A-C1A-NA	-2.24	108.47	111.93
22	BA	407	CLA	C6-C5-C3	2.24	117.73	112.62
29	BA	401	SQD	O5-C5-C4	2.24	113.90	109.73
22	AC	503	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
22	AC	512	CLA	C2A-C3A-C4A	2.24	105.51	101.89
26	BZ	101	BCR	C1-C6-C7	2.24	121.89	115.69
26	BB	622	BCR	C1-C6-C7	2.24	121.89	115.69
22	AB	606	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
22	AC	511	CLA	CAA-C2A-C3A	-2.23	107.72	113.32
22	AC	501	CLA	O2D-CGD-CBD	2.23	115.85	111.34
22	BB	614	CLA	C1D-C2D-C3D	-2.23	104.78	106.97
22	BB	615	CLA	C2A-C3A-C4A	2.23	105.50	101.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AH	101	BCR	C37-C22-C23	2.23	121.69	118.09
22	BC	505	CLA	C4D-CHA-CBD	-2.23	104.21	109.45
34	BV	201	HEM	C3A-C4A-NA	-2.23	108.01	109.50
22	AB	611	CLA	C1D-C2D-C3D	-2.23	104.79	106.97
27	BH	101	DGD	C3G-O3G-C1D	-2.23	109.33	113.80
22	BC	508	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
22	BC	506	CLA	C6-C5-C3	2.23	117.70	112.62
29	AA	415	SQD	C15-C14-C13	2.23	126.39	114.56
26	AT	102	BCR	C19-C18-C17	-2.23	115.55	118.98
22	BD	402	CLA	C1-C2-C3	2.23	130.09	126.23
22	BB	611	CLA	C2A-C3A-C4A	2.23	105.49	101.89
22	AB	606	CLA	C2A-C3A-C4A	2.22	105.49	101.89
26	AB	619	BCR	C1-C6-C7	2.22	121.86	115.69
22	BD	402	CLA	C4D-CHA-CBD	-2.22	104.23	109.45
22	AB	615	CLA	C1D-C2D-C3D	-2.22	104.79	106.97
26	BA	410	BCR	C23-C22-C21	-2.22	115.56	118.98
22	AB	605	CLA	C4D-CHA-CBD	-2.22	104.23	109.45
26	AB	618	BCR	C35-C13-C12	2.22	121.68	118.09
22	AC	512	CLA	C2A-C1A-CHA	2.22	127.92	123.87
26	AA	409	BCR	C1-C6-C7	2.22	121.84	115.69
22	BD	402	CLA	C6-C5-C3	2.22	117.69	112.62
23	AD	403	PHO	O2D-CGD-CBD	2.22	115.82	111.34
26	AB	617	BCR	C36-C18-C19	2.22	121.67	118.09
22	AC	503	CLA	C4D-CHA-CBD	-2.22	104.24	109.45
22	BB	606	CLA	C4D-CHA-CBD	-2.22	104.24	109.45
26	AB	620	BCR	C32-C1-C6	2.22	114.00	110.33
34	BE	101	HEM	C1B-NB-C4B	2.22	107.41	105.11
30	BE	102	LMG	O7-C8-C7	2.22	116.70	108.50
22	BB	607	CLA	CED-O2D-CGD	2.21	121.27	116.00
22	AB	610	CLA	C16-C15-C13	2.21	122.33	115.44
22	BC	505	CLA	C2A-C3A-C4A	2.21	105.47	101.89
26	BC	515	BCR	C35-C13-C12	2.21	121.67	118.09
22	AB	613	CLA	C4D-CHA-CBD	-2.21	104.26	109.45
22	BA	407	CLA	C1D-C2D-C3D	-2.21	104.81	106.97
22	BD	402	CLA	C2A-C1A-NA	-2.21	108.51	111.33
29	BA	401	SQD	C34-C33-C32	2.21	126.30	114.56
22	AB	612	CLA	CBA-CAA-C2A	2.21	119.35	113.95
22	AB	614	CLA	C4D-CHA-CBD	-2.21	104.27	109.45
26	BZ	101	BCR	C28-C27-C26	2.20	117.44	113.81
22	BB	614	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
26	BK	102	BCR	C8-C7-C6	2.20	133.74	127.23
34	AE	101	HEM	C1B-NB-C4B	2.21	107.40	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	513	CLA	CBA-CAA-C2A	2.20	119.34	113.95
22	BB	609	CLA	C4D-CHA-CBD	-2.20	104.28	109.45
22	BC	503	CLA	C4D-CHA-CBD	-2.20	104.28	109.45
26	BA	410	BCR	C35-C13-C12	2.20	121.65	118.09
30	BI	101	LMG	O6-C1-C2	2.20	114.81	110.30
24	AJ	101	PL9	C10-C9-C8	-2.20	119.14	123.52
26	BB	622	BCR	C32-C1-C6	2.20	113.97	110.33
26	AK	102	BCR	C8-C7-C6	2.20	133.72	127.23
22	BB	607	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
26	BK	102	BCR	C19-C18-C17	-2.20	115.59	118.98
22	BB	615	CLA	O2D-CGD-CBD	2.20	115.78	111.34
22	BB	613	CLA	C4B-NB-C1B	2.20	109.23	107.12
26	BC	515	BCR	C12-C13-C14	-2.20	115.59	118.98
22	BB	611	CLA	C1-C2-C3	2.20	130.04	126.23
22	AB	609	CLA	C4D-CHA-CBD	-2.19	104.30	109.45
22	BC	513	CLA	C4D-CHA-CBD	-2.20	104.29	109.45
22	BC	504	CLA	C2A-C3A-C4A	2.19	105.44	101.89
26	AB	620	BCR	C30-C25-C24	2.19	121.77	115.69
30	AB	623	LMG	O6-C5-C6	2.19	111.80	106.34
22	BB	618	CLA	O2D-CGD-CBD	2.19	115.77	111.34
22	BC	503	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
29	BF	101	SQD	C15-C14-C13	2.19	126.21	114.56
26	AA	409	BCR	C34-C9-C8	2.19	121.63	118.09
26	AA	409	BCR	C8-C9-C10	-2.19	115.60	118.98
26	AH	101	BCR	C32-C1-C6	2.19	113.95	110.33
27	AH	102	DGD	C3G-O3G-C1D	-2.19	109.41	113.80
22	BC	508	CLA	O2D-CGD-CBD	2.19	115.76	111.34
22	AB	604	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
22	AC	512	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
26	BB	621	BCR	C1-C6-C7	2.19	121.75	115.69
22	BC	504	CLA	C4D-CHA-CBD	-2.19	104.31	109.45
26	AC	515	BCR	C37-C22-C23	2.19	121.62	118.09
22	AA	402	CLA	C4D-CHA-CBD	-2.19	104.32	109.45
22	BB	605	CLA	C4D-CHA-CBD	-2.18	104.32	109.45
22	AB	608	CLA	O2A-C1-C2	2.18	113.12	108.12
22	AB	605	CLA	C2A-C3A-C4A	2.18	105.42	101.89
27	BA	411	DGD	C3G-O3G-C1D	-2.18	109.42	113.80
22	AC	504	CLA	C2A-C3A-C4A	2.18	105.42	101.89
22	AC	504	CLA	C4D-CHA-CBD	-2.18	104.33	109.45
22	AD	404	CLA	C1-C2-C3	2.18	130.01	126.23
22	BA	403	CLA	C4D-CHA-CBD	-2.18	104.33	109.45
22	BB	618	CLA	C1D-C2D-C3D	-2.18	104.84	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	406	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
22	BB	608	CLA	C4D-CHA-CBD	-2.18	104.34	109.45
22	BB	616	CLA	C4B-NB-C1B	2.18	109.22	107.12
22	BC	512	CLA	C2A-C1A-NA	-2.18	108.55	111.33
22	BB	612	CLA	C4D-CHA-CBD	-2.18	104.34	109.45
22	AC	513	CLA	C4D-CHA-CBD	-2.18	104.34	109.45
22	AC	502	CLA	C2A-C3A-C4A	2.18	105.41	101.89
22	AB	607	CLA	C1D-C2D-C3D	-2.18	104.84	106.97
22	AC	512	CLA	C1D-C2D-C3D	-2.17	104.84	106.97
22	BC	504	CLA	C1D-C2D-C3D	-2.17	104.84	106.97
22	AB	615	CLA	C2A-C1A-CHA	2.17	127.83	123.87
22	AB	615	CLA	O2D-CGD-CBD	2.17	115.73	111.34
22	AC	510	CLA	O2D-CGD-CBD	2.17	115.73	111.34
22	AB	609	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
29	BF	101	SQD	O48-C46-C45	2.17	114.50	108.80
22	BC	506	CLA	C2A-C3A-C4A	2.17	105.40	101.89
22	AA	406	CLA	C2A-C3A-C4A	2.17	105.40	101.89
22	AD	402	CLA	CMB-C2B-C3B	2.17	129.25	125.16
22	AB	612	CLA	C7-C6-C5	-2.17	106.64	112.97
26	AH	101	BCR	C36-C18-C19	2.17	121.59	118.09
22	BB	610	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
22	AB	602	CLA	C1D-C2D-C3D	-2.16	104.85	106.97
26	AK	102	BCR	C19-C18-C17	-2.16	115.65	118.98
22	BC	508	CLA	C1D-C2D-C3D	-2.16	104.85	106.97
22	AB	603	CLA	C7-C6-C5	-2.16	106.66	112.97
29	AA	412	SQD	C17-C16-C15	2.16	126.04	114.56
22	BC	505	CLA	C4B-NB-C1B	2.16	109.20	107.12
22	BB	613	CLA	C1D-C2D-C3D	-2.16	104.86	106.97
29	AF	101	SQD	C15-C14-C13	2.16	126.04	114.56
22	AB	602	CLA	C2A-C3A-C4A	2.16	105.39	101.89
26	BZ	101	BCR	C34-C9-C8	2.16	121.58	118.09
22	AB	601	CLA	C2A-C3A-C4A	2.16	105.38	101.89
26	AB	620	BCR	C1-C6-C7	2.16	121.67	115.69
26	BB	621	BCR	C7-C8-C9	2.15	129.44	126.22
22	AB	613	CLA	C4B-NB-C1B	2.15	109.19	107.12
22	AB	603	CLA	C4D-CHA-CBD	-2.16	104.39	109.45
22	BB	604	CLA	C2A-C1A-CHA	2.16	127.80	123.87
22	AC	512	CLA	O2D-CGD-CBD	2.16	115.69	111.34
22	BB	619	CLA	O2A-C1-C2	2.16	113.06	108.12
27	BC	516	DGD	O3G-C1D-C2D	2.15	110.91	108.15
24	BJ	101	PL9	C10-C9-C8	-2.15	119.23	123.52
27	AA	410	DGD	C3G-O3G-C1D	-2.15	109.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	508	CLA	C2A-C1A-NA	-2.15	108.58	111.33
22	BA	407	CLA	C2A-C3A-C4A	2.15	105.37	101.89
22	AC	508	CLA	C2A-C3A-C4A	2.15	105.37	101.89
22	BC	512	CLA	C6-C5-C3	2.15	117.53	112.62
22	BB	612	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
22	BC	508	CLA	C2A-C3A-C4A	2.15	105.36	101.89
22	AB	601	CLA	C2A-C1A-CHA	2.15	127.79	123.87
22	AB	610	CLA	C4B-NB-C1B	2.15	109.19	107.12
22	AB	610	CLA	CMB-C2B-C3B	2.15	129.21	125.16
22	AC	507	CLA	O2D-CGD-CBD	2.15	115.68	111.34
22	AC	506	CLA	C2A-C3A-C4A	2.15	105.36	101.89
32	BB	625	LMT	C1'-O5'-C5'	-2.14	109.58	113.73
22	BC	512	CLA	C2A-C3A-C4A	2.15	105.36	101.89
22	AD	404	CLA	C4D-CHA-CBD	-2.14	104.42	109.45
22	BA	404	CLA	C4D-CHA-CBD	-2.14	104.41	109.45
29	AF	101	SQD	O48-C46-C45	2.15	114.44	108.80
22	AC	506	CLA	C1D-C2D-C3D	-2.14	104.87	106.97
22	BB	610	CLA	C2A-C3A-C4A	2.14	105.36	101.89
26	BK	102	BCR	C40-C30-C25	2.14	113.88	110.33
22	AC	503	CLA	CAA-C2A-C3A	-2.14	107.96	113.32
22	AC	512	CLA	C6-C5-C3	2.14	117.51	112.62
22	BC	511	CLA	C2A-C1A-NA	-2.14	108.59	111.33
22	BC	511	CLA	C6-C7-C8	2.14	122.11	115.44
34	BV	201	HEM	C4C-NC-C1C	2.14	107.69	105.51
26	BJ	102	BCR	C34-C9-C8	2.14	121.55	118.09
22	BC	513	CLA	CAA-C2A-C3A	-2.14	107.96	113.32
24	AJ	101	PL9	C25-C24-C23	-2.14	119.26	123.52
23	BD	403	PHO	CMB-C2B-C3B	2.14	129.19	125.16
23	BD	403	PHO	O2D-CGD-CBD	2.14	115.67	111.34
22	BC	501	CLA	C2A-C3A-C4A	2.14	105.35	101.89
22	BB	612	CLA	C2A-C3A-C4A	2.14	105.35	101.89
23	BD	403	PHO	CHC-C1C-NC	-2.14	124.86	128.68
24	AA	407	PL9	C30-C29-C28	-2.14	119.27	123.52
22	BC	509	CLA	C7-C6-C5	-2.14	106.73	112.97
22	BB	605	CLA	C2A-C3A-C4A	2.14	105.35	101.89
32	AB	624	LMT	C1'-O5'-C5'	-2.13	109.60	113.73
22	AB	604	CLA	C2A-C1A-NA	-2.13	108.61	111.33
22	AD	402	CLA	C4D-CHA-CBD	-2.13	104.44	109.45
26	BC	515	BCR	C36-C18-C19	2.13	121.54	118.09
34	BE	101	HEM	CAD-CBD-CGD	2.13	117.55	113.53
22	AC	512	CLA	C4B-NB-C1B	2.13	109.17	107.12
32	BB	625	LMT	C6'-C5'-C4'	-2.13	107.17	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	510	CLA	O2D-CGD-CBD	2.13	115.65	111.34
27	BA	411	DGD	C3G-C2G-C1G	-2.13	106.97	111.86
22	BC	509	CLA	O2D-CGD-CBD	2.13	115.64	111.34
32	BB	626	LMT	O1B-C1B-C2B	2.13	113.21	108.11
22	BC	501	CLA	C4D-CHA-CBD	-2.13	104.45	109.45
22	BB	611	CLA	O2A-C1-C2	2.13	112.99	108.12
22	AC	513	CLA	CAA-C2A-C3A	-2.13	107.99	113.32
26	AT	102	BCR	C37-C22-C23	2.13	121.53	118.09
26	BB	622	BCR	C28-C27-C26	2.13	117.31	113.81
22	AC	507	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
22	AB	611	CLA	O2D-CGD-CBD	2.13	115.64	111.34
29	BA	413	SQD	C17-C16-C15	2.13	125.86	114.56
26	AB	620	BCR	C16-C17-C18	2.13	130.36	127.29
26	BD	406	BCR	C7-C8-C9	2.13	129.40	126.22
22	BA	407	CLA	C4D-CHA-CBD	-2.12	104.46	109.45
30	BA	414	LMG	C9-C8-C7	-2.12	106.98	111.86
22	BB	607	CLA	C1-C2-C3	2.12	129.91	126.23
26	BC	514	BCR	C11-C10-C9	2.12	130.36	127.29
26	BB	621	BCR	C35-C13-C12	2.12	121.52	118.09
26	BA	410	BCR	C12-C13-C14	-2.12	115.71	118.98
22	AB	603	CLA	C2A-C3A-C4A	2.12	105.33	101.89
29	BL	101	SQD	C15-C14-C13	2.12	125.84	114.56
22	BB	614	CLA	C2A-C3A-C4A	2.12	105.33	101.89
26	BK	102	BCR	C36-C18-C19	2.12	121.52	118.09
34	BE	101	HEM	C4D-ND-C1D	2.12	107.31	105.11
22	AB	615	CLA	CAA-C2A-C3A	-2.12	108.01	113.32
22	BB	609	CLA	C2A-C1A-CHA	2.12	127.74	123.87
27	AC	516	DGD	O3E-C3E-C2E	-2.12	105.62	110.36
22	BD	404	CLA	C4D-CHA-CBD	-2.12	104.47	109.45
22	AB	601	CLA	C6-C5-C3	2.12	117.45	112.62
22	AB	604	CLA	CED-O2D-CGD	2.12	121.05	116.00
22	AB	604	CLA	C6-C5-C3	2.12	117.46	112.62
22	BB	614	CLA	O2D-CGD-CBD	2.12	115.62	111.34
22	BA	403	CLA	C2A-C3A-C4A	2.12	105.32	101.89
30	AB	622	LMG	O8-C9-C8	-2.12	103.23	108.80
22	BA	405	CLA	C4D-CHA-CBD	-2.11	104.48	109.45
26	AB	618	BCR	C16-C17-C18	2.12	130.35	127.29
26	AT	102	BCR	C32-C1-C6	2.12	113.83	110.33
22	BC	511	CLA	C4B-NB-C1B	2.12	109.16	107.12
22	BC	509	CLA	CAA-C2A-C3A	-2.11	108.03	113.32
28	AA	411	LHG	P-O6-C4	-2.11	106.84	122.03
22	BB	618	CLA	C2A-C1A-CHA	2.11	127.72	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BA	412	LHG	P-O6-C4	-2.11	106.83	122.03
29	BA	413	SQD	O3-C3-C2	-2.11	105.64	110.36
23	AD	403	PHO	C1D-C2D-C3D	-2.11	105.07	107.12
22	AC	501	CLA	C4D-CHA-CBD	-2.11	104.50	109.45
22	BB	610	CLA	C1D-C2D-C3D	-2.11	104.91	106.97
26	AC	515	BCR	C36-C18-C19	2.11	121.49	118.09
22	AB	604	CLA	C2A-C1A-CHA	2.11	127.71	123.87
22	AB	602	CLA	C4D-CHA-CBD	-2.11	104.50	109.45
30	AC	520	LMG	C7-O1-C1	-2.11	109.58	113.80
22	BB	615	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
22	BC	512	CLA	C4B-NB-C1B	2.10	109.15	107.12
22	BB	616	CLA	CMB-C2B-C3B	2.11	129.13	125.16
22	AC	502	CLA	C4D-CHA-CBD	-2.10	104.51	109.45
22	AC	510	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
22	BB	610	CLA	CBA-CAA-C2A	2.10	119.09	113.95
26	BC	515	BCR	C23-C22-C21	-2.10	115.74	118.98
22	BA	407	CLA	C16-C15-C13	2.10	121.98	115.44
29	BD	409	SQD	C15-C14-C13	2.10	125.71	114.56
26	AB	618	BCR	C34-C9-C8	2.10	121.48	118.09
29	AF	101	SQD	O47-C7-C8	2.10	116.01	111.54
22	AC	505	CLA	C4B-NB-C1B	2.10	109.14	107.12
22	BB	608	CLA	C1D-C2D-C3D	-2.10	104.92	106.97
26	BB	620	BCR	C19-C18-C17	-2.10	115.75	118.98
26	AB	618	BCR	C19-C18-C17	-2.10	115.75	118.98
26	AC	514	BCR	C40-C30-C25	2.10	113.80	110.33
22	BB	606	CLA	C2A-C1A-NA	-2.10	108.65	111.33
26	AT	102	BCR	C20-C21-C22	2.10	130.32	127.29
22	BD	404	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
22	AB	611	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
32	AB	624	LMT	C6'-C5'-C4'	-2.09	107.28	113.27
30	AA	413	LMG	C9-C8-C7	-2.09	107.05	111.86
23	BA	406	PHO	C6-C7-C8	2.09	121.95	115.44
30	AD	408	LMG	O8-C9-C8	-2.09	103.30	108.80
22	AC	501	CLA	C2A-C3A-C4A	2.09	105.28	101.89
22	AB	616	CLA	C1D-C2D-C3D	-2.09	104.92	106.97
22	AA	406	CLA	C1D-C2D-C3D	-2.09	104.92	106.97
22	BB	609	CLA	C2A-C3A-C4A	2.09	105.27	101.89
22	BC	503	CLA	O2D-CGD-CBD	2.09	115.56	111.34
22	AC	511	CLA	C6-C7-C8	2.09	121.95	115.44
26	BA	410	BCR	C36-C18-C19	2.09	121.47	118.09
22	BB	613	CLA	C16-C15-C13	2.09	121.94	115.44
29	AF	101	SQD	O8-S-O9	-2.09	107.04	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	607	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
24	BA	408	PL9	C30-C29-C28	-2.09	119.36	123.52
22	AC	504	CLA	CED-O2D-CGD	2.09	120.97	116.00
26	BD	406	BCR	C16-C17-C18	2.09	130.31	127.29
26	BA	410	BCR	C1-C6-C7	2.09	121.47	115.69
22	AB	603	CLA	O2D-CGD-CBD	2.09	115.56	111.34
22	BB	605	CLA	C1-C2-C3	2.09	129.85	126.23
22	AB	610	CLA	CBA-CAA-C2A	2.09	119.05	113.95
23	BA	406	PHO	O2D-CGD-CBD	2.08	115.55	111.34
22	BC	507	CLA	C2A-C3A-C4A	2.08	105.26	101.89
22	AB	607	CLA	C7-C6-C5	-2.09	106.88	112.97
22	AD	402	CLA	C6-C5-C3	2.08	117.38	112.62
22	AC	507	CLA	C2A-C3A-C4A	2.08	105.26	101.89
23	AD	403	PHO	CHC-C1C-NC	-2.08	124.97	128.68
27	BC	516	DGD	C3G-C2G-C1G	-2.08	107.08	111.86
22	BB	613	CLA	C4D-CHA-CBD	-2.08	104.57	109.45
22	AB	616	CLA	O2A-C1-C2	2.08	112.88	108.12
26	AC	514	BCR	C11-C10-C9	2.08	130.29	127.29
22	BB	606	CLA	C7-C6-C5	-2.08	106.91	112.97
22	BB	604	CLA	C2A-C3A-C4A	2.07	105.25	101.89
26	AZ	101	BCR	C28-C27-C26	2.08	117.22	113.81
22	AB	602	CLA	CMB-C2B-C3B	2.08	129.07	125.16
22	AA	406	CLA	C16-C15-C13	2.07	121.90	115.44
22	AC	503	CLA	C1D-C2D-C3D	-2.07	104.94	106.97
22	AC	509	CLA	C4D-CHA-CBD	-2.07	104.58	109.45
22	BC	503	CLA	CAA-C2A-C3A	-2.07	108.13	113.32
32	AT	101	LMT	C1B-O1B-C4'	-2.07	112.74	118.00
22	BC	513	CLA	C4B-NB-C1B	2.07	109.11	107.12
26	BX	101	BCR	C34-C9-C8	2.07	121.43	118.09
22	AB	612	CLA	C4D-CHA-CBD	-2.07	104.59	109.45
22	AB	614	CLA	C6-C7-C8	2.07	121.87	115.44
22	BC	510	CLA	C4B-NB-C1B	2.07	109.11	107.12
22	AC	510	CLA	CMA-C3A-C2A	-2.06	105.29	114.45
29	BL	101	SQD	O3-C3-C2	-2.06	105.74	110.36
22	AC	501	CLA	C6-C5-C3	2.06	117.33	112.62
32	AB	625	LMT	O1B-C1B-C2B	2.06	113.06	108.11
22	BB	607	CLA	C2A-C1A-CHA	2.06	127.63	123.87
22	BC	503	CLA	CBA-CAA-C2A	2.06	118.99	113.95
23	AA	405	PHO	C6-C7-C8	2.06	121.86	115.44
22	BC	510	CLA	C4D-CHA-CBD	-2.06	104.61	109.45
22	AB	614	CLA	C1-O2A-CGA	2.06	122.99	117.00
26	AK	102	BCR	C40-C30-C25	2.06	113.74	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	610	CLA	C7-C6-C5	-2.06	106.95	112.97
22	BB	618	CLA	C2A-C1A-NA	-2.06	108.70	111.33
27	AA	410	DGD	C6D-O5D-C1E	2.06	117.94	113.80
22	AB	607	CLA	C2D-C1D-ND	2.06	111.91	109.56
32	AB	625	LMT	C1-O1'-C1'	-2.06	110.28	113.91
26	BD	406	BCR	C8-C9-C10	-2.06	115.81	118.98
22	BA	404	CLA	C1D-C2D-C3D	-2.06	104.95	106.97
22	AC	509	CLA	CBA-CAA-C2A	2.06	118.98	113.95
29	AD	409	SQD	C15-C14-C13	2.06	125.48	114.56
26	BZ	101	BCR	C7-C8-C9	2.06	129.29	126.22
26	AB	618	BCR	C28-C27-C26	2.06	117.19	113.81
26	BB	622	BCR	C37-C22-C23	2.06	121.41	118.09
30	BM	102	LMG	C7-O1-C1	-2.06	109.67	113.80
22	AC	508	CLA	C1-C2-C3	2.06	129.79	126.23
22	BB	617	CLA	C7-C6-C5	-2.05	106.97	112.97
26	AK	102	BCR	C36-C18-C19	2.05	121.41	118.09
26	AB	620	BCR	C12-C13-C14	-2.05	115.81	118.98
22	AA	403	CLA	C4D-CHA-CBD	-2.05	104.63	109.45
26	AZ	101	BCR	C7-C8-C9	2.05	129.29	126.22
22	BC	510	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
22	AB	614	CLA	C7-C6-C5	-2.05	106.98	112.97
22	BB	617	CLA	C6-C7-C8	2.05	121.82	115.44
22	BB	607	CLA	C2A-C1A-NA	-2.05	108.71	111.33
22	BB	619	CLA	C2A-C1A-CHA	2.05	127.61	123.87
22	AB	606	CLA	C2A-C1A-CHA	2.05	127.61	123.87
22	BC	503	CLA	C2A-C3A-C4A	2.05	105.21	101.89
22	AB	607	CLA	C2A-C3A-C4A	2.05	105.21	101.89
27	BC	517	DGD	C6E-C5E-C4E	-2.05	108.04	113.04
26	BJ	102	BCR	C3-C4-C5	2.05	117.18	113.81
22	BB	606	CLA	C1-C2-C3	2.05	129.78	126.23
22	AB	614	CLA	C2A-C3A-C4A	2.05	105.20	101.89
26	AA	409	BCR	C12-C13-C14	-2.05	115.83	118.98
26	BK	102	BCR	C28-C27-C26	2.04	117.17	113.81
22	AC	508	CLA	C1D-C2D-C3D	-2.04	104.97	106.97
22	AC	507	CLA	C1D-C2D-C3D	-2.04	104.97	106.97
29	BF	101	SQD	O47-C7-C8	2.04	115.89	111.54
22	AC	501	CLA	C2A-C1A-CHA	2.04	127.59	123.87
22	AB	608	CLA	C4B-NB-C1B	2.04	109.08	107.12
24	BJ	101	PL9	C25-C24-C23	-2.04	119.45	123.52
22	AB	613	CLA	CMB-C2B-C3B	2.04	129.00	125.16
22	BC	508	CLA	C2D-C1D-ND	2.04	111.89	109.56
22	BB	610	CLA	C2A-C1A-NA	-2.04	108.72	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	503	CLA	C4B-NB-C1B	2.04	109.08	107.12
30	AE	102	LMG	C8-O7-C10	2.04	122.64	117.86
22	AA	402	CLA	C2A-C3A-C4A	2.04	105.19	101.89
27	AA	410	DGD	C6D-C5D-C4D	2.04	116.60	111.98
22	AB	615	CLA	C4B-NB-C1B	2.04	109.08	107.12
22	BC	503	CLA	C1D-C2D-C3D	-2.04	104.98	106.97
27	AC	517	DGD	C6E-C5E-C4E	-2.03	108.07	113.04
34	BE	101	HEM	C2A-C1A-NA	-2.03	106.91	109.73
26	AB	619	BCR	C37-C22-C23	2.04	121.38	118.09
24	AA	407	PL9	C15-C14-C13	-2.04	119.47	123.52
22	BB	605	CLA	CMB-C2B-C3B	2.03	128.99	125.16
26	AD	406	BCR	C16-C17-C18	2.03	130.23	127.29
22	AC	510	CLA	C4B-NB-C1B	2.03	109.08	107.12
22	BB	613	CLA	C12-C11-C10	-2.03	102.98	113.00
22	AC	509	CLA	O2D-CGD-CBD	2.03	115.45	111.34
22	AA	402	CLA	C4B-NB-C1B	2.03	109.08	107.12
22	AC	501	CLA	C1-C2-C3	2.03	129.75	126.23
29	BB	601	SQD	O3-C3-C2	-2.03	105.82	110.36
26	BX	101	BCR	C32-C1-C6	2.03	113.69	110.33
22	BD	404	CLA	O2D-CGD-CBD	2.03	115.44	111.34
26	AB	619	BCR	C7-C8-C9	2.03	129.25	126.22
22	BB	617	CLA	C1D-C2D-C3D	-2.03	104.98	106.97
22	BB	613	CLA	CMB-C2B-C3B	2.03	128.98	125.16
22	AB	601	CLA	C4B-NB-C1B	2.03	109.07	107.12
22	AC	511	CLA	C2A-C3A-C4A	2.03	105.18	101.89
22	BB	615	CLA	C7-C6-C5	-2.03	107.05	112.97
22	AD	404	CLA	C2A-C1A-CHA	2.03	127.57	123.87
22	AB	605	CLA	O2D-CGD-CBD	2.03	115.44	111.34
22	BB	617	CLA	C1-O2A-CGA	2.03	122.89	117.00
22	BB	604	CLA	C4B-NB-C1B	2.03	109.07	107.12
22	AB	614	CLA	C2A-C1A-NA	-2.03	108.74	111.33
26	AC	514	BCR	C32-C1-C2	-2.03	100.73	108.78
22	BC	509	CLA	C12-C11-C10	-2.03	103.01	113.00
22	AB	616	CLA	C2A-C1A-CHA	2.02	127.56	123.87
26	BD	406	BCR	C32-C1-C6	2.02	113.68	110.33
22	AB	609	CLA	CMA-C3A-C2A	-2.02	105.48	114.45
26	AD	406	BCR	C36-C18-C19	2.02	121.36	118.09
32	BT	101	LMT	C1B-O1B-C4'	-2.02	112.86	118.00
22	BB	617	CLA	C2A-C1A-NA	-2.02	108.75	111.33
26	AB	617	BCR	C16-C17-C18	2.02	130.21	127.29
22	AB	613	CLA	C1-C2-C3	2.02	129.73	126.23
22	AB	612	CLA	C6-C7-C8	2.02	121.73	115.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BD	409	SQD	C6-C5-C4	-2.02	107.60	111.86
29	BA	401	SQD	O48-C23-O10	-2.02	118.20	123.48
30	AI	101	LMG	O6-C1-C2	2.02	114.44	110.30
26	BB	621	BCR	C37-C22-C23	2.02	121.35	118.09
23	BA	406	PHO	CAA-C2A-C3A	-2.02	108.27	113.32
22	BC	509	CLA	CBA-CAA-C2A	2.02	118.88	113.95
26	AA	409	BCR	C36-C18-C19	2.02	121.35	118.09
22	AC	503	CLA	C4B-NB-C1B	2.01	109.06	107.12
29	BA	401	SQD	O8-S-O7	2.01	116.17	111.69
22	BC	508	CLA	C2A-C1A-CHA	2.01	127.54	123.87
22	AC	513	CLA	C4B-NB-C1B	2.01	109.06	107.12
22	AA	404	CLA	C4D-CHA-CBD	-2.01	104.72	109.45
32	BI	102	LMT	C1B-O1B-C4'	-2.01	112.89	118.00
22	AA	402	CLA	C6-C7-C8	2.01	121.70	115.44
22	BB	606	CLA	C2A-C3A-C4A	2.01	105.15	101.89
22	BC	501	CLA	C1-C2-C3	2.01	129.72	126.23
22	AC	510	CLA	C4D-CHA-CBD	-2.01	104.73	109.45
26	AC	514	BCR	C36-C18-C19	2.01	121.34	118.09
30	BD	408	LMG	O1-C1-C2	2.01	110.73	108.15
22	AB	610	CLA	C12-C11-C10	-2.01	103.08	113.00
22	AC	508	CLA	C2A-C1A-CHA	2.01	127.54	123.87
22	BC	507	CLA	C1D-C2D-C3D	-2.01	105.00	106.97
22	BA	404	CLA	O2A-C1-C2	2.01	112.72	108.12
27	BA	411	DGD	C6D-C5D-C4D	2.01	116.53	111.98
22	AA	406	CLA	C4D-CHA-CBD	-2.01	104.73	109.45
22	AC	502	CLA	O2D-CGD-CBD	2.01	115.40	111.34
24	BA	408	PL9	C7-C3-C4	2.01	118.53	116.92
22	BD	402	CLA	C4B-NB-C1B	2.01	109.05	107.12
22	AA	406	CLA	C6-C5-C3	2.00	117.20	112.62
22	AC	513	CLA	C2A-C3A-C4A	2.00	105.14	101.89
22	AD	402	CLA	C2A-C1A-NA	-2.01	108.77	111.33
26	BB	622	BCR	C16-C17-C18	2.01	130.19	127.29
22	AB	613	CLA	C1D-C2D-C3D	-2.00	105.01	106.97
22	AD	404	CLA	CBA-CAA-C2A	2.00	118.85	113.95
34	AV	201	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
22	BC	508	CLA	C2A-C1A-NA	-2.00	108.78	111.33
22	BC	511	CLA	CBA-CAA-C2A	2.00	118.84	113.95

All (98) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	AC	520	LMG	C2

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Mol	Chain	Res	Type	Atom
30	AC	520	LMG	C5
27	AB	626	DGD	C2D
27	AB	626	DGD	C5D
27	AB	626	DGD	C5E
27	AH	102	DGD	C2D
27	AH	102	DGD	C5D
27	AH	102	DGD	C5E
30	AB	623	LMG	C2
30	AB	623	LMG	C5
30	AM	101	LMG	C2
30	AM	101	LMG	C5
30	AE	102	LMG	C2
30	AE	102	LMG	C5
27	AC	517	DGD	C2D
27	AC	517	DGD	C5D
27	AC	517	DGD	C5E
30	AB	622	LMG	C2
30	AB	622	LMG	C5
27	BC	518	DGD	C2D
27	BC	518	DGD	C5D
27	BC	518	DGD	C5E
30	BA	414	LMG	C2
30	BA	414	LMG	C5
30	BE	102	LMG	C2
30	BE	102	LMG	C5
27	AA	410	DGD	C2D
27	AA	410	DGD	C5D
27	AA	410	DGD	C5E
23	AD	403	PHO	C2A
23	AD	403	PHO	C13
23	AD	403	PHO	C8
27	AC	518	DGD	C2D
27	AC	518	DGD	C5D
27	AC	518	DGD	C5E
30	BB	623	LMG	C2
30	BB	623	LMG	C5
27	BD	410	DGD	C2D
27	BD	410	DGD	C5D
27	BD	410	DGD	C5E
27	BC	516	DGD	C2D
27	BC	516	DGD	C5D
27	BC	516	DGD	C5E

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Mol	Chain	Res	Type	Atom
30	BI	101	LMG	C2
30	BI	101	LMG	C5
27	BC	517	DGD	C2D
27	BC	517	DGD	C5D
27	BC	517	DGD	C5E
27	BA	411	DGD	C2D
27	BA	411	DGD	C5D
27	BA	411	DGD	C5E
30	AA	413	LMG	C2
30	AA	413	LMG	C5
27	BH	101	DGD	C2D
27	BH	101	DGD	C5D
27	BH	101	DGD	C5E
30	BD	408	LMG	C2
30	BD	408	LMG	C5
30	AB	621	LMG	C2
30	AB	621	LMG	C5
30	BC	520	LMG	C2
30	BC	520	LMG	C5
23	BA	406	PHO	C2A
23	BA	406	PHO	C13
23	BA	406	PHO	C8
23	AA	405	PHO	C2A
23	AA	405	PHO	C13
23	AA	405	PHO	C8
30	AC	519	LMG	C2
30	AC	519	LMG	C5
30	BB	624	LMG	C2
30	BB	624	LMG	C5
27	AC	516	DGD	C2D
27	AC	516	DGD	C5D
27	AC	516	DGD	C5E
30	AA	416	LMG	C2
30	AA	416	LMG	C5
27	AD	410	DGD	C2D
27	AD	410	DGD	C5D
27	AD	410	DGD	C5E
30	BD	407	LMG	C2
30	BD	407	LMG	C5
30	BM	102	LMG	C2
30	BM	102	LMG	C5
30	AD	408	LMG	C2

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Mol	Chain	Res	Type	Atom
30	AD	408	LMG	C5
30	BC	519	LMG	C2
30	BC	519	LMG	C5
27	BB	602	DGD	C2D
27	BB	602	DGD	C5D
27	BB	602	DGD	C5E
30	AI	101	LMG	C2
30	AI	101	LMG	C5
30	AD	407	LMG	C2
30	AD	407	LMG	C5
23	BD	403	PHO	C2A
23	BD	403	PHO	C13
23	BD	403	PHO	C8

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	AD	409	SQD	C45-O47-C7-C8
29	BD	409	SQD	C45-O47-C7-C8
29	AD	409	SQD	C45-O47-C7-O49
29	BD	409	SQD	C45-O47-C7-O49
30	BM	102	LMG	C8-O7-C10-C11
30	AM	101	LMG	C8-O7-C10-C11
22	AC	502	CLA	C1-C2-C3-C4
22	BC	502	CLA	C1-C2-C3-C4
30	BD	408	LMG	C7-O1-C1-O6
30	AD	408	LMG	C7-O1-C1-O6
22	AC	509	CLA	C1-C2-C3-C4
22	BC	509	CLA	C1-C2-C3-C4
22	BB	605	CLA	C1-C2-C3-C4
22	BA	404	CLA	C1-C2-C3-C4
22	AA	403	CLA	C1-C2-C3-C4
22	AB	602	CLA	C1-C2-C3-C4
22	AB	606	CLA	C1-C2-C3-C4
22	BB	609	CLA	C1-C2-C3-C4
23	AA	405	PHO	C1-C2-C3-C4
23	BA	406	PHO	C1-C2-C3-C4
22	AC	510	CLA	C1-C2-C3-C4
22	BC	510	CLA	C1-C2-C3-C4
22	BC	513	CLA	C1-C2-C3-C4
22	AC	513	CLA	C1-C2-C3-C4
22	BB	614	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	AB	611	CLA	C1-C2-C3-C4

There are no ring outliers.

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	AA	335/344 (97%)	-0.43	6 (1%) 65 74	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.23	5 (1%) 70 79	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.23	6 (1%) 75 83	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.23	11 (2%) 59 67	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.14	15 (3%) 43 51	43, 72, 87, 102	0
3	BC	447/473 (94%)	0.13	22 (4%) 28 34	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.39	4 (1%) 75 83	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.27	7 (2%) 60 69	40, 69, 91, 101	0
5	AE	82/84 (97%)	0.11	7 (8%) 11 13	54, 75, 93, 99	0
5	BE	82/84 (97%)	0.50	10 (12%) 5 6	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.01	2 (5%) 23 28	56, 73, 94, 97	0
6	BF	35/45 (77%)	0.33	3 (8%) 11 13	75, 82, 97, 99	0
7	AH	65/66 (98%)	0.14	3 (4%) 31 38	57, 76, 92, 97	0
7	BH	65/66 (98%)	0.32	8 (12%) 5 6	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.04	3 (8%) 11 13	57, 70, 87, 94	0
8	BI	35/38 (92%)	0.04	1 (2%) 49 58	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.42	1 (2%) 49 58	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.04	4 (11%) 5 7	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.35	2 (5%) 25 30	67, 75, 87, 93	0
10	BK	37/37 (100%)	-0.00	2 (5%) 25 30	84, 90, 96, 101	0
11	AL	37/37 (100%)	0.26	5 (13%) 4 5	45, 60, 98, 107	0
11	BL	37/37 (100%)	0.39	6 (16%) 2 3	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.03	2 (5%) 22 25	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.12	2 (5%) 22 25	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.10	12 (4%) 28 34	39, 70, 93, 107	0
13	BO	243/247 (98%)	0.18	16 (6%) 18 21	48, 76, 97, 107	0
14	AT	32/32 (100%)	0.19	3 (9%) 9 11	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.02	2 (6%) 19 23	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.06	1 (1%) 79 86	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.19	1 (1%) 79 86	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.21	0 100 100	49, 66, 76, 79	0
16	BV	137/137 (100%)	0.12	8 (5%) 22 26	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.30	4 (14%) 3 5	79, 91, 97, 99	0
17	By	28/46 (60%)	0.34	3 (10%) 6 8	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.15	2 (5%) 25 30	70, 79, 93, 95	0
18	BX	37/50 (74%)	0.25	5 (13%) 4 5	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.24	10 (16%) 2 3	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.62	10 (16%) 2 3	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.09	214 (4%) 35 43	23, 71, 94, 110	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	65	LEU	8.7
5	BE	4	THR	7.2
12	AM	33	GLN	6.2
11	BL	1	MET	6.1
20	BZ	1	MET	6.0
20	BZ	62	VAL	6.0
20	AZ	1	MET	5.9
3	BC	473	ASP	5.8
6	AF	12	SER	5.7
7	BH	66	GLY	5.7
5	AE	6	GLY	5.4
20	BZ	60	PHE	5.4
11	BL	2	GLU	5.4
13	AO	272	ALA	5.3
13	BO	49	ASP	5.2
20	AZ	34	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
14	AT	30	THR	5.2
3	BC	253	LEU	5.1
14	BT	32	LYS	4.9
5	BE	84	LYS	4.9
20	AZ	33	TRP	4.9
6	BF	11	VAL	4.7
4	BD	227	GLU	4.6
2	BB	128	THR	4.6
3	AC	192	GLY	4.6
18	BX	12	ILE	4.5
3	BC	204	LEU	4.4
13	AO	87	GLN	4.4
7	BH	64	ALA	4.4
5	AE	17	VAL	4.4
12	BM	33	GLN	4.4
1	BA	10	SER	4.3
5	AE	84	LYS	4.3
4	AD	227	GLU	4.3
13	BO	50	ASP	4.3
3	BC	142	GLU	4.3
3	AC	27	ASP	4.2
18	BX	46	VAL	4.2
13	BO	51	THR	4.1
11	BL	3	PRO	4.0
6	AF	11	VAL	4.0
5	BE	3	GLY	4.0
1	AA	10	SER	4.0
5	BE	17	VAL	4.0
20	BZ	61	VAL	4.0
14	AT	31	LYS	4.0
18	BX	47	GLN	4.0
4	BD	239	GLN	3.9
11	AL	1	MET	3.9
2	BB	85	GLY	3.9
11	AL	2	GLU	3.9
9	BJ	7	ARG	3.9
18	AX	47	GLN	3.8
1	AA	11	ALA	3.8
20	AZ	62	VAL	3.8
1	BA	11	ALA	3.8
4	BD	226	GLY	3.8
3	BC	207	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
5	BE	6	GLY	3.7
14	AT	32	LYS	3.7
13	BO	84	ASN	3.7
3	BC	252	ILE	3.7
13	AO	115	SER	3.6
18	BX	11	THR	3.6
13	AO	84	ASN	3.6
6	BF	13	TYR	3.5
18	AX	46	VAL	3.5
20	BZ	34	ASP	3.5
1	BA	12	ASN	3.5
3	AC	182	PHE	3.5
13	BO	48	LEU	3.4
2	BB	488	PRO	3.4
7	BH	6	TRP	3.4
10	BK	10	LYS	3.4
11	BL	7	ARG	3.3
5	AE	5	THR	3.3
5	BE	60	GLN	3.3
3	BC	182	PHE	3.3
17	By	19	ILE	3.3
5	AE	83	LEU	3.2
10	BK	46	ARG	3.2
13	BO	52	ALA	3.2
4	AD	228	GLY	3.2
11	BL	5	PRO	3.2
13	AO	88	GLU	3.2
3	BC	30	SER	3.2
3	BC	145	SER	3.2
2	AB	85	GLY	3.2
3	AC	102	GLY	3.2
3	BC	146	PHE	3.1
17	By	46	LEU	3.1
13	AO	114	ASN	3.1
20	AZ	35	ARG	3.1
15	BU	53	GLU	3.1
13	BO	30	THR	3.1
20	BZ	35	ARG	3.0
20	AZ	60	PHE	3.0
3	BC	208	VAL	3.0
17	Ay	41	VAL	3.0
1	AA	12	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
15	AU	38	GLU	3.0
13	BO	87	GLN	3.0
13	AO	271	PRO	3.0
12	AM	34	LYS	3.0
2	BB	127	ARG	3.0
16	BV	50	LYS	3.0
8	AI	34	ARG	3.0
11	AL	3	PRO	2.9
13	BO	232	GLY	2.9
20	AZ	38	GLN	2.9
9	BJ	40	LEU	2.9
5	AE	12	ASP	2.9
12	BM	34	LYS	2.9
5	BE	61	ARG	2.8
3	AC	198	VAL	2.8
3	AC	143	TYR	2.8
20	AZ	4	LEU	2.8
13	BO	60	SER	2.8
1	BA	15	GLU	2.8
2	AB	127	ARG	2.8
7	AH	6	TRP	2.8
20	AZ	30	PRO	2.7
7	AH	2	ALA	2.7
9	BJ	8	ILE	2.7
13	BO	228	ALA	2.7
16	BV	39	ASN	2.7
3	AC	255	THR	2.7
6	BF	12	SER	2.7
13	BO	61	SER	2.7
4	BD	233	ARG	2.6
2	BB	161	LEU	2.6
3	BC	472	LEU	2.6
17	Ay	45	ASN	2.6
13	BO	112	LYS	2.6
11	AL	7	ARG	2.6
16	BV	42	GLY	2.6
13	BO	35	ASP	2.6
8	AI	33	LYS	2.6
3	AC	214	LEU	2.6
20	BZ	31	GLN	2.6
1	BA	100	ALA	2.6
3	BC	471	SER	2.5

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Mol	Chain	Res	Type	RSRZ
18	BX	45	LYS	2.5
20	BZ	3	ILE	2.5
14	BT	31	LYS	2.5
20	BZ	38	GLN	2.5
3	BC	255	THR	2.5
16	BV	43	LYS	2.4
2	BB	491	VAL	2.4
2	BB	490	GLN	2.4
3	BC	32	GLY	2.4
17	By	22	LEU	2.4
5	BE	5	THR	2.4
1	AA	243	GLU	2.4
4	AD	226	GLY	2.4
2	AB	405	GLU	2.4
3	AC	181	PHE	2.4
13	AO	51	THR	2.4
7	BH	23	PRO	2.4
2	AB	86	ILE	2.4
13	BO	88	GLU	2.4
4	BD	225	ASP	2.4
17	Ay	19	ILE	2.4
2	BB	86	ILE	2.3
13	BO	89	ALA	2.3
3	BC	33	PHE	2.3
3	AC	236	GLY	2.3
8	AI	35	LYS	2.3
8	BI	34	ARG	2.3
5	BE	21	VAL	2.3
3	AC	207	ARG	2.3
4	AD	13	GLY	2.3
1	AA	16	ARG	2.3
2	BB	350	GLU	2.3
3	AC	191	PRO	2.3
3	BC	194	GLY	2.3
10	AK	10	LYS	2.2
4	BD	240	ALA	2.2
5	BE	59	GLU	2.2
16	BV	83	GLU	2.2
3	BC	195	ASP	2.2
20	BZ	4	LEU	2.2
7	AH	4	ARG	2.2
2	AB	114	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	BC	138	GLU	2.2
3	BC	191	PRO	2.2
7	BH	7	LEU	2.2
11	BL	8	GLN	2.2
13	AO	31	LEU	2.2
16	BV	116	GLU	2.2
11	AL	5	PRO	2.2
3	BC	262	ARG	2.1
3	AC	138	GLU	2.1
1	AA	31	GLY	2.1
7	BH	18	TYR	2.1
13	AO	35	ASP	2.1
13	AO	255	GLU	2.1
3	BC	144	SER	2.1
20	AZ	3	ILE	2.1
3	AC	416	SER	2.1
2	BB	295	GLY	2.1
2	BB	114	HIS	2.1
2	AB	487	SER	2.1
7	BH	3	ARG	2.1
9	BJ	9	PRO	2.1
10	AK	46	ARG	2.1
4	BD	241	GLU	2.1
9	AJ	7	ARG	2.1
16	BV	31	PRO	2.1
3	AC	460	ASP	2.0
17	Ay	21	GLN	2.0
16	BV	61	TYR	2.0
5	AE	32	ILE	2.0
13	AO	234	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	CL	AA	414	1/1	0.70	26.23	73,73,73,73	0
27	DGD	AD	410	63/66	0.51	11.93	91,97,107,108	0
26	BCR	BJ	102	40/40	0.50	8.56	93,98,101,102	0
24	PL9	AJ	101	35/55	0.53	7.92	93,101,107,109	0
30	LMG	AA	416	42/55	0.36	6.71	67,92,96,99	0
26	BCR	AJ	102	40/40	0.44	6.71	85,91,101,102	0
27	DGD	BD	410	63/66	0.50	6.43	84,100,105,105	0
22	CLA	AD	404	65/65	0.32	6.26	80,83,102,103	0
24	PL9	BA	408	45/55	0.34	6.24	82,88,90,92	0
24	PL9	BJ	101	35/55	0.41	6.18	78,99,111,112	0
24	PL9	AA	407	45/55	0.35	5.75	83,87,94,95	0
30	LMG	AB	623	42/55	0.38	5.75	70,89,92,93	0
30	LMG	AI	101	43/55	0.49	5.74	83,92,97,98	0
30	LMG	AC	520	45/55	0.40	5.57	75,92,97,98	0
32	LMT	BI	102	35/35	0.55	5.57	90,104,106,106	0
31	CL	BA	415	1/1	0.37	5.53	81,81,81,81	0
32	LMT	AI	102	35/35	0.47	5.24	74,92,95,95	0
22	CLA	BA	407	65/65	0.35	5.17	72,76,103,104	0
26	BCR	AK	102	40/40	0.34	4.99	73,77,81,81	0
32	LMT	AD	411	31/35	0.47	4.84	52,96,104,104	0
28	LHG	BC	521	37/49	0.57	4.76	90,100,113,114	0
22	CLA	AB	601	65/65	0.37	4.71	88,97,102,105	0
32	LMT	AB	625	35/35	0.42	4.57	82,98,100,101	0
32	LMT	AT	101	35/35	0.36	4.51	72,91,97,98	0
27	DGD	BB	602	52/66	0.30	4.33	71,85,104,105	0
28	LHG	AC	521	37/49	0.45	4.28	78,99,109,109	0
32	LMT	BD	411	31/35	0.52	4.24	67,91,99,100	0
22	CLA	AA	406	65/65	0.30	4.22	54,60,89,90	0
32	LMT	AB	624	35/35	0.59	4.02	71,100,106,107	0
27	DGD	AB	626	52/66	0.31	3.95	79,94,105,107	0
30	LMG	BC	520	45/55	0.44	3.94	86,93,101,102	0
26	BCR	BK	102	40/40	0.37	3.90	76,81,85,85	0
29	SQD	BA	401	54/54	0.35	3.76	82,91,107,108	0
32	LMT	BB	625	35/35	0.49	3.74	66,103,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CA	BO	301	1/1	0.32	3.74	100,100,100,100	0
26	BCR	AZ	101	40/40	0.30	3.53	75,82,90,91	0
33	BCT	AD	401	4/4	0.24	3.48	90,91,91,92	0
29	SQD	AA	415	54/54	0.28	3.34	71,87,105,105	0
30	LMG	BE	102	44/55	0.38	3.18	75,92,98,99	0
22	CLA	AB	604	65/65	0.24	3.13	67,73,91,91	0
30	LMG	BC	519	48/55	0.34	2.98	83,90,94,95	0
30	LMG	AD	408	48/55	0.23	2.85	63,68,74,80	0
27	DGD	BA	411	56/66	0.35	2.84	76,85,103,104	0
30	LMG	BD	408	48/55	0.24	2.80	68,75,85,87	0
22	CLA	AC	512	65/65	0.32	2.73	91,95,106,106	0
30	LMG	BI	101	43/55	0.35	2.70	84,90,99,100	0
22	CLA	BB	612	65/65	0.27	2.69	82,89,92,95	0
26	BCR	BC	514	40/40	0.26	2.68	81,83,87,87	0
30	LMG	BD	407	46/55	0.24	2.68	70,80,92,94	0
32	LMT	AB	627	35/35	0.50	2.64	73,103,106,107	0
26	BCR	AH	101	40/40	0.32	2.61	76,88,95,95	0
29	SQD	AF	101	45/54	0.35	2.47	82,97,102,103	0
29	SQD	BF	101	45/54	0.37	2.42	95,98,103,104	0
22	CLA	AC	507	65/65	0.28	2.28	83,90,95,97	0
26	BCR	BB	622	40/40	0.27	2.24	67,71,79,80	0
30	LMG	BB	623	49/55	0.25	2.21	70,78,88,91	0
22	CLA	BC	513	65/65	0.35	2.18	96,99,106,107	0
23	PHO	BD	403	64/64	0.22	2.17	77,88,92,93	0
32	LMT	BT	101	35/35	0.37	2.17	77,91,94,95	0
22	CLA	AB	614	65/65	0.24	2.15	78,85,98,99	0
22	CLA	AC	513	65/65	0.37	2.14	92,98,104,106	0
22	CLA	AC	504	65/65	0.22	2.11	78,86,107,107	0
26	BCR	BZ	101	40/40	0.29	2.08	81,90,93,94	0
32	LMT	BB	626	35/35	0.35	2.05	76,93,101,102	0
22	CLA	BA	405	65/65	0.19	2.05	72,76,104,105	0
26	BCR	AC	514	40/40	0.21	1.92	56,66,73,74	0
30	LMG	AC	519	48/55	0.30	1.90	75,84,89,90	0
22	CLA	AC	505	65/65	0.21	1.90	69,73,77,79	0
22	CLA	AB	609	65/65	0.23	1.85	76,87,91,92	0
27	DGD	AC	516	53/66	0.23	1.85	57,72,91,92	0
27	DGD	AC	517	62/66	0.20	1.78	70,78,91,92	0
30	LMG	AB	621	49/55	0.23	1.74	62,75,80,83	0
22	CLA	AB	602	65/65	0.22	1.72	81,85,88,90	0
24	PL9	AD	405	55/55	0.21	1.71	52,67,71,73	0
27	DGD	BC	517	62/66	0.22	1.71	78,82,100,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	PL9	BD	405	55/55	0.21	1.70	63,70,76,78	0
27	DGD	AA	410	56/66	0.32	1.68	78,86,91,92	0
22	CLA	AC	503	65/65	0.22	1.67	78,86,92,95	0
26	BCR	AB	620	40/40	0.26	1.64	75,77,83,84	0
34	HEM	AE	101	43/43	0.28	1.63	85,92,103,106	0
32	LMT	BM	101	35/35	0.29	1.60	70,88,97,101	0
22	CLA	BB	609	65/65	0.25	1.57	72,80,96,96	0
22	CLA	AB	606	65/65	0.26	1.56	73,87,96,96	0
29	SQD	AD	409	43/54	0.25	1.54	68,92,108,111	0
22	CLA	BD	404	65/65	0.25	1.53	89,92,101,102	0
22	CLA	BB	606	65/65	0.20	1.53	58,61,74,76	0
22	CLA	BC	510	65/65	0.22	1.48	79,83,92,92	0
30	LMG	AA	413	51/55	0.22	1.42	70,74,77,79	0
26	BCR	AT	102	40/40	0.20	1.40	72,79,91,91	0
27	DGD	BC	516	53/66	0.23	1.39	69,77,96,97	0
22	CLA	AD	402	65/65	0.20	1.37	47,58,69,71	0
26	BCR	BD	406	40/40	0.22	1.35	66,78,92,92	0
28	LHG	AA	411	39/49	0.22	1.34	63,68,76,78	0
30	LMG	AE	102	44/55	0.30	1.33	81,91,96,96	0
34	HEM	BE	101	43/43	0.27	1.29	93,95,104,107	0
30	LMG	AD	407	46/55	0.19	1.27	63,71,90,92	0
22	CLA	AB	616	65/65	0.29	1.26	73,85,105,106	0
34	HEM	AV	201	43/43	0.21	1.24	60,63,66,67	0
26	BCR	AB	618	40/40	0.18	1.24	75,78,82,83	0
22	CLA	BB	608	65/65	0.19	1.23	45,53,76,78	0
32	LMT	BB	603	35/35	0.35	1.23	68,86,95,96	0
22	CLA	BC	505	65/65	0.23	1.22	88,93,94,95	0
22	CLA	BC	512	65/65	0.32	1.21	95,99,109,110	0
22	CLA	AA	404	65/65	0.20	1.18	63,72,97,99	0
22	CLA	BD	402	65/65	0.18	1.17	50,57,79,83	0
29	SQD	BB	601	47/54	0.28	1.16	74,87,109,111	0
22	CLA	AB	605	65/65	0.21	1.15	68,76,84,85	0
22	CLA	BB	604	65/65	0.34	1.14	86,98,107,109	0
22	CLA	BB	613	65/65	0.21	1.13	69,77,82,84	0
30	LMG	AB	622	49/55	0.19	1.13	64,73,80,83	0
29	SQD	AA	412	51/54	0.25	1.13	73,83,98,99	0
22	CLA	BB	617	65/65	0.23	1.12	75,79,99,100	0
30	LMG	BM	102	42/55	0.30	1.10	72,90,95,98	0
27	DGD	BH	101	58/66	0.20	1.09	66,73,80,81	0
26	BCR	BC	515	40/40	0.29	1.09	74,80,91,92	0
26	BCR	AA	409	40/40	0.21	1.07	59,67,70,71	0
26	BCR	BX	101	40/40	0.34	1.04	76,79,89,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	BCR	AB	619	40/40	0.18	1.04	62,70,82,83	0
32	LMT	AM	102	35/35	0.28	1.02	67,89,93,96	0
27	DGD	AC	518	66/66	0.21	1.00	62,68,84,86	0
29	SQD	BL	101	47/54	0.29	0.99	75,91,115,116	0
27	DGD	BC	518	66/66	0.23	0.99	71,78,89,90	0
22	CLA	BB	605	65/65	0.20	0.95	77,82,86,89	0
22	CLA	BB	619	65/65	0.29	0.92	75,81,93,95	0
26	BCR	BB	620	40/40	0.20	0.88	66,69,72,73	0
22	CLA	AA	402	65/65	0.17	0.87	51,58,66,69	0
28	LHG	BA	412	39/49	0.24	0.86	72,77,80,81	0
22	CLA	AB	612	65/65	0.22	0.85	63,75,81,83	0
22	CLA	BC	504	65/65	0.20	0.80	87,92,102,102	0
22	CLA	BB	615	65/65	0.18	0.80	60,72,77,81	0
22	CLA	AC	501	65/65	0.21	0.80	78,83,85,86	0
22	CLA	BC	507	65/65	0.23	0.79	84,92,96,97	0
22	CLA	AA	403	65/65	0.16	0.78	41,48,56,60	0
30	LMG	BB	624	49/55	0.18	0.77	68,72,78,79	0
23	PHO	AA	405	64/64	0.17	0.77	40,64,67,69	0
23	PHO	AD	403	64/64	0.17	0.76	39,56,70,72	0
29	SQD	BA	413	51/54	0.25	0.75	73,90,103,104	0
22	CLA	AC	506	65/65	0.23	0.75	83,87,101,102	0
26	BCR	BA	410	40/40	0.20	0.71	61,74,82,83	0
22	CLA	AB	611	65/65	0.19	0.66	62,68,71,73	0
22	CLA	BC	509	65/65	0.23	0.66	73,83,93,94	0
22	CLA	BC	508	65/65	0.23	0.62	92,97,101,106	0
26	BCR	AD	406	40/40	0.16	0.61	64,72,85,85	0
27	DGD	AH	102	58/66	0.20	0.60	57,72,85,86	0
22	CLA	BB	607	65/65	0.19	0.59	53,64,86,87	0
34	HEM	BV	201	43/43	0.19	0.59	58,67,76,79	0
30	LMG	BA	414	51/55	0.20	0.57	62,71,78,80	0
23	PHO	BA	406	64/64	0.17	0.57	54,61,70,74	0
22	CLA	AB	608	65/65	0.18	0.52	72,79,87,91	0
29	SQD	BD	409	43/54	0.24	0.50	73,88,110,111	0
26	BCR	BB	621	40/40	0.18	0.48	57,69,82,83	0
22	CLA	AB	610	65/65	0.20	0.46	60,67,79,80	0
22	CLA	BB	610	65/65	0.17	0.46	60,70,77,81	0
22	CLA	AB	613	65/65	0.17	0.46	65,69,84,87	0
30	LMG	AM	101	42/55	0.28	0.46	68,86,93,95	0
22	CLA	AB	615	65/65	0.21	0.44	83,93,97,99	0
22	CLA	BC	502	65/65	0.22	0.43	81,85,101,103	0
26	BCR	AC	515	40/40	0.22	0.43	69,75,80,81	0
22	CLA	AC	508	65/65	0.19	0.41	80,86,99,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	AC	511	65/65	0.24	0.40	77,85,89,90	0
22	CLA	BC	511	65/65	0.25	0.37	91,99,104,105	0
33	BCT	BD	401	4/4	0.17	0.37	84,86,87,88	0
26	BCR	AB	617	40/40	0.18	0.35	56,67,75,76	0
22	CLA	AC	509	65/65	0.21	0.34	59,74,86,89	0
35	CA	AO	301	1/1	0.22	0.31	87,87,87,87	0
22	CLA	BB	618	65/65	0.21	0.29	69,84,87,88	0
22	CLA	BA	403	65/65	0.18	0.28	57,64,71,75	0
22	CLA	AB	607	65/65	0.15	0.27	50,55,74,74	0
22	CLA	BC	506	65/65	0.23	0.24	81,85,97,99	0
22	CLA	AB	603	65/65	0.17	0.19	54,60,72,74	0
22	CLA	BC	503	65/65	0.21	0.13	82,97,100,101	0
22	CLA	BC	501	65/65	0.19	0.02	76,80,87,88	0
22	CLA	BB	616	65/65	0.15	-0.02	49,54,79,82	0
22	CLA	BA	404	65/65	0.15	-0.06	55,60,68,70	0
22	CLA	BB	614	65/65	0.16	-0.13	59,68,75,77	0
22	CLA	BB	611	65/65	0.16	-0.21	67,74,81,85	0
25	OEC	AA	408	5/9	0.14	-0.25	56,62,67,75	0
25	OEC	BA	409	5/9	0.15	-0.27	30,74,79,92	0
22	CLA	AC	502	65/65	0.16	-0.29	50,58,81,84	0
35	CA	BK	101	1/1	0.12	-0.92	90,90,90,90	0
22	CLA	AC	510	65/65	0.14	-1.36	48,56,70,72	0
21	FE2	AA	401	1/1	0.12	-1.61	69,69,69,69	0
35	CA	AK	101	1/1	0.10	-2.63	95,95,95,95	0
21	FE2	BA	402	1/1	0.11	-4.20	81,81,81,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.