



Full wwPDB X-ray Structure Validation Report

Jun 17, 2014 – 05:46 AM BST

PDB ID : 4V82
Title : Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors : Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.;
Saenger, W.; Zouni, A.
Deposited on : 2010-11-30
Resolution : 3.20 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>

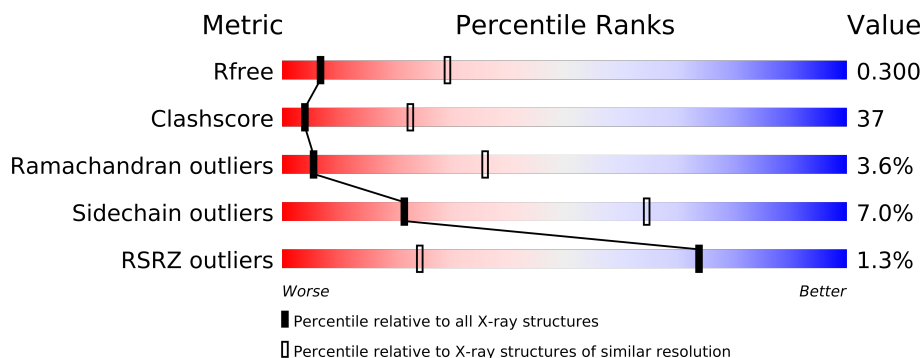
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	461	
3	BC	461	
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	41	
18	BX	41	
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
24	CLA	AA	406	-	X
24	CLA	AA	407	-	X
24	CLA	AB	601	-	X
24	CLA	AB	605	-	X
24	CLA	AB	608	-	X
24	CLA	AB	615	-	X
24	CLA	AB	616	-	X
24	CLA	AC	504	-	X
24	CLA	AD	404	-	X
24	CLA	BA	5408	-	X
24	CLA	BB	5605	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
24	CLA	BB	5609	-	X
24	CLA	BB	5612	-	X
24	CLA	BC	5504	-	X
24	CLA	BC	5513	-	X
24	CLA	BD	5405	-	X
27	BCR	AB	617	-	X
27	BCR	AC	515	-	X
27	BCR	AC	516	-	X
27	BCR	AD	406	-	X
27	BCR	AJ	101	-	X
27	BCR	AK	102	-	X
27	BCR	AT	101	-	X
27	BCR	AX	101	-	X
27	BCR	BB	5621	-	X
27	BCR	BB	5623	-	X
27	BCR	BC	5515	-	X
27	BCR	BD	5407	-	X
27	BCR	BJ	5101	-	X
27	BCR	BT	5101	-	X
27	BCR	BX	5101	-	X
28	DGD	AA	411	-	X
28	DGD	AB	628	-	X
28	DGD	AC	517	-	X
28	DGD	AC	518	-	X
28	DGD	AC	519	-	X
28	DGD	AE	101	-	X
28	DGD	BA	5412	-	X
28	DGD	BB	5602	-	X
28	DGD	BC	5518	-	X
28	DGD	BC	5519	-	X
28	DGD	BE	5102	-	X
29	LHG	BA	5415	-	X
30	SQD	AB	622	-	X
30	SQD	AF	102	-	X
30	SQD	BA	5401	-	X
30	SQD	BB	5625	-	X
31	LMG	AA	414	-	X
31	LMG	AA	417	-	X
31	LMG	AB	620	-	X
31	LMG	AB	621	-	X
31	LMG	AC	520	-	X
31	LMG	AC	521	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
31	LMG	AD	407	-	X
31	LMG	AD	408	-	X
31	LMG	AI	101	-	X
31	LMG	AJ	102	-	X
31	LMG	BA	5402	-	X
31	LMG	BB	5624	-	X
31	LMG	BC	5520	-	X
31	LMG	BD	5408	-	X
31	LMG	BD	5410	-	X
31	LMG	BE	5101	-	X
31	LMG	BI	5101	-	X
31	LMG	BL	5101	-	X
32	LMT	AB	623	-	X
32	LMT	AB	624	-	X
32	LMT	AB	629	-	X
32	LMT	AB	630	-	X
32	LMT	AD	409	-	X
32	LMT	AI	102	-	X
32	LMT	AI	103	-	X
32	LMT	AM	102	-	X
32	LMT	BB	5603	-	X
32	LMT	BB	5604	-	X
32	LMT	BB	5626	-	X
32	LMT	BB	5627	-	X
32	LMT	BC	5522	-	X
32	LMT	BI	5102	-	X
32	LMT	BM	5101	-	X
33	DMS	AB	625	-	X
33	DMS	AB	626	-	X
33	DMS	AV	202	-	X
33	DMS	BB	5628	-	X
33	DMS	BV	5203	-	X
35	PL9	AD	405	-	X
37	CA	BO	5301	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 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 1.

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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	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	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			
9	BJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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 Photosystem II reaction center 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 reaction center X 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 PSBX PROTEIN.

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				

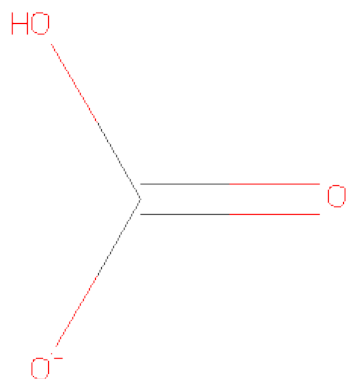
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	BD	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

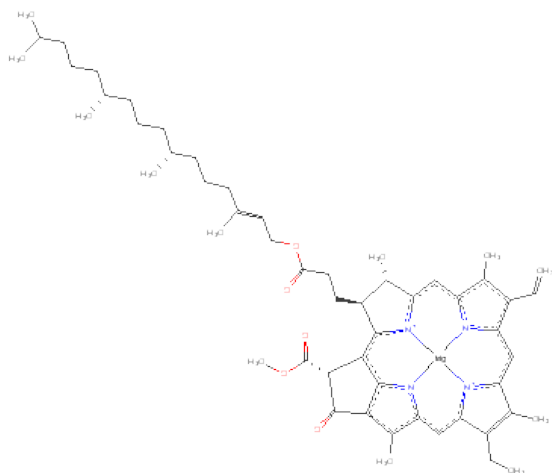


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	AA	1	Total	Cl	0	1
			2	2		
23	BA	1	Total	Cl	0	1
			2	2		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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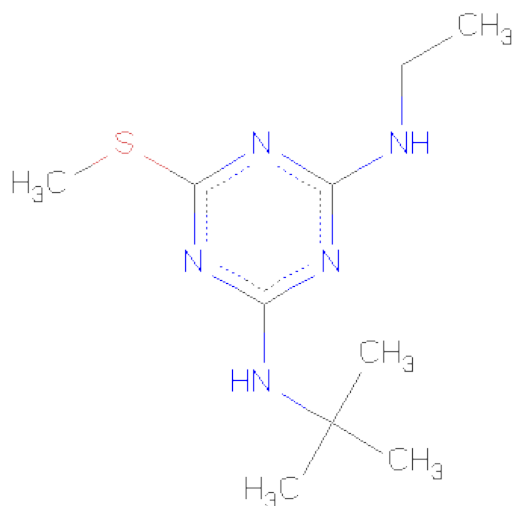
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55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

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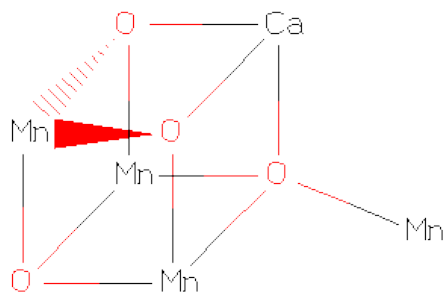
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55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

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: C₁₀H₁₉N₅S).



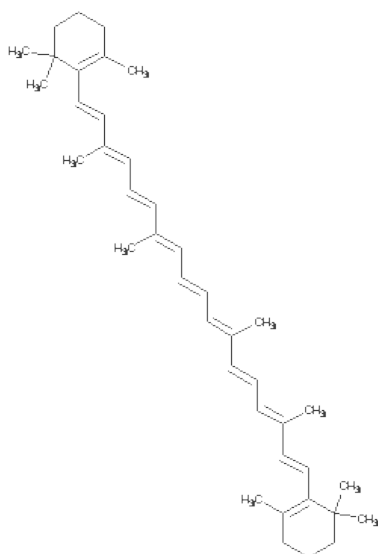
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



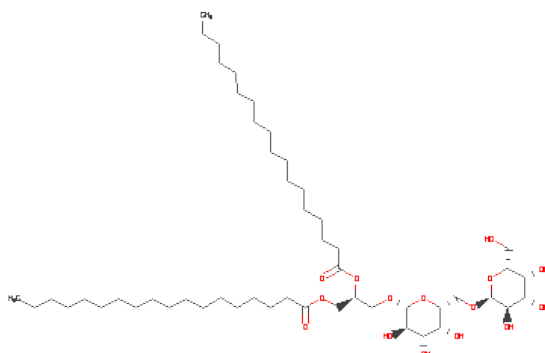
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

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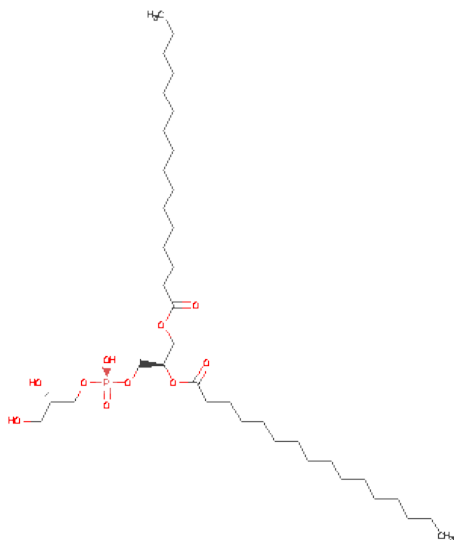
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



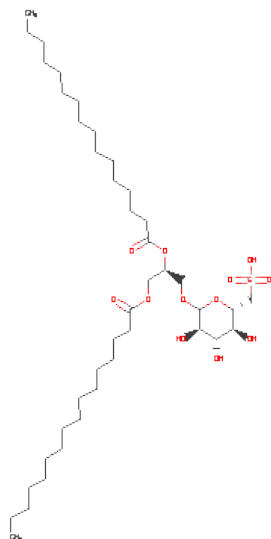
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



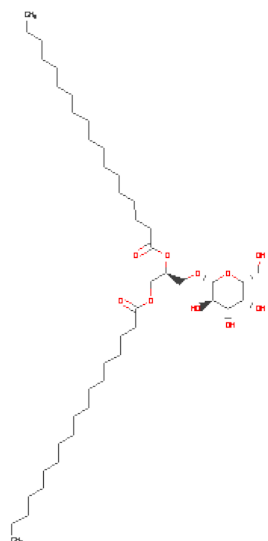
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

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

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



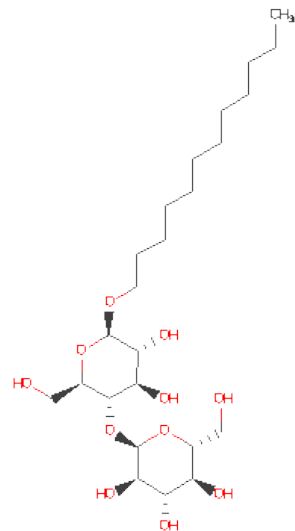
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			42	32	10		
31	AB	1	Total	C	O	0	0
			51	41	10		
31	AB	1	Total	C	O	0	0
			49	39	10		
31	AC	1	Total	C	O	0	0
			48	38	10		
31	AC	1	Total	C	O	0	0
			45	35	10		
31	AD	1	Total	C	O	0	0
			49	39	10		
31	AD	1	Total	C	O	0	0
			48	38	10		
31	AI	1	Total	C	O	0	0
			43	33	10		
31	AJ	1	Total	C	O	0	0
			46	36	10		
31	AM	1	Total	C	O	0	0
			42	32	10		
31	BA	1	Total	C	O	0	0
			42	32	10		
31	BB	1	Total	C	O	0	0
			49	39	10		
31	BC	1	Total	C	O	0	0
			48	38	10		
31	BC	1	Total	C	O	0	0
			45	35	10		
31	BD	1	Total	C	O	0	0
			46	36	10		
31	BD	1	Total	C	O	0	0
			49	39	10		
31	BD	1	Total	C	O	0	0
			48	38	10		
31	BE	1	Total	C	O	0	0
			44	34	10		
31	BI	1	Total	C	O	0	0
			43	33	10		
31	BL	1	Total	C	O	0	0
			51	41	10		
31	BM	1	Total	C	O	0	0
			42	32	10		

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



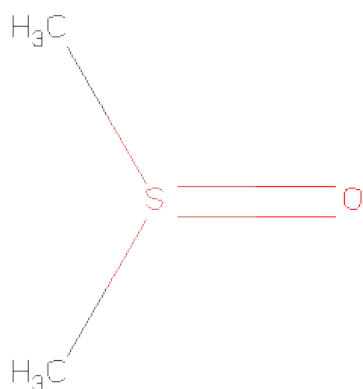
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BC	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



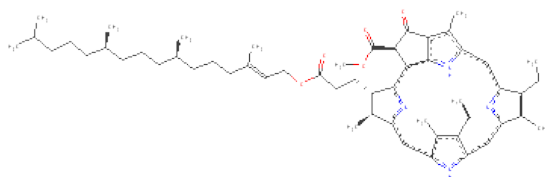
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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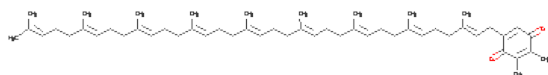
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



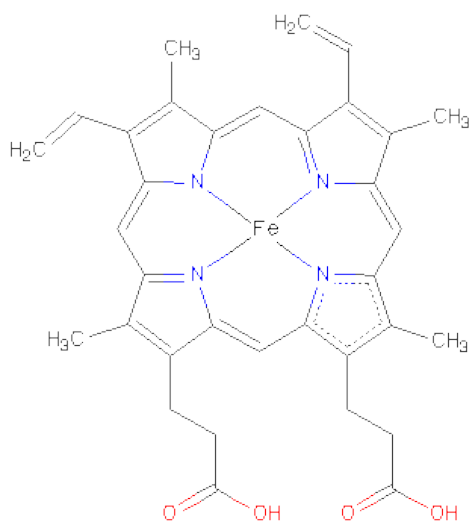
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 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: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	AD	1	Total	C	O	0	0
			55	53	2		
35	BD	1	Total	C	O	0	0
			55	53	2		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

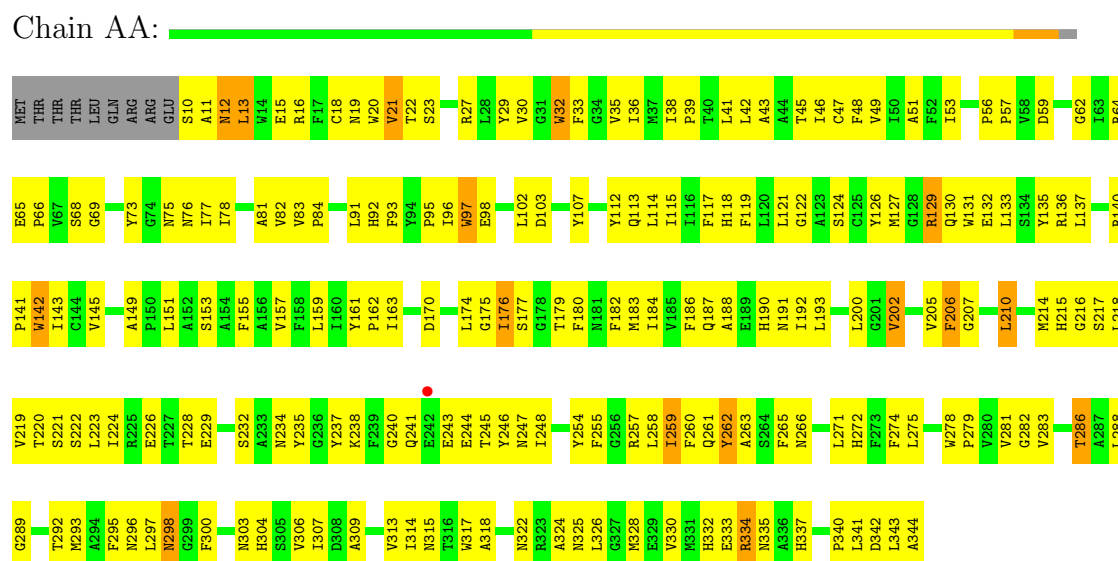
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	BO	1	Total 1	Ca 1	0	0
37	AK	1	Total 1	Ca 1	0	0
37	BF	1	Total 1	Ca 1	0	0
37	BK	1	Total 1	Ca 1	0	0
37	AO	1	Total 1	Ca 1	0	0
37	AF	1	Total 1	Ca 1	0	0

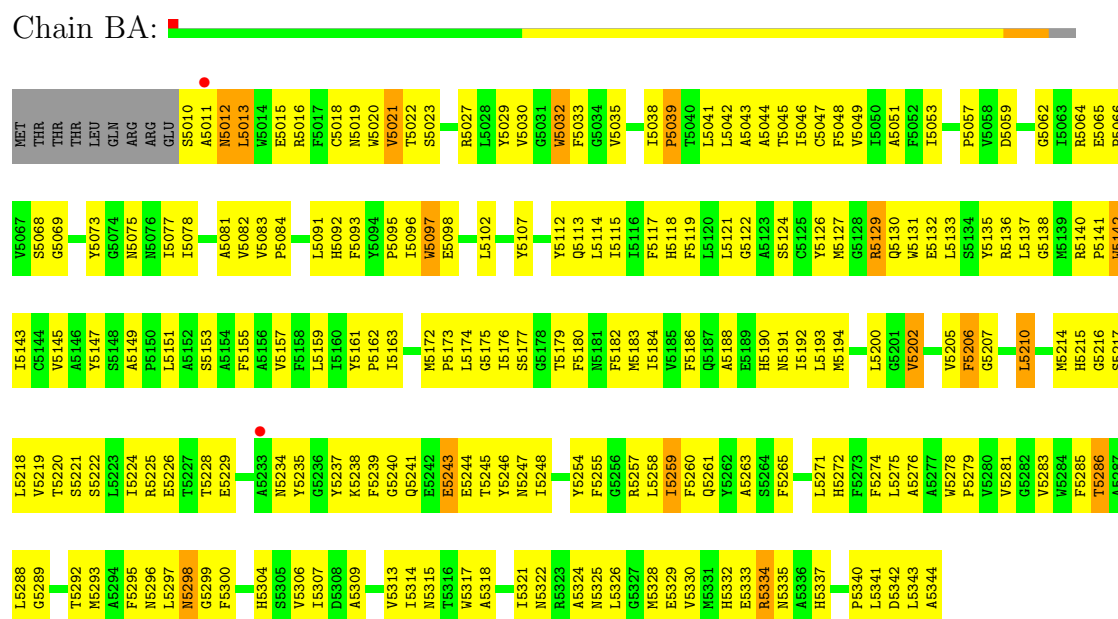
3 Residue-property plots

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 1

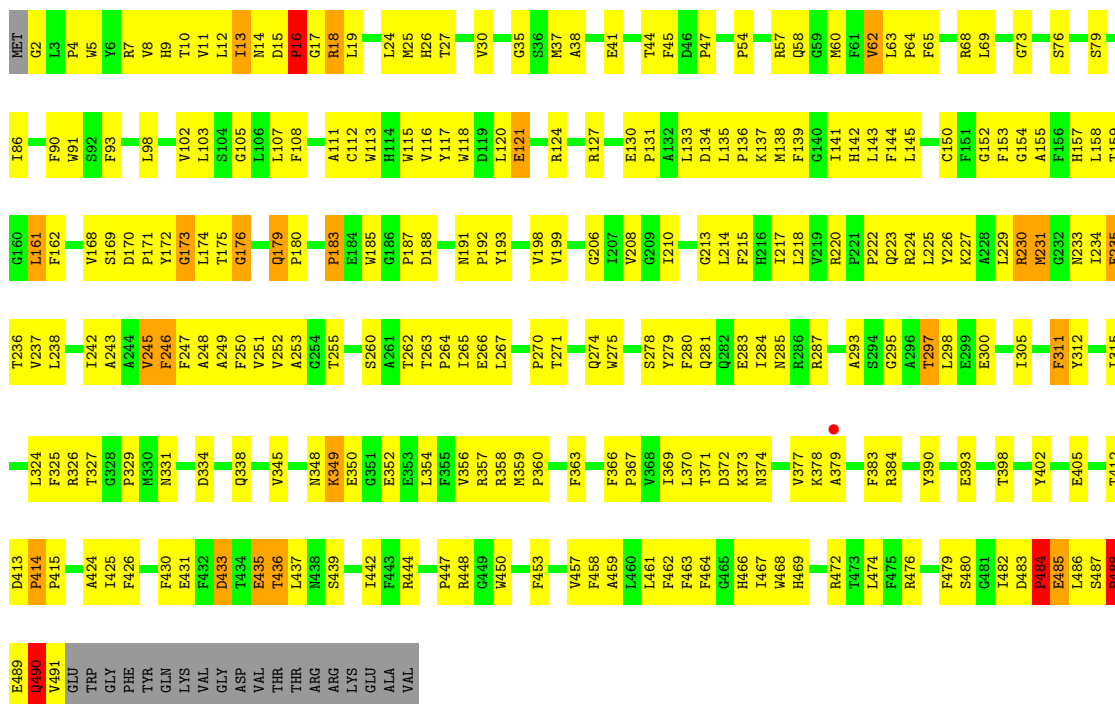


• Molecule 1: Photosystem Q(B) protein 1



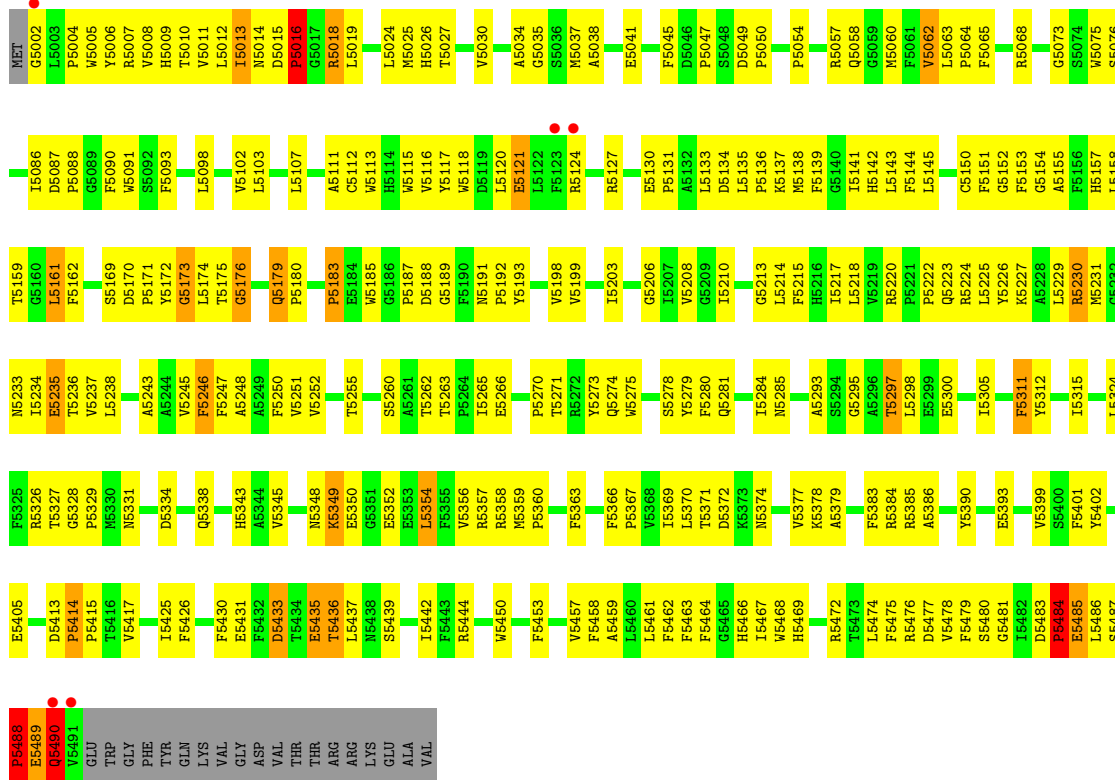
• Molecule 2: Photosystem II core light harvesting protein

Chain AB:



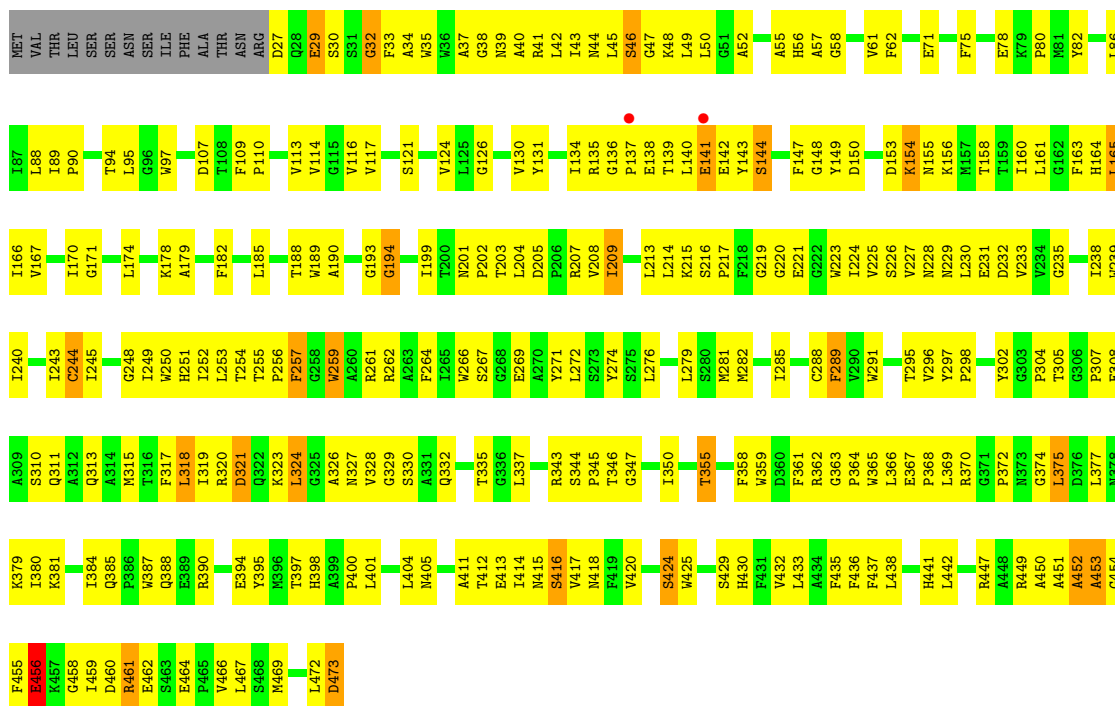
• Molecule 2: Photosystem II core light harvesting protein

Chain BB:



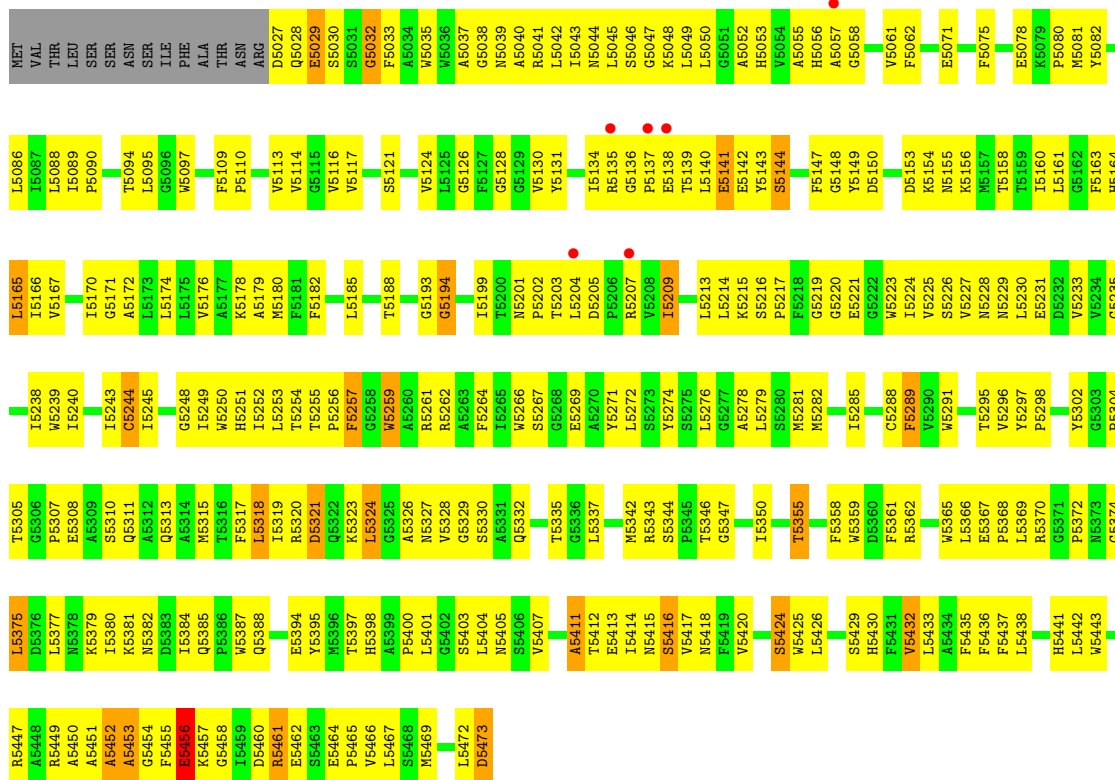
• Molecule 3: Photosystem II CP43 protein

Chain AC:



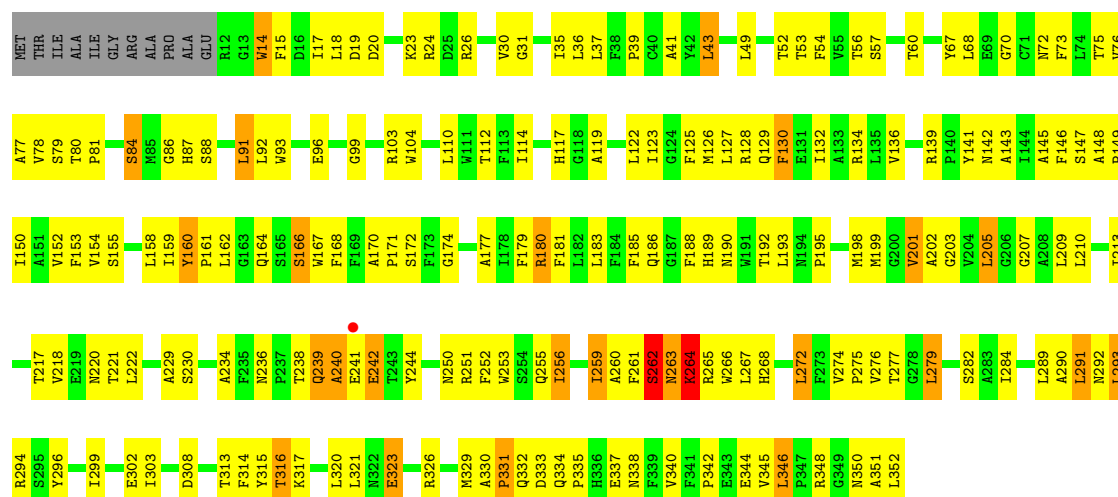
- Molecule 3: Photosystem II CP43 protein

Chain BC:



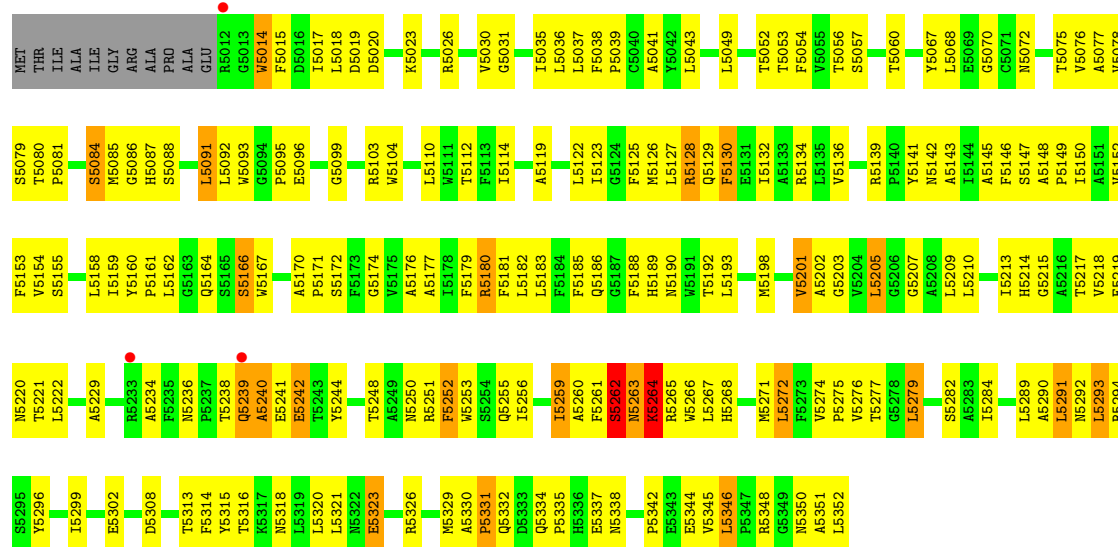
- Molecule 4: Photosystem II D2 protein

Chain AD:



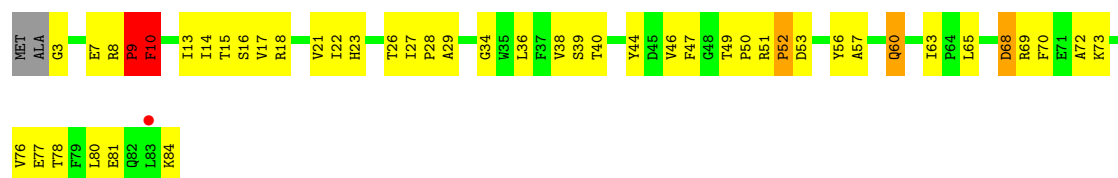
• Molecule 4: Photosystem II D2 protein

Chain BD:



• Molecule 5: Cytochrome b559 subunit alpha

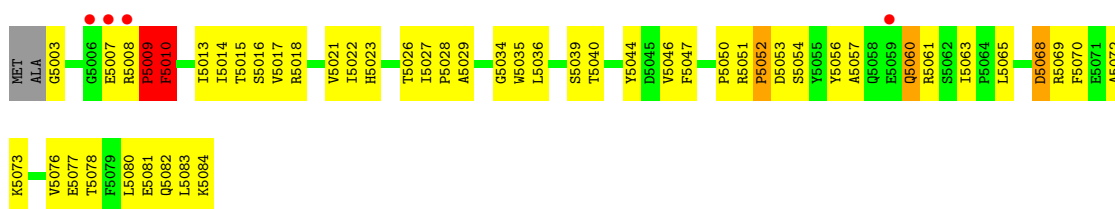
Chain AE:



• Molecule 5: Cytochrome b559 subunit alpha

Chain BE:





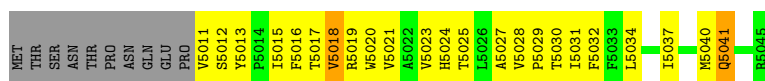
- Molecule 6: Cytochrome b559 subunit beta

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:



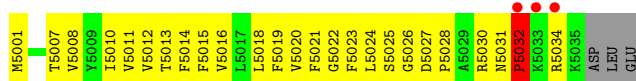
- Molecule 8: Photosystem II reaction center protein I

Chain AI:



- Molecule 8: Photosystem II reaction center protein I

Chain BI:



- Molecule 9: Photosystem II reaction center protein J

Chain AJ:



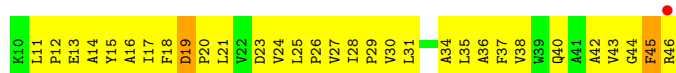
- Molecule 9: Photosystem II reaction center protein J

Chain BJ:



- Molecule 10: Photosystem II reaction center protein K

Chain AK:



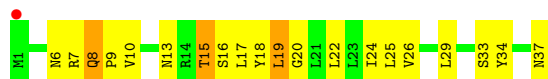
- Molecule 10: Photosystem II reaction center protein K

Chain BK:



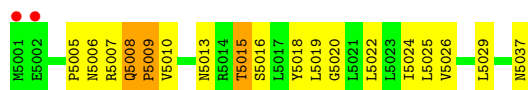
- Molecule 11: Photosystem II reaction center protein L

Chain AL:



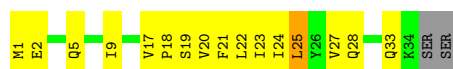
- Molecule 11: Photosystem II reaction center protein L

Chain BL:



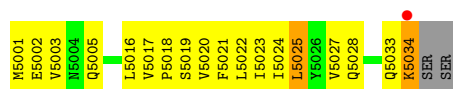
- Molecule 12: Photosystem II reaction center protein M

Chain AM:



- Molecule 12: Photosystem II reaction center protein M

Chain BM:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

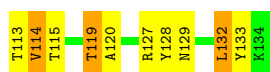
Y266	P271	A272	G170	E171	N173	R178	T179	A180	N181	F182	L183	D184	P185	K186	G187	R188	G189	L190	A191	S192	G193	Y194	Q202	E206	E207	R210	K214	R215	L218	T219	K220	G221	Q222	I223	S224	L225	V230	D231	G232	R233	T234	G235	G236	T240	G252	V259	K260	G263	V264	T265	T98	T101	L104	D105	Q106	T107	Q108	G109	M114	S115	D116	G117	S118	L119	T120	F121	V122	E123	E124	D125	G126	I127	D128	F129	Q130	P131	V132	T133	V134	Q135	R141	L144	F145	L146	T147	V148	K149	N150	L151	V152	A153	K154	T155	Q156	P157	N158	V159	T160	S161	S165	T166	D167	F168	V169	A1A	L1A	G1A	T30	L31	T32	Y33	D34	D35	I36	T39	G40	L41	A42	M43	P46	T51	A52	A55	Y56	P57	L58	D59	S60	S61	Y64	R65	I66	L69	C70	L71	Q72	P73	L77	E80	E81	P82	K83	N84	K85	R86	Q87	O88	A89	E90	F91	V92	P93	T94	V02
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|-------|-------|-------|-------|
| V5264 | D5167 | V5097 | ALA |
| F5265 | K5168 | T5098 | ALA |
| Y5266 | K5169 | | LYS |
| | G5170 | T5101 | GLN |
| P5271 | E5171 | | T5030 |
| A5272 | F5172 | L5104 | L5031 |
| | N5173 | D5105 | T5032 |
| | | Q5106 | T5033 |
| | R5178 | T5107 | D5034 |
| | T5179 | Q5108 | D5035 |
| | A5180 | G5109 | I5036 |
| | N5181 | | |
| | F5182 | K5112 | T5039 |
| | L5183 | N5113 | G5040 |
| | D5184 | N5114 | L5041 |
| | P5185 | S5115 | A5042 |
| | K5186 | D5116 | N5043 |
| | G5187 | G5117 | |
| | R5188 | S5118 | P5046 |
| | G5189 | L5119 | |
| | L5190 | T5120 | T5061 |
| | A5191 | F5121 | A5062 |
| | S5192 | V5122 | |
| | G5193 | E5123 | A5065 |
| | Y5194 | E5124 | Y5066 |
| | | D5125 | |
| | Q5202 | G5126 | D5069 |
| | | T5127 | S5060 |
| | E5206 | D5128 | S5061 |
| | E5207 | F5129 | |
| | | Q5130 | Y5064 |
| | R5210 | P5131 | R5065 |
| | K5214 | V5132 | I5066 |
| | R5215 | T5133 | |
| | | V5134 | L5069 |
| | | Q5135 | G5070 |
| | L5218 | | L5071 |
| | T5219 | R5141 | Q5072 |
| | K5220 | | |
| | Q5221 | L5144 | T5075 |
| | S5223 | | F5076 |
| | S5224 | T5147 | L5077 |
| | L5225 | V5148 | V5078 |
| | | K5149 | S5079 |
| | V5230 | N5150 | E5080 |
| | D5231 | L5151 | E5081 |
| | | V5152 | P5082 |
| | T5234 | A5153 | K5083 |
| | G5235 | S5154 | N5084 |
| | E5236 | T5155 | K5085 |
| | | Q5156 | R5086 |
| | | P5157 | Q5087 |
| | T5240 | N5158 | E5088 |
| | | V5159 | A5089 |
| | G5252 | T5160 | T5090 |
| | V5259 | S5161 | F5091 |
| | K5260 | T5162 | P5092 |
| | | | P5093 |
| | | S5165 | T5094 |
| | C5263 | | |

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|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | I4 | I14 | I15 | I16 | I17 | I18 | I19 | A20 | I21 | F22 | F23 | R24 | E25 | P26 | I29 | T30 | K31 | K32 |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

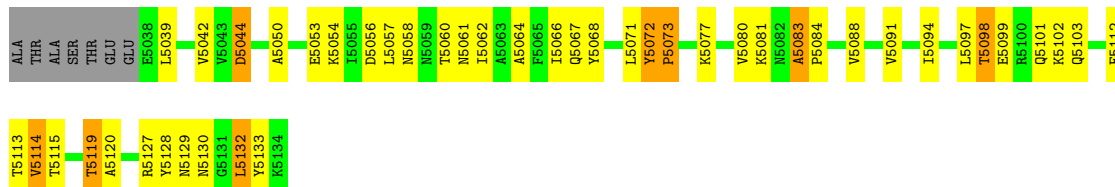
- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|--|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| M5001 | E5002 | T5003 | I5004 | T5005 | Y5006 | | I5014 | A5015 | L5016 | F5017 | F5018 | F5019 | A5020 | I5021 | F5022 | F5023 | R5024 | E5025 | P5026 | P5027 | R5028 | I5029 | T5030 | K5031 | K5032 |
|-------|-------|-------|-------|-------|-------|--|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|
| ALA | THR | ALA | SER | THR | GLU | GLU | E38 | L39 | V42 | V43 | D44 | A50 | Y51 | G52 | E53 | K54 | I55 | D56 | L57 | N58 | N59 | T60 | N61 | I62 | A63 | A64 | F65 | I66 | Q67 | Y68 | L71 | Y72 | P73 | T74 | L75 | V80 | A83 | P84 | V88 | E89 | D90 | V91 | I94 | L97 | T98 | Q101 | K102 | Q103 | F104 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|



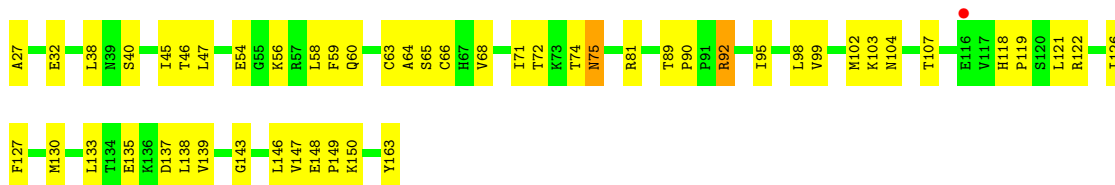
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU:



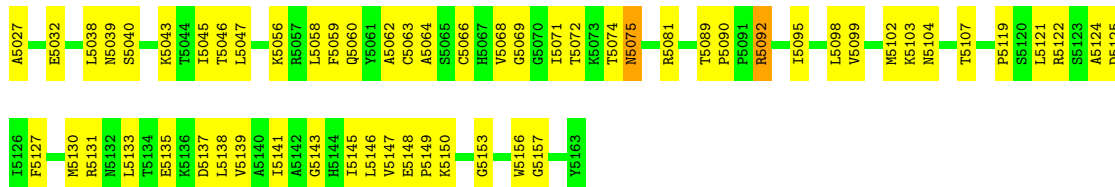
- Molecule 16: Cytochrome c-550

Chain AV:



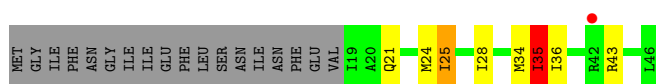
- Molecule 16: Cytochrome c-550

Chain BV:



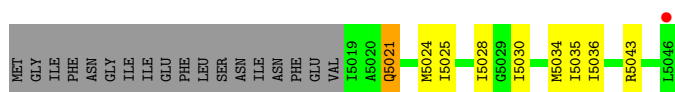
- Molecule 17: Photosystem II reaction center protein ycf12

Chain Ay:



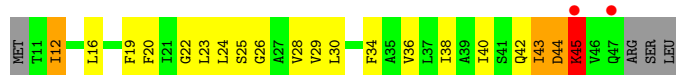
- Molecule 17: Photosystem II reaction center protein ycf12

Chain By:



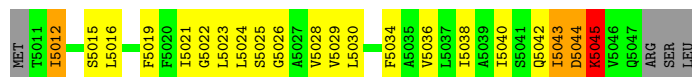
- Molecule 18: Photosystem II reaction center X protein

Chain AX:



- Molecule 18: Photosystem II reaction center X protein

Chain BX:



- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain AY:



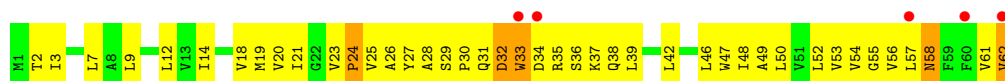
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:



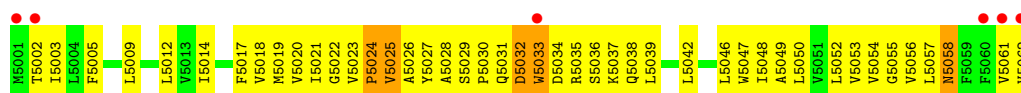
- Molecule 20: Photosystem II reaction center protein Z

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	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 39.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.1 (39.38-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.281 , 0.300	Depositor DCC
R_{free} test set	3179 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 159033 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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, MST, LMT, CLA, PL9, BCT, DMS, 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	0.50	0/2713	0.72	0/3700
1	BA	0.52	0/2713	0.72	0/3700
2	AB	0.51	0/3986	0.73	0/5433
2	BB	0.52	0/3986	0.73	3/5433 (0.1%)
3	AC	0.46	0/3556	0.71	1/4842 (0.0%)
3	BC	0.47	0/3556	0.71	1/4842 (0.0%)
4	AD	0.53	0/2806	0.73	0/3825
4	BD	0.55	0/2806	0.73	0/3825
5	AE	0.51	0/685	0.76	0/933
5	BE	0.54	0/685	0.77	0/933
6	AF	0.75	0/291	0.78	0/397
6	BF	0.71	0/291	0.74	0/397
7	AH	0.47	0/520	0.78	0/709
7	BH	0.49	0/520	0.79	0/709
8	AI	0.58	0/293	0.77	0/395
8	BI	0.64	0/293	0.81	0/395
9	AJ	0.55	0/277	0.86	0/375
9	BJ	0.67	0/277	0.88	0/375
10	AK	0.54	0/303	0.73	0/416
10	BK	0.62	0/303	0.73	0/416
11	AL	0.58	0/311	0.78	1/422 (0.2%)
11	BL	0.57	0/311	0.81	0/422
12	AM	0.65	0/270	0.87	0/367
12	BM	0.66	0/270	0.85	0/367
13	AO	0.49	0/1876	0.76	0/2548
13	BO	0.48	0/1876	0.76	1/2548 (0.0%)
14	AT	0.80	1/284 (0.4%)	0.82	0/381
14	BT	0.81	1/284 (0.4%)	0.87	2/381 (0.5%)
15	AU	0.54	0/785	0.84	2/1064 (0.2%)
15	BU	0.52	0/785	0.83	0/1064
16	AV	0.46	0/1081	0.70	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BV	0.46	0/1081	0.70	0/1468
17	Ay	1.12	1/202 (0.5%)	1.24	1/272 (0.4%)
17	By	1.03	1/202 (0.5%)	1.22	1/272 (0.4%)
18	AX	0.57	0/273	0.76	0/370
18	BX	0.63	0/273	0.69	0/370
20	AZ	0.53	0/490	0.75	1/669 (0.1%)
20	BZ	0.60	0/490	0.80	0/669
All	All	0.53	4/42004 (0.0%)	0.75	14/57172 (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
2	BB	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-5.67	1.41	1.54
14	BT	5032	LYS	C-OXT	5.50	1.33	1.23
17	Ay	35	ILE	CA-CB	-5.35	1.42	1.54
14	AT	32	LYS	CA-CB	5.19	1.65	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BO	5030	THR	N-CA-CB	-5.76	99.35	110.30
2	BB	5488	PRO	N-CA-C	5.72	126.97	112.10
2	BB	5489	GLU	N-CA-C	5.65	126.27	111.00
14	BT	5004	ILE	CB-CA-C	-5.65	100.31	111.60
3	AC	32	GLY	N-CA-C	-5.56	99.19	113.10
17	By	5021	GLN	N-CA-CB	-5.41	100.87	110.60
14	BT	5032	LYS	CB-CA-C	-5.38	99.64	110.40
17	Ay	25	ILE	CB-CA-C	-5.38	100.84	111.60
11	AL	19	LEU	CA-CB-CG	5.35	127.61	115.30
15	AU	57	LEU	CA-CB-CG	-5.30	103.11	115.30
3	BC	5032	GLY	N-CA-C	-5.08	100.39	113.10
15	AU	72	TYR	N-CA-C	5.08	124.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	5354	LEU	CA-CB-CG	-5.07	103.64	115.30
20	AZ	7	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain
2	BB	5273	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	300	0
1	BA	2628	0	2524	309	0
2	AB	3850	0	3718	344	0
2	BB	3850	0	3718	351	0
3	AC	3444	0	3365	350	0
3	BC	3444	0	3365	358	0
4	AD	2711	0	2610	245	0
4	BD	2711	0	2610	255	0
5	AE	666	0	651	68	0
5	BE	666	0	651	76	0
6	AF	282	0	291	36	0
6	BF	282	0	291	32	0
7	AH	507	0	521	65	0
7	BH	507	0	521	69	0
8	AI	286	0	308	34	0
8	BI	286	0	305	37	0
9	AJ	271	0	276	36	0
9	BJ	271	0	276	38	0
10	AK	293	0	305	48	0
10	BK	293	0	305	45	0
11	AL	304	0	316	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BL	304	0	313	35	0
12	AM	267	0	289	26	0
12	BM	267	0	286	26	0
13	AO	1845	0	1801	137	0
13	BO	1845	0	1801	142	0
14	AT	275	0	288	28	0
14	BT	275	0	285	27	0
15	AU	774	0	773	52	0
15	BU	774	0	773	51	0
16	AV	1060	0	1068	48	0
16	BV	1060	0	1068	48	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	33	0
18	BX	270	0	299	27	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	53	0
20	BZ	479	0	513	55	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0
24	AA	260	0	288	41	0
24	AB	1040	0	1152	133	0
24	AC	845	0	936	91	0
24	AD	130	0	144	17	0
24	BA	260	0	288	44	0
24	BB	1040	0	1152	142	0
24	BC	845	0	936	94	0
24	BD	130	0	144	18	0
25	AA	16	0	19	9	0
25	BA	16	0	19	9	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	8	0
27	AC	120	0	168	24	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AK	40	0	56	5	0
27	AT	40	0	56	10	0
27	AX	40	0	56	8	0
27	BA	40	0	56	3	0
27	BB	120	0	168	8	0
27	BC	120	0	168	25	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	6	0
27	BX	40	0	56	4	0
28	AA	56	0	70	9	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	9	0
28	BA	56	0	70	9	0
28	BB	52	0	62	5	0
28	BC	181	0	243	64	0
28	BE	63	0	87	1	0
28	BH	58	0	74	8	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	17	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	15	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	4	0
31	BI	43	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	1	0
32	BB	140	0	184	16	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	2	0
33	AB	8	0	12	0	0
33	AU	4	0	6	0	0
33	AV	4	0	6	0	0
33	BB	8	0	12	0	0
33	BV	8	0	12	0	0
34	AD	128	0	148	14	0
34	BD	128	0	148	15	0
35	AD	55	0	80	15	0
35	BD	55	0	80	16	0
36	AF	43	0	30	8	0
36	AV	43	0	30	4	0
36	BF	43	0	30	7	0
36	BV	43	0	30	6	0
37	AF	1	0	0	0	0
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3700	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 37.

All (3700) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:BU:5083:ALA:HB1	15:BU:5084:PRO:HD2	1.29	1.09
10:AK:28:ILE:HA	10:AK:31:LEU:HD12	1.35	1.09
1:BA:5325:ASN:HA	1:BA:5328:MET:HE3	1.34	1.08
1:AA:102:LEU:HB2	31:AA:417:LMG:H351	1.10	1.08
10:BK:5028:ILE:HA	10:BK:5031:LEU:HD12	1.35	1.08
2:BB:5027:THR:HG22	2:BB:5107:LEU:HD13	1.36	1.08
1:AA:278:TRP:CE3	28:AC:519:DGD:CIA	2.38	1.07
13:BO:5087:GLN:O	13:BO:5088:GLU:HG3	1.54	1.07
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.33	1.06
16:AV:63:CYS:SG	36:AV:201:HEM:HAB	1.96	1.06
1:BA:5200:LEU:HD11	28:BC:5519:DGD:HAW2	1.38	1.05
28:BA:5412:DGD:O2D	3:BC:5216:SER:HB2	1.57	1.04
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.35	1.04
9:BJ:5015:THR:HG21	10:BK:5038:VAL:HG13	1.35	1.04
13:BO:5082:PRO:HG3	13:BO:5089:ALA:HB2	1.34	1.04
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.22	1.04
1:AA:200:LEU:CD1	28:AC:519:DGD:HAW2	1.88	1.03
13:AO:87:GLN:O	13:AO:88:GLU:HG3	1.56	1.03
3:AC:52:ALA:HA	24:AC:511:CLA:HMB3	1.42	1.02
1:BA:5200:LEU:CD1	28:BC:5519:DGD:HAW2	1.89	1.01
2:BB:5260:SER:OG	2:BB:5262:THR:HG22	1.61	1.00
3:BC:5254:THR:HG22	3:BC:5255:THR:H	1.26	1.00
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.40	1.00
28:AA:411:DGD:O2D	3:AC:216:SER:HB2	1.61	1.00
1:AA:200:LEU:HD11	28:AC:519:DGD:HAW2	1.42	0.99
2:AB:260:SER:OG	2:AB:262:THR:HG22	1.60	0.99
1:AA:325:ASN:HA	1:AA:328:MET:HE3	1.41	0.99
3:BC:5052:ALA:HA	24:BC:5511:CLA:HMB3	1.43	0.98
4:AD:14:TRP:HE1	7:AH:25:TRP:HH2	1.12	0.97
3:AC:254:THR:HG22	3:AC:255:THR:H	1.26	0.97
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.47	0.97
5:BE:5056:TYR:O	16:BV:5027:ALA:HB2	1.64	0.96
1:BA:5278:TRP:CE3	28:BC:5519:DGD:CIA	2.48	0.96
2:BB:5476:ARG:HB3	2:BB:5476:ARG:HH11	1.31	0.95
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:H403	1.48	0.95
4:BD:5014:TRP:HE1	7:BH:5025:TRP:HH2	1.14	0.95
16:BV:5063:CYS:SG	36:BV:5201:HEM:HAB	2.07	0.94
13:BO:5069:LEU:HB3	13:BO:5107:ILE:HB	1.48	0.94
2:AB:476:ARG:HH11	2:AB:476:ARG:HB3	1.32	0.94
3:AC:305:THR:HG22	3:AC:308:GLU:CB	1.97	0.94
2:BB:5476:ARG:NH1	2:BB:5476:ARG:HB3	1.82	0.94
2:AB:248:ALA:HA	24:AB:603:CLA:H42	1.49	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.31	0.93
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	1.48	0.93
3:AC:461:ARG:HG3	3:AC:461:ARG:HH11	1.31	0.93
4:BD:5274:VAL:HA	35:BD:5406:PL9:H253	1.51	0.93
3:BC:5461:ARG:HG3	3:BC:5461:ARG:HH11	1.33	0.93
1:BA:5341:LEU:HB2	3:BC:5313:GLN:HE22	1.30	0.92
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.35	0.92
5:AE:15:THR:HG22	9:AJ:7:ARG:H	1.34	0.92
2:AB:476:ARG:NH1	2:AB:476:ARG:HB3	1.84	0.92
18:BX:5026:GLY:O	18:BX:5029:VAL:HG12	1.70	0.92
3:BC:5305:THR:HG22	3:BC:5308:GLU:CB	2.00	0.92
3:BC:5239:TRP:HE3	3:BC:5243:ILE:HD11	1.34	0.91
2:BB:5248:ALA:HA	24:BB:5607:CLA:H42	1.52	0.91
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB2	1.50	0.91
1:BA:5102:LEU:HB2	31:BA:5402:LMG:H351	1.51	0.91
5:BE:5015:THR:HG22	9:BJ:5007:ARG:H	1.35	0.91
4:BD:5103:ARG:HG3	5:BE:5073:LYS:HG3	1.52	0.91
24:BB:5607:CLA:HBB1	24:BB:5609:CLA:H171	1.52	0.91
24:AA:405:CLA:HED1	35:AD:405:PL9:H372	1.53	0.90
24:AC:501:CLA:HMB3	27:AC:516:BCR:H403	1.54	0.90
2:BB:5016:PRO:HG3	2:BB:5133:LEU:HD11	1.49	0.90
15:BU:5088:VAL:O	15:BU:5091:VAL:HG12	1.72	0.90
24:AB:603:CLA:HBB1	24:AB:605:CLA:H171	1.52	0.90
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.51	0.90
1:AA:102:LEU:CB	31:AA:417:LMG:H351	2.00	0.90
2:AB:12:LEU:HD13	2:AB:19:LEU:HA	1.53	0.89
2:BB:5004:PRO:HG2	2:BB:5007:ARG:HD2	1.55	0.89
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	2.02	0.89
18:AX:26:GLY:O	18:AX:29:VAL:HG12	1.72	0.89
4:AD:87:HIS:CD2	4:AD:166:SER:HA	2.07	0.89
14:AT:18:PHE:HB2	27:AT:101:BCR:H10C	1.54	0.89
4:BD:5087:HIS:CD2	4:BD:5166:SER:HA	2.07	0.88
1:BA:5278:TRP:HH2	28:BC:5519:DGD:HBG1	1.38	0.88
24:BA:5406:CLA:HED1	35:BD:5406:PL9:H372	1.55	0.88
5:AE:46:VAL:HG13	28:AE:101:DGD:HG31	1.53	0.88
2:BB:5012:LEU:HD13	2:BB:5019:LEU:HA	1.56	0.88
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.35	0.88
3:BC:5451:ALA:HA	3:BC:5456:GLU:OE2	1.73	0.88
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.56	0.88
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	1.88	0.87
7:BH:5061:SER:HA	28:BH:5101:DGD:HE4	1.54	0.87
13:BO:5230:VAL:HG12	13:BO:5231:ASP:H	1.39	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:451:ALA:HA	3:AC:456:GLU:OE2	1.74	0.87
15:AU:88:VAL:O	15:AU:91:VAL:HG12	1.74	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.56	0.86
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	1.90	0.86
5:BE:5046:VAL:HG13	28:BE:5102:DGD:HG31	1.56	0.86
15:BU:5083:ALA:HB1	15:BU:5084:PRO:CD	2.04	0.86
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.75	0.85
2:BB:5179:GLN:HA	2:BB:5179:GLN:HE21	1.41	0.85
3:BC:5380:ILE:HA	3:BC:5384:ILE:HD11	1.55	0.85
3:BC:5117:VAL:HG11	31:BC:5521:LMG:H192	1.58	0.85
4:BD:5122:LEU:HD21	24:BD:5402:CLA:H92	1.58	0.85
3:AC:130:VAL:HG13	24:AC:511:CLA:H92	1.59	0.85
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.58	0.85
3:BC:5113:VAL:O	3:BC:5117:VAL:HG23	1.75	0.85
1:AA:341:LEU:HB2	3:AC:313:GLN:HE22	1.40	0.85
3:AC:113:VAL:O	3:AC:117:VAL:HG23	1.75	0.85
4:BD:5148:ALA:HB3	4:BD:5149:PRO:HD3	1.59	0.84
7:AH:61:SER:HA	28:AH:101:DGD:HE4	1.59	0.84
2:AB:179:GLN:HE21	2:AB:179:GLN:HA	1.43	0.84
4:AD:274:VAL:HA	35:AD:405:PL9:H253	1.57	0.84
1:BA:5033:PHE:HE1	24:BC:5505:CLA:H92	1.41	0.84
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.58	0.84
1:AA:177:SER:HA	1:AA:180:PHE:HD2	1.42	0.84
5:BE:5015:THR:HG22	9:BJ:5007:ARG:N	1.93	0.84
5:BE:5015:THR:HG23	9:BJ:5008:ILE:O	1.77	0.84
2:BB:5383:PHE:O	13:BO:5192:SER:HA	1.78	0.84
2:AB:223:GLN:HG3	2:AB:227:LYS:HE3	1.60	0.84
16:BV:5066:CYS:SG	36:BV:5201:HEM:HAC	2.18	0.84
24:BA:5406:CLA:H93	34:BD:5403:PHO:HMA1	1.60	0.83
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.78	0.83
1:AA:278:TRP:CZ3	28:AC:519:DGD:HAG2	2.12	0.83
1:BA:5289:GLY:O	1:BA:5292:THR:HG22	1.77	0.83
24:AA:405:CLA:H93	34:AD:402:PHO:HMA1	1.60	0.83
2:BB:5464:PHE:HD2	24:BB:5615:CLA:HAC2	1.43	0.83
13:AO:32:THR:O	13:AO:36:ILE:HD12	1.79	0.83
13:BO:5032:THR:O	13:BO:5036:ILE:HD12	1.77	0.83
3:BC:5130:VAL:HG13	24:BC:5511:CLA:H92	1.60	0.83
5:AE:15:THR:HG22	9:AJ:7:ARG:N	1.93	0.83
4:BD:5148:ALA:HB2	4:BD:5276:VAL:HG13	1.58	0.83
13:BO:5031:LEU:HD12	13:BO:5031:LEU:H	1.44	0.83
31:AD:408:LMG:HC8	11:AL:19:LEU:HD23	1.60	0.83
3:AC:307:PRO:HB3	3:AC:358:PHE:CD1	2.14	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:BC:5504:CLA:C15	28:BC:5519:DGD:HA91	2.08	0.82
1:BA:5278:TRP:CH2	28:BC:5519:DGD:HBG1	2.13	0.82
7:AH:55:LEU:HD21	18:AX:16:LEU:HD23	1.59	0.82
4:BD:5088:SER:HB2	5:BE:5069:ARG:NH2	1.94	0.82
16:AV:66:CYS:SG	36:AV:201:HEM:HAC	2.20	0.82
2:AB:464:PHE:HD2	24:AB:611:CLA:HAC2	1.45	0.82
32:AB:629:LMT:H51	14:BT:5004:ILE:HG13	1.60	0.82
35:BD:5406:PL9:H201	31:BL:5101:LMG:H182	1.61	0.82
1:AA:278:TRP:HH2	28:AC:519:DGD:HBG1	1.42	0.82
3:BC:5116:VAL:HG21	27:BC:5515:BCR:H323	1.62	0.82
2:AB:155:ALA:O	2:AB:161:LEU:HD22	1.79	0.82
1:AA:192:ILE:HA	1:AA:293:MET:HE3	1.62	0.81
2:AB:121:GLU:HG3	7:AH:4:ARG:HA	1.60	0.81
2:BB:5357:ARG:HH11	2:BB:5357:ARG:HG3	1.45	0.81
3:AC:385:GLN:H	3:AC:388:GLN:NE2	1.79	0.81
2:BB:5155:ALA:O	2:BB:5161:LEU:HD22	1.80	0.81
1:BA:5214:MET:HA	1:BA:5214:MET:CE	2.10	0.81
10:AK:19:ASP:N	10:AK:20:PRO:HD2	1.96	0.81
2:BB:5354:LEU:HD23	2:BB:5378:LYS:HB2	1.62	0.81
4:AD:17:ILE:HG21	18:AX:42:GLN:HG2	1.63	0.81
2:BB:5354:LEU:CD2	2:BB:5378:LYS:HB2	2.11	0.81
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.80	0.81
1:BA:5084:PRO:HA	1:BA:5112:TYR:CD2	2.15	0.81
1:AA:214:MET:HA	1:AA:214:MET:CE	2.11	0.81
3:BC:5029:GLU:HB3	10:BK:5046:ARG:HH11	1.46	0.81
31:BD:5410:LMG:HC8	11:BL:5019:LEU:HD23	1.61	0.81
3:BC:5307:PRO:HB3	3:BC:5358:PHE:CD1	2.15	0.80
1:BA:5214:MET:HA	1:BA:5214:MET:HE3	1.63	0.80
3:BC:5310:SER:OG	3:BC:5355:THR:HG23	1.82	0.80
5:BE:5036:LEU:O	5:BE:5040:THR:HG23	1.82	0.80
24:AB:603:CLA:HAC2	24:AB:606:CLA:HBB2	1.64	0.80
31:AB:620:LMG:H182	35:AD:405:PL9:H201	1.63	0.80
31:BI:5101:LMG:H152	32:BI:5102:LMT:H52	1.62	0.80
1:BA:5281:VAL:CG1	28:BC:5519:DGD:HAG3	2.11	0.80
1:AA:33:PHE:HE1	24:AC:505:CLA:H92	1.45	0.80
2:AB:354:LEU:CD2	2:AB:378:LYS:HB2	2.12	0.80
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.82	0.80
14:AT:4:ILE:HG13	32:BB:5603:LMT:H51	1.64	0.80
3:BC:5464:GLU:HB3	3:BC:5467:LEU:HD12	1.64	0.80
4:AD:122:LEU:HD21	24:AD:401:CLA:H92	1.64	0.80
31:AA:414:LMG:O3	5:AE:9:PRO:HB3	1.81	0.80
4:BD:5221:THR:HG23	4:BD:5244:TYR:HB2	1.63	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:357:ARG:HH11	2:AB:357:ARG:HG3	1.46	0.80
2:AB:297:THR:HG23	2:AB:300:GLU:H	1.47	0.80
18:BX:5034:PHE:O	18:BX:5038:ILE:HG12	1.82	0.79
2:BB:5135:LEU:HB2	2:BB:5136:PRO:HD3	1.62	0.79
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.63	0.79
24:BB:5607:CLA:HAC2	24:BB:5610:CLA:HBB2	1.65	0.79
3:BC:5155:ASN:HA	3:BC:5158:THR:HG22	1.65	0.79
2:AB:383:PHE:O	13:AO:192:SER:HA	1.82	0.79
31:AI:101:LMG:H152	32:AI:102:LMT:H52	1.64	0.79
4:BD:5152:VAL:HG21	4:BD:5279:LEU:HD13	1.64	0.79
24:BD:5405:CLA:H41	18:BX:5023:LEU:HD12	1.64	0.79
3:AC:116:VAL:HG21	27:AC:515:BCR:H323	1.63	0.79
1:BA:5143:ILE:HD11	4:BD:5217:THR:HA	1.64	0.79
5:BE:5009:PRO:HB3	31:BE:5101:LMG:O3	1.81	0.79
1:BA:5177:SER:HA	1:BA:5180:PHE:HD2	1.47	0.79
3:AC:372:PRO:O	13:AO:36:ILE:HD13	1.82	0.79
1:AA:84:PRO:HA	1:AA:112:TYR:CD2	2.16	0.79
1:AA:278:TRP:CH2	28:AC:519:DGD:HGB1	2.18	0.79
24:AA:407:CLA:H43	24:AC:505:CLA:H201	1.64	0.79
16:AV:63:CYS:SG	36:AV:201:HEM:CAB	2.71	0.79
2:BB:5173:GLY:HA3	2:BB:5265:ILE:HD11	1.64	0.79
7:AH:21:VAL:HG23	7:AH:22:ALA:O	1.83	0.78
1:BA:5258:LEU:HB3	1:BA:5259:ILE:HD13	1.65	0.78
1:AA:258:LEU:HB3	1:AA:259:ILE:HD13	1.63	0.78
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HD1	1.46	0.78
20:AZ:19:MET:O	20:AZ:23:VAL:HG23	1.83	0.78
2:AB:354:LEU:HD23	2:AB:378:LYS:HB2	1.63	0.78
20:BZ:5036:SER:HA	20:BZ:5039:LEU:HG	1.65	0.78
24:BC:5504:CLA:H151	28:BC:5519:DGD:HA91	1.64	0.78
1:BA:5192:ILE:HA	1:BA:5293:MET:HE3	1.66	0.78
4:BD:5017:ILE:HG21	18:BX:5042:GLN:HG2	1.63	0.78
31:BC:5520:LMG:O9	31:BC:5520:LMG:O8	2.01	0.78
15:BU:5072:TYR:HB3	15:BU:5073:PRO:HD3	1.66	0.78
1:BA:5278:TRP:HB3	1:BA:5279:PRO:HD3	1.64	0.78
7:BH:5042:LEU:HD12	7:BH:5045:ILE:HD11	1.64	0.78
1:AA:289:GLY:O	1:AA:292:THR:HG22	1.82	0.78
31:AC:520:LMG:O8	31:AC:520:LMG:O9	2.01	0.78
24:BA:5408:CLA:H43	24:BC:5505:CLA:H201	1.66	0.78
3:AC:461:ARG:CG	3:AC:461:ARG:HH11	1.96	0.78
1:BA:5083:VAL:HG22	4:BD:5314:PHE:HE2	1.49	0.78
13:BO:5032:THR:HG22	13:BO:5035:ASP:OD2	1.83	0.77
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.65	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5133:LEU:HD23	4:BD:5252:PHE:CD1	2.18	0.77
2:BB:5489:GLU:HB2	5:BE:5003:GLY:N	1.98	0.77
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:H	1.87	0.77
28:BA:5412:DGD:O2D	3:BC:5216:SER:CB	2.32	0.77
7:BH:5055:LEU:HD21	18:BX:5016:LEU:HD23	1.64	0.77
10:AK:27:VAL:O	10:AK:30:VAL:HG12	1.82	0.77
1:AA:127:MET:HE3	3:AC:442:LEU:HD21	1.67	0.77
3:AC:48:LYS:HE2	3:AC:138:GLU:HG3	1.67	0.77
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.65	0.77
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.85	0.77
3:BC:5219:GLY:HA2	28:BC:5517:DGD:O3D	1.85	0.77
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	2.00	0.77
3:AC:464:GLU:HB3	3:AC:467:LEU:HD12	1.65	0.77
24:AC:511:CLA:H202	20:AZ:20:VAL:HA	1.66	0.77
3:AC:117:VAL:HG11	31:AC:521:LMG:H192	1.67	0.77
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.14	0.77
2:BB:5068:ARG:HH22	24:BB:5608:CLA:HED1	1.49	0.77
2:BB:5223:GLN:HG3	2:BB:5227:LYS:HE3	1.66	0.76
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.51	0.76
13:AO:32:THR:HG22	13:AO:35:ASP:OD2	1.83	0.76
2:BB:5297:THR:HG23	2:BB:5300:GLU:H	1.50	0.76
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.67	0.76
24:AC:504:CLA:C15	28:AC:519:DGD:HA91	2.14	0.76
24:BA:5405:CLA:H13	24:BA:5406:CLA:H91	1.67	0.76
3:BC:5062:PHE:HE2	10:BK:5029:PRO:HD3	1.50	0.76
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.67	0.76
28:AA:411:DGD:O2D	3:AC:216:SER:CB	2.33	0.76
24:AD:404:CLA:H41	18:AX:23:LEU:HD12	1.65	0.76
2:BB:5461:LEU:HD11	31:BB:5624:LMG:H412	1.68	0.76
12:AM:33:GLN:HB3	12:BM:5033:GLN:HB3	1.65	0.76
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.66	0.76
1:AA:262:TYR:CE1	31:AA:414:LMG:HC5	2.21	0.76
1:BA:5259:ILE:N	1:BA:5259:ILE:HD13	2.01	0.76
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.49	0.76
2:AB:121:GLU:CG	7:AH:4:ARG:HA	2.16	0.76
2:AB:4:PRO:HG2	2:AB:7:ARG:HD2	1.66	0.76
27:BC:5514:BCR:H353	27:BK:5102:BCR:H321	1.68	0.76
3:BC:5461:ARG:CG	3:BC:5461:ARG:HH11	1.97	0.76
5:BE:5078:THR:HA	5:BE:5081:GLU:HG2	1.68	0.76
12:BM:5001:MET:HG2	12:BM:5002:GLU:H	1.51	0.76
13:AO:128:ASP:OD2	13:AO:149:LYS:HG2	1.86	0.75
7:AH:42:LEU:HD12	7:AH:45:ILE:HD11	1.67	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:5016:PRO:CG	2:BB:5133:LEU:HD11	2.16	0.75
1:BA:5255:PHE:CE1	1:BA:5259:ILE:HD11	2.21	0.75
2:AB:468:TRP:HD1	2:AB:469:HIS:HD1	1.31	0.75
24:AB:604:CLA:H11	24:AB:612:CLA:H152	1.68	0.75
3:BC:5372:PRO:O	13:BO:5036:ILE:HD13	1.86	0.75
2:BB:5121:GLU:HG3	7:BH:5004:ARG:HA	1.67	0.75
24:AC:503:CLA:H191	24:AC:503:CLA:HMD2	1.67	0.75
27:AC:514:BCR:H353	27:AK:102:BCR:H321	1.68	0.75
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.17	0.75
2:BB:5414:PRO:HB2	2:BB:5415:PRO:HD3	1.68	0.75
1:BA:5049:VAL:O	1:BA:5053:ILE:HG13	1.87	0.75
3:BC:5048:LYS:HE2	3:BC:5138:GLU:HG3	1.66	0.75
4:BD:5091:LEU:HD22	7:BH:5052:THR:HG21	1.69	0.75
2:BB:5462:PHE:HA	24:BB:5615:CLA:HMC1	1.69	0.74
10:BK:5027:VAL:O	10:BK:5030:VAL:HG12	1.86	0.74
4:BD:5103:ARG:NH1	5:BE:5077:GLU:HG3	2.02	0.74
3:BC:5385:GLN:H	3:BC:5388:GLN:NE2	1.85	0.74
31:AA:417:LMG:H201	2:BB:5098:LEU:HD13	1.69	0.74
1:BA:5315:ASN:HD21	4:BD:5332:GLN:HE22	1.35	0.74
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.69	0.74
1:BA:5064:ARG:O	13:BO:5178:ARG:NH2	2.21	0.74
4:AD:152:VAL:HG21	4:AD:279:LEU:HD13	1.67	0.74
2:BB:5121:GLU:CG	7:BH:5004:ARG:HA	2.18	0.74
3:AC:219:GLY:HA2	28:AC:517:DGD:O3D	1.86	0.74
13:BO:5171:GLU:HG2	13:BO:5172:PHE:N	2.02	0.74
13:AO:230:VAL:HG12	13:AO:231:ASP:N	2.03	0.74
1:AA:13:LEU:HA	1:AA:16:ARG:HD3	1.69	0.74
10:AK:18:PHE:HE1	20:AZ:9:LEU:HG	1.51	0.74
13:BO:5178:ARG:HH11	13:BO:5178:ARG:HG3	1.53	0.74
13:AO:31:LEU:HD12	13:AO:31:LEU:H	1.51	0.74
13:AO:178:ARG:HH11	13:AO:178:ARG:HG3	1.53	0.74
2:AB:474:LEU:HD13	30:AB:622:SQD:H81	1.69	0.74
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG21	2.23	0.74
3:BC:5453:ALA:O	8:BI:5034:ARG:HB2	1.87	0.74
24:AB:608:CLA:H52	24:AB:609:CLA:H8	1.70	0.73
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.53	0.73
3:BC:5209:ILE:HG23	27:BC:5516:BCR:H382	1.70	0.73
13:BO:5031:LEU:HD12	13:BO:5031:LEU:N	2.03	0.73
2:AB:16:PRO:CG	2:AB:133:LEU:HD11	2.17	0.73
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.21	0.73
2:BB:5483:ASP:CB	2:BB:5484:PRO:HD2	2.16	0.73
13:AO:171:GLU:HG2	13:AO:172:PHE:N	2.02	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.70	0.73
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.22	0.73
2:AB:224:ARG:HG3	7:AH:25:TRP:HD1	1.51	0.73
24:BB:5608:CLA:H11	24:BB:5616:CLA:H152	1.71	0.73
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.69	0.73
10:BK:5018:PHE:HE1	20:BZ:5009:LEU:HG	1.53	0.73
2:BB:5474:LEU:HD13	30:BB:5625:SQD:H81	1.68	0.73
3:AC:397:THR:HG21	16:AV:66:CYS:SG	2.27	0.73
24:AC:513:CLA:HMC2	27:AC:515:BCR:H372	1.70	0.73
2:BB:5324:LEU:HA	4:BD:5293:LEU:CD2	2.18	0.73
2:AB:248:ALA:HA	24:AB:603:CLA:C4	2.19	0.73
24:BB:5612:CLA:H52	24:BB:5613:CLA:H8	1.71	0.73
3:AC:55:ALA:HB1	27:AC:514:BCR:H373	1.69	0.73
3:AC:248:GLY:O	3:AC:252:ILE:HG12	1.89	0.73
1:AA:300:PHE:HE2	28:AC:519:DGD:O1A	1.71	0.73
1:AA:18:CYS:O	1:AA:22:THR:HG22	1.89	0.73
4:AD:103:ARG:NH1	5:AE:77:GLU:HG3	2.04	0.73
1:BA:5127:MET:HE3	3:BC:5442:LEU:HD21	1.71	0.73
5:BE:5018:ARG:O	5:BE:5022:ILE:HG13	1.89	0.73
8:AI:16:VAL:O	8:AI:20:VAL:HG23	1.87	0.72
14:AT:21:ILE:HD12	27:AT:101:BCR:H332	1.71	0.72
24:BC:5509:CLA:H121	24:BC:5509:CLA:HBD	1.71	0.72
1:AA:259:ILE:HD13	1:AA:259:ILE:N	2.03	0.72
3:BC:5055:ALA:HB1	27:BC:5514:BCR:H373	1.68	0.72
1:AA:278:TRP:HB3	1:AA:279:PRO:HD3	1.70	0.72
3:BC:5029:GLU:HB3	10:BK:5046:ARG:NH1	2.04	0.72
3:AC:429:SER:O	3:AC:432:VAL:HG12	1.89	0.72
1:AA:260:PHE:CE1	1:AA:263:ALA:HB2	2.25	0.72
1:AA:315:ASN:HD21	4:AD:332:GLN:HE22	1.37	0.72
2:BB:5371:THR:HG22	2:BB:5377:VAL:HA	1.71	0.72
2:BB:5086:ILE:HD12	2:BB:5086:ILE:O	1.89	0.72
3:BC:5117:VAL:CG1	31:BC:5521:LMG:H192	2.20	0.72
35:BD:5406:PL9:H23	35:BD:5406:PL9:H303	1.71	0.72
4:BD:5018:LEU:HD22	18:BX:5038:ILE:HD13	1.71	0.72
2:BB:5214:LEU:O	2:BB:5218:LEU:HG	1.89	0.72
8:BI:5016:VAL:O	8:BI:5020:VAL:HG23	1.90	0.72
7:BH:5021:VAL:HG23	7:BH:5022:ALA:O	1.88	0.72
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.90	0.72
3:BC:5254:THR:HG22	3:BC:5255:THR:N	2.04	0.72
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD23	1.72	0.72
1:BA:5334:ARG:HD3	4:BD:5320:LEU:CD1	2.20	0.72
1:BA:5013:LEU:HA	1:BA:5016:ARG:HD3	1.69	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:86:ILE:HD12	2:AB:86:ILE:O	1.90	0.72
13:BO:5120:THR:HG22	13:BO:5154:SER:OG	1.90	0.72
24:AC:504:CLA:H151	28:AC:519:DGD:HA91	1.69	0.72
1:AA:83:VAL:HG22	4:AD:314:PHE:HE2	1.53	0.72
3:BC:5318:LEU:HG	3:BC:5328:VAL:HG11	1.69	0.71
3:BC:5418:ASN:CB	28:BC:5519:DGD:HE2	2.19	0.71
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:N	2.06	0.71
4:AD:91:LEU:HD22	7:AH:52:THR:HG21	1.70	0.71
35:AD:405:PL9:H303	35:AD:405:PL9:H23	1.70	0.71
4:BD:5053:THR:HG22	4:BD:5067:TYR:CE2	2.25	0.71
2:BB:5425:ILE:HG22	2:BB:5426:PHE:CD2	2.25	0.71
2:AB:137:LYS:O	2:AB:141:ILE:HG13	1.90	0.71
3:BC:5397:THR:HG21	16:BV:5066:CYS:SG	2.30	0.71
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.55	0.71
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.72	0.71
1:AA:133:LEU:HD23	4:AD:252:PHE:CD1	2.26	0.71
1:AA:234:ASN:HD21	4:AD:266:TRP:HB2	1.56	0.71
3:AC:254:THR:HG22	3:AC:255:THR:N	2.04	0.71
20:BZ:5019:MET:O	20:BZ:5023:VAL:HG23	1.90	0.71
1:AA:255:PHE:CE1	1:AA:259:ILE:HD11	2.25	0.71
3:AC:344:SER:O	13:AO:101:THR:HG22	1.90	0.71
12:AM:20:VAL:HG21	12:BM:5020:VAL:HG21	1.72	0.71
4:AD:134:ARG:HA	4:AD:134:ARG:HE	1.56	0.71
4:AD:274:VAL:HB	4:AD:275:PRO:HD3	1.73	0.71
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.73	0.71
2:AB:425:ILE:HG22	2:AB:426:PHE:CD2	2.26	0.71
15:AU:94:ILE:O	15:AU:97:LEU:HG	1.91	0.71
24:AC:509:CLA:HBD	24:AC:509:CLA:H121	1.71	0.71
7:AH:58:VAL:HG13	7:AH:58:VAL:O	1.91	0.71
11:BL:5013:ASN:HD21	11:BL:5015:THR:HG22	1.56	0.71
20:AZ:52:LEU:O	20:AZ:56:VAL:HG23	1.91	0.71
20:AZ:2:THR:HG23	20:AZ:3:ILE:N	2.06	0.71
3:BC:5344:SER:O	13:BO:5101:THR:HG22	1.91	0.71
2:BB:5004:PRO:HD2	2:BB:5007:ARG:HB2	1.71	0.70
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.91	0.70
5:BE:5034:GLY:HA2	6:BF:5032:PHE:CE1	2.26	0.70
2:AB:235:GLU:HG2	2:AB:235:GLU:O	1.91	0.70
5:AE:18:ARG:O	5:AE:22:ILE:HG13	1.90	0.70
24:AA:404:CLA:H13	24:AA:405:CLA:H91	1.73	0.70
2:BB:5235:GLU:HG2	2:BB:5235:GLU:O	1.91	0.70
3:BC:5337:LEU:HD12	13:BO:5131:PRO:HG3	1.73	0.70
10:BK:5028:ILE:HA	10:BK:5031:LEU:CD1	2.18	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:305:THR:HG23	3:AC:308:GLU:H	1.55	0.70
2:BB:5130:GLU:HB2	2:BB:5131:PRO:HD2	1.73	0.70
2:AB:461:LEU:HD11	31:AB:621:LMG:H412	1.71	0.70
2:BB:5121:GLU:HG2	7:BH:5004:ARG:HD2	1.73	0.70
1:AA:39:PRO:HB2	24:AA:407:CLA:HBB1	1.74	0.70
24:AB:610:CLA:H111	24:AB:615:CLA:HAA1	1.74	0.70
2:AB:116:VAL:HG21	27:AB:619:BCR:H271	1.73	0.70
24:BB:5618:CLA:OBD	11:BL:5010:VAL:HG21	1.90	0.70
2:AB:98:LEU:HD13	31:BA:5402:LMG:H201	1.73	0.70
2:BB:5116:VAL:HG21	27:BB:5623:BCR:H271	1.71	0.70
3:BC:5429:SER:O	3:BC:5432:VAL:HG12	1.90	0.70
1:AA:49:VAL:O	1:AA:53:ILE:HG13	1.92	0.70
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.04	0.70
16:BV:5066:CYS:SG	36:BV:5201:HEM:CAC	2.79	0.70
2:AB:183:PRO:HG3	2:AB:199:VAL:CG1	2.21	0.70
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	1.92	0.70
2:BB:5068:ARG:HH12	24:BB:5608:CLA:HED1	1.56	0.70
1:AA:288:LEU:HD13	3:AC:432:VAL:HG23	1.74	0.70
1:BA:5260:PHE:CE1	1:BA:5263:ALA:HB2	2.27	0.70
4:BD:5189:HIS:HA	4:BD:5294:ARG:HD2	1.74	0.70
2:BB:5191:ASN:HB2	7:BH:5058:VAL:CG2	2.20	0.70
24:BC:5511:CLA:H202	20:BZ:5020:VAL:HA	1.74	0.70
24:BC:5503:CLA:H191	24:BC:5503:CLA:HMD2	1.72	0.69
4:BD:5088:SER:HB2	5:BE:5069:ARG:CZ	2.22	0.69
16:BV:5135:GLU:O	16:BV:5139:VAL:HG23	1.91	0.69
2:BB:5137:LYS:O	2:BB:5141:ILE:HG13	1.92	0.69
1:BA:5032:TRP:HA	1:BA:5032:TRP:CE3	2.27	0.69
7:BH:5058:VAL:O	7:BH:5058:VAL:HG13	1.92	0.69
2:BB:5297:THR:HG22	2:BB:5300:GLU:OE1	1.92	0.69
20:BZ:5052:LEU:O	20:BZ:5056:VAL:HG23	1.93	0.69
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.93	0.69
11:AL:13:ASN:HD21	11:AL:15:THR:HG22	1.56	0.69
12:AM:33:GLN:CB	12:BM:5033:GLN:HB3	2.21	0.69
15:BU:5094:ILE:O	15:BU:5097:LEU:HG	1.92	0.69
2:AB:298:LEU:HD23	2:AB:402:TYR:CZ	2.28	0.69
4:BD:5018:LEU:HD22	18:BX:5038:ILE:CD1	2.22	0.69
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.75	0.69
1:AA:334:ARG:HD3	4:AD:320:LEU:CD1	2.23	0.69
2:BB:5120:LEU:HD13	24:BB:5620:CLA:HMD2	1.75	0.69
24:BB:5614:CLA:H111	24:BB:5619:CLA:HAA1	1.75	0.69
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.93	0.69
1:BA:5261:GLN:NE2	2:BB:5489:GLU:HG3	2.07	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5154:LYS:HE2	3:BC:5261:ARG:HD2	1.74	0.69
7:AH:55:LEU:O	7:AH:58:VAL:HG12	1.92	0.69
4:BD:5274:VAL:HB	4:BD:5275:PRO:HD3	1.74	0.69
3:BC:5158:THR:O	3:BC:5251:HIS:HB3	1.92	0.69
6:AF:27:ALA:HB1	36:AF:101:HEM:HBC2	1.74	0.69
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.27	0.69
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.22	0.69
3:BC:5113:VAL:HG11	31:BC:5521:LMG:H132	1.74	0.69
4:BD:5103:ARG:HH12	5:BE:5077:GLU:HG3	1.58	0.69
1:BA:5271:LEU:HD12	25:BA:5409:MST:H162	1.73	0.69
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.93	0.69
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.23	0.69
1:AA:278:TRP:CD2	28:AC:519:DGD:HAG2	2.25	0.69
1:BA:5300:PHE:HE2	28:BC:5519:DGD:O1A	1.75	0.69
1:AA:177:SER:HA	1:AA:180:PHE:CD2	2.28	0.69
24:BC:5502:CLA:HBB2	24:BC:5510:CLA:H152	1.74	0.69
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.75	0.69
4:BD:5054:PHE:HB3	5:BE:5047:PHE:CD2	2.28	0.69
30:BB:5625:SQD:H172	32:BB:5627:LMT:H101	1.74	0.69
13:BO:5230:VAL:HG12	13:BO:5231:ASP:N	2.08	0.69
3:BC:5415:ASN:O	3:BC:5416:SER:HB3	1.93	0.68
1:AA:234:ASN:ND2	4:AD:266:TRP:HB2	2.08	0.68
2:AB:462:PHE:HA	24:AB:611:CLA:HMC1	1.74	0.68
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.96	0.68
6:BF:5027:ALA:HB1	36:BF:5101:HEM:HBC2	1.73	0.68
1:BA:5018:CYS:O	1:BA:5022:THR:HG22	1.93	0.68
2:BB:5248:ALA:HA	24:BB:5607:CLA:C4	2.22	0.68
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.74	0.68
4:AD:192:THR:HG23	24:AD:401:CLA:HBC2	1.74	0.68
3:BC:5472:LEU:HG	4:BD:5251:ARG:NH1	2.08	0.68
1:BA:5278:TRP:CZ3	28:BC:5519:DGD:HAG2	2.27	0.68
1:BA:5038:ILE:HG23	30:BA:5401:SQD:H131	1.76	0.68
4:BD:5250:ASN:HD22	4:BD:5262:SER:HB3	1.57	0.68
1:BA:5234:ASN:HD21	4:BD:5266:TRP:HB2	1.57	0.68
27:AC:515:BCR:H312	20:AZ:55:GLY:HA2	1.74	0.68
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.75	0.68
2:AB:250:PHE:CD2	2:AB:459:ALA:HB1	2.29	0.68
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.76	0.68
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.93	0.68
8:AI:11:VAL:HG22	32:AI:102:LMT:H101	1.76	0.68
1:BA:5234:ASN:ND2	4:BD:5266:TRP:HB2	2.09	0.68
24:BC:5513:CLA:HMC2	27:BC:5515:BCR:H372	1.76	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5192:THR:HG23	24:BD:5402:CLA:HBC2	1.75	0.68
4:BD:5129:GLN:NE2	4:BD:5143:ALA:HA	2.08	0.68
1:BA:5288:LEU:HD13	3:BC:5432:VAL:HG23	1.76	0.68
5:AE:23:HIS:HA	5:AE:26:THR:OG1	1.93	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HB2	1.76	0.68
3:AC:209:ILE:HG23	27:AC:516:BCR:H382	1.76	0.68
18:AX:12:ILE:HG13	18:AX:12:ILE:O	1.94	0.68
3:AC:385:GLN:H	3:AC:388:GLN:HE21	1.41	0.68
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.29	0.68
2:BB:5005:TRP:O	2:BB:5008:VAL:HG13	1.93	0.68
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.93	0.68
30:AB:622:SQD:H172	32:AB:624:LMT:H101	1.75	0.68
2:BB:5357:ARG:NH1	2:BB:5357:ARG:HG3	2.06	0.68
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.08	0.68
1:BA:5039:PRO:HB2	24:BA:5408:CLA:HBB1	1.74	0.68
3:BC:5062:PHE:HE2	10:BK:5028:ILE:HB	1.58	0.68
16:AV:66:CYS:SG	36:AV:201:HEM:CAC	2.81	0.68
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.59	0.68
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	1.94	0.67
12:AM:33:GLN:HB3	12:BM:5033:GLN:CB	2.23	0.67
3:AC:62:PHE:HE2	10:AK:28:ILE:HB	1.59	0.67
3:BC:5150:ASP:HB3	3:BC:5153:ASP:HB2	1.75	0.67
3:AC:262:ARG:HH21	32:AI:103:LMT:H5'	1.59	0.67
2:BB:5065:PHE:O	24:BB:5609:CLA:HBA1	1.94	0.67
2:AB:121:GLU:HG2	7:AH:4:ARG:HD2	1.74	0.67
10:BK:5040:GLN:HA	10:BK:5043:VAL:HG12	1.74	0.67
2:BB:5010:THR:O	2:BB:5013:ILE:HG13	1.94	0.67
3:BC:5305:THR:CG2	3:BC:5308:GLU:H	2.08	0.67
4:AD:103:ARG:HH12	5:AE:77:GLU:HG3	1.60	0.67
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.76	0.67
1:BA:5239:PHE:O	14:BT:5029:ILE:HA	1.95	0.67
12:BM:5025:LEU:O	12:BM:5028:GLN:HG3	1.95	0.67
2:BB:5068:ARG:HH12	24:BB:5608:CLA:CED	2.07	0.67
27:AC:515:BCR:C31	20:AZ:55:GLY:HA2	2.24	0.67
2:AB:297:THR:HG22	2:AB:300:GLU:OE1	1.94	0.67
13:AO:114:ASN:HD21	13:AO:120:THR:HG23	1.59	0.67
13:BO:5092:VAL:CG1	13:BO:5093:PRO:HD2	2.24	0.67
2:BB:5250:PHE:CD2	2:BB:5459:ALA:HB1	2.30	0.67
3:AC:52:ALA:HA	24:AC:511:CLA:CMB	2.23	0.67
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.30	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:HD23	1.76	0.67
1:AA:214:MET:HE3	1:AA:214:MET:HA	1.74	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:103:LEU:HD21	24:AB:605:CLA:HMC3	1.76	0.67
24:AC:502:CLA:HBB2	24:AC:510:CLA:H152	1.76	0.67
14:BT:5029:ILE:HD12	14:BT:5029:ILE:H	1.58	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:CD2	2.24	0.67
2:BB:5379:ALA:HA	2:BB:5390:TYR:HB3	1.76	0.67
7:AH:9:ASP:O	7:AH:12:ARG:HB2	1.95	0.67
2:AB:130:GLU:HB2	2:AB:131:PRO:HD2	1.76	0.67
2:AB:8:VAL:HB	24:AB:614:CLA:O1D	1.95	0.67
2:BB:5233:ASN:O	2:BB:5236:THR:HG22	1.95	0.67
1:BA:5136:ARG:NH2	8:BI:5027:ASP:OD1	2.27	0.67
1:BA:5190:HIS:HB3	1:BA:5293:MET:HE2	1.76	0.67
2:AB:234:ILE:HD12	2:AB:237:VAL:HG21	1.77	0.67
3:BC:5215:LYS:HB3	3:BC:5223:TRP:HA	1.75	0.67
3:BC:5240:ILE:O	3:BC:5244:CYS:HB2	1.95	0.67
31:AA:414:LMG:HO2	5:AE:10:PHE:HD2	1.43	0.67
3:BC:5347:GLY:HA3	13:BO:5043:ASN:HB2	1.75	0.67
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.77	0.67
4:BD:5134:ARG:HA	4:BD:5134:ARG:HE	1.60	0.67
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.67
3:BC:5089:ILE:N	3:BC:5090:PRO:HD2	2.10	0.67
13:BO:5128:ASP:OD2	13:BO:5149:LYS:HG2	1.93	0.67
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.30	0.67
16:BV:5063:CYS:SG	36:BV:5201:HEM:CAB	2.81	0.67
3:BC:5308:GLU:HB2	3:BC:5361:PHE:CE1	2.29	0.67
3:BC:5199:ILE:H	3:BC:5199:ILE:HD12	1.60	0.67
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CZ	2.29	0.67
1:AA:33:PHE:CE1	24:AC:505:CLA:H92	2.29	0.66
2:AB:62:VAL:HG13	24:AB:605:CLA:HED3	1.77	0.66
13:BO:5169:LYS:HG2	13:BO:5224:SER:HB3	1.77	0.66
3:AC:199:ILE:HD12	3:AC:199:ILE:H	1.60	0.66
1:BA:5297:LEU:HD11	3:BC:5404:LEU:HD12	1.77	0.66
2:BB:5224:ARG:HG3	7:BH:5025:TRP:CD1	2.30	0.66
2:BB:5222:PRO:HG3	7:BH:5027:THR:H	1.58	0.66
3:AC:134:ILE:HD11	24:AC:511:CLA:H93	1.77	0.66
15:AU:66:ILE:HG22	15:AU:66:ILE:O	1.95	0.66
3:BC:5040:ALA:O	3:BC:5043:ILE:HG13	1.95	0.66
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
24:AB:613:CLA:HED3	24:AB:613:CLA:H2	1.76	0.66
24:BB:5612:CLA:H18	24:BB:5613:CLA:H192	1.77	0.66
3:BC:5062:PHE:CE2	10:BK:5029:PRO:HD3	2.29	0.66
3:BC:5254:THR:CG2	3:BC:5255:THR:H	2.06	0.66
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:BV:5133:LEU:H	16:BV:5133:LEU:HD12	1.59	0.66
3:BC:5248:GLY:O	3:BC:5252:ILE:HG12	1.94	0.66
2:AB:233:ASN:O	2:AB:236:THR:HG22	1.95	0.66
24:AB:608:CLA:H18	24:AB:609:CLA:H192	1.77	0.66
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.60	0.66
4:BD:5261:PHE:HA	31:BD:5410:LMG:O2	1.96	0.66
10:AK:28:ILE:HA	10:AK:31:LEU:CD1	2.17	0.66
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.59	0.66
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.76	0.66
5:BE:5027:ILE:HB	5:BE:5028:PRO:HD3	1.78	0.66
18:AX:36:VAL:O	18:AX:40:ILE:HG22	1.96	0.66
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.76	0.66
2:AB:5:TRP:O	2:AB:8:VAL:HG13	1.95	0.66
1:BA:5033:PHE:CE1	24:BC:5505:CLA:H92	2.27	0.66
2:AB:357:ARG:HG3	2:AB:357:ARG:NH1	2.06	0.66
20:AZ:32:ASP:HA	20:AZ:34:ASP:OD2	1.95	0.66
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.77	0.66
24:BC:5504:CLA:H172	28:BC:5519:DGD:HAE1	1.76	0.66
2:AB:120:LEU:HD13	24:AB:616:CLA:HMD2	1.78	0.66
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.29	0.66
10:BK:5019:ASP:N	10:BK:5020:PRO:HD2	2.10	0.66
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	1.96	0.66
13:AO:31:LEU:N	13:AO:31:LEU:HD12	2.11	0.66
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.77	0.66
1:BA:5330:VAL:HG11	4:BD:5348:ARG:HG2	1.77	0.66
30:BB:5601:SQD:H81	30:BB:5601:SQD:H242	1.78	0.66
2:BB:5208:VAL:HG21	24:BB:5606:CLA:HMC1	1.78	0.66
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.61	0.66
3:BC:5453:ALA:HA	8:BI:5034:ARG:O	1.95	0.66
15:BU:5057:LEU:HD11	15:BU:5112:PHE:HB3	1.76	0.66
1:AA:102:LEU:HB2	31:AA:417:LMG:C35	2.06	0.66
3:BC:5224:ILE:O	3:BC:5227:VAL:HG23	1.94	0.66
1:BA:5221:SER:HB2	4:BD:5139:ARG:O	1.96	0.66
3:BC:5305:THR:HG23	3:BC:5308:GLU:H	1.59	0.66
2:BB:5008:VAL:HB	24:BB:5618:CLA:O1D	1.95	0.66
13:AO:87:GLN:O	13:AO:88:GLU:CG	2.41	0.66
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.17	0.66
1:AA:39:PRO:HB2	24:AA:407:CLA:CBB	2.25	0.66
1:BA:5176:ILE:HG22	1:BA:5180:PHE:CE2	2.30	0.66
24:BB:5617:CLA:H2	24:BB:5617:CLA:HED3	1.77	0.66
3:AC:254:THR:CG2	3:AC:255:THR:H	2.07	0.66
4:BD:5103:ARG:HG3	5:BE:5073:LYS:CG	2.26	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:5114:ASN:HD21	13:BO:5120:THR:HG23	1.60	0.66
16:AV:133:LEU:HD12	16:AV:133:LEU:H	1.61	0.66
1:BA:5081:ALA:HB2	1:BA:5175:GLY:HA3	1.77	0.66
30:AB:627:SQD:H242	30:AB:627:SQD:H81	1.76	0.66
3:AC:405:ASN:HB2	28:AC:519:DGD:HG32	1.77	0.65
1:BA:5278:TRP:CD2	28:BC:5519:DGD:HAG2	2.29	0.65
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.25	0.65
1:BA:5180:PHE:CD1	4:BD:5192:THR:HB	2.31	0.65
4:BD:5122:LEU:HB3	4:BD:5150:ILE:CD1	2.26	0.65
15:BU:5068:TYR:HB2	15:BU:5071:LEU:HD12	1.77	0.65
24:AB:614:CLA:OBD	11:AL:10:VAL:HG21	1.95	0.65
2:AB:65:PHE:O	24:AB:605:CLA:HBA1	1.96	0.65
31:AI:101:LMG:O9	31:AI:101:LMG:O8	2.14	0.65
3:BC:5282:MET:HG2	24:BC:5501:CLA:H71	1.78	0.65
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.79	0.65
15:BU:5066:ILE:O	15:BU:5066:ILE:HG22	1.95	0.65
3:BC:5262:ARG:HH21	32:BC:5522:LMT:H5'	1.61	0.65
2:AB:489:GLU:HB2	5:AE:3:GLY:N	2.11	0.65
4:AD:261:PHE:HA	31:AD:408:LMG:O2	1.96	0.65
11:AL:16:SER:HA	11:AL:19:LEU:HG	1.75	0.65
11:BL:5026:VAL:HG21	31:BL:5101:LMG:H202	1.78	0.65
2:AB:468:TRP:HD1	2:AB:469:HIS:ND1	1.94	0.65
8:AI:19:PHE:CE1	8:AI:23:PHE:HE2	2.14	0.65
1:BA:5039:PRO:HB2	24:BA:5408:CLA:CBB	2.27	0.65
2:BB:5183:PRO:HG3	2:BB:5199:VAL:CG1	2.27	0.65
13:BO:5087:GLN:O	13:BO:5088:GLU:CG	2.41	0.65
5:BE:5017:VAL:O	5:BE:5021:VAL:HG23	1.95	0.65
4:BD:5103:ARG:CG	5:BE:5073:LYS:HG3	2.26	0.65
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.10	0.65
20:AZ:2:THR:HG23	20:AZ:3:ILE:H	1.60	0.65
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.60	0.65
3:BC:5416:SER:C	28:BC:5519:DGD:O3E	2.35	0.65
1:BA:5093:PHE:CD2	1:BA:5095:PRO:HD3	2.31	0.65
3:BC:5134:ILE:HD11	24:BC:5511:CLA:H93	1.79	0.65
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	1.97	0.65
2:AB:183:PRO:HG3	2:AB:199:VAL:HG11	1.78	0.65
1:BA:5057:PRO:HG3	1:BA:5068:SER:HB3	1.77	0.65
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG1	2.30	0.65
3:AC:416:SER:N	28:AC:519:DGD:O3E	2.30	0.65
3:BC:5405:ASN:HB2	28:BC:5519:DGD:HG32	1.77	0.65
31:BI:5101:LMG:O8	31:BI:5101:LMG:O9	2.15	0.65
5:BE:5010:PHE:HD2	31:BE:5101:LMG:HO2	1.45	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:5023:HIS:HA	5:BE:5026:THR:OG1	1.96	0.65
16:AV:71:ILE:HD12	16:AV:72:THR:N	2.11	0.65
2:AB:187:PRO:HB3	24:AB:601:CLA:HMB2	1.78	0.65
2:AB:68:ARG:HH12	24:AB:604:CLA:CED	2.09	0.65
2:BB:5062:VAL:HG13	24:BB:5609:CLA:HED3	1.78	0.65
31:BD:5410:LMG:O6	11:BL:5015:THR:HG21	1.97	0.65
3:BC:5062:PHE:CE2	10:BK:5028:ILE:HB	2.32	0.65
3:AC:110:PRO:O	3:AC:114:VAL:HG23	1.97	0.65
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.12	0.65
1:AA:271:LEU:HD12	25:AA:408:MST:H162	1.78	0.65
1:BA:5097:TRP:HA	8:BI:5001:MET:SD	2.36	0.65
2:AB:213:GLY:O	2:AB:217:ILE:HG13	1.97	0.65
1:AA:32:TRP:CE3	1:AA:32:TRP:HA	2.32	0.65
2:AB:10:THR:O	2:AB:13:ILE:HG13	1.95	0.65
16:BV:5071:ILE:HD12	16:BV:5072:THR:N	2.12	0.65
3:BC:5320:ARG:O	3:BC:5324:LEU:HD23	1.96	0.65
3:AC:282:MET:HG2	24:AC:501:CLA:H71	1.79	0.65
2:BB:5009:HIS:HB2	24:BB:5615:CLA:HBA2	1.79	0.65
2:BB:5234:ILE:HD12	2:BB:5237:VAL:HG21	1.78	0.65
3:BC:5223:TRP:CD2	3:BC:5224:ILE:HG13	2.32	0.65
4:BD:5153:PHE:HB2	24:BD:5402:CLA:H41	1.79	0.65
2:BB:5222:PRO:HG3	7:BH:5026:GLY:HA3	1.78	0.65
3:AC:179:ALA:HB1	3:AC:199:ILE:HD13	1.79	0.65
5:AE:51:ARG:HG3	5:AE:51:ARG:HH11	1.62	0.65
4:AD:153:PHE:HB2	24:AD:401:CLA:H41	1.79	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.97	0.65
5:AE:78:THR:HA	5:AE:81:GLU:HG2	1.78	0.65
2:BB:5150:CYS:HB2	24:BB:5607:CLA:HMC3	1.78	0.64
15:BU:5058:ASN:ND2	15:BU:5114:VAL:HG13	2.11	0.64
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.32	0.64
1:AA:257:ARG:HG3	1:AA:257:ARG:HH11	1.62	0.64
3:AC:362:ARG:HE	3:AC:370:ARG:HH11	1.45	0.64
2:BB:5393:GLU:HG2	15:BU:5044:ASP:O	1.97	0.64
1:AA:300:PHE:CE2	28:AC:519:DGD:O1A	2.50	0.64
3:BC:5416:SER:C	28:BC:5519:DGD:HO3E	2.01	0.64
1:AA:288:LEU:HD22	3:AC:432:VAL:HG23	1.80	0.64
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.79	0.64
3:BC:5437:PHE:HA	24:BC:5508:CLA:CMC	2.27	0.64
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:H	1.60	0.64
3:AC:320:ARG:O	3:AC:324:LEU:HD23	1.97	0.64
3:BC:5052:ALA:HA	24:BC:5511:CLA:CMB	2.24	0.64
16:AV:135:GLU:O	16:AV:139:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5149:TYR:HA	3:BC:5156:LYS:HD3	1.77	0.64
1:BA:5048:PHE:HB2	1:BA:5115:ILE:HD13	1.79	0.64
24:AC:503:CLA:H171	24:AC:510:CLA:HBB2	1.79	0.64
10:AK:24:VAL:O	10:AK:27:VAL:HG12	1.98	0.64
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	1.98	0.64
2:AB:384:ARG:HD3	15:AU:132:LEU:CD1	2.28	0.64
2:BB:5213:GLY:O	2:BB:5217:ILE:HG13	1.96	0.64
10:BK:5017:ILE:H	10:BK:5017:ILE:HD12	1.62	0.64
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.62	0.64
31:AD:408:LMG:O6	11:AL:15:THR:HG21	1.98	0.64
3:BC:5179:ALA:HB1	3:BC:5199:ILE:HD13	1.77	0.64
1:BA:5228:THR:HG22	1:BA:5229:GLU:H	1.61	0.64
1:BA:5010:SER:HB3	1:BA:5016:ARG:NH1	2.13	0.64
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.12	0.64
2:BB:5246:PHE:CD1	2:BB:5246:PHE:C	2.71	0.64
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.31	0.64
3:BC:5418:ASN:CA	28:BC:5519:DGD:HE2	2.27	0.64
2:AB:9:HIS:HB2	24:AB:611:CLA:HBA2	1.79	0.64
3:BC:5030:SER:HB3	10:BK:5046:ARG:O	1.98	0.64
2:AB:278:SER:HB3	2:AB:281:GLN:HE21	1.63	0.64
1:AA:281:VAL:CG1	28:AC:519:DGD:HAG3	2.27	0.64
2:AB:247:PHE:HB2	24:AB:608:CLA:HBC1	1.80	0.64
2:AB:68:ARG:HH22	24:AB:604:CLA:HED1	1.62	0.64
7:AH:38:PHE:HB2	27:AX:101:BCR:H10C	1.78	0.64
2:BB:5103:LEU:HD21	24:BB:5609:CLA:HMC3	1.80	0.64
3:AC:42:LEU:HD23	24:AC:511:CLA:HED3	1.79	0.64
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	1.98	0.64
2:AB:214:LEU:O	2:AB:218:LEU:HG	1.97	0.64
1:BA:5077:ILE:HD11	14:BT:5006:TYR:HB3	1.79	0.64
4:BD:5261:PHE:CD2	4:BD:5267:LEU:HD12	2.33	0.63
31:BB:5624:LMG:H411	4:BD:5284:ILE:HG12	1.80	0.63
13:BO:5039:THR:OG1	13:BO:5041:LEU:HB2	1.98	0.63
2:AB:208:VAL:HG21	24:AB:602:CLA:HMC1	1.79	0.63
31:AB:620:LMG:H202	11:AL:26:VAL:HG21	1.79	0.63
3:AC:437:PHE:HA	24:AC:508:CLA:CMC	2.28	0.63
28:AH:101:DGD:O1B	28:AH:101:DGD:C1G	2.46	0.63
3:BC:5449:ARG:HG2	24:BC:5505:CLA:HED1	1.80	0.63
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.81	0.63
8:BI:5014:PHE:CZ	8:BI:5018:LEU:HD11	2.33	0.63
28:BC:5518:DGD:HG11	31:BC:5520:LMG:H301	1.81	0.63
2:BB:5187:PRO:HB3	24:BB:5605:CLA:HMB2	1.79	0.63
2:BB:5191:ASN:HB2	7:BH:5058:VAL:HG23	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:C40	2.26	0.63
8:BI:5011:VAL:HG22	32:BI:5102:LMT:H101	1.80	0.63
4:BD:5236:ASN:ND2	4:BD:5239:GLN:O	2.29	0.63
13:BO:5144:LEU:CD1	13:BO:5259:VAL:HG11	2.29	0.63
13:BO:5218:LEU:HD22	15:BU:5119:THR:HG21	1.80	0.63
1:AA:176:ILE:HG22	1:AA:180:PHE:CE2	2.34	0.63
4:BD:5041:ALA:HB1	34:BD:5404:PHO:H42	1.81	0.63
4:AD:103:ARG:CG	5:AE:73:LYS:HG3	2.28	0.63
8:AI:8:VAL:O	8:AI:12:VAL:HG23	1.97	0.63
16:AV:95:ILE:O	16:AV:99:VAL:HG23	1.99	0.63
3:AC:304:PRO:HB3	3:AC:395:TYR:CD1	2.33	0.63
28:AC:518:DGD:HG11	31:AC:520:LMG:H301	1.81	0.63
2:AB:68:ARG:HH12	24:AB:604:CLA:HED1	1.64	0.63
3:AC:288:CYS:SG	28:AC:517:DGD:HA21	2.39	0.63
28:BH:5101:DGD:O1B	28:BH:5101:DGD:C1G	2.45	0.63
15:BU:5058:ASN:OD1	15:BU:5084:PRO:HA	1.98	0.63
3:AC:117:VAL:CG1	31:AC:521:LMG:H192	2.28	0.63
3:BC:5385:GLN:H	3:BC:5388:GLN:HE21	1.46	0.63
4:BD:5080:THR:HG23	4:BD:5172:SER:OG	1.99	0.63
2:AB:191:ASN:HB2	7:AH:58:VAL:HG23	1.80	0.63
3:BC:5437:PHE:CZ	24:BC:5502:CLA:HMC1	2.34	0.63
3:AC:461:ARG:CG	3:AC:461:ARG:NH1	2.60	0.63
5:BE:5076:VAL:O	5:BE:5080:LEU:HD22	1.98	0.63
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.63
2:AB:124:ARG:HH11	2:AB:124:ARG:HG3	1.63	0.63
1:AA:274:PHE:CE2	25:AA:408:MST:H133	2.33	0.63
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	1.99	0.63
1:AA:221:SER:HB2	4:AD:139:ARG:O	1.99	0.63
11:BL:5016:SER:HA	11:BL:5019:LEU:HG	1.80	0.63
1:BA:5343:LEU:O	1:BA:5344:ALA:HB2	1.99	0.63
13:BO:5206:GLU:CD	13:BO:5206:GLU:H	2.01	0.63
1:BA:5304:HIS:CE1	3:BC:5414:ILE:HD12	2.33	0.63
6:BF:5028:VAL:HB	6:BF:5029:PRO:HD3	1.81	0.63
13:BO:5234:THR:OG1	13:BO:5236:GLU:HG2	1.99	0.63
11:BL:5008:GLN:HE21	11:BL:5008:GLN:N	1.97	0.62
1:BA:5177:SER:HA	1:BA:5180:PHE:CD2	2.32	0.62
2:BB:5118:TRP:CH2	11:BL:5005:PRO:HD2	2.34	0.62
13:BO:5069:LEU:HD12	13:BO:5070:CYS:H	1.63	0.62
16:BV:5095:ILE:O	16:BV:5099:VAL:HG23	1.98	0.62
7:BH:5038:PHE:HB2	27:BX:5101:BCR:H10C	1.81	0.62
4:BD:5053:THR:HG22	4:BD:5067:TYR:CD2	2.34	0.62
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.29	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5413:GLU:HG3	3:BC:5414:ILE:H	1.64	0.62
2:AB:150:CYS:HB2	24:AB:603:CLA:HMC3	1.82	0.62
2:BB:5224:ARG:HG2	7:BH:5024:GLY:O	1.99	0.62
8:BI:5019:PHE:CE1	8:BI:5023:PHE:HE2	2.17	0.62
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.14	0.62
4:AD:207:GLY:HA3	4:AD:275:PRO:HG3	1.80	0.62
35:AD:405:PL9:C23	35:AD:405:PL9:H303	2.30	0.62
2:BB:5008:VAL:HG23	2:BB:5009:HIS:CD2	2.34	0.62
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.34	0.62
1:BA:5228:THR:HG22	1:BA:5229:GLU:N	2.15	0.62
16:BV:5047:LEU:HD11	16:BV:5143:GLY:HA3	1.81	0.62
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.62
11:BL:5018:TYR:CE2	14:BT:5020:ALA:HA	2.35	0.62
4:BD:5241:GLU:H	4:BD:5241:GLU:CD	2.01	0.62
4:AD:103:ARG:HG3	5:AE:73:LYS:CG	2.28	0.62
4:AD:80:THR:HB	4:AD:81:PRO:HD2	1.80	0.62
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.34	0.62
5:BE:5008:ARG:HH22	5:BE:5016:SER:HB3	1.64	0.62
4:AD:261:PHE:CD2	4:AD:267:LEU:HD12	2.35	0.62
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CZ	2.35	0.62
5:AE:34:GLY:CA	6:AF:32:PHE:CE1	2.83	0.62
3:AC:432:VAL:CG1	3:AC:433:LEU:N	2.63	0.62
1:BA:5193:LEU:HD13	4:BD:5179:PHE:HB3	1.81	0.62
16:BV:5092:ARG:HG3	16:BV:5092:ARG:HH11	1.65	0.62
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.30	0.62
11:AL:13:ASN:ND2	11:AL:15:THR:HG22	2.15	0.62
3:BC:5039:ASN:HB3	24:BC:5509:CLA:CBB	2.30	0.62
3:BC:5062:PHE:HD2	10:BK:5029:PRO:HG3	1.65	0.62
1:AA:48:PHE:HB2	1:AA:115:ILE:HD13	1.81	0.62
15:AU:58:ASN:HD22	15:AU:114:VAL:HG13	1.64	0.62
4:AD:14:TRP:CD1	4:AD:15:PHE:N	2.68	0.62
2:AB:179:GLN:HE21	2:AB:180:PRO:HD2	1.64	0.62
18:BX:5036:VAL:O	18:BX:5040:ILE:HG22	1.99	0.62
1:BA:5296:ASN:HB2	3:BC:5400:PRO:O	2.00	0.62
2:BB:5284:ILE:HG23	2:BB:5305:ILE:HD12	1.82	0.62
1:BA:5306:VAL:HG13	1:BA:5314:ILE:O	2.00	0.62
3:AC:416:SER:C	28:AC:519:DGD:O3E	2.38	0.62
1:AA:200:LEU:HD13	28:AC:519:DGD:HAW2	1.76	0.62
2:AB:329:PRO:HD3	24:AB:607:CLA:HED1	1.82	0.62
2:AB:8:VAL:HG23	2:AB:9:HIS:CD2	2.34	0.62
1:BA:5161:TYR:HB3	1:BA:5162:PRO:HD3	1.82	0.62
3:BC:5288:CYS:SG	28:BC:5517:DGD:HA21	2.39	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:62:PHE:HD2	10:AK:29:PRO:HG3	1.65	0.62
6:BF:5017:THR:HG23	6:BF:5020:TRP:H	1.65	0.62
4:BD:5080:THR:HB	4:BD:5081:PRO:HD2	1.81	0.62
3:AC:40:ALA:O	3:AC:43:ILE:HG13	2.00	0.62
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.00	0.62
24:AB:608:CLA:H143	24:AD:404:CLA:HMB2	1.82	0.61
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.34	0.61
3:BC:5041:ARG:NH1	24:BC:5511:CLA:OBD	2.33	0.61
5:AE:26:THR:HB	36:AF:101:HEM:HAB	1.81	0.61
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.15	0.61
3:BC:5047:GLY:O	3:BC:5050:LEU:HB3	2.00	0.61
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.65	0.61
1:BA:5012:ASN:HD22	1:BA:5015:GLU:HB2	1.66	0.61
4:BD:5239:GLN:O	4:BD:5240:ALA:HB3	2.00	0.61
16:AV:99:VAL:O	16:AV:103:LYS:HG3	2.00	0.61
2:BB:5284:ILE:HG23	2:BB:5305:ILE:CD1	2.30	0.61
31:AB:621:LMG:H411	4:AD:284:ILE:HG12	1.82	0.61
2:BB:5068:ARG:HH22	24:BB:5608:CLA:CED	2.12	0.61
2:BB:5027:THR:CG2	2:BB:5107:LEU:HD13	2.21	0.61
2:BB:5134:ASP:OD2	2:BB:5137:LYS:HB2	2.00	0.61
2:AB:453:PHE:HB2	4:AD:291:LEU:HD23	1.82	0.61
11:BL:5007:ARG:O	11:BL:5007:ARG:HD2	2.00	0.61
3:AC:62:PHE:CE2	10:AK:28:ILE:HB	2.34	0.61
1:BA:5064:ARG:HD3	1:BA:5064:ARG:N	2.14	0.61
2:AB:142:HIS:HA	2:AB:145:LEU:HD12	1.83	0.61
13:BO:5151:LEU:HD12	13:BO:5152:VAL:H	1.65	0.61
5:BE:5051:ARG:HG3	5:BE:5051:ARG:HH11	1.65	0.61
2:BB:5247:PHE:HB2	24:BB:5612:CLA:HBC1	1.81	0.61
1:BA:5200:LEU:HD13	28:BC:5519:DGD:HAW2	1.78	0.61
24:AB:611:CLA:H201	24:AB:613:CLA:H92	1.82	0.61
29:AA:412:LHG:HC11	3:AC:447:ARG:NH2	2.16	0.61
2:BB:5468:TRP:HD1	2:BB:5469:HIS:ND1	1.98	0.61
28:BA:5412:DGD:HO2D	3:BC:5216:SER:HB2	1.64	0.61
3:BC:5114:VAL:HG22	31:BC:5521:LMG:H141	1.81	0.61
4:BD:5207:GLY:HA3	4:BD:5275:PRO:HG3	1.83	0.61
3:BC:5324:LEU:N	3:BC:5324:LEU:HD22	2.15	0.61
3:BC:5033:PHE:CE1	4:BD:5229:ALA:CB	2.84	0.61
24:BB:5612:CLA:H143	24:BD:5405:CLA:HMB2	1.83	0.61
3:BC:5264:PHE:HE1	27:BC:5516:BCR:H321	1.66	0.61
2:AB:179:GLN:NE2	2:AB:180:PRO:HD2	2.15	0.61
1:AA:10:SER:HB3	1:AA:16:ARG:NH1	2.14	0.61
3:AC:324:LEU:HD22	3:AC:324:LEU:N	2.16	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5131:TRP:CE3	1:BA:5132:GLU:N	2.69	0.61
24:BC:5511:CLA:H151	20:BZ:5024:PRO:HG3	1.83	0.61
2:BB:5383:PHE:CZ	13:BO:5193:GLY:HA2	2.35	0.61
27:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.81	0.61
1:AA:133:LEU:O	1:AA:137:LEU:HG	2.00	0.61
3:AC:472:LEU:HG	4:AD:251:ARG:NH1	2.16	0.61
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.36	0.61
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG13	2.36	0.61
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.29	0.61
7:BH:5009:ASP:O	7:BH:5012:ARG:HB2	2.01	0.61
2:BB:5278:SER:HB3	2:BB:5281:GLN:HE21	1.65	0.61
3:AC:30:SER:HB3	10:AK:46:ARG:O	2.00	0.61
2:BB:5173:GLY:CA	2:BB:5265:ILE:HD11	2.31	0.61
13:AO:169:LYS:HG2	13:AO:224:SER:HB3	1.82	0.61
2:AB:246:PHE:C	2:AB:246:PHE:CD1	2.72	0.61
13:AO:151:LEU:HD12	13:AO:152:VAL:H	1.64	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.01	0.61
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG11	1.83	0.60
1:AA:262:TYR:CZ	31:AA:414:LMG:HC5	2.36	0.60
6:BF:5017:THR:O	6:BF:5021:VAL:HG23	2.00	0.60
8:BI:5008:VAL:O	8:BI:5012:VAL:HG23	2.01	0.60
2:AB:222:PRO:HD2	2:AB:225:LEU:HD12	1.83	0.60
2:BB:5133:LEU:HB3	2:BB:5138:MET:CE	2.30	0.60
3:AC:113:VAL:HG11	31:AC:521:LMG:H132	1.83	0.60
1:BA:5300:PHE:CE2	28:BC:5519:DGD:O1A	2.54	0.60
2:AB:153:PHE:N	24:AB:606:CLA:HMC3	2.16	0.60
1:AA:262:TYR:OH	31:AA:414:LMG:HC5	2.00	0.60
16:AV:92:ARG:HH11	16:AV:92:ARG:HG3	1.66	0.60
7:BH:5006:TRP:CE2	7:BH:5010:ILE:HD11	2.36	0.60
35:BD:5406:PL9:C23	35:BD:5406:PL9:H303	2.31	0.60
16:BV:5038:LEU:HD12	16:BV:5095:ILE:HB	1.83	0.60
4:BD:5253:TRP:HA	4:BD:5256:ILE:HG22	1.84	0.60
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.70	0.60
2:AB:479:PHE:O	2:AB:480:SER:HB2	2.01	0.60
24:BC:5504:CLA:H152	28:BC:5519:DGD:HA91	1.84	0.60
24:AB:610:CLA:H121	24:AB:610:CLA:O1D	2.01	0.60
28:AA:411:DGD:HO2D	3:AC:216:SER:HB2	1.65	0.60
12:AM:19:SER:O	12:AM:23:ILE:HD13	2.01	0.60
15:BU:5113:THR:O	15:BU:5114:VAL:HG23	2.01	0.60
10:BK:5018:PHE:CE1	20:BZ:5009:LEU:HG	2.36	0.60
9:AJ:17:ALA:O	9:AJ:21:VAL:HG23	2.01	0.60
1:AA:324:ALA:HB2	4:AD:329:MET:SD	2.42	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.02	0.60
2:BB:5068:ARG:NH2	24:BB:5608:CLA:HED1	2.17	0.60
4:AD:80:THR:HG23	4:AD:172:SER:OG	2.01	0.60
3:AC:437:PHE:CZ	24:AC:502:CLA:HMC1	2.36	0.60
24:BC:5503:CLA:H171	24:BC:5510:CLA:HBB2	1.83	0.60
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.36	0.60
29:AA:415:LHG:HC41	29:AA:415:LHG:O9	2.02	0.60
12:BM:5001:MET:CG	12:BM:5002:GLU:H	2.13	0.60
16:AV:104:ASN:HA	16:AV:122:ARG:HD3	1.83	0.60
3:BC:5044:ASN:C	3:BC:5045:LEU:HD12	2.21	0.60
1:AA:297:LEU:HD11	3:AC:404:LEU:HD12	1.84	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.31	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.82	0.60
2:BB:5384:ARG:HD3	15:BU:5132:LEU:CD1	2.32	0.60
1:BA:5289:GLY:O	1:BA:5292:THR:CG2	2.49	0.60
24:AB:603:CLA:H161	7:AH:38:PHE:HE2	1.65	0.60
24:BB:5608:CLA:HMD2	24:BB:5616:CLA:H193	1.83	0.60
3:AC:41:ARG:NH1	24:AC:511:CLA:OBD	2.34	0.60
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.84	0.60
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.83	0.60
4:BD:5145:ALA:HB2	4:BD:5272:LEU:HD21	1.83	0.60
2:BB:5124:ARG:HH11	2:BB:5124:ARG:HG3	1.67	0.60
13:BO:5118:SER:HB3	13:BO:5157:PRO:HA	1.84	0.60
2:AB:113:TRP:CE2	2:AB:117:TYR:HD1	2.20	0.60
30:AB:622:SQD:H442	4:AD:23:LYS:HE2	1.82	0.60
3:BC:5156:LYS:O	3:BC:5160:ILE:HG13	2.02	0.60
2:BB:5142:HIS:HA	2:BB:5145:LEU:HD12	1.83	0.60
13:AO:64:TYR:HD1	13:AO:271:PRO:HA	1.67	0.60
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.84	0.60
3:BC:5216:SER:HB3	3:BC:5221:GLU:HB2	1.84	0.60
27:BC:5516:BCR:HC41	8:BI:5020:VAL:HG13	1.82	0.60
27:BC:5514:BCR:H391	10:BK:5036:ALA:HB2	1.83	0.60
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.37	0.60
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NH2	2.17	0.60
3:BC:5143:TYR:O	3:BC:5144:SER:HB2	2.02	0.60
3:BC:5413:GLU:HG3	3:BC:5414:ILE:N	2.17	0.59
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.84	0.59
3:AC:233:VAL:HA	27:AC:516:BCR:H281	1.84	0.59
3:AC:52:ALA:CA	24:AC:511:CLA:HMB3	2.27	0.59
3:BC:5042:LEU:HD23	24:BC:5511:CLA:HED3	1.82	0.59
3:AC:167:VAL:HG11	24:AC:512:CLA:H3A	1.84	0.59
9:BJ:5017:ALA:O	9:BJ:5021:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.25	0.59
24:AA:405:CLA:HBA2	31:AB:620:LMG:C25	2.32	0.59
10:BK:5024:VAL:O	10:BK:5027:VAL:HG12	2.02	0.59
5:AE:8:ARG:HH22	5:AE:16:SER:HB3	1.67	0.59
2:BB:5265:ILE:HG13	2:BB:5266:GLU:N	2.17	0.59
2:AB:359:MET:HB2	2:AB:425:ILE:HG23	1.84	0.59
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HG23	1.82	0.59
1:BA:5265:PHE:CD1	1:BA:5271:LEU:HA	2.36	0.59
2:AB:280:PHE:CE2	2:AB:312:TYR:HB3	2.36	0.59
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.02	0.59
16:AV:47:LEU:HD11	16:AV:143:GLY:HA3	1.83	0.59
8:AI:1:MET:HE1	32:BB:5604:LMT:H41	1.84	0.59
3:BC:5178:LYS:HA	3:BC:5182:PHE:HB2	1.83	0.59
2:BB:5188:ASP:OD1	7:BH:5058:VAL:HA	2.03	0.59
13:BO:5083:LYS:HG2	13:BO:5084:ASN:H	1.66	0.59
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.13	0.59
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.38	0.59
3:BC:5415:ASN:HB3	9:BJ:5039:SER:OG	2.03	0.59
4:BD:5014:TRP:CD1	4:BD:5015:PHE:N	2.70	0.59
6:AF:19:ARG:HH11	6:AF:19:ARG:HG3	1.67	0.59
3:AC:324:LEU:CD2	3:AC:324:LEU:N	2.66	0.59
10:BK:5017:ILE:N	10:BK:5017:ILE:HD12	2.17	0.59
1:BA:5257:ARG:HH11	1:BA:5257:ARG:HG3	1.66	0.59
13:AO:206:GLU:CD	13:AO:206:GLU:H	2.05	0.59
24:AB:604:CLA:H121	24:AB:615:CLA:HBA1	1.83	0.59
1:BA:5220:THR:HG23	4:BD:5141:TYR:HD1	1.68	0.59
3:AC:362:ARG:HE	3:AC:370:ARG:NH1	1.99	0.59
2:BB:5487:SER:N	2:BB:5488:PRO:HD2	2.17	0.59
35:BD:5406:PL9:H262	35:BD:5406:PL9:C30	2.32	0.59
11:BL:5013:ASN:ND2	11:BL:5015:THR:HG22	2.18	0.59
3:AC:305:THR:HG22	3:AC:308:GLU:HB3	1.81	0.59
1:BA:5083:VAL:HG22	4:BD:5314:PHE:CE2	2.36	0.59
16:BV:5099:VAL:O	16:BV:5103:LYS:HG3	2.02	0.59
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.84	0.59
24:BC:5504:CLA:H151	28:BC:5519:DGD:C9A	2.31	0.59
24:BB:5607:CLA:H161	7:BH:5038:PHE:HE2	1.68	0.59
3:BC:5037:ALA:C	24:BC:5508:CLA:HBA1	2.23	0.59
24:AC:511:CLA:H151	20:AZ:24:PRO:HG3	1.84	0.59
5:BE:5026:THR:HB	36:BF:5101:HEM:HAB	1.85	0.59
5:AE:51:ARG:NH1	5:AE:51:ARG:HG3	2.15	0.59
1:AA:97:TRP:HA	8:AI:1:MET:SD	2.43	0.59
6:BF:5037:ILE:HA	6:BF:5040:MET:SD	2.43	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:AI:14:PHE:CZ	8:AI:18:LEU:HD11	2.38	0.59
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.84	0.59
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.02	0.59
4:AD:299:ILE:HG13	11:AL:37:ASN:HD21	1.67	0.59
1:BA:5032:TRP:HA	1:BA:5032:TRP:HE3	1.67	0.59
2:AB:483:ASP:HB3	2:AB:484:PRO:HD2	1.85	0.59
3:BC:5033:PHE:CE1	4:BD:5229:ALA:HB3	2.38	0.59
3:BC:5170:ILE:HG22	3:BC:5174:LEU:CD2	2.33	0.59
3:BC:5405:ASN:HB2	28:BC:5519:DGD:C3G	2.32	0.59
35:AD:405:PL9:H262	35:AD:405:PL9:C30	2.33	0.59
7:BH:5055:LEU:O	7:BH:5058:VAL:HG12	2.02	0.59
1:BA:5188:ALA:HB2	1:BA:5328:MET:HB2	1.85	0.59
10:BK:5031:LEU:O	10:BK:5034:ALA:HB3	2.03	0.59
2:AB:384:ARG:HD3	15:AU:132:LEU:HD11	1.85	0.59
15:AU:68:TYR:HB2	15:AU:71:LEU:HD12	1.84	0.59
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.18	0.59
3:AC:418:ASN:CB	28:AC:519:DGD:HE2	2.32	0.59
24:AA:405:CLA:H92	34:AD:402:PHO:HMB3	1.85	0.59
4:AD:150:ILE:O	4:AD:154:VAL:HG23	2.03	0.59
24:BB:5612:CLA:H202	7:BH:5043:LEU:HD11	1.83	0.59
1:AA:64:ARG:HD3	1:AA:64:ARG:N	2.17	0.59
6:AF:15:ILE:HG22	6:AF:16:PHE:HD1	1.68	0.59
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.85	0.59
15:AU:98:THR:HG23	15:AU:101:GLN:OE1	2.03	0.59
1:AA:180:PHE:CD1	4:AD:192:THR:HB	2.38	0.58
2:BB:5458:PHE:HB3	24:BB:5608:CLA:HBC2	1.84	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
1:BA:5013:LEU:CA	1:BA:5016:ARG:HD3	2.33	0.58
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.03	0.58
3:BC:5324:LEU:CD2	3:BC:5324:LEU:N	2.65	0.58
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.85	0.58
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.03	0.58
24:AC:501:CLA:HMB3	27:AC:516:BCR:C40	2.31	0.58
3:AC:264:PHE:HE1	27:AC:516:BCR:H321	1.67	0.58
10:BK:5026:PRO:O	10:BK:5029:PRO:HD2	2.02	0.58
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.02	0.58
7:BH:5012:ARG:N	7:BH:5013:PRO:HD2	2.18	0.58
6:BF:5015:ILE:HG22	6:BF:5016:PHE:HD1	1.68	0.58
4:BD:5299:ILE:HG13	11:BL:5037:ASN:HD21	1.68	0.58
28:BC:5519:DGD:HG2	9:BJ:5033:TYR:OH	2.03	0.58
1:BA:5020:TRP:CD1	1:BA:5020:TRP:C	2.75	0.58
9:BJ:5011:TRP:CE3	10:BK:5042:ALA:HB2	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:AU:54:LYS:HD2	15:AU:113:THR:HG23	1.86	0.58
24:BB:5615:CLA:H201	24:BB:5617:CLA:H92	1.84	0.58
3:BC:5167:VAL:HG11	24:BC:5512:CLA:H3A	1.83	0.58
1:BA:5163:ILE:HG12	28:BC:5517:DGD:HB31	1.85	0.58
35:BD:5406:PL9:H301	35:BD:5406:PL9:C33	2.34	0.58
5:BE:5026:THR:O	5:BE:5029:ALA:HB3	2.02	0.58
2:AB:490:GLN:OE1	2:AB:490:GLN:O	2.21	0.58
2:AB:144:PHE:CE1	2:AB:210:ILE:HG23	2.39	0.58
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.68	0.58
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.03	0.58
3:BC:5110:PRO:O	3:BC:5114:VAL:HG23	2.02	0.58
3:BC:5116:VAL:HG23	3:BC:5117:VAL:N	2.19	0.58
2:BB:5359:MET:HB2	2:BB:5425:ILE:HG23	1.85	0.58
1:AA:271:LEU:C	1:AA:271:LEU:HD23	2.24	0.58
2:BB:5246:PHE:C	2:BB:5246:PHE:HD1	2.07	0.58
16:BV:5056:LYS:O	16:BV:5060:GLN:HG3	2.03	0.58
4:AD:41:ALA:HB1	34:AD:403:PHO:H42	1.85	0.58
14:BT:5018:PHE:HB2	27:BT:5101:BCR:HC8	1.84	0.58
20:BZ:5033:TRP:HD1	20:BZ:5033:TRP:O	1.87	0.58
3:BC:5432:VAL:CG1	3:BC:5433:LEU:N	2.65	0.58
2:BB:5349:LYS:HG3	2:BB:5350:GLU:OE1	2.03	0.58
6:BF:5011:VAL:HG12	6:BF:5012:SER:H	1.69	0.58
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.04	0.58
3:AC:279:LEU:HD23	3:AC:282:MET:HE3	1.85	0.58
3:AC:39:ASN:HB3	24:AC:509:CLA:CBB	2.33	0.58
14:AT:18:PHE:HB2	27:AT:101:BCR:HC8	1.84	0.58
1:BA:5274:PHE:CE2	25:BA:5409:MST:H133	2.37	0.58
3:AC:257:PHE:O	3:AC:261:ARG:HG3	2.03	0.58
2:BB:5170:ASP:HB2	2:BB:5171:PRO:CD	2.32	0.58
3:AC:39:ASN:HB2	24:AC:508:CLA:HBA2	1.84	0.58
24:BB:5608:CLA:H121	24:BB:5619:CLA:HBA1	1.85	0.58
3:BC:5279:LEU:HD12	3:BC:5437:PHE:HE1	1.69	0.58
4:BD:5086:GLY:CA	4:BD:5166:SER:HB2	2.34	0.58
4:BD:5267:LEU:HD23	4:BD:5267:LEU:C	2.24	0.58
1:BA:5272:HIS:HD2	4:BD:5218:VAL:HG21	1.68	0.58
4:AD:244:TYR:OH	4:AD:264:LYS:HD2	2.03	0.58
16:BV:5133:LEU:H	16:BV:5133:LEU:CD1	2.16	0.58
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.38	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.03	0.58
2:BB:5479:PHE:O	2:BB:5480:SER:HB2	2.03	0.58
6:BF:5018:VAL:HG12	6:BF:5019:ARG:N	2.19	0.58
8:BI:5027:ASP:N	8:BI:5028:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:BB:5618:CLA:H202	31:BL:5101:LMG:H422	1.86	0.58
2:BB:5179:GLN:NE2	2:BB:5180:PRO:HD2	2.18	0.58
4:BD:5244:TYR:OH	4:BD:5264:LYS:HD2	2.04	0.58
4:AD:171:PRO:HG3	4:AD:181:PHE:CZ	2.39	0.58
3:BC:5367:GLU:HB2	3:BC:5368:PRO:HD3	1.86	0.58
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.03	0.58
1:AA:219:VAL:HG11	4:AD:268:HIS:CD2	2.38	0.58
1:BA:5307:ILE:HG22	1:BA:5313:VAL:HA	1.86	0.58
24:BA:5406:CLA:HBA2	31:BL:5101:LMG:C25	2.33	0.58
2:AB:383:PHE:CZ	13:AO:193:GLY:HA2	2.39	0.58
1:BA:5190:HIS:HB3	1:BA:5293:MET:CE	2.34	0.58
1:BA:5219:VAL:HG11	4:BD:5268:HIS:CD2	2.38	0.58
2:BB:5113:TRP:CE2	2:BB:5117:TYR:HD1	2.22	0.58
2:AB:135:LEU:HD23	2:AB:138:MET:HE1	1.86	0.57
3:AC:37:ALA:C	24:AC:508:CLA:HBA1	2.25	0.57
18:AX:16:LEU:O	18:AX:16:LEU:HD13	2.04	0.57
3:BC:5226:SER:O	28:BC:5517:DGD:HE62	2.04	0.57
1:BA:5341:LEU:HB2	3:BC:5313:GLN:NE2	2.10	0.57
1:AA:330:VAL:CG1	4:AD:348:ARG:HG2	2.34	0.57
3:BC:5377:LEU:O	3:BC:5381:LYS:HB2	2.04	0.57
14:BT:5022:PHE:C	14:BT:5023:PHE:HD2	2.06	0.57
6:BF:5037:ILE:HG22	9:BJ:5028:PHE:CE1	2.38	0.57
13:BO:5123:GLU:HG2	13:BO:5124:GLU:N	2.17	0.57
24:AB:604:CLA:HMD2	24:AB:612:CLA:H193	1.86	0.57
1:BA:5283:VAL:HG21	34:BD:5403:PHO:HBC3	1.86	0.57
2:BB:5153:PHE:N	24:BB:5610:CLA:HMC3	2.19	0.57
24:BC:5505:CLA:O1A	8:BI:5023:PHE:CE1	2.57	0.57
1:AA:260:PHE:CZ	1:AA:263:ALA:HB2	2.39	0.57
3:AC:449:ARG:HG2	24:AC:505:CLA:HED1	1.86	0.57
8:AI:13:THR:HA	8:AI:16:VAL:HG12	1.86	0.57
30:BB:5625:SQD:H442	4:BD:5023:LYS:HE2	1.85	0.57
24:BB:5606:CLA:H11	7:BH:5049:TYR:HD2	1.69	0.57
3:BC:5297:TYR:HA	3:BC:5302:TYR:HE2	1.69	0.57
6:AF:37:ILE:HA	6:AF:40:MET:SD	2.44	0.57
24:AB:602:CLA:HBD	24:AB:602:CLA:H43	1.86	0.57
3:AC:279:LEU:HA	3:AC:282:MET:HE3	1.86	0.57
1:BA:5045:THR:HG23	1:BA:5046:ILE:N	2.18	0.57
24:BC:5512:CLA:H203	31:BC:5521:LMG:H381	1.86	0.57
11:BL:5008:GLN:N	11:BL:5008:GLN:NE2	2.52	0.57
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.05	0.57
13:AO:32:THR:O	13:AO:36:ILE:CD1	2.52	0.57
2:AB:458:PHE:HB3	24:AB:604:CLA:HBC2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:226:SER:O	28:AC:517:DGD:HE62	2.04	0.57
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.52	0.57
2:BB:5135:LEU:HD23	2:BB:5138:MET:HE1	1.86	0.57
32:BB:5627:LMT:H112	7:BH:5035:MET:HE2	1.87	0.57
2:BB:5262:THR:HG23	2:BB:5263:THR:HG23	1.86	0.57
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.69	0.57
3:BC:5220:GLY:N	28:BC:5517:DGD:O3D	2.35	0.57
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.24	0.57
1:AA:13:LEU:CA	1:AA:16:ARG:HD3	2.34	0.57
1:AA:57:PRO:HD3	1:AA:73:TYR:CD2	2.40	0.57
1:BA:5317:TRP:CD1	4:BD:5177:ALA:HB2	2.38	0.57
3:BC:5039:ASN:HB2	24:BC:5508:CLA:HBA2	1.85	0.57
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	2.05	0.57
1:BA:5315:ASN:HD21	4:BD:5332:GLN:NE2	2.02	0.57
2:BB:5483:ASP:HB3	2:BB:5484:PRO:HD2	1.85	0.57
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.87	0.57
3:AC:199:ILE:HD12	3:AC:199:ILE:N	2.18	0.57
4:BD:5056:THR:HG21	5:BE:5050:PRO:HD3	1.87	0.57
4:AD:335:PRO:HB2	5:AE:65:LEU:HD21	1.86	0.57
1:BA:5289:GLY:HA2	1:BA:5292:THR:HG22	1.86	0.57
2:BB:5237:VAL:HG22	24:BB:5614:CLA:HBC2	1.86	0.57
5:BE:5015:THR:HB	9:BJ:5006:GLY:HA2	1.87	0.57
24:AC:504:CLA:H2	28:AC:518:DGD:HA21	1.87	0.57
3:BC:5405:ASN:HA	28:BC:5519:DGD:HG11	1.87	0.57
28:BC:5519:DGD:O3D	9:BJ:5037:GLY:O	2.20	0.57
24:BB:5614:CLA:O1D	24:BB:5614:CLA:H121	2.04	0.57
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.87	0.57
13:BO:5114:ASN:ND2	13:BO:5120:THR:HG23	2.20	0.57
2:AB:246:PHE:C	2:AB:246:PHE:HD1	2.08	0.57
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.38	0.57
24:AC:504:CLA:H172	28:AC:519:DGD:HAE1	1.85	0.57
24:BB:5613:CLA:HMC2	27:BX:5101:BCR:H343	1.85	0.57
3:BC:5233:VAL:HA	27:BC:5516:BCR:H281	1.87	0.57
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:HD11	1.87	0.57
13:BO:5218:LEU:CD2	15:BU:5119:THR:HG21	2.35	0.57
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.05	0.57
2:AB:327:THR:O	2:AB:444:ARG:NE	2.36	0.57
18:BX:5045:LYS:N	18:BX:5045:LYS:HD3	2.19	0.57
1:BA:5191:ASN:HB2	3:BC:5411:ALA:HB1	1.85	0.57
1:BA:5278:TRP:O	1:BA:5281:VAL:HG12	2.05	0.56
32:AB:624:LMT:H92	7:AH:35:MET:CE	2.35	0.56
24:BB:5606:CLA:HBD	24:BB:5606:CLA:H43	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5057:ALA:HB1	24:BC:5512:CLA:HED2	1.85	0.56
4:BD:5150:ILE:O	4:BD:5154:VAL:HG23	2.06	0.56
32:BB:5627:LMT:H92	7:BH:5035:MET:CE	2.35	0.56
3:BC:5062:PHE:HZ	10:BK:5028:ILE:HD12	1.69	0.56
5:BE:5077:GLU:HA	5:BE:5080:LEU:HD23	1.87	0.56
13:BO:5098:THR:HG23	13:BO:5133:THR:HB	1.87	0.56
25:AA:408:MST:N3	25:AA:408:MST:H122	2.20	0.56
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.05	0.56
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.04	0.56
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.35	0.56
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.87	0.56
28:AA:411:DGD:O1B	28:AA:411:DGD:C1G	2.53	0.56
1:BA:5180:PHE:CE1	4:BD:5192:THR:HB	2.40	0.56
7:BH:5058:VAL:O	7:BH:5058:VAL:CG1	2.53	0.56
13:AO:114:ASN:ND2	13:AO:120:THR:HG23	2.19	0.56
27:AC:516:BCR:HC41	8:AI:20:VAL:HG13	1.86	0.56
2:AB:462:PHE:CZ	24:AB:613:CLA:HMB3	2.40	0.56
24:AB:609:CLA:HMC2	27:AX:101:BCR:H343	1.87	0.56
2:BB:5462:PHE:HA	24:BB:5615:CLA:CMC	2.35	0.56
4:BD:5086:GLY:C	4:BD:5166:SER:HB2	2.25	0.56
4:BD:5158:LEU:O	4:BD:5162:LEU:HG	2.06	0.56
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.06	0.56
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.06	0.56
3:BC:5375:LEU:HB3	3:BC:5380:ILE:HD11	1.87	0.56
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.20	0.56
5:AE:56:TYR:HE1	5:AE:63:ILE:HD12	1.69	0.56
1:AA:262:TYR:CE1	31:AA:414:LMG:C5	2.89	0.56
4:BD:5221:THR:CG2	4:BD:5244:TYR:HB2	2.35	0.56
2:BB:5271:THR:OG1	2:BB:5274:GLN:HG3	2.05	0.56
1:AA:15:GLU:O	1:AA:19:ASN:OD1	2.23	0.56
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.56
3:BC:5199:ILE:N	3:BC:5199:ILE:HD12	2.20	0.56
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.68	0.56
2:BB:5453:PHE:HB2	4:BD:5291:LEU:HD23	1.87	0.56
3:BC:5304:PRO:HB3	3:BC:5395:TYR:CD1	2.40	0.56
20:BZ:5014:ILE:O	20:BZ:5018:VAL:HG23	2.05	0.56
3:BC:5362:ARG:HE	3:BC:5370:ARG:HH11	1.52	0.56
1:AA:278:TRP:O	1:AA:281:VAL:HG12	2.04	0.56
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.21	0.56
2:BB:5027:THR:HG22	2:BB:5107:LEU:CD1	2.24	0.56
8:BI:5013:THR:HA	8:BI:5016:VAL:HG12	1.85	0.56
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:5154:SER:O	13:BO:5168:PHE:HA	2.05	0.56
5:BE:5051:ARG:HG3	5:BE:5051:ARG:NH1	2.19	0.56
3:BC:5297:TYR:HA	3:BC:5302:TYR:CE2	2.40	0.56
1:AA:126:TYR:O	1:AA:130:GLN:HG3	2.06	0.56
1:BA:5326:LEU:HD21	3:BC:5412:THR:HB	1.87	0.56
5:BE:5014:ILE:CG2	9:BJ:5013:VAL:HG11	2.35	0.56
24:AB:611:CLA:C5	24:AB:614:CLA:HBC2	2.36	0.56
3:BC:5149:TYR:HA	3:BC:5156:LYS:CD	2.35	0.56
2:AB:262:THR:HG23	2:AB:263:THR:HG23	1.88	0.56
16:AV:133:LEU:CD1	16:AV:133:LEU:H	2.18	0.56
2:AB:271:THR:OG1	2:AB:274:GLN:HG3	2.05	0.56
13:BO:5173:ASN:ND2	13:BO:5220:LYS:HD3	2.20	0.56
24:AC:505:CLA:O1A	8:AI:23:PHE:CE1	2.59	0.56
8:AI:13:THR:O	8:AI:16:VAL:HG12	2.06	0.56
1:BA:5221:SER:HB3	4:BD:5141:TYR:HB2	1.86	0.56
15:BU:5083:ALA:CB	15:BU:5084:PRO:CD	2.82	0.56
3:BC:5158:THR:HG21	3:BC:5254:THR:O	2.06	0.56
3:BC:5461:ARG:NH2	4:BD:5242:GLU:O	2.38	0.56
4:AD:145:ALA:HB2	4:AD:272:LEU:HD21	1.86	0.56
3:AC:114:VAL:HG22	31:AC:521:LMG:H141	1.87	0.56
13:AO:148:VAL:HA	13:AO:172:PHE:CD2	2.40	0.56
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.39	0.56
2:BB:5206:GLY:O	2:BB:5210:ILE:HG13	2.05	0.56
2:BB:5280:PHE:CE2	2:BB:5312:TYR:HB3	2.40	0.56
2:BB:5270:PRO:HG3	2:BB:5312:TYR:HD2	1.70	0.56
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	2.05	0.56
13:BO:5215:ARG:NH1	13:BO:5252:GLY:O	2.38	0.56
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.88	0.56
2:AB:250:PHE:CE2	2:AB:459:ALA:HB1	2.41	0.56
2:BB:5329:PRO:HD3	24:BB:5611:CLA:HED1	1.86	0.56
1:BA:5092:HIS:HD2	3:BC:5219:GLY:HA3	1.71	0.56
10:BK:5035:LEU:HA	10:BK:5038:VAL:HG23	1.88	0.56
13:BO:5080:GLU:O	13:BO:5089:ALA:HB1	2.05	0.56
3:AC:42:LEU:CD2	24:AC:511:CLA:HED3	2.36	0.56
5:BE:5056:TYR:HE1	5:BE:5063:ILE:HD12	1.71	0.56
2:BB:5179:GLN:HE21	2:BB:5180:PRO:HD2	1.71	0.56
4:BD:5129:GLN:HE22	4:BD:5143:ALA:HA	1.70	0.56
1:BA:5133:LEU:O	1:BA:5137:LEU:HG	2.06	0.56
1:BA:5124:SER:O	1:BA:5127:MET:HB3	2.06	0.56
3:AC:44:ASN:O	3:AC:45:LEU:HD12	2.05	0.56
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.88	0.56
3:AC:170:ILE:HG22	3:AC:174:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:AE:57:ALA:H	5:AE:60:GLN:NE2	2.04	0.56
4:AD:241:GLU:H	4:AD:241:GLU:CD	2.08	0.56
1:AA:157:VAL:HG21	24:AA:405:CLA:CMC	2.36	0.56
1:AA:180:PHE:CE1	4:AD:192:THR:HB	2.41	0.56
2:BB:5462:PHE:CZ	24:BB:5617:CLA:HMB3	2.41	0.56
5:BE:5069:ARG:HG3	5:BE:5070:PHE:N	2.20	0.56
5:AE:15:THR:HB	9:AJ:6:GLY:HA2	1.87	0.56
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB3	1.83	0.56
3:AC:57:ALA:HB1	24:AC:512:CLA:HED2	1.88	0.56
15:AU:66:ILE:HG12	15:AU:72:TYR:CG	2.41	0.56
2:BB:5369:ILE:O	2:BB:5370:LEU:HD23	2.04	0.56
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.56
3:BC:5343:ARG:NH1	3:BC:5347:GLY:O	2.39	0.56
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CD2	2.41	0.56
4:BD:5092:LEU:HA	4:BD:5104:TRP:CD1	2.41	0.56
24:AB:608:CLA:H203	24:AD:404:CLA:HBA2	1.89	0.56
32:AB:624:LMT:H112	7:AH:35:MET:HE2	1.89	0.56
24:BA:5406:CLA:H93	34:BD:5403:PHO:HHB	1.88	0.56
15:BU:5058:ASN:HD22	15:BU:5114:VAL:HG13	1.69	0.56
3:BC:5374:GLY:O	3:BC:5375:LEU:C	2.44	0.56
4:BD:5346:LEU:O	4:BD:5348:ARG:HG3	2.06	0.56
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.87	0.56
3:AC:405:ASN:HA	28:AC:519:DGD:HG11	1.88	0.55
28:BC:5518:DGD:HB22	28:BC:5519:DGD:HA21	1.88	0.55
2:AB:133:LEU:HB3	2:AB:138:MET:HE2	1.88	0.55
3:AC:233:VAL:HA	27:AC:516:BCR:C28	2.36	0.55
3:AC:95:LEU:HD13	24:AC:502:CLA:H143	1.89	0.55
35:AD:405:PL9:H301	35:AD:405:PL9:C33	2.34	0.55
18:AX:12:ILE:HA	27:AX:101:BCR:H401	1.88	0.55
3:BC:5124:VAL:HB	27:BC:5515:BCR:H362	1.88	0.55
14:AT:29:ILE:N	14:AT:29:ILE:HD12	2.06	0.55
24:AC:513:CLA:H42	24:AC:513:CLA:HAA1	1.88	0.55
1:BA:5048:PHE:HA	1:BA:5115:ILE:HD11	1.88	0.55
3:BC:5416:SER:N	28:BC:5519:DGD:O3E	2.37	0.55
24:BA:5406:CLA:H92	34:BD:5403:PHO:HMB3	1.87	0.55
24:BB:5605:CLA:HMB1	27:BX:5101:BCR:H393	1.88	0.55
5:BE:5076:VAL:O	5:BE:5080:LEU:CD2	2.54	0.55
2:BB:5483:ASP:CG	2:BB:5484:PRO:HD2	2.26	0.55
2:BB:5144:PHE:CE1	2:BB:5210:ILE:HG23	2.41	0.55
3:BC:5033:PHE:HE1	4:BD:5229:ALA:CB	2.19	0.55
16:AV:81:ARG:HH11	16:AV:81:ARG:HG2	1.70	0.55
1:AA:304:HIS:CE1	3:AC:414:ILE:HD12	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CIA	2.36	0.55
24:AB:601:CLA:HMB1	27:AX:101:BCR:H393	1.88	0.55
8:BI:5013:THR:O	8:BI:5016:VAL:HG12	2.06	0.55
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.89	0.55
25:BA:5409:MST:N3	25:BA:5409:MST:H131	2.20	0.55
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.55
4:AD:86:GLY:C	4:AD:166:SER:HB2	2.26	0.55
24:AA:405:CLA:H201	14:AT:14:ILE:HD11	1.86	0.55
3:BC:5225:VAL:HG22	3:BC:5289:PHE:CD1	2.42	0.55
4:BD:5014:TRP:NE1	7:BH:5025:TRP:HH2	1.95	0.55
2:BB:5154:GLY:O	2:BB:5159:THR:HG23	2.06	0.55
13:BO:5092:VAL:HG13	13:BO:5093:PRO:HD2	1.87	0.55
4:BD:5239:GLN:O	4:BD:5240:ALA:CB	2.54	0.55
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD11	1.89	0.55
3:BC:5170:ILE:HG22	3:BC:5174:LEU:HD23	1.88	0.55
9:BJ:5011:TRP:CG	10:BK:5042:ALA:HA	2.41	0.55
15:BU:5098:THR:HG23	15:BU:5101:GLN:OE1	2.07	0.55
12:BM:5005:GLN:HE22	32:BM:5101:LMT:H3'	1.71	0.55
2:AB:231:MET:HG2	24:AB:610:CLA:HMC1	1.89	0.55
4:BD:5266:TRP:CD1	31:BD:5410:LMG:HC1	2.42	0.55
3:BC:5155:ASN:O	3:BC:5158:THR:HG22	2.07	0.55
20:BZ:5033:TRP:CD1	20:BZ:5033:TRP:O	2.60	0.55
15:BU:5066:ILE:HG12	15:BU:5072:TYR:CG	2.42	0.55
4:AD:253:TRP:HA	4:AD:256:ILE:HG22	1.89	0.55
1:AA:205:VAL:HG21	24:AA:404:CLA:CMA	2.37	0.55
24:AB:602:CLA:H11	7:AH:49:TYR:HD2	1.71	0.55
1:BA:5176:ILE:HG22	1:BA:5180:PHE:HE2	1.71	0.55
27:BC:5515:BCR:H312	20:BZ:5055:GLY:HA2	1.88	0.55
3:BC:5461:ARG:CG	3:BC:5461:ARG:NH1	2.61	0.55
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.06	0.55
2:AB:121:GLU:HG3	7:AH:4:ARG:CA	2.36	0.55
2:BB:5176:GLY:HA3	2:BB:5266:GLU:OE1	2.06	0.55
1:AA:124:SER:O	1:AA:127:MET:HB3	2.07	0.55
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.36	0.55
4:BD:5049:LEU:O	4:BD:5053:THR:HG23	2.06	0.55
1:BA:5271:LEU:HD21	25:BA:5409:MST:H83	1.89	0.55
2:BB:5275:TRP:CH2	2:BB:5358:ARG:HD3	2.41	0.55
1:AA:191:ASN:HB2	3:AC:411:ALA:HB1	1.89	0.55
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.07	0.55
1:AA:340:PRO:HG2	3:AC:317:PHE:CZ	2.42	0.55
1:AA:20:TRP:C	1:AA:20:TRP:CD1	2.80	0.55
31:AB:620:LMG:H191	11:AL:22:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:BH:5055:LEU:HB2	7:BH:5058:VAL:HG12	1.89	0.55
29:BA:5415:LHG:HC41	29:BA:5415:LHG:O9	2.05	0.55
12:AM:20:VAL:HG22	12:BM:5020:VAL:HG11	1.89	0.55
3:BC:5257:PHE:O	3:BC:5261:ARG:HG3	2.06	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:CE	2.36	0.55
2:BB:5348:ASN:OD1	2:BB:5352:GLU:HB2	2.06	0.55
1:BA:5289:GLY:C	1:BA:5292:THR:HG22	2.27	0.55
2:AB:90:PHE:CE2	2:AB:91:TRP:CZ3	2.94	0.55
4:AD:259:ILE:HG12	31:AD:408:LMG:H301	1.89	0.55
12:AM:23:ILE:HG12	31:AM:101:LMG:H212	1.89	0.55
1:BA:5217:SER:HA	1:BA:5220:THR:HG22	1.89	0.55
1:BA:5157:VAL:HG21	24:BA:5406:CLA:CMC	2.36	0.55
24:BC:5513:CLA:H42	24:BC:5513:CLA:HAA1	1.88	0.55
3:AC:35:TRP:O	24:AC:511:CLA:HMD3	2.07	0.55
1:AA:341:LEU:HB2	3:AC:313:GLN:NE2	2.17	0.55
2:BB:5354:LEU:HD21	2:BB:5378:LYS:HB2	1.89	0.55
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:N	2.57	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:HE1	1.89	0.55
13:AO:64:TYR:CD1	13:AO:271:PRO:HA	2.41	0.55
3:BC:5281:MET:O	3:BC:5285:ILE:HG13	2.06	0.55
13:BO:5064:TYR:HD1	13:BO:5271:PRO:HA	1.72	0.55
4:BD:5313:THR:OG1	4:BD:5315:TYR:HB3	2.07	0.55
2:BB:5230:ARG:O	2:BB:5233:ASN:HB3	2.07	0.55
30:BB:5625:SQD:H152	32:BB:5627:LMT:H81	1.89	0.55
3:AC:62:PHE:HZ	10:AK:28:ILE:HD12	1.71	0.55
3:BC:5453:ALA:C	8:BI:5034:ARG:HB2	2.27	0.55
7:BH:5011:LEU:C	7:BH:5013:PRO:HD2	2.28	0.55
25:AA:408:MST:N3	25:AA:408:MST:H131	2.21	0.55
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.22	0.55
1:BA:5281:VAL:CG1	28:BC:5519:DGD:CIA	2.84	0.55
24:AB:613:CLA:H203	31:AD:407:LMG:H401	1.89	0.55
28:BA:5412:DGD:C1G	28:BA:5412:DGD:O1B	2.55	0.55
27:BC:5515:BCR:C31	20:BZ:5055:GLY:HA2	2.37	0.55
2:AB:76:SER:HB3	31:BA:5402:LMG:H301	1.88	0.55
24:AC:512:CLA:H203	31:AC:521:LMG:H381	1.88	0.55
1:BA:5064:ARG:HD3	1:BA:5064:ARG:H	1.72	0.55
1:AA:288:LEU:HD13	3:AC:432:VAL:CG2	2.37	0.55
4:BD:5053:THR:HG22	4:BD:5067:TYR:HE2	1.72	0.55
4:BD:5077:ALA:HB2	4:BD:5174:GLY:HA3	1.88	0.55
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.88	0.55
1:BA:5330:VAL:HG12	4:BD:5348:ARG:HA	1.87	0.55
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5326:ALA:HB2	15:BU:5128:TYR:CG	2.42	0.55
28:AC:519:DGD:HE62	9:AJ:40:LEU:HD11	1.89	0.54
1:AA:38:ILE:HB	1:AA:39:PRO:HD3	1.89	0.54
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	1.87	0.54
1:BA:5234:ASN:HB2	31:BL:5101:LMG:O3	2.05	0.54
30:AA:416:SQD:H302	24:BB:5620:CLA:H51	1.88	0.54
3:BC:5095:LEU:HD13	24:BC:5502:CLA:H143	1.87	0.54
4:BD:5086:GLY:HA2	4:BD:5166:SER:HB2	1.88	0.54
15:AU:57:LEU:HD11	15:AU:112:PHE:HB3	1.89	0.54
13:AO:116:ASP:C	13:AO:116:ASP:OD2	2.46	0.54
3:BC:5259:TRP:HD1	3:BC:5259:TRP:H	1.55	0.54
13:BO:5086:ARG:O	13:BO:5086:ARG:NE	2.40	0.54
1:AA:289:GLY:HA2	1:AA:292:THR:HG22	1.90	0.54
1:AA:32:TRP:HE3	1:AA:32:TRP:HA	1.72	0.54
3:AC:279:LEU:HD12	3:AC:437:PHE:HE1	1.73	0.54
2:AB:222:PRO:CG	7:AH:27:THR:H	2.20	0.54
2:BB:5068:ARG:NH1	24:BB:5608:CLA:HED1	2.22	0.54
2:BB:5222:PRO:HD2	2:BB:5225:LEU:HD12	1.88	0.54
24:BB:5617:CLA:H203	31:BD:5409:LMG:H401	1.88	0.54
3:BC:5279:LEU:HD23	3:BC:5282:MET:HE3	1.89	0.54
3:BC:5279:LEU:HA	3:BC:5282:MET:HE3	1.89	0.54
8:BI:5010:ILE:HG21	32:BI:5102:LMT:H82	1.88	0.54
3:BC:5035:TRP:O	24:BC:5511:CLA:HMD3	2.07	0.54
7:BH:5017:GLU:CD	7:BH:5017:GLU:H	2.10	0.54
20:BZ:5012:LEU:HD12	20:BZ:5012:LEU:O	2.08	0.54
24:AB:609:CLA:OBD	7:AH:27:THR:HB	2.06	0.54
24:BB:5615:CLA:C5	24:BB:5618:CLA:HBC2	2.38	0.54
3:BC:5279:LEU:HD22	24:BC:5503:CLA:H143	1.89	0.54
20:BZ:5023:VAL:O	20:BZ:5026:ALA:HB3	2.08	0.54
3:AC:466:VAL:HA	3:AC:469:MET:HE1	1.89	0.54
15:BU:5064:ALA:O	15:BU:5067:GLN:HG2	2.06	0.54
4:BD:5330:ALA:HB3	4:BD:5331:PRO:HD3	1.89	0.54
24:AB:610:CLA:HBB1	24:AB:610:CLA:HHC	1.89	0.54
4:AD:14:TRP:NE1	7:AH:25:TRP:HH2	1.93	0.54
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.88	0.54
2:BB:5183:PRO:HB2	2:BB:5185:TRP:CH2	2.42	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
5:BE:5034:GLY:CA	6:BF:5032:PHE:CE1	2.90	0.54
1:BA:5069:GLY:HA2	1:BA:5075:ASN:ND2	2.22	0.54
13:AO:117:GLY:O	13:AO:159:VAL:HG12	2.07	0.54
1:AA:214:MET:HE2	1:AA:214:MET:HA	1.90	0.54
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.28	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:AB:603:CLA:H161	7:AH:38:PHE:CE2	2.43	0.54
4:AD:152:VAL:HG11	24:AD:401:CLA:H11	1.88	0.54
2:BB:5018:ARG:HD3	2:BB:5118:TRP:HB3	1.89	0.54
31:BD:5410:LMG:H192	31:BL:5101:LMG:H201	1.89	0.54
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.07	0.54
20:BZ:5032:ASP:C	20:BZ:5034:ASP:N	2.60	0.54
4:AD:128:ARG:HG2	4:AD:129:GLN:N	2.22	0.54
1:AA:261:GLN:NE2	2:AB:489:GLU:HG3	2.22	0.54
16:AV:71:ILE:C	16:AV:71:ILE:HD12	2.28	0.54
27:BD:5407:BCR:H343	27:BD:5407:BCR:H321	1.89	0.54
3:AC:281:MET:O	3:AC:285:ILE:HG13	2.07	0.54
13:BO:5180:ALA:HB1	13:BO:5191:ALA:HB2	1.90	0.54
28:AA:411:DGD:O1B	28:AA:411:DGD:HG12	2.07	0.54
24:AB:614:CLA:H202	31:AB:620:LMG:H422	1.90	0.54
12:AM:33:GLN:HA	31:AM:101:LMG:HC62	1.90	0.54
2:BB:5058:GLN:O	24:BB:5611:CLA:HED3	2.07	0.54
20:AZ:33:TRP:O	20:AZ:33:TRP:HD1	1.90	0.54
4:BD:5185:PHE:CE2	4:BD:5289:LEU:HD12	2.42	0.54
2:AB:12:LEU:CD1	2:AB:19:LEU:HD12	2.38	0.54
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE2	1.89	0.54
35:BD:5406:PL9:H401	11:BL:5029:LEU:HD23	1.90	0.54
3:BC:5042:LEU:CD2	24:BC:5511:CLA:HED3	2.37	0.54
1:BA:5315:ASN:ND2	4:BD:5332:GLN:NE2	2.56	0.54
1:BA:5064:ARG:HG3	1:BA:5064:ARG:HH11	1.71	0.54
1:BA:5240:GLY:HA3	14:BT:5029:ILE:HG22	1.88	0.54
24:AA:405:CLA:H93	34:AD:402:PHO:HHB	1.89	0.54
2:AB:237:VAL:HG22	24:AB:610:CLA:HBC2	1.88	0.54
35:AD:405:PL9:H401	11:AL:29:LEU:HD23	1.90	0.54
24:BA:5405:CLA:H202	34:BD:5403:PHO:HMA2	1.89	0.54
24:BA:5406:CLA:C9	34:BD:5403:PHO:HHB	2.37	0.54
4:BD:5259:ILE:HG12	31:BD:5410:LMG:H301	1.89	0.54
3:BC:5155:ASN:CA	3:BC:5158:THR:HG22	2.36	0.54
3:BC:5311:GLN:OE1	3:BC:5355:THR:HG22	2.08	0.54
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.90	0.54
1:BA:5013:LEU:N	1:BA:5016:ARG:HH11	2.06	0.54
1:BA:5081:ALA:CB	1:BA:5175:GLY:HA3	2.37	0.54
2:BB:5011:VAL:HG23	11:BL:5006:ASN:O	2.07	0.54
6:BF:5011:VAL:HG12	6:BF:5012:SER:N	2.23	0.54
4:BD:5335:PRO:HB2	5:BE:5065:LEU:HD21	1.89	0.54
11:AL:18:TYR:CE2	14:AT:20:ALA:HA	2.43	0.54
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG1	2.41	0.54
1:BA:5119:PHE:HZ	24:BA:5405:CLA:H101	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5223:TRP:CE3	3:BC:5224:ILE:HG13	2.43	0.54
5:AE:76:VAL:O	5:AE:80:LEU:CD2	2.56	0.54
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.73	0.54
1:BA:5012:ASN:ND2	1:BA:5015:GLU:HB2	2.22	0.54
2:BB:5246:PHE:CE2	2:BB:5463:PHE:HA	2.43	0.54
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.08	0.54
10:AK:43:VAL:HG21	10:AK:46:ARG:HE	1.72	0.54
1:AA:64:ARG:HH11	1:AA:64:ARG:HG3	1.73	0.54
12:BM:5023:ILE:HG12	31:BM:5102:LMG:H212	1.90	0.54
1:BA:5260:PHE:CZ	1:BA:5263:ALA:HB2	2.43	0.54
3:BC:5472:LEU:HG	4:BD:5251:ARG:HH12	1.72	0.54
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.21	0.54
4:BD:5238:THR:O	4:BD:5239:GLN:O	2.26	0.54
2:BB:5356:VAL:HA	2:BB:5370:LEU:HD22	1.90	0.54
2:BB:5331:ASN:HB3	2:BB:5437:LEU:HD22	1.88	0.54
18:BX:5022:GLY:HA2	18:BX:5025:SER:OG	2.08	0.54
16:BV:5104:ASN:HA	16:BV:5122:ARG:HD3	1.90	0.54
1:BA:5340:PRO:HG2	3:BC:5317:PHE:CZ	2.43	0.54
3:BC:5250:TRP:C	3:BC:5250:TRP:CD1	2.81	0.54
3:AC:259:TRP:HD1	3:AC:259:TRP:H	1.56	0.54
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.08	0.53
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	1.90	0.53
1:BA:5244:GLU:OE2	4:BD:5264:LYS:NZ	2.41	0.53
1:BA:5271:LEU:HD23	1:BA:5271:LEU:C	2.28	0.53
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53
16:AV:38:LEU:HD12	16:AV:95:ILE:HB	1.89	0.53
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.91	0.53
1:BA:5126:TYR:O	1:BA:5130:GLN:HG3	2.07	0.53
2:AB:157:HIS:HD2	2:AB:158:LEU:HD23	1.73	0.53
24:AA:404:CLA:H202	34:AD:402:PHO:HMA2	1.89	0.53
2:BB:5250:PHE:CE2	2:BB:5459:ALA:HB1	2.43	0.53
24:BB:5609:CLA:H141	24:BB:5614:CLA:HED2	1.88	0.53
24:BB:5612:CLA:H203	24:BD:5405:CLA:HBA2	1.89	0.53
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.70	0.53
3:AC:163:PHE:O	3:AC:167:VAL:HG23	2.09	0.53
1:AA:262:TYR:HE1	31:AA:414:LMG:HC5	1.72	0.53
3:AC:170:ILE:HG22	3:AC:174:LEU:HD23	1.91	0.53
16:BV:5146:LEU:O	16:BV:5150:LYS:HG3	2.08	0.53
1:AA:119:PHE:HZ	24:AA:404:CLA:H101	1.74	0.53
9:AJ:19:MET:O	9:AJ:23:VAL:HG23	2.07	0.53
3:BC:5155:ASN:HA	3:BC:5158:THR:CG2	2.34	0.53
3:AC:432:VAL:HG13	3:AC:433:LEU:N	2.23	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:315:ASN:HD21	4:AD:332:GLN:NE2	2.05	0.53
3:BC:5044:ASN:O	3:BC:5045:LEU:HD12	2.08	0.53
9:BJ:5011:TRP:CE2	9:BJ:5012:ILE:HG13	2.42	0.53
1:BA:5332:HIS:HB3	4:BD:5321:LEU:HD21	1.90	0.53
4:BD:5068:LEU:HD11	5:BE:5044:TYR:CE1	2.43	0.53
2:AB:215:PHE:C	2:AB:215:PHE:CD2	2.82	0.53
3:AC:415:ASN:O	3:AC:416:SER:CB	2.55	0.53
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.72	0.53
4:AD:86:GLY:CA	4:AD:166:SER:HB2	2.38	0.53
24:BA:5406:CLA:H201	14:BT:5014:ILE:HD11	1.90	0.53
3:AC:311:GLN:OE1	3:AC:355:THR:HG22	2.08	0.53
20:BZ:5049:ALA:O	20:BZ:5053:VAL:HG23	2.07	0.53
4:AD:26:ARG:HH11	4:AD:26:ARG:HG3	1.72	0.53
24:BC:5504:CLA:H2	28:BC:5518:DGD:HA21	1.89	0.53
2:AB:462:PHE:CE1	24:AB:613:CLA:HMB3	2.44	0.53
24:AB:608:CLA:H202	7:AH:43:LEU:HD11	1.90	0.53
31:AD:408:LMG:H392	27:AT:101:BCR:HC32	1.91	0.53
18:AX:12:ILE:HG23	18:AX:12:ILE:O	2.09	0.53
4:BD:5088:SER:CB	5:BE:5069:ARG:NH2	2.69	0.53
3:AC:124:VAL:HB	27:AC:515:BCR:H362	1.89	0.53
5:BE:5010:PHE:HD2	31:BE:5101:LMG:O2	1.92	0.53
1:BA:5190:HIS:O	1:BA:5298:ASN:HB3	2.09	0.53
13:AO:98:THR:HG23	13:AO:133:THR:HB	1.89	0.53
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.08	0.53
1:BA:5324:ALA:HB2	4:BD:5329:MET:SD	2.49	0.53
2:BB:5327:THR:O	2:BB:5444:ARG:NE	2.39	0.53
15:AU:64:ALA:O	15:AU:67:GLN:HG2	2.08	0.53
3:AC:437:PHE:CZ	24:AC:510:CLA:HMB3	2.44	0.53
2:BB:5231:MET:HG2	24:BB:5614:CLA:HMC1	1.90	0.53
11:BL:5022:LEU:HG	31:BL:5101:LMG:H191	1.89	0.53
11:BL:5022:LEU:O	11:BL:5026:VAL:HG22	2.08	0.53
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.43	0.53
3:AC:405:ASN:HB2	28:AC:519:DGD:C3G	2.38	0.53
3:AC:279:LEU:HD22	24:AC:503:CLA:H143	1.90	0.53
1:BA:5155:PHE:CE1	28:BA:5412:DGD:HBE1	2.44	0.53
2:BB:5030:VAL:HG12	24:BB:5609:CLA:HHH	1.91	0.53
3:BC:5149:TYR:CA	3:BC:5156:LYS:HD3	2.38	0.53
1:BA:5254:TYR:CD1	4:BD:5132:ILE:HG22	2.43	0.53
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.90	0.53
8:AI:1:MET:CE	32:BB:5604:LMT:H41	2.39	0.53
3:BC:5368:PRO:O	3:BC:5379:LYS:HE2	2.08	0.53
2:BB:5087:ASP:OD1	28:BB:5602:DGD:HD62	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:AD:406:BCR:H321	27:AD:406:BCR:H343	1.91	0.53
2:BB:5363:PHE:HD1	4:BD:5326:ARG:HD2	1.74	0.53
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.39	0.53
16:BV:5074:THR:O	16:BV:5075:ASN:HB2	2.08	0.53
4:BD:5037:LEU:HD13	4:BD:5125:PHE:N	2.24	0.53
2:AB:462:PHE:HA	24:AB:611:CLA:CMC	2.37	0.53
24:AB:616:CLA:H51	30:BA:5401:SQD:H302	1.90	0.53
2:BB:5062:VAL:CG1	24:BB:5609:CLA:HED3	2.39	0.53
3:BC:5387:TRP:CE2	3:BC:5388:GLN:HG3	2.44	0.53
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.44	0.53
2:AB:183:PRO:HG3	2:AB:199:VAL:HG12	1.90	0.53
13:AO:218:LEU:CD2	15:AU:119:THR:HG21	2.39	0.53
1:AA:332:HIS:HB3	4:AD:321:LEU:HD21	1.91	0.53
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.08	0.53
1:BA:5333:GLU:HB2	1:BA:5337:HIS:HE1	1.74	0.53
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.91	0.53
1:AA:307:ILE:HG22	1:AA:313:VAL:HA	1.89	0.53
20:AZ:12:LEU:O	20:AZ:12:LEU:HD12	2.08	0.53
1:AA:289:GLY:O	1:AA:292:THR:CG2	2.53	0.53
24:AC:504:CLA:H151	28:AC:519:DGD:C9A	2.36	0.53
1:AA:234:ASN:HB2	31:AB:620:LMG:O3	2.09	0.53
2:AB:68:ARG:HH22	24:AB:604:CLA:CED	2.21	0.53
1:AA:220:THR:HG23	4:AD:141:TYR:HD1	1.73	0.53
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.89	0.53
4:BD:5076:VAL:O	4:BD:5077:ALA:HB2	2.09	0.53
4:AD:313:THR:OG1	4:AD:315:TYR:HB3	2.09	0.53
2:AB:135:LEU:HD13	2:AB:237:VAL:CG2	2.39	0.53
2:AB:91:TRP:CD1	24:AB:606:CLA:HBD	2.43	0.53
2:AB:225:LEU:HD23	32:AB:624:LMT:H42	1.91	0.53
24:BA:5406:CLA:H152	24:BA:5406:CLA:H102	1.91	0.53
3:BC:5233:VAL:HA	27:BC:5516:BCR:C28	2.38	0.53
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.09	0.53
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:CD1	2.38	0.53
12:AM:20:VAL:O	12:AM:24:ILE:HG13	2.07	0.53
4:BD:5134:ARG:HE	4:BD:5134:ARG:CA	2.21	0.53
3:BC:5166:ILE:HG23	3:BC:5245:ILE:HG23	1.91	0.53
5:BE:5008:ARG:HD3	5:BE:5013:ILE:HG12	1.91	0.53
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.09	0.53
1:BA:5142:TRP:HB2	4:BD:5220:ASN:OD1	2.09	0.53
24:AA:405:CLA:C9	34:AD:402:PHO:HHB	2.39	0.52
2:BB:5005:TRP:CH2	31:BL:5101:LMG:H291	2.44	0.52
24:BB:5614:CLA:HHC	24:BB:5614:CLA:HBB1	1.89	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:BZ:5030:PRO:C	20:BZ:5032:ASP:H	2.12	0.52
20:BZ:5035:ARG:O	20:BZ:5038:GLN:HB3	2.09	0.52
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.56	0.52
3:BC:5137:PRO:HB2	3:BC:5139:THR:O	2.09	0.52
6:BF:5041:GLN:HE21	6:BF:5041:GLN:N	2.07	0.52
1:AA:234:ASN:HD21	4:AD:266:TRP:CB	2.21	0.52
24:AA:405:CLA:H102	24:AA:405:CLA:H152	1.91	0.52
30:AB:622:SQD:H152	32:AB:624:LMT:H81	1.90	0.52
4:AD:267:LEU:C	4:AD:267:LEU:HD23	2.30	0.52
3:BC:5113:VAL:CG1	31:BC:5521:LMG:H132	2.40	0.52
3:BC:5279:LEU:HD23	3:BC:5282:MET:CE	2.39	0.52
3:BC:5042:LEU:HD13	24:BC:5511:CLA:HMA3	1.90	0.52
3:BC:5126:GLY:O	3:BC:5130:VAL:HG23	2.09	0.52
1:BA:5254:TYR:OH	4:BD:5129:GLN:HB3	2.09	0.52
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.52
20:AZ:34:ASP:OD1	20:AZ:35:ARG:N	2.42	0.52
13:BO:5223:ILE:HG12	13:BO:5224:SER:N	2.25	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:N	2.72	0.52
3:BC:5337:LEU:HD12	13:BO:5131:PRO:CG	2.39	0.52
2:AB:246:PHE:CE2	2:AB:463:PHE:HA	2.44	0.52
4:AD:238:THR:O	4:AD:239:GLN:O	2.28	0.52
1:BA:5202:VAL:HG11	24:BA:5407:CLA:OBD	2.10	0.52
24:AC:504:CLA:H152	28:AC:519:DGD:HA91	1.90	0.52
24:AC:504:CLA:H61	28:AC:518:DGD:HA61	1.89	0.52
24:AB:611:CLA:H51	24:AB:614:CLA:HBC2	1.92	0.52
24:BB:5613:CLA:OBD	7:BH:5027:THR:HB	2.10	0.52
2:BB:5030:VAL:HG22	24:BB:5617:CLA:C3C	2.39	0.52
3:AC:38:GLY:HA3	24:AC:511:CLA:HMD3	1.92	0.52
3:AC:149:TYR:HA	3:AC:156:LYS:CD	2.40	0.52
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD21	1.91	0.52
14:BT:5022:PHE:C	14:BT:5023:PHE:CD2	2.83	0.52
13:BO:5144:LEU:HD13	13:BO:5259:VAL:HG11	1.90	0.52
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.10	0.52
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.21	0.52
3:AC:259:TRP:N	3:AC:259:TRP:CD1	2.78	0.52
1:BA:5035:VAL:HA	27:BA:5411:BCR:H333	1.90	0.52
16:AV:56:LYS:O	16:AV:60:GLN:HG3	2.09	0.52
2:BB:5143:LEU:HD12	2:BB:5143:LEU:O	2.10	0.52
4:BD:5302:GLU:OE2	4:BD:5302:GLU:HA	2.10	0.52
2:AB:62:VAL:CG1	24:AB:605:CLA:HED3	2.39	0.52
2:BB:5238:LEU:HB2	24:BB:5616:CLA:HMD3	1.91	0.52
15:BU:5054:LYS:HD2	15:BU:5113:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:AA:414:LMG:O2	5:AE:10:PHE:HD2	1.92	0.52
16:AV:133:LEU:N	16:AV:133:LEU:HD12	2.24	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.25	0.52
13:BO:5210:ARG:HA	15:BU:5039:LEU:CD1	2.40	0.52
16:BV:5081:ARG:HH11	16:BV:5081:ARG:HG2	1.73	0.52
1:AA:155:PHE:CE1	28:AA:411:DGD:HBE1	2.44	0.52
24:AB:615:CLA:H142	24:AB:616:CLA:H151	1.91	0.52
3:AC:220:GLY:N	28:AC:517:DGD:O3D	2.42	0.52
1:BA:5220:THR:CG2	4:BD:5141:TYR:HD1	2.23	0.52
1:BA:5157:VAL:HG11	24:BA:5406:CLA:HMC3	1.92	0.52
2:BB:5010:THR:HG22	2:BB:5013:ILE:HD11	1.92	0.52
2:BB:5090:PHE:CE2	2:BB:5091:TRP:CZ3	2.97	0.52
2:BB:5157:HIS:HD2	2:BB:5158:LEU:HD23	1.75	0.52
24:BB:5612:CLA:C4	4:BD:5127:LEU:HD11	2.20	0.52
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.45	0.52
12:AM:27:VAL:HG12	12:BM:5028:GLN:HB3	1.90	0.52
10:AK:17:ILE:N	10:AK:17:ILE:HD12	2.23	0.52
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.44	0.52
4:AD:308:ASP:OD1	4:AD:308:ASP:C	2.47	0.52
2:AB:10:THR:C	2:AB:12:LEU:H	2.11	0.52
31:AB:620:LMG:H201	31:AD:408:LMG:H192	1.90	0.52
11:AL:22:LEU:O	11:AL:26:VAL:HG22	2.10	0.52
2:BB:5139:PHE:CZ	24:BB:5613:CLA:HMB3	2.45	0.52
2:AB:260:SER:HG	2:AB:262:THR:HG22	1.70	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:H	2.22	0.52
2:AB:331:ASN:HB3	2:AB:437:LEU:HD22	1.92	0.52
13:AO:215:ARG:NH1	13:AO:252:GLY:O	2.43	0.52
3:BC:5141:GLU:CD	3:BC:5141:GLU:H	2.13	0.52
3:BC:5140:LEU:HB2	3:BC:5148:GLY:HA2	1.91	0.52
1:BA:5289:GLY:CA	1:BA:5292:THR:HG22	2.38	0.52
3:BC:5418:ASN:HA	28:BC:5519:DGD:HE2	1.91	0.52
2:AB:238:LEU:N	24:AB:612:CLA:HMD3	2.25	0.52
3:AC:279:LEU:HD23	3:AC:282:MET:CE	2.39	0.52
3:AC:437:PHE:HA	24:AC:508:CLA:HMC3	1.91	0.52
2:BB:5010:THR:C	2:BB:5012:LEU:H	2.11	0.52
31:BL:5101:LMG:H302	12:BM:5022:LEU:HD21	1.91	0.52
4:BD:5128:ARG:HG2	4:BD:5129:GLN:N	2.24	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.52
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.10	0.52
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	1.92	0.52
3:AC:250:TRP:C	3:AC:250:TRP:CD1	2.82	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:AB:601:CLA:HBB1	24:AB:601:CLA:HHC	1.91	0.52
2:AB:30:VAL:HG22	24:AB:613:CLA:C3C	2.40	0.52
1:BA:5093:PHE:CZ	24:BA:5408:CLA:HBA1	2.45	0.52
3:BC:5149:TYR:CB	3:BC:5156:LYS:HD3	2.40	0.52
4:BD:5154:VAL:O	4:BD:5158:LEU:HB2	2.10	0.52
2:AB:354:LEU:HD21	2:AB:378:LYS:HB2	1.90	0.52
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.40	0.52
4:AD:236:ASN:ND2	4:AD:239:GLN:O	2.37	0.52
3:BC:5366:LEU:C	3:BC:5366:LEU:HD23	2.30	0.52
1:AA:193:LEU:HD13	4:AD:179:PHE:HB3	1.91	0.52
13:AO:91:PHE:CE1	13:AO:260:LYS:HB2	2.45	0.52
20:BZ:5042:LEU:O	20:BZ:5046:LEU:HB2	2.10	0.52
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.92	0.52
13:AO:46:PRO:HD2	13:AO:266:TYR:HD2	1.74	0.52
3:AC:366:LEU:HD23	3:AC:366:LEU:C	2.29	0.52
1:AA:176:ILE:HG22	1:AA:180:PHE:HE2	1.73	0.52
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.10	0.52
4:AD:158:LEU:O	4:AD:162:LEU:HG	2.09	0.52
4:AD:88:SER:CB	5:AE:69:ARG:NH2	2.69	0.52
3:BC:5037:ALA:O	24:BC:5508:CLA:HBA1	2.10	0.52
3:BC:5052:ALA:CA	24:BC:5511:CLA:HMB3	2.28	0.52
5:AE:8:ARG:HD3	5:AE:13:ILE:HG12	1.92	0.52
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.92	0.52
3:AC:149:TYR:CB	3:AC:156:LYS:HD3	2.40	0.52
1:BA:5315:ASN:ND2	4:BD:5332:GLN:HE22	2.06	0.52
1:BA:5064:ARG:HG3	1:BA:5064:ARG:NH1	2.25	0.52
3:AC:252:ILE:HG22	3:AC:253:LEU:HD23	1.91	0.52
5:AE:26:THR:HB	36:AF:101:HEM:CAB	2.40	0.52
25:BA:5409:MST:H122	25:BA:5409:MST:N3	2.24	0.52
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.25	0.52
3:BC:5362:ARG:HE	3:BC:5370:ARG:NH1	2.07	0.52
4:BD:5072:ASN:HA	31:BD:5408:LMG:HC72	1.92	0.52
13:BO:5059:ASP:C	13:BO:5061:SER:H	2.13	0.52
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.52
27:AT:101:BCR:H19C	27:BB:5622:BCR:H363	1.91	0.52
2:BB:5091:TRP:CD1	24:BB:5610:CLA:HBD	2.45	0.52
2:BB:5461:LEU:HD21	31:BB:5624:LMG:C43	2.39	0.52
13:BO:5230:VAL:CG1	13:BO:5231:ASP:H	2.17	0.52
2:AB:369:ILE:O	2:AB:370:LEU:HD23	2.09	0.52
4:BD:5201:VAL:O	4:BD:5205:LEU:HB2	2.09	0.52
1:BA:5027:ARG:NH1	1:BA:5027:ARG:O	2.43	0.52
3:BC:5214:LEU:N	3:BC:5214:LEU:HD22	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5026:ARG:HG3	4:BD:5026:ARG:HH11	1.75	0.52
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:HD11	1.93	0.51
1:BA:5159:LEU:HD11	28:BC:5517:DGD:HB51	1.92	0.51
4:BD:5274:VAL:HA	35:BD:5406:PL9:C25	2.34	0.51
3:BC:5038:GLY:HA3	24:BC:5511:CLA:HMD3	1.92	0.51
10:AK:18:PHE:C	10:AK:20:PRO:HD2	2.29	0.51
20:BZ:5031:GLN:O	20:BZ:5032:ASP:HB3	2.11	0.51
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.20	0.51
2:BB:5121:GLU:HG3	7:BH:5004:ARG:CA	2.39	0.51
1:AA:315:ASN:ND2	4:AD:332:GLN:NE2	2.57	0.51
13:AO:84:ASN:ND2	2:BB:5431:GLU:OE2	2.43	0.51
1:BA:5082:VAL:HB	1:BA:5174:LEU:HB2	1.91	0.51
4:BD:5350:ASN:O	4:BD:5352:LEU:N	2.42	0.51
2:BB:5192:PRO:HD2	7:BH:5060:VAL:HG12	1.93	0.51
4:AD:35:ILE:O	24:AD:404:CLA:HBB2	2.11	0.51
1:AA:283:VAL:HG21	34:AD:402:PHO:HBC3	1.91	0.51
11:BL:5008:GLN:HB3	11:BL:5009:PRO:HD2	1.93	0.51
10:BK:5020:PRO:O	10:BK:5023:ASP:HB2	2.11	0.51
20:AZ:42:LEU:O	20:AZ:46:LEU:HB2	2.09	0.51
27:BK:5102:BCR:H331	27:BK:5102:BCR:HC8	1.92	0.51
1:BA:5011:ALA:O	1:BA:5012:ASN:CB	2.58	0.51
12:BM:5020:VAL:O	12:BM:5024:ILE:HG13	2.11	0.51
1:BA:5288:LEU:HD13	3:BC:5432:VAL:CG2	2.37	0.51
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.51
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE2	2.46	0.51
13:BO:5180:ALA:HB2	15:BU:5120:ALA:O	2.09	0.51
4:BD:5188:PHE:CZ	4:BD:5326:ARG:HG2	2.46	0.51
13:BO:5046:PRO:HD2	13:BO:5266:TYR:HD2	1.75	0.51
4:AD:92:LEU:HA	4:AD:104:TRP:CD1	2.45	0.51
1:AA:289:GLY:C	1:AA:292:THR:HG22	2.31	0.51
3:AC:415:ASN:HB3	9:AJ:39:SER:OG	2.08	0.51
24:AA:405:CLA:HMD2	24:AD:401:CLA:CBB	2.40	0.51
1:AA:38:ILE:HG23	30:AA:416:SQD:H131	1.93	0.51
1:AA:93:PHE:CZ	24:AA:407:CLA:HBA1	2.44	0.51
2:AB:10:THR:HG22	2:AB:13:ILE:HD11	1.92	0.51
2:AB:58:GLN:O	24:AB:607:CLA:HED3	2.10	0.51
2:BB:5012:LEU:CD1	2:BB:5019:LEU:HD12	2.40	0.51
2:BB:5027:THR:HG23	24:BB:5609:CLA:HMC1	1.93	0.51
2:BB:5135:LEU:HD13	2:BB:5237:VAL:CG2	2.41	0.51
3:BC:5163:PHE:O	3:BC:5167:VAL:HG23	2.09	0.51
4:BD:5259:ILE:HD13	14:BT:5021:ILE:HG12	1.93	0.51
24:BD:5405:CLA:H42	18:BX:5023:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.09	0.51
1:BA:5271:LEU:HD21	25:BA:5409:MST:C8	2.40	0.51
3:BC:5259:TRP:N	3:BC:5259:TRP:CD1	2.77	0.51
9:BJ:5019:MET:O	9:BJ:5023:VAL:HG23	2.10	0.51
3:AC:297:TYR:HA	3:AC:302:TYR:CE2	2.46	0.51
24:BC:5504:CLA:H61	28:BC:5518:DGD:HA61	1.92	0.51
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.14	0.51
1:BA:5020:TRP:O	1:BA:5021:VAL:C	2.49	0.51
24:BB:5607:CLA:H161	7:BH:5038:PHE:CE2	2.45	0.51
15:BU:5050:ALA:HB1	15:BU:5113:THR:HG21	1.93	0.51
3:AC:377:LEU:O	3:AC:381:LYS:HB2	2.10	0.51
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.51
4:BD:5334:GLN:N	4:BD:5335:PRO:HD3	2.24	0.51
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	1.93	0.51
16:BV:5058:LEU:HD13	16:BV:5137:ASP:HB3	1.92	0.51
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.51
2:BB:5433:ASP:OD1	2:BB:5433:ASP:C	2.47	0.51
3:BC:5204:LEU:HD21	3:BC:5238:ILE:HG21	1.92	0.51
2:AB:461:LEU:HD21	31:AB:621:LMG:C43	2.41	0.51
28:BA:5412:DGD:HG12	28:BA:5412:DGD:O1B	2.11	0.51
2:BB:5462:PHE:CE1	24:BB:5617:CLA:HMB3	2.44	0.51
24:BB:5619:CLA:H142	24:BB:5620:CLA:H151	1.92	0.51
4:BD:5266:TRP:HE1	31:BD:5410:LMG:HC72	1.74	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.41	0.51
1:AA:64:ARG:HD3	1:AA:64:ARG:H	1.75	0.51
1:AA:83:VAL:HG22	4:AD:314:PHE:CE2	2.41	0.51
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.59	0.51
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.75	0.51
1:BA:5129:ARG:NH2	4:BD:5256:ILE:HA	2.26	0.51
3:AC:453:ALA:HA	8:AI:34:ARG:O	2.10	0.51
18:BX:5022:GLY:HA2	18:BX:5025:SER:HG	1.75	0.51
3:BC:5458:GLY:HA2	4:BD:5222:LEU:O	2.11	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
3:AC:158:THR:HG21	3:AC:254:THR:O	2.09	0.51
5:BE:5072:ALA:O	5:BE:5076:VAL:HG23	2.10	0.51
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.92	0.51
4:AD:302:GLU:OE2	4:AD:302:GLU:HA	2.11	0.51
24:AB:611:CLA:H142	31:AB:620:LMG:H371	1.92	0.51
2:BB:5187:PRO:HB3	24:BB:5605:CLA:CMB	2.41	0.51
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	1.93	0.51
2:BB:5315:ILE:HG22	2:BB:5426:PHE:HB3	1.92	0.51
2:AB:173:GLY:CA	2:AB:265:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:5280:PHE:O	2:BB:5284:ILE:HG13	2.10	0.51
3:BC:5297:TYR:HD1	3:BC:5302:TYR:CE2	2.29	0.51
18:BX:5024:LEU:O	18:BX:5028:VAL:HG23	2.10	0.51
15:BU:5080:VAL:HG22	15:BU:5127:ARG:HH21	1.76	0.51
13:BO:5071:LEU:HD23	13:BO:5265:PHE:HB3	1.91	0.51
3:AC:321:ASP:OD2	15:AU:129:ASN:HB2	2.11	0.51
32:AB:624:LMT:H92	7:AH:35:MET:HE2	1.92	0.51
3:AC:37:ALA:O	24:AC:508:CLA:HBA1	2.11	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB2	1.93	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.41	0.51
24:BB:5615:CLA:H142	31:BL:5101:LMG:H371	1.92	0.51
3:AC:42:LEU:HD13	24:AC:511:CLA:HMA3	1.93	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.93	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CE2	2.29	0.51
1:AA:244:GLU:OE2	4:AD:264:LYS:NZ	2.43	0.51
20:AZ:2:THR:CG2	20:AZ:3:ILE:H	2.23	0.51
2:AB:356:VAL:HA	2:AB:370:LEU:HD22	1.93	0.51
3:AC:171:GLY:O	3:AC:174:LEU:HB2	2.11	0.51
3:AC:327:ASN:HB3	13:AO:125:ASP:OD1	2.11	0.51
11:AL:8:GLN:HE21	11:AL:8:GLN:N	2.08	0.51
31:AC:520:LMG:H292	27:AJ:101:BCR:H363	1.93	0.51
3:AC:264:PHE:HE1	27:AC:516:BCR:C32	2.24	0.51
2:BB:5015:ASP:N	2:BB:5016:PRO:HD3	2.26	0.51
2:BB:5091:TRP:CZ3	24:BB:5610:CLA:O1A	2.64	0.51
2:BB:5225:LEU:HD23	32:BB:5627:LMT:H42	1.92	0.51
14:BT:5018:PHE:HB2	27:BT:5101:BCR:H10C	1.93	0.51
3:BC:5028:GLN:HB2	24:BC:5511:CLA:CED	2.41	0.51
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CE2	2.29	0.51
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CE2	2.45	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CD2	2.29	0.51
20:BZ:5034:ASP:OD1	20:BZ:5035:ARG:N	2.44	0.51
4:AD:134:ARG:CA	4:AD:134:ARG:HE	2.20	0.51
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.26	0.51
2:BB:5251:VAL:O	2:BB:5255:THR:HG23	2.11	0.51
2:BB:5366:PHE:CD1	2:BB:5367:PRO:HD2	2.46	0.51
3:BC:5315:MET:HE1	3:BC:5369:LEU:HD12	1.92	0.51
3:BC:5094:THR:HG22	3:BC:5298:PRO:HD2	1.93	0.51
2:BB:5063:LEU:N	2:BB:5064:PRO:HD2	2.26	0.51
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.46	0.51
2:AB:30:VAL:HG12	24:AB:605:CLA:HHD	1.93	0.51
2:AB:238:LEU:HB2	24:AB:612:CLA:HMD3	1.93	0.51
3:BC:5288:CYS:HB3	28:BC:5517:DGD:HG2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.51
15:AU:66:ILE:CG1	15:AU:72:TYR:CD1	2.94	0.51
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.25	0.51
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.10	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:HE2	1.75	0.51
13:BO:5092:VAL:HG12	13:BO:5093:PRO:HD2	1.91	0.51
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.46	0.51
4:AD:87:HIS:HB2	28:AH:101:DGD:O2D	2.11	0.50
31:AB:620:LMG:HC91	11:AL:19:LEU:CD1	2.41	0.50
1:BA:5205:VAL:HG21	24:BA:5405:CLA:CMA	2.41	0.50
3:BC:5264:PHE:HE1	27:BC:5516:BCR:C32	2.25	0.50
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.10	0.50
1:AA:262:TYR:HE1	31:AA:414:LMG:C5	2.24	0.50
2:AB:2:GLY:HA3	11:AL:9:PRO:HG2	1.93	0.50
2:AB:176:GLY:HA3	2:AB:266:GLU:OE1	2.12	0.50
18:BX:5044:ASP:O	18:BX:5045:LYS:HB3	2.11	0.50
3:AC:458:GLY:HA2	4:AD:222:LEU:O	2.10	0.50
27:AB:618:BCR:H363	27:BT:5101:BCR:H19C	1.92	0.50
31:AM:101:LMG:O2	11:BL:5009:PRO:HB3	2.11	0.50
2:BB:5354:LEU:N	2:BB:5354:LEU:HD12	2.26	0.50
2:BB:5172:TYR:OH	7:BH:5063:LYS:HE2	2.11	0.50
4:BD:5253:TRP:HB2	4:BD:5260:ALA:HB2	1.93	0.50
29:BA:5413:LHG:HC11	3:BC:5447:ARG:CZ	2.41	0.50
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.41	0.50
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.92	0.50
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.45	0.50
24:BC:5505:CLA:H2	24:BC:5505:CLA:HAA1	1.94	0.50
20:AZ:23:VAL:HG12	20:AZ:27:TYR:CE2	2.46	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:H83	1.93	0.50
16:BV:5133:LEU:N	16:BV:5133:LEU:HD12	2.24	0.50
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CE2	2.47	0.50
3:BC:5033:PHE:CD1	4:BD:5229:ALA:HB3	2.45	0.50
3:AC:321:ASP:OD1	3:AC:321:ASP:N	2.42	0.50
4:AD:37:LEU:HD13	4:AD:125:PHE:N	2.26	0.50
1:AA:200:LEU:HD11	28:AC:519:DGD:CCA	2.29	0.50
3:BC:5415:ASN:CB	9:BJ:5039:SER:OG	2.60	0.50
24:AB:612:CLA:H171	24:AB:613:CLA:HBB2	1.92	0.50
24:AC:502:CLA:H122	24:AC:503:CLA:HMB2	1.93	0.50
24:AA:405:CLA:H92	34:AD:402:PHO:CMB	2.41	0.50
7:AH:50:ASN:HD22	28:AH:101:DGD:HA21	1.76	0.50
8:AI:19:PHE:CZ	8:AI:23:PHE:HE2	2.29	0.50
24:BA:5406:CLA:H92	34:BD:5403:PHO:CMB	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:5139:PHE:HZ	24:BB:5613:CLA:HMB3	1.77	0.50
3:BC:5437:PHE:CZ	24:BC:5510:CLA:HMB3	2.47	0.50
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC3	1.92	0.50
11:BL:5019:LEU:CD1	31:BL:5101:LMG:HC91	2.42	0.50
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.60	0.50
3:AC:262:ARG:HH21	32:AI:103:LMT:C5'	2.25	0.50
8:AI:21:PHE:HE1	32:AI:103:LMT:H41	1.75	0.50
10:AK:14:ALA:O	10:AK:17:ILE:HD13	2.10	0.50
1:AA:48:PHE:HA	1:AA:115:ILE:HD11	1.92	0.50
13:AO:46:PRO:HD2	13:AO:266:TYR:CD2	2.45	0.50
13:BO:5046:PRO:HD2	13:BO:5266:TYR:CD2	2.46	0.50
16:BV:5119:PRO:HA	16:BV:5127:PHE:CD2	2.46	0.50
2:BB:5215:PHE:C	2:BB:5215:PHE:CD2	2.85	0.50
2:BB:5405:GLU:HA	2:BB:5405:GLU:OE1	2.10	0.50
24:AC:501:CLA:CAD	24:AC:503:CLA:H12	2.42	0.50
24:AD:401:CLA:H2	34:AD:403:PHO:HBB1	1.92	0.50
24:BB:5616:CLA:H171	24:BB:5617:CLA:HBB2	1.93	0.50
18:BX:5012:ILE:O	18:BX:5012:ILE:HG13	2.11	0.50
13:BO:5032:THR:O	13:BO:5036:ILE:CD1	2.54	0.50
20:BZ:5033:TRP:O	20:BZ:5037:LYS:HB2	2.12	0.50
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.11	0.50
3:BC:5377:LEU:CD2	13:BO:5126:GLY:HA2	2.41	0.50
3:AC:326:ALA:HB2	15:AU:128:TYR:CG	2.46	0.50
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.93	0.50
3:BC:5193:GLY:O	3:BC:5194:GLY:C	2.48	0.50
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.12	0.50
3:BC:5321:ASP:OD1	3:BC:5321:ASP:N	2.44	0.50
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CB	2.23	0.50
2:BB:5377:VAL:HG11	4:BD:5342:PRO:HG2	1.93	0.50
13:AO:155:THR:HG23	13:AO:168:PHE:CE2	2.47	0.50
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.39	0.50
14:BT:5022:PHE:O	14:BT:5023:PHE:CD2	2.64	0.50
1:BA:5182:PHE:O	1:BA:5186:PHE:HB2	2.12	0.50
13:BO:5091:PHE:CE1	13:BO:5260:LYS:HB2	2.47	0.50
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.50
2:AB:5:TRP:CH2	31:AB:620:LMG:H291	2.47	0.50
3:AC:225:VAL:CG2	28:AC:517:DGD:HG11	2.41	0.50
4:BD:5279:LEU:HD22	24:BD:5402:CLA:HMA2	1.93	0.50
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.24	0.50
1:AA:190:HIS:HB3	1:AA:293:MET:CE	2.41	0.50
27:AK:102:BCR:HC8	27:AK:102:BCR:H331	1.93	0.50
3:BC:5335:THR:HA	13:BO:5178:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:AH:11:LEU:HA	7:AH:14:LEU:HD12	1.93	0.50
13:AO:234:THR:HG1	13:AO:236:GLU:HG2	1.76	0.50
10:BK:5017:ILE:H	10:BK:5017:ILE:CD1	2.25	0.50
3:AC:368:PRO:O	3:AC:379:LYS:HE2	2.12	0.50
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.47	0.50
3:AC:418:ASN:CA	28:AC:519:DGD:HE2	2.42	0.50
2:AB:25:MET:HE2	27:AB:617:BCR:H393	1.93	0.50
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.12	0.50
27:BC:5516:BCR:HC41	8:BI:5020:VAL:CG1	2.41	0.50
24:BA:5406:CLA:HMD2	24:BD:5402:CLA:CBB	2.42	0.50
14:AT:29:ILE:N	14:AT:29:ILE:CD1	2.71	0.50
1:BA:5258:LEU:HB3	1:BA:5259:ILE:CD1	2.40	0.50
3:BC:5055:ALA:CB	27:BC:5514:BCR:H373	2.38	0.50
12:BM:5025:LEU:N	12:BM:5025:LEU:HD23	2.27	0.50
5:BE:5014:ILE:O	5:BE:5014:ILE:HG22	2.12	0.50
13:BO:5225:LEU:N	13:BO:5225:LEU:HD12	2.27	0.50
31:AB:620:LMG:H302	12:AM:22:LEU:HD21	1.93	0.50
24:BB:5615:CLA:H51	24:BB:5618:CLA:HBC2	1.94	0.50
3:BC:5276:LEU:HD21	24:BC:5508:CLA:HBB1	1.93	0.50
11:BL:5022:LEU:HD13	14:BT:5016:LEU:HD23	1.94	0.50
3:AC:109:PHE:O	3:AC:113:VAL:HG23	2.11	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:C8	2.42	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.23	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
6:BF:5018:VAL:CG1	6:BF:5019:ARG:N	2.74	0.50
13:BO:5064:TYR:CD1	13:BO:5271:PRO:HA	2.47	0.50
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.50
13:AO:86:ARG:NE	13:AO:86:ARG:O	2.45	0.50
29:AA:412:LHG:HC11	3:AC:447:ARG:CZ	2.41	0.49
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.46	0.49
3:AC:29:GLU:CB	10:AK:46:ARG:NH1	2.71	0.49
1:AA:258:LEU:HB3	1:AA:259:ILE:CD1	2.39	0.49
3:BC:5171:GLY:O	3:BC:5174:LEU:HB2	2.12	0.49
13:BO:5117:GLY:O	13:BO:5159:VAL:HG12	2.11	0.49
1:AA:200:LEU:HD21	28:AC:519:DGD:HAW1	1.94	0.49
1:AA:289:GLY:CA	1:AA:292:THR:HG22	2.42	0.49
28:AC:519:DGD:HG2	9:AJ:33:TYR:OH	2.12	0.49
4:AD:141:TYR:OH	31:AD:407:LMG:HC2	2.11	0.49
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.12	0.49
1:BA:5043:ALA:HB3	1:BA:5118:HIS:HD2	1.77	0.49
3:BC:5225:VAL:CG2	28:BC:5517:DGD:HG11	2.42	0.49
4:BD:5141:TYR:OH	31:BD:5409:LMG:HC2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:AJ:18:GLY:HA3	27:AK:102:BCR:H371	1.94	0.49
4:BD:5053:THR:HA	4:BD:5067:TYR:CD2	2.47	0.49
2:BB:5235:GLU:OE1	2:BB:5472:ARG:NH1	2.44	0.49
1:AA:271:LEU:HD21	25:AA:408:MST:C8	2.41	0.49
1:BA:5257:ARG:NH1	1:BA:5257:ARG:HG3	2.26	0.49
15:BU:5080:VAL:HG22	15:BU:5127:ARG:NH2	2.27	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
1:AA:69:GLY:HA2	1:AA:75:ASN:ND2	2.27	0.49
2:BB:5311:PHE:HA	2:BB:5430:PHE:CZ	2.47	0.49
2:AB:311:PHE:HA	2:AB:430:PHE:CZ	2.47	0.49
4:AD:193:LEU:O	4:AD:193:LEU:HG	2.11	0.49
13:BO:5186:LYS:HA	13:BO:5186:LYS:HE2	1.92	0.49
2:AB:91:TRP:CZ3	24:AB:606:CLA:O1A	2.65	0.49
3:AC:225:VAL:HG22	3:AC:289:PHE:CD1	2.47	0.49
24:AB:608:CLA:C4	4:AD:127:LEU:HD11	2.21	0.49
24:BB:5605:CLA:HBC3	7:BH:5041:PHE:CE1	2.47	0.49
3:BC:5109:PHE:O	3:BC:5113:VAL:HG23	2.12	0.49
5:AE:7:GLU:O	5:AE:9:PRO:HD3	2.12	0.49
20:BZ:5029:SER:C	20:BZ:5031:GLN:H	2.16	0.49
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.49
2:AB:371:THR:HG22	2:AB:377:VAL:CA	2.41	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
31:BC:5520:LMG:H292	27:BJ:5101:BCR:H363	1.93	0.49
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.80	0.49
2:AB:243:ALA:HB2	2:AB:466:HIS:ND1	2.27	0.49
2:BB:5450:TRP:HB3	24:BB:5611:CLA:HMB2	1.95	0.49
3:BC:5114:VAL:CG2	31:BC:5521:LMG:H141	2.41	0.49
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HA	1.94	0.49
12:BM:5017:VAL:HG12	12:BM:5018:PRO:N	2.26	0.49
3:AC:55:ALA:CB	27:AC:514:BCR:H373	2.40	0.49
13:AO:225:LEU:N	13:AO:225:LEU:HD12	2.28	0.49
20:AZ:2:THR:CG2	20:AZ:3:ILE:N	2.73	0.49
14:BT:5025:GLU:O	14:BT:5026:PRO:C	2.50	0.49
2:AB:384:ARG:HD3	15:AU:132:LEU:HD13	1.94	0.49
3:BC:5332:GLN:HG3	13:BO:5129:PHE:CE2	2.47	0.49
2:BB:5372:ASP:OD1	2:BB:5374:ASN:N	2.44	0.49
4:AD:57:SER:HA	4:AD:60:THR:HG22	1.95	0.49
6:AF:41:GLN:HE21	6:AF:41:GLN:N	2.10	0.49
28:AC:519:DGD:O3D	9:AJ:37:GLY:O	2.25	0.49
1:AA:163:ILE:HG12	28:AC:517:DGD:HB31	1.93	0.49
4:AD:279:LEU:HD22	24:AD:401:CLA:HMA2	1.94	0.49
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC1	1.93	0.49
11:BL:5020:GLY:HA3	12:BM:5022:LEU:CD1	2.43	0.49
13:BO:5178:ARG:HD2	13:BO:5182:PHE:CD1	2.46	0.49
3:BC:5452:ALA:O	3:BC:5454:GLY:N	2.44	0.49
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.46	0.49
1:AA:57:PRO:HD3	1:AA:73:TYR:CE2	2.48	0.49
6:AF:19:ARG:HG3	6:AF:19:ARG:NH1	2.28	0.49
3:BC:5252:ILE:HG22	3:BC:5253:LEU:HD23	1.95	0.49
1:AA:257:ARG:NH1	1:AA:257:ARG:HG3	2.24	0.49
16:BV:5090:PRO:O	16:BV:5092:ARG:HD3	2.13	0.49
13:AO:186:LYS:HE2	13:AO:186:LYS:HA	1.95	0.49
3:AC:276:LEU:HD21	24:AC:508:CLA:HBB1	1.94	0.49
28:AH:101:DGD:O1B	28:AH:101:DGD:HG12	2.12	0.49
2:BB:5252:VAL:HG12	24:BB:5607:CLA:O1A	2.13	0.49
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.95	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
2:AB:44:THR:HB	32:AB:629:LMT:O6'	2.13	0.49
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.48	0.49
1:BA:5077:ILE:HG12	14:BT:5006:TYR:CD1	2.47	0.49
2:BB:5305:ILE:HG22	2:BB:5305:ILE:O	2.11	0.49
4:BD:5161:PRO:HB3	4:BD:5170:ALA:HB2	1.94	0.49
2:AB:41:GLU:HB3	2:AB:60:MET:SD	2.52	0.49
18:AX:24:LEU:O	18:AX:28:VAL:HG23	2.12	0.49
2:AB:251:VAL:O	2:AB:255:THR:HG23	2.12	0.49
24:AB:605:CLA:H141	24:AB:610:CLA:HED2	1.94	0.49
1:BA:5038:ILE:HB	1:BA:5039:PRO:HD3	1.93	0.49
15:BU:5072:TYR:CB	15:BU:5073:PRO:HD3	2.40	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
13:BO:5148:VAL:HA	13:BO:5172:PHE:CD2	2.47	0.49
3:BC:5337:LEU:CD1	13:BO:5131:PRO:HG3	2.41	0.49
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NE	2.27	0.49
9:BJ:5024:ILE:HG23	9:BJ:5025:VAL:N	2.27	0.49
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.12	0.49
4:BD:5308:ASP:C	4:BD:5308:ASP:OD1	2.49	0.49
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.94	0.49
2:BB:5008:VAL:HG23	2:BB:5009:HIS:HD2	1.76	0.49
24:BB:5608:CLA:HMC2	24:BB:5615:CLA:H191	1.95	0.49
2:BB:5115:TRP:CZ2	24:BB:5618:CLA:HBA2	2.47	0.49
3:BC:5049:LEU:HD23	3:BC:5149:TYR:OH	2.12	0.49
24:BB:5612:CLA:HMA1	4:BD:5130:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5186:GLN:HB2	24:BD:5402:CLA:HBC1	1.95	0.49
13:AO:83:LYS:HE2	2:BB:5338:GLN:HA	1.94	0.49
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.48	0.49
3:BC:5089:ILE:N	3:BC:5090:PRO:CD	2.74	0.49
16:BV:5071:ILE:C	16:BV:5071:ILE:HD12	2.33	0.49
3:AC:297:TYR:HA	3:AC:302:TYR:HE2	1.77	0.49
7:AH:44:ILE:HG12	18:AX:19:PHE:CE2	2.48	0.49
10:AK:12:PRO:HB3	20:AZ:62:VAL:HG11	1.93	0.49
9:BJ:5034:ALA:O	9:BJ:5035:GLY:O	2.31	0.49
28:AC:518:DGD:HB22	28:AC:519:DGD:HA21	1.95	0.49
1:AA:22:THR:HG21	8:AI:30:ARG:HE	1.78	0.49
24:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.48	0.49
24:AD:404:CLA:C4	18:AX:23:LEU:HA	2.43	0.49
28:BH:5101:DGD:O1B	28:BH:5101:DGD:HG12	2.12	0.49
2:BB:5002:GLY:HA3	11:BL:5009:PRO:HG2	1.94	0.49
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.12	0.49
13:BO:5155:THR:HG23	13:BO:5168:PHE:CE2	2.48	0.49
4:BD:5052:THR:HG22	4:BD:5067:TYR:CE2	2.48	0.49
4:AD:57:SER:CA	4:AD:60:THR:HG22	2.43	0.49
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.48	0.49
13:BO:5240:THR:HA	13:BO:5264:VAL:HA	1.95	0.49
13:AO:71:LEU:HD23	13:AO:265:PHE:HB3	1.94	0.49
2:AB:27:THR:HG23	24:AB:605:CLA:HMC1	1.94	0.49
2:AB:187:PRO:HB3	24:AB:601:CLA:CMB	2.42	0.49
2:AB:8:VAL:HG23	2:AB:9:HIS:HD2	1.77	0.49
3:BC:5271:TYR:CE1	24:BC:5507:CLA:HAC2	2.48	0.49
3:AC:149:TYR:CA	3:AC:156:LYS:HD3	2.42	0.49
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.61	0.49
1:AA:59:ASP:OD1	1:AA:64:ARG:N	2.46	0.49
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.43	0.49
13:AO:210:ARG:HA	15:AU:39:LEU:CD1	2.43	0.49
3:BC:5346:THR:O	13:BO:5040:GLY:HA2	2.13	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.27	0.49
18:BX:5043:ILE:HG22	18:BX:5043:ILE:O	2.13	0.49
2:AB:139:PHE:CZ	24:AB:609:CLA:HMB3	2.48	0.48
24:AC:505:CLA:HAA1	24:AC:505:CLA:H2	1.95	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:HA	1.94	0.48
1:BA:5159:LEU:C	1:BA:5162:PRO:HD2	2.34	0.48
24:BA:5408:CLA:HBA2	28:BA:5412:DGD:HB22	1.95	0.48
24:BB:5606:CLA:H191	4:BD:5158:LEU:HB3	1.96	0.48
20:BZ:5023:VAL:HB	20:BZ:5024:PRO:HD3	1.95	0.48
3:BC:5380:ILE:CA	3:BC:5384:ILE:HD11	2.37	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:BZ:5032:ASP:OD1	20:BZ:5036:SER:HB2	2.13	0.48
1:AA:64:ARG:NH1	1:AA:64:ARG:HG3	2.27	0.48
20:AZ:48:ILE:O	20:AZ:52:LEU:HG	2.13	0.48
20:BZ:5048:ILE:O	20:BZ:5052:LEU:HG	2.13	0.48
5:BE:5026:THR:HB	36:BF:5101:HEM:CAB	2.43	0.48
2:BB:5270:PRO:HG3	2:BB:5312:TYR:CD2	2.48	0.48
2:BB:5384:ARG:HH11	15:BU:5132:LEU:HD13	1.77	0.48
3:BC:5296:VAL:HG23	3:BC:5297:TYR:CD2	2.48	0.48
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.78	0.48
2:BB:5293:ALA:C	2:BB:5295:GLY:H	2.15	0.48
13:BO:5116:ASP:C	13:BO:5116:ASP:OD2	2.50	0.48
24:AB:604:CLA:HMC2	24:AB:611:CLA:H191	1.95	0.48
4:AD:266:TRP:CD1	31:AD:408:LMG:HC1	2.47	0.48
2:BB:5238:LEU:N	24:BB:5616:CLA:HMD3	2.28	0.48
4:BD:5266:TRP:NE1	31:BD:5410:LMG:HC72	2.28	0.48
3:AC:49:LEU:HD23	3:AC:149:TYR:OH	2.13	0.48
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.48
2:BB:5324:LEU:CA	4:BD:5293:LEU:HD23	2.38	0.48
3:BC:5249:ILE:O	3:BC:5253:LEU:HG	2.13	0.48
15:BU:5057:LEU:HD11	15:BU:5112:PHE:CB	2.42	0.48
1:BA:5057:PRO:HG3	1:BA:5068:SER:CB	2.43	0.48
2:AB:384:ARG:NH1	15:AU:132:LEU:HD13	2.28	0.48
3:BC:5235:GLY:O	3:BC:5238:ILE:HB	2.13	0.48
13:AO:71:LEU:HD12	13:AO:104:LEU:HD12	1.95	0.48
16:AV:146:LEU:O	16:AV:150:LYS:HG3	2.13	0.48
13:BO:5066:ILE:HD12	13:BO:5121:PHE:CD1	2.48	0.48
1:BA:5092:HIS:CD2	3:BC:5219:GLY:HA3	2.48	0.48
24:BB:5605:CLA:HHC	24:BB:5605:CLA:HBB1	1.94	0.48
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.48
15:AU:73:PRO:HG2	16:AV:107:THR:HB	1.95	0.48
13:BO:5147:THR:OG1	13:BO:5148:VAL:N	2.47	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	2.97	0.48
29:BA:5413:LHG:C1	3:BC:5447:ARG:HE	2.26	0.48
29:BA:5413:LHG:HC11	3:BC:5447:ARG:HH21	1.78	0.48
13:AO:159:VAL:HG13	13:AO:159:VAL:O	2.13	0.48
13:BO:5065:ARG:NH1	13:BO:5065:ARG:HB2	2.28	0.48
24:AB:611:CLA:H92	31:AD:407:LMG:H232	1.95	0.48
7:AH:35:MET:SD	27:AX:101:BCR:H322	2.53	0.48
8:BI:5019:PHE:CZ	8:BI:5023:PHE:HE2	2.30	0.48
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CD2	2.30	0.48
2:AB:354:LEU:N	2:AB:354:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:BZ:5032:ASP:OD1	20:BZ:5033:TRP:N	2.41	0.48
1:AA:254:TYR:CD1	4:AD:132:ILE:HG22	2.48	0.48
1:BA:5330:VAL:CG1	4:BD:5348:ARG:HG2	2.42	0.48
1:AA:318:ALA:HB2	4:AD:75:THR:HG22	1.95	0.48
1:AA:27:ARG:NH1	1:AA:27:ARG:O	2.47	0.48
1:AA:45:THR:CG2	1:AA:46:ILE:N	2.76	0.48
24:AC:506:CLA:HMC2	24:AC:507:CLA:H8	1.95	0.48
2:BB:5004:PRO:CG	2:BB:5007:ARG:HD2	2.35	0.48
4:BD:5087:HIS:HB2	28:BH:5101:DGD:O2D	2.12	0.48
4:BD:5210:LEU:HA	4:BD:5213:ILE:HG22	1.95	0.48
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.48
7:BH:5011:LEU:HA	7:BH:5014:LEU:HD12	1.94	0.48
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.34	0.48
3:AC:337:LEU:HD12	13:AO:131:PRO:CG	2.44	0.48
5:BE:5061:ARG:NH2	16:BV:5153:GLY:HA3	2.28	0.48
13:BO:5135:GLN:HG2	13:BO:5141:ARG:HG3	1.96	0.48
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.44	0.48
2:BB:5012:LEU:HD12	2:BB:5019:LEU:HD12	1.96	0.48
1:BA:5220:THR:HG23	4:BD:5141:TYR:CD1	2.49	0.48
24:BC:5511:CLA:H143	20:BZ:5024:PRO:HG2	1.96	0.48
5:BE:5078:THR:O	5:BE:5081:GLU:HB2	2.14	0.48
13:BO:5120:THR:HA	13:BO:5153:ALA:O	2.14	0.48
6:BF:5015:ILE:HG22	6:BF:5016:PHE:CD1	2.47	0.48
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.14	0.48
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
2:AB:372:ASP:OD1	2:AB:374:ASN:N	2.46	0.48
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.49	0.48
1:BA:5278:TRP:HA	28:BC:5519:DGD:HAG1	1.96	0.48
1:BA:5022:THR:HG21	8:BI:5030:ARG:HE	1.78	0.48
3:AC:147:PHE:CD2	24:AC:513:CLA:H3A	2.49	0.48
13:AO:155:THR:HG22	13:AO:167:ASP:O	2.14	0.48
3:BC:5418:ASN:HB2	28:BC:5519:DGD:HE2	1.92	0.48
1:BA:5281:VAL:HG13	28:BC:5519:DGD:HAG3	1.93	0.48
2:AB:245:VAL:HG22	24:AB:612:CLA:H192	1.95	0.48
3:AC:271:TYR:CE1	24:AC:507:CLA:HAC2	2.49	0.48
3:BC:5350:ILE:HG21	3:BC:5359:TRP:HB2	1.96	0.48
24:BC:5501:CLA:CAD	24:BC:5503:CLA:H12	2.44	0.48
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.96	0.48
3:AC:461:ARG:NH2	4:AD:242:GLU:O	2.46	0.48
7:BH:5013:PRO:HG2	7:BH:5014:LEU:H	1.78	0.48
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.48
16:AV:143:GLY:O	16:AV:147:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:188:PHE:CZ	4:AD:326:ARG:HG2	2.49	0.48
18:AX:22:GLY:HA2	18:AX:25:SER:HG	1.79	0.48
1:AA:248:ILE:CG1	1:AA:248:ILE:O	2.61	0.48
3:AC:214:LEU:HD22	3:AC:214:LEU:N	2.28	0.48
2:BB:5107:LEU:HD21	24:BB:5619:CLA:H42	1.95	0.48
3:BC:5436:PHE:O	24:BC:5508:CLA:HAC1	2.14	0.48
24:BC:5507:CLA:HHC	24:BC:5507:CLA:HBB1	1.96	0.48
5:BE:5069:ARG:HG3	5:BE:5070:PHE:H	1.79	0.48
11:BL:5016:SER:HA	11:BL:5019:LEU:CG	2.44	0.48
15:BU:5066:ILE:O	15:BU:5066:ILE:CG2	2.61	0.48
1:AA:315:ASN:ND2	4:AD:332:GLN:HE22	2.07	0.48
1:BA:5131:TRP:CE3	1:BA:5132:GLU:CA	2.97	0.48
1:BA:5047:CYS:SG	1:BA:5114:LEU:HD22	2.53	0.48
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.79	0.48
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	1.95	0.48
4:BD:5209:LEU:HD23	4:BD:5209:LEU:C	2.34	0.48
2:AB:222:PRO:HG3	7:AH:27:THR:N	2.25	0.48
2:AB:234:ILE:HD12	2:AB:237:VAL:CG2	2.43	0.48
24:BB:5610:CLA:H52	27:BB:5623:BCR:H321	1.96	0.48
2:BB:5329:PRO:HD2	31:BB:5624:LMG:O4	2.14	0.48
4:BD:5152:VAL:HG11	24:BD:5402:CLA:H11	1.94	0.48
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.48
4:AD:218:VAL:HG22	4:AD:244:TYR:CE2	2.49	0.48
18:AX:44:ASP:N	18:AX:44:ASP:OD1	2.46	0.48
2:AB:326:ARG:HD3	2:AB:442:ILE:HG22	1.95	0.48
16:BV:5121:LEU:CD2	16:BV:5138:LEU:HD11	2.44	0.48
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.16	0.48
1:AA:183:MET:HA	24:AA:404:CLA:HMD2	1.96	0.47
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.47
2:AB:15:ASP:N	2:AB:16:PRO:HD3	2.29	0.47
2:AB:12:LEU:HD12	2:AB:19:LEU:HD12	1.94	0.47
3:AC:256:PRO:HG2	3:AC:266:TRP:CH2	2.49	0.47
5:AE:69:ARG:HG3	5:AE:70:PHE:H	1.78	0.47
11:AL:20:GLY:HA3	12:AM:22:LEU:CD1	2.44	0.47
24:BA:5406:CLA:HED2	4:BD:5198:MET:SD	2.54	0.47
3:BC:5365:TRP:HA	3:BC:5387:TRP:CH2	2.49	0.47
1:BA:5048:PHE:CA	1:BA:5115:ILE:HD11	2.44	0.47
13:AO:236:GLU:O	13:AO:236:GLU:HG3	2.14	0.47
5:BE:5051:ARG:O	5:BE:5053:ASP:N	2.47	0.47
13:BO:5157:PRO:O	13:BO:5158:ASN:O	2.32	0.47
1:BA:5322:ASN:OD1	3:BC:5412:THR:HA	2.14	0.47
16:AV:81:ARG:NH1	16:AV:81:ARG:HG2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:AU:38:GLU:O	15:AU:39:LEU:O	2.32	0.47
13:BO:5071:LEU:HD12	13:BO:5104:LEU:HD12	1.96	0.47
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.14	0.47
4:BD:5096:GLU:H	4:BD:5096:GLU:CD	2.17	0.47
1:BA:5281:VAL:HG11	28:BC:5519:DGD:HAV1	1.96	0.47
24:BC:5504:CLA:H192	28:BC:5518:DGD:HBN2	1.96	0.47
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.49	0.47
24:AC:507:CLA:HBB1	24:AC:507:CLA:HHC	1.96	0.47
4:AD:261:PHE:HE1	4:AD:266:TRP:CD1	2.33	0.47
2:BB:5012:LEU:HD22	2:BB:5018:ARG:HB2	1.95	0.47
11:BL:5026:VAL:HG11	31:BL:5101:LMG:H202	1.96	0.47
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.96	0.47
20:BZ:5036:SER:HA	20:BZ:5039:LEU:CG	2.40	0.47
4:AD:221:THR:HG23	4:AD:221:THR:O	2.13	0.47
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.47
3:BC:5441:HIS:HD2	3:BC:5442:LEU:HD12	1.78	0.47
1:AA:275:LEU:HD13	25:AA:408:MST:C8	2.44	0.47
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.13	0.47
4:BD:5160:TYR:HB3	4:BD:5161:PRO:CD	2.44	0.47
1:AA:295:PHE:O	3:AC:424:SER:OG	2.32	0.47
20:BZ:5047:TRP:O	20:BZ:5050:LEU:HB2	2.14	0.47
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.29	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
24:AA:407:CLA:HBA2	28:AA:411:DGD:HB22	1.96	0.47
2:AB:457:VAL:HG12	2:AB:458:PHE:N	2.29	0.47
2:AB:450:TRP:HB3	24:AB:607:CLA:HMB2	1.95	0.47
3:AC:437:PHE:HA	24:AC:508:CLA:HMC1	1.95	0.47
3:AC:330:SER:HB2	13:AO:149:LYS:NZ	2.29	0.47
6:BF:5016:PHE:N	6:BF:5016:PHE:CD1	2.82	0.47
6:BF:5019:ARG:HH11	6:BF:5019:ARG:HG3	1.78	0.47
3:AC:297:TYR:HD1	3:AC:302:TYR:CE2	2.33	0.47
3:AC:450:ALA:HA	3:AC:455:PHE:CE2	2.49	0.47
4:BD:5084:SER:HB3	5:BE:5068:ASP:HA	1.95	0.47
24:AC:504:CLA:H192	28:AC:518:DGD:HBN2	1.96	0.47
1:AA:153:SER:CB	24:AA:404:CLA:H11	2.45	0.47
24:AB:603:CLA:H2	24:AB:605:CLA:H91	1.96	0.47
24:AB:608:CLA:C1	24:AB:608:CLA:HAA1	2.44	0.47
1:BA:5091:LEU:HD11	1:BA:5163:ILE:HA	1.94	0.47
24:BC:5502:CLA:H122	24:BC:5503:CLA:HMB2	1.96	0.47
3:BC:5147:PHE:CD2	24:BC:5513:CLA:H3A	2.49	0.47
1:BA:5119:PHE:HD1	34:BD:5403:PHO:H92	1.78	0.47
7:BH:5050:ASN:HD22	28:BH:5101:DGD:HA21	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:5039:THR:HB	13:BO:5041:LEU:HD22	1.95	0.47
13:AO:155:THR:HG23	13:AO:168:PHE:CD2	2.50	0.47
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HA	1.95	0.47
8:BI:5014:PHE:CE2	8:BI:5018:LEU:HD11	2.49	0.47
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.14	0.47
28:AC:519:DGD:HE62	9:AJ:40:LEU:CD1	2.45	0.47
29:AA:412:LHG:HC11	3:AC:447:ARG:HH21	1.78	0.47
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.67	0.47
4:AD:274:VAL:HA	35:AD:405:PL9:C25	2.37	0.47
1:BA:5039:PRO:CB	24:BA:5408:CLA:HBB1	2.44	0.47
2:BB:5198:VAL:HG11	24:BB:5607:CLA:HED2	1.97	0.47
24:BC:5506:CLA:HMC2	24:BC:5507:CLA:H8	1.96	0.47
1:BA:5029:TYR:CD2	1:BA:5133:LEU:HD13	2.49	0.47
1:AA:272:HIS:HD2	4:AD:218:VAL:HG21	1.76	0.47
11:BL:5024:ILE:HG21	12:BM:5019:SER:OG	2.14	0.47
12:AM:24:ILE:HD13	31:BM:5102:LMG:H351	1.96	0.47
20:AZ:53:VAL:O	20:AZ:57:LEU:HB2	2.14	0.47
5:BE:5027:ILE:CB	5:BE:5028:PRO:HD3	2.43	0.47
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	1.96	0.47
1:AA:326:LEU:CD2	3:AC:412:THR:HB	2.44	0.47
4:AD:299:ILE:HG13	11:AL:37:ASN:ND2	2.29	0.47
16:BV:5045:ILE:HG12	16:BV:5046:THR:N	2.29	0.47
19:BY:5011:UNK:C	19:BY:5013:UNK:N	2.76	0.47
3:BC:5327:ASN:HB3	13:BO:5125:ASP:OD1	2.14	0.47
3:BC:5131:TYR:HE1	3:BC:5135:ARG:HD2	1.80	0.47
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.79	0.47
2:AB:54:PRO:HD2	2:AB:57:ARG:HG3	1.95	0.47
4:AD:96:GLU:H	4:AD:96:GLU:CD	2.18	0.47
7:AH:17:GLU:H	7:AH:17:GLU:CD	2.16	0.47
31:AB:620:LMG:H202	11:AL:26:VAL:HG11	1.95	0.47
4:BD:5087:HIS:HD2	4:BD:5166:SER:HA	1.72	0.47
7:BH:5025:TRP:O	7:BH:5026:GLY:C	2.53	0.47
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.14	0.47
13:AO:36:ILE:HG23	13:AO:41:LEU:CB	2.44	0.47
13:AO:39:THR:HB	13:AO:41:LEU:HD22	1.96	0.47
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.47
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.47
1:AA:13:LEU:N	1:AA:16:ARG:HH11	2.13	0.47
3:BC:5330:SER:HB2	13:BO:5149:LYS:NZ	2.29	0.47
4:BD:5180:ARG:HG3	4:BD:5181:PHE:N	2.29	0.47
5:AE:27:ILE:CB	5:AE:28:PRO:HD3	2.44	0.47
1:AA:43:ALA:HB3	1:AA:118:HIS:HD2	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:BU:5099:GLU:HA	15:BU:5102:LYS:HE3	1.97	0.47
1:AA:223:LEU:O	2:AB:482:ILE:HG12	2.13	0.47
2:AB:405:GLU:OE1	2:AB:405:GLU:HA	2.14	0.47
3:AC:416:SER:CA	28:AC:519:DGD:O3E	2.62	0.47
3:AC:437:PHE:HZ	24:AC:510:CLA:HMB3	1.79	0.47
1:AA:119:PHE:HD1	34:AD:402:PHO:H92	1.79	0.47
24:AB:602:CLA:H93	7:AH:46:LEU:HD13	1.96	0.47
1:AA:32:TRP:HB2	8:AI:23:PHE:CZ	2.49	0.47
1:BA:5183:MET:HG3	24:BA:5406:CLA:HBC1	1.96	0.47
24:BC:5510:CLA:H122	24:BC:5510:CLA:H161	1.81	0.47
24:BB:5615:CLA:H92	31:BD:5409:LMG:H232	1.95	0.47
2:BB:5250:PHE:O	28:BH:5101:DGD:HB82	2.15	0.47
2:AB:9:HIS:HB2	24:AB:611:CLA:CBA	2.44	0.47
4:AD:274:VAL:CB	4:AD:275:PRO:HD3	2.44	0.47
24:AD:404:CLA:H42	18:AX:23:LEU:HA	1.96	0.47
1:BA:5153:SER:HB2	24:BA:5405:CLA:H11	1.97	0.47
2:BB:5187:PRO:HG2	2:BB:5188:ASP:H	1.80	0.47
24:BB:5611:CLA:H41	24:BB:5611:CLA:H61	1.74	0.47
3:BC:5271:TYR:HA	3:BC:5274:TYR:CD2	2.49	0.47
4:BD:5263:ASN:O	4:BD:5266:TRP:N	2.47	0.47
5:BE:5015:THR:O	9:BJ:5008:ILE:CD1	2.63	0.47
3:BC:5318:LEU:HD21	3:BC:5380:ILE:HG23	1.97	0.47
1:BA:5059:ASP:OD2	1:BA:5062:GLY:HA2	2.15	0.47
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.29	0.47
1:AA:288:LEU:HD22	3:AC:432:VAL:HA	1.96	0.47
1:BA:5015:GLU:O	1:BA:5019:ASN:OD1	2.32	0.47
3:AC:472:LEU:O	3:AC:473:ASP:O	2.32	0.47
2:AB:324:LEU:CA	4:AD:293:LEU:HD23	2.43	0.47
3:BC:5262:ARG:HH21	32:BC:5522:LMT:C5'	2.26	0.47
13:BO:5236:GLU:HG3	13:BO:5236:GLU:O	2.14	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.95	0.47
3:BC:5075:PHE:CD1	3:BC:5086:LEU:HD21	2.50	0.47
2:AB:325:PHE:CD1	11:AL:34:TYR:HB3	2.49	0.47
2:AB:279:TYR:HE1	7:AH:63:LYS:HE3	1.80	0.47
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.50	0.47
3:BC:5394:GLU:OE2	3:BC:5398:HIS:CD2	2.68	0.47
13:AO:65:ARG:NH1	13:AO:65:ARG:HB2	2.29	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
1:AA:47:CYS:SG	1:AA:114:LEU:HD22	2.54	0.47
1:BA:5248:ILE:O	1:BA:5248:ILE:CG1	2.62	0.47
2:AB:143:LEU:HD12	2:AB:143:LEU:O	2.14	0.47
15:AU:58:ASN:OD1	15:AU:84:PRO:CA	2.61	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:39:PRO:CB	24:AA:407:CLA:HBB1	2.44	0.47
2:AB:329:PRO:HD2	31:AB:621:LMG:O4	2.15	0.47
1:AA:214:MET:HE1	4:AD:142:ASN:OD1	2.14	0.47
2:AB:250:PHE:O	28:AH:101:DGD:HB82	2.15	0.47
11:AL:17:LEU:HD11	12:AM:23:ILE:HD12	1.97	0.47
1:BA:5135:TYR:HE1	3:BC:5449:ARG:O	1.97	0.47
2:BB:5250:PHE:HD1	28:BH:5101:DGD:HB92	1.80	0.47
4:BD:5086:GLY:O	4:BD:5166:SER:HB2	2.15	0.47
24:BB:5618:CLA:H162	31:BL:5101:LMG:H422	1.96	0.47
3:AC:387:TRP:CE2	3:AC:388:GLN:HG3	2.49	0.47
29:BA:5415:LHG:H102	31:BE:5101:LMG:H142	1.97	0.47
2:AB:384:ARG:HH11	15:AU:132:LEU:HD13	1.79	0.47
16:BV:5143:GLY:O	16:BV:5147:VAL:HG23	2.14	0.47
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.79	0.47
2:AB:356:VAL:HA	2:AB:370:LEU:CD2	2.45	0.47
4:AD:68:LEU:HD11	5:AE:44:TYR:CE1	2.49	0.47
11:AL:8:GLN:N	11:AL:8:GLN:NE2	2.62	0.47
3:AC:319:ILE:O	3:AC:323:LYS:HG3	2.15	0.47
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.35	0.47
2:AB:329:PRO:HD3	24:AB:607:CLA:CED	2.44	0.47
3:AC:436:PHE:O	24:AC:508:CLA:HAC1	2.15	0.47
8:AI:11:VAL:CG2	32:AI:102:LMT:H101	2.44	0.47
1:BA:5183:MET:HA	24:BA:5405:CLA:HMD2	1.97	0.47
2:BB:5025:MET:HE2	27:BB:5621:BCR:H393	1.97	0.47
24:BB:5614:CLA:H111	24:BB:5619:CLA:CAA	2.44	0.47
13:BO:5070:CYS:SG	13:BO:5105:ASP:OD1	2.72	0.47
13:BO:5031:LEU:N	13:BO:5031:LEU:CD1	2.72	0.47
13:BO:5171:GLU:HA	13:BO:5221:GLY:O	2.15	0.47
2:AB:425:ILE:HG22	2:AB:426:PHE:HD2	1.75	0.47
5:BE:5014:ILE:HG22	9:BJ:5013:VAL:HG11	1.96	0.47
2:BB:5369:ILE:C	2:BB:5370:LEU:HD23	2.35	0.47
1:BA:5329:GLU:O	1:BA:5332:HIS:ND1	2.45	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
10:BK:5015:TYR:OH	20:BZ:5058:ASN:ND2	2.48	0.47
2:AB:485:GLU:HG2	2:AB:486:LEU:N	2.29	0.47
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.47
28:BC:5518:DGD:O3D	27:BJ:5101:BCR:H382	2.14	0.47
24:AB:601:CLA:HBC3	7:AH:41:PHE:CE1	2.50	0.47
2:AB:115:TRP:CZ2	24:AB:614:CLA:HBA2	2.50	0.47
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG12	1.95	0.47
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CBA	2.45	0.47
3:BC:5042:LEU:HD21	24:BC:5511:CLA:H2A	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:375:LEU:HB3	3:AC:380:ILE:HD11	1.96	0.47
2:BB:5175:THR:O	2:BB:5176:GLY:O	2.33	0.47
5:BE:5078:THR:HA	5:BE:5081:GLU:CG	2.43	0.47
1:AA:13:LEU:HD12	1:AA:16:ARG:NH1	2.29	0.47
3:BC:5473:ASP:HB2	14:BT:5026:PRO:HB3	1.96	0.47
3:BC:5143:TYR:O	3:BC:5144:SER:CB	2.62	0.47
16:BV:5081:ARG:CZ	16:BV:5157:GLY:HA3	2.45	0.47
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.97	0.47
13:BO:5077:LEU:HB3	13:BO:5091:PHE:HB3	1.97	0.47
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.30	0.47
1:AA:202:VAL:HG11	24:AA:406:CLA:OBD	2.14	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.97	0.47
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.68	0.47
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.15	0.46
3:AC:264:PHE:CE1	27:AC:516:BCR:H321	2.50	0.46
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.46
2:BB:5112:CYS:HB3	27:BB:5623:BCR:H393	1.96	0.46
24:BC:5510:CLA:HBB1	24:BC:5510:CLA:HHC	1.96	0.46
11:BL:5016:SER:O	11:BL:5019:LEU:HD12	2.14	0.46
24:BD:5405:CLA:C4	18:BX:5023:LEU:HA	2.45	0.46
2:BB:5193:TYR:CD1	2:BB:5260:SER:HA	2.50	0.46
3:BC:5038:GLY:HA3	24:BC:5511:CLA:C2D	2.45	0.46
20:BZ:5023:VAL:HG12	20:BZ:5027:TYR:CE2	2.49	0.46
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.15	0.46
13:AO:36:ILE:HG23	13:AO:41:LEU:HB2	1.97	0.46
5:BE:5036:LEU:HA	5:BE:5039:SER:OG	2.15	0.46
1:BA:5222:SER:O	1:BA:5246:TYR:HB2	2.14	0.46
15:BU:5072:TYR:O	15:BU:5073:PRO:C	2.51	0.46
3:BC:5432:VAL:HG13	3:BC:5433:LEU:N	2.29	0.46
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.46
3:BC:5420:VAL:HB	3:BC:5425:TRP:HE1	1.80	0.46
24:AB:602:CLA:H191	4:AD:158:LEU:HB3	1.97	0.46
2:BB:5007:ARG:HA	24:BB:5615:CLA:HBA1	1.97	0.46
2:BB:5153:PHE:CZ	2:BB:5158:LEU:HD21	2.50	0.46
18:BX:5012:ILE:CD1	18:BX:5016:LEU:HD12	2.44	0.46
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.98	0.46
10:BK:5043:VAL:HG21	10:BK:5046:ARG:HE	1.80	0.46
15:BU:5073:PRO:HG2	16:BV:5107:THR:HB	1.97	0.46
1:AA:12:ASN:ND2	1:AA:15:GLU:HB2	2.29	0.46
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	1.97	0.46
2:AB:489:GLU:C	2:AB:490:GLN:HG3	2.36	0.46
5:AE:78:THR:O	5:AE:81:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5131:TRP:CE3	1:BA:5132:GLU:HA	2.51	0.46
1:BA:5140:ARG:HB2	4:BD:5220:ASN:HA	1.96	0.46
18:BX:5024:LEU:HA	18:BX:5024:LEU:HD12	1.74	0.46
1:AA:210:LEU:HD23	1:AA:210:LEU:C	2.36	0.46
8:AI:33:LYS:O	8:AI:35:LYS:HG2	2.14	0.46
4:BD:5093:TRP:HA	4:BD:5099:GLY:H	1.81	0.46
16:BV:5098:LEU:O	16:BV:5102:MET:HG3	2.14	0.46
1:AA:35:VAL:HA	27:AA:410:BCR:H333	1.95	0.46
24:AB:608:CLA:CAB	4:AD:123:ILE:HG23	2.45	0.46
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.16	0.46
7:AH:43:LEU:O	7:AH:47:GLU:HG3	2.14	0.46
1:BA:5021:VAL:HG12	1:BA:5022:THR:N	2.30	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:ND1	2.30	0.46
2:BB:5245:VAL:HG22	24:BB:5616:CLA:H192	1.96	0.46
4:BD:5036:LEU:O	4:BD:5039:PRO:HD2	2.15	0.46
2:BB:5005:TRP:CZ2	31:BL:5101:LMG:H291	2.50	0.46
5:BE:5017:VAL:HA	9:BJ:5008:ILE:HD11	1.96	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.30	0.46
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.15	0.46
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.29	0.46
6:BF:5023:VAL:O	6:BF:5027:ALA:CB	2.63	0.46
2:BB:5384:ARG:NH1	15:BU:5132:LEU:HD13	2.30	0.46
4:BD:5299:ILE:HG13	11:BL:5037:ASN:ND2	2.30	0.46
1:BA:5326:LEU:CD2	3:BC:5412:THR:HB	2.46	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CG	2.63	0.46
1:BA:5138:GLY:HA3	8:BI:5032:PRO:HG2	1.98	0.46
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.46
1:AA:21:VAL:HG12	1:AA:22:THR:N	2.29	0.46
31:AA:417:LMG:H301	2:BB:5076:SER:HB3	1.96	0.46
2:AB:112:CYS:HB3	27:AB:619:BCR:H393	1.98	0.46
2:AB:242:ILE:HG22	2:AB:466:HIS:HB2	1.96	0.46
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.15	0.46
3:BC:5057:ALA:O	3:BC:5061:VAL:HG23	2.15	0.46
24:BC:5511:CLA:H141	20:BZ:5020:VAL:O	2.16	0.46
1:BA:5244:GLU:HG3	1:BA:5246:TYR:H	1.80	0.46
2:AB:298:LEU:HD23	2:AB:402:TYR:CE1	2.51	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.46
1:BA:5064:ARG:NH1	13:BO:5098:THR:HG21	2.31	0.46
4:AD:251:ARG:HG2	4:AD:255:GLN:OE1	2.16	0.46
1:AA:275:LEU:HD13	25:AA:408:MST:H83	1.96	0.46
1:AA:48:PHE:CA	1:AA:115:ILE:HD11	2.45	0.46
3:BC:5094:THR:CG2	3:BC:5298:PRO:HD2	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:420:VAL:HB	3:AC:425:TRP:HE1	1.79	0.46
16:BV:5148:GLU:OE1	16:BV:5148:GLU:HA	2.15	0.46
4:BD:5136:VAL:O	4:BD:5136:VAL:HG12	2.15	0.46
1:AA:220:THR:CG2	4:AD:141:TYR:HD1	2.29	0.46
2:AB:237:VAL:HB	24:AB:612:CLA:CMD	2.46	0.46
29:AA:412:LHG:HC11	3:AC:447:ARG:NE	2.31	0.46
4:AD:279:LEU:CD2	24:AD:401:CLA:HMA2	2.45	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:CE1	2.50	0.46
4:BD:5250:ASN:ND2	4:BD:5262:SER:HB3	2.28	0.46
20:BZ:5021:ILE:O	20:BZ:5025:VAL:HG22	2.16	0.46
3:BC:5380:ILE:HA	3:BC:5384:ILE:CD1	2.37	0.46
2:AB:179:GLN:HE21	2:AB:179:GLN:CA	2.18	0.46
3:BC:5029:GLU:HA	10:BK:5046:ARG:HH12	1.80	0.46
6:BF:5021:VAL:HG21	30:BF:5102:SQD:H101	1.97	0.46
1:AA:131:TRP:CE3	1:AA:132:GLU:HA	2.50	0.46
13:BO:5072:GLN:O	13:BO:5263:GLY:HA3	2.14	0.46
4:AD:209:LEU:HD23	4:AD:209:LEU:C	2.35	0.46
4:AD:72:ASN:HA	31:AJ:102:LMG:HC72	1.97	0.46
24:AA:407:CLA:HMA2	28:AA:411:DGD:HB42	1.98	0.46
24:AB:610:CLA:H111	24:AB:615:CLA:CAA	2.43	0.46
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.28	0.46
3:AC:288:CYS:HB3	28:AC:517:DGD:HG2	1.98	0.46
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.97	0.46
1:AA:214:MET:HE1	34:AD:403:PHO:OBD	2.14	0.46
4:AD:88:SER:HA	7:AH:50:ASN:OD1	2.15	0.46
30:BB:5601:SQD:H141	24:BB:5618:CLA:H143	1.97	0.46
3:BC:5266:TRP:HZ3	24:BC:5507:CLA:HBC2	1.80	0.46
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.50	0.46
20:BZ:5032:ASP:C	20:BZ:5034:ASP:H	2.17	0.46
1:BA:5010:SER:C	1:BA:5012:ASN:H	2.19	0.46
2:BB:5124:ARG:HD3	2:BB:5131:PRO:N	2.30	0.46
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.46
4:BD:5253:TRP:HA	4:BD:5256:ILE:CG2	2.45	0.46
1:BA:5140:ARG:HD3	4:BD:5219:GLU:O	2.15	0.46
13:BO:5071:LEU:HD23	13:BO:5265:PHE:CB	2.45	0.46
2:AB:334:ASP:HB3	13:AO:202:GLN:HG3	1.98	0.46
4:AD:155:SER:HA	4:AD:159:ILE:HG13	1.98	0.46
3:AC:418:ASN:HB2	28:AC:519:DGD:HE2	1.98	0.46
1:AA:153:SER:HB2	24:AA:404:CLA:H11	1.98	0.46
24:AA:405:CLA:H72	31:AB:620:LMG:C25	2.46	0.46
2:AB:135:LEU:HD21	2:AB:234:ILE:HD13	1.98	0.46
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:119:ALA:O	4:AD:123:ILE:HG13	2.16	0.46
1:AA:32:TRP:CB	8:AI:23:PHE:CZ	2.98	0.46
1:BA:5149:ALA:HB1	1:BA:5283:VAL:CG1	2.45	0.46
2:BB:5012:LEU:HB2	24:BB:5616:CLA:HMC2	1.98	0.46
3:BC:5213:LEU:HD21	27:BC:5516:BCR:C19	2.46	0.46
3:BC:5267:SER:O	3:BC:5271:TYR:CD2	2.69	0.46
4:BD:5210:LEU:HD13	4:BD:5271:MET:HG2	1.98	0.46
16:BV:5059:PHE:HA	16:BV:5063:CYS:SG	2.56	0.46
3:AC:57:ALA:O	3:AC:61:VAL:HG23	2.16	0.46
2:BB:5371:THR:HG22	2:BB:5377:VAL:CA	2.42	0.46
5:AE:26:THR:HB	36:AF:101:HEM:C3B	2.51	0.46
6:BF:5031:ILE:HG12	36:BF:5101:HEM:HMC2	1.97	0.46
4:BD:5057:SER:HA	4:BD:5060:THR:HG22	1.97	0.46
1:AA:210:LEU:C	1:AA:210:LEU:CD2	2.84	0.46
2:BB:5490:GLN:OE1	2:BB:5490:GLN:O	2.33	0.46
3:BC:5319:ILE:O	3:BC:5323:LYS:HG3	2.15	0.46
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.96	0.46
2:AB:107:LEU:HD21	24:AB:615:CLA:H42	1.97	0.46
1:AA:135:TYR:HE1	3:AC:449:ARG:O	1.99	0.46
4:AD:162:LEU:HD21	4:AD:167:TRP:CH2	2.50	0.46
1:BA:5179:THR:HG22	1:BA:5183:MET:CE	2.46	0.46
3:BC:5272:LEU:HA	24:BC:5509:CLA:HMD3	1.97	0.46
24:BB:5612:CLA:CAB	4:BD:5123:ILE:HG23	2.46	0.46
24:BA:5406:CLA:H61	34:BD:5403:PHO:HMB3	1.97	0.46
3:AC:62:PHE:HZ	10:AK:28:ILE:CD1	2.29	0.46
2:BB:5179:GLN:CA	2:BB:5179:GLN:HE21	2.17	0.46
3:AC:164:HIS:HA	3:AC:167:VAL:HG23	1.97	0.46
4:BD:5217:THR:O	4:BD:5221:THR:HB	2.15	0.46
4:AD:180:ARG:HG3	4:AD:181:PHE:N	2.31	0.46
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD13	1.98	0.46
2:BB:5356:VAL:HG22	2:BB:5370:LEU:HD21	1.97	0.46
2:AB:363:PHE:HD1	4:AD:326:ARG:HD2	1.80	0.46
4:AD:30:VAL:HG12	4:AD:31:GLY:N	2.30	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
2:AB:152:GLY:C	24:AB:606:CLA:HMC3	2.36	0.46
2:AB:187:PRO:HG2	2:AB:188:ASP:H	1.80	0.46
3:AC:215:LYS:HZ3	3:AC:226:SER:CB	2.28	0.46
3:AC:271:TYR:HA	3:AC:274:TYR:CD2	2.50	0.46
11:AL:22:LEU:HD13	14:AT:16:LEU:HD23	1.98	0.46
1:BA:5151:LEU:HD21	1:BA:5155:PHE:HE2	1.81	0.46
2:BB:5012:LEU:O	2:BB:5014:ASN:N	2.49	0.46
30:BB:5601:SQD:H92	24:BB:5618:CLA:H42	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:AJ:11:TRP:CE3	10:AK:42:ALA:HB2	2.51	0.46
9:BJ:5003:SER:CA	9:BJ:5007:ARG:HH22	2.29	0.46
4:BD:5323:GLU:HG2	13:BO:5194:TYR:OH	2.16	0.46
2:AB:121:GLU:HG2	7:AH:4:ARG:CD	2.43	0.46
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.67	0.46
2:BB:5121:GLU:HG2	7:BH:5004:ARG:CD	2.42	0.46
3:BC:5335:THR:HA	13:BO:5178:ARG:CD	2.46	0.46
2:BB:5425:ILE:HG22	2:BB:5426:PHE:HD2	1.78	0.46
3:BC:5465:PRO:O	3:BC:5469:MET:HE3	2.16	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CD	2.64	0.46
13:BO:5159:VAL:O	13:BO:5159:VAL:HG13	2.16	0.46
1:BA:5114:LEU:HD23	1:BA:5114:LEU:C	2.37	0.46
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.84	0.46
4:BD:5193:LEU:O	4:BD:5193:LEU:HG	2.16	0.46
2:AB:226:TYR:HA	2:AB:231:MET:HE2	1.97	0.46
2:AB:9:HIS:HB2	24:AB:611:CLA:CGA	2.46	0.46
3:AC:272:LEU:HA	24:AC:509:CLA:HMD3	1.97	0.46
1:AA:159:LEU:HD11	28:AC:517:DGD:HB51	1.97	0.46
1:BA:5021:VAL:HG11	1:BA:5032:TRP:CE3	2.51	0.46
35:BD:5406:PL9:H303	35:BD:5406:PL9:H262	1.97	0.46
3:BC:5460:ASP:O	3:BC:5461:ARG:C	2.54	0.46
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	2.16	0.46
13:BO:5036:ILE:HG23	13:BO:5041:LEU:CB	2.46	0.46
2:BB:5354:LEU:HD21	2:BB:5378:LYS:CB	2.46	0.46
12:BM:5019:SER:O	12:BM:5023:ILE:HD13	2.16	0.46
7:BH:5006:TRP:O	7:BH:5010:ILE:HG13	2.16	0.46
13:BO:5271:PRO:HG2	13:BO:5272:ALA:H	1.81	0.46
4:BD:5084:SER:HB3	5:BE:5068:ASP:CA	2.46	0.46
2:AB:485:GLU:CG	2:AB:486:LEU:N	2.78	0.46
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.81	0.46
2:BB:5485:GLU:CG	2:BB:5486:LEU:N	2.79	0.46
1:BA:5318:ALA:HB2	4:BD:5075:THR:HG22	1.97	0.46
2:BB:5285:ASN:HD22	2:BB:5285:ASN:N	2.14	0.46
3:BC:5185:LEU:HD12	3:BC:5230:LEU:HD12	1.97	0.46
31:AC:520:LMG:H202	9:AJ:22:ILE:HG21	1.97	0.45
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	1.99	0.45
24:AB:604:CLA:H111	24:AB:615:CLA:H2	1.97	0.45
3:BC:5229:ASN:ND2	3:BC:5231:GLU:HB2	2.31	0.45
14:BT:5014:ILE:HD13	14:BT:5017:PHE:CD2	2.52	0.45
1:BA:5084:PRO:HA	1:BA:5112:TYR:CG	2.49	0.45
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.80	0.45
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:5215:ARG:HD2	15:BU:5039:LEU:HD22	1.98	0.45
2:BB:5356:VAL:HA	2:BB:5370:LEU:CD2	2.45	0.45
2:AB:398:THR:HG22	2:AB:412:THR:HG22	1.96	0.45
4:AD:136:VAL:HG12	4:AD:136:VAL:O	2.16	0.45
11:AL:7:ARG:HD2	11:AL:7:ARG:O	2.16	0.45
3:BC:5414:ILE:HG22	3:BC:5415:ASN:N	2.32	0.45
1:BA:5214:MET:HE1	34:BD:5404:PHO:OBD	2.16	0.45
1:BA:5042:LEU:HD21	30:BA:5401:SQD:H152	1.97	0.45
2:BB:5016:PRO:HB3	2:BB:5133:LEU:HD21	1.97	0.45
2:BB:5329:PRO:HD3	24:BB:5611:CLA:CED	2.46	0.45
3:BC:5435:PHE:O	3:BC:5438:LEU:N	2.47	0.45
4:BD:5119:ALA:O	4:BD:5123:ILE:HG13	2.16	0.45
3:AC:55:ALA:HB1	27:AC:514:BCR:C37	2.43	0.45
1:AA:29:TYR:HD2	1:AA:133:LEU:HB2	1.80	0.45
6:BF:5016:PHE:N	6:BF:5016:PHE:HD1	2.14	0.45
2:AB:144:PHE:CE1	2:AB:210:ILE:CG2	2.99	0.45
3:AC:75:PHE:CD1	3:AC:86:LEU:HD21	2.51	0.45
16:BV:5141:ILE:O	16:BV:5145:ILE:HG13	2.16	0.45
4:AD:126:MET:HE1	4:AD:147:SER:HA	1.99	0.45
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.52	0.45
3:BC:5450:ALA:HA	3:BC:5455:PHE:CE2	2.51	0.45
14:AT:18:PHE:CB	27:AT:101:BCR:HC8	2.47	0.45
2:BB:5102:VAL:HB	24:BB:5610:CLA:H91	1.98	0.45
3:BC:5438:LEU:HD23	28:BC:5517:DGD:HAW2	1.97	0.45
11:BL:5022:LEU:HG	31:BL:5101:LMG:C19	2.46	0.45
2:AB:179:GLN:HA	2:AB:179:GLN:NE2	2.22	0.45
3:AC:318:LEU:HD21	3:AC:380:ILE:HG23	1.97	0.45
20:BZ:5036:SER:C	20:BZ:5038:GLN:N	2.70	0.45
3:BC:5055:ALA:HB1	27:BC:5514:BCR:C37	2.41	0.45
13:BO:5114:ASN:HD21	13:BO:5120:THR:CG2	2.29	0.45
16:BV:5130:MET:SD	16:BV:5133:LEU:HD22	2.56	0.45
4:BD:5079:SER:HA	4:BD:5172:SER:HB3	1.97	0.45
3:BC:5202:PRO:HB2	3:BC:5235:GLY:HA2	1.98	0.45
7:BH:5044:ILE:HG12	18:BX:5019:PHE:CE2	2.51	0.45
1:BA:5292:THR:HB	28:BC:5518:DGD:HAH2	1.99	0.45
2:AB:112:CYS:O	2:AB:116:VAL:HG23	2.16	0.45
24:AC:510:CLA:HHC	24:AC:510:CLA:HBB1	1.98	0.45
35:AD:405:PL9:H262	35:AD:405:PL9:H303	1.98	0.45
24:BA:5408:CLA:HMA2	28:BA:5412:DGD:HB42	1.98	0.45
24:BB:5612:CLA:HAA1	24:BB:5612:CLA:C1	2.45	0.45
4:BD:5088:SER:HA	7:BH:5050:ASN:OD1	2.16	0.45
6:AF:24:HIS:NE2	36:AF:101:HEM:NB	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.16	0.45
4:BD:5057:SER:CA	4:BD:5060:THR:HG22	2.46	0.45
16:AV:118:HIS:ND1	16:AV:119:PRO:HD2	2.31	0.45
1:AA:342:ASP:HB2	4:AD:352:LEU:HD21	1.98	0.45
13:AO:135:GLN:HB3	13:AO:135:GLN:HE21	1.48	0.45
8:BI:5024:LEU:O	8:BI:5026:GLY:N	2.41	0.45
1:BA:5041:LEU:HD21	1:BA:5122:GLY:HA3	1.99	0.45
2:BB:5041:GLU:HB3	2:BB:5060:MET:SD	2.55	0.45
1:AA:234:ASN:HD21	4:AD:266:TRP:CA	2.30	0.45
2:AB:153:PHE:O	2:AB:157:HIS:HB3	2.17	0.45
24:AB:612:CLA:H13	24:AB:613:CLA:CBB	2.47	0.45
24:AC:507:CLA:O1D	24:AC:509:CLA:H101	2.17	0.45
3:AC:213:LEU:HD21	27:AC:516:BCR:C19	2.47	0.45
1:BA:5045:THR:CG2	1:BA:5046:ILE:N	2.79	0.45
1:BA:5096:ILE:HD12	24:BA:5408:CLA:HMD1	1.98	0.45
1:BA:5216:GLY:O	1:BA:5220:THR:HG22	2.17	0.45
2:BB:5007:ARG:HG2	24:BB:5615:CLA:HED1	1.97	0.45
24:BB:5608:CLA:H111	24:BB:5619:CLA:H2	1.99	0.45
5:AE:17:VAL:HG22	9:AJ:8:ILE:CD1	2.47	0.45
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.64	0.45
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.16	0.45
2:BB:5172:TYR:O	2:BB:5173:GLY:C	2.52	0.45
10:BK:5021:LEU:HD11	27:BK:5102:BCR:HC42	1.99	0.45
13:AO:215:ARG:HD2	15:AU:39:LEU:HD22	1.97	0.45
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.45
1:AA:65:GLU:N	1:AA:66:PRO:HD3	2.32	0.45
2:AB:226:TYR:HA	2:AB:231:MET:CE	2.47	0.45
2:BB:5153:PHE:O	2:BB:5157:HIS:HB3	2.17	0.45
2:BB:5234:ILE:HD12	2:BB:5237:VAL:CG2	2.45	0.45
32:BB:5627:LMT:H92	7:BH:5035:MET:HE2	1.98	0.45
24:BA:5408:CLA:HBC1	31:BI:5101:LMG:H361	1.98	0.45
9:BJ:5003:SER:CB	9:BJ:5007:ARG:HH22	2.30	0.45
3:AC:365:TRP:HA	3:AC:387:TRP:CH2	2.51	0.45
2:BB:5279:TYR:HE1	7:BH:5063:LYS:HE3	1.80	0.45
4:BD:5038:PHE:CE2	4:BD:5128:ARG:NH2	2.85	0.45
20:AZ:30:PRO:HA	20:AZ:33:TRP:CE3	2.51	0.45
1:AA:29:TYR:CD2	1:AA:133:LEU:HB2	2.51	0.45
4:BD:5251:ARG:HG2	4:BD:5255:GLN:OE1	2.17	0.45
2:BB:5390:TYR:HD2	4:BD:5344:GLU:OE1	2.00	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.17	0.45
4:BD:5176:ALA:HA	4:BD:5179:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:5278:SER:HB3	2:BB:5281:GLN:NE2	2.31	0.45
13:BO:5210:ARG:HA	15:BU:5039:LEU:HD13	1.97	0.45
16:BV:5081:ARG:HG2	16:BV:5081:ARG:NH1	2.31	0.45
5:AE:14:ILE:HG22	9:AJ:13:VAL:HG11	1.99	0.45
3:BC:5193:GLY:O	3:BC:5194:GLY:O	2.34	0.45
15:BU:5056:ASP:OD2	15:BU:5115:THR:OG1	2.34	0.45
32:BD:5411:LMT:O2'	18:BX:5021:ILE:HG21	2.15	0.45
6:BF:5030:THR:HG22	6:BF:5034:LEU:CD1	2.47	0.45
12:BM:5003:VAL:HG11	14:BT:5002:GLU:HG2	1.99	0.45
13:BO:5184:ASP:HB2	13:BO:5185:PRO:HD2	1.99	0.45
28:AC:518:DGD:O3D	27:AJ:101:BCR:H382	2.16	0.45
1:AA:157:VAL:HG11	24:AA:405:CLA:HMC3	1.99	0.45
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA2	1.99	0.45
8:AI:10:ILE:HG21	32:AI:102:LMT:H82	1.98	0.45
27:AB:617:BCR:HC41	12:AM:9:ILE:HG23	1.98	0.45
1:BA:5180:PHE:O	1:BA:5184:ILE:HG13	2.17	0.45
2:BB:5010:THR:C	2:BB:5012:LEU:N	2.70	0.45
2:BB:5112:CYS:O	2:BB:5116:VAL:HG23	2.16	0.45
3:BC:5276:LEU:HD23	3:BC:5276:LEU:HA	1.75	0.45
4:BD:5035:ILE:O	24:BD:5405:CLA:HBB2	2.16	0.45
12:BM:5033:GLN:HG2	12:BM:5034:LYS:N	2.32	0.45
10:BK:5011:LEU:HD12	10:BK:5019:ASP:HA	1.98	0.45
20:BZ:5009:LEU:HD13	20:BZ:5054:VAL:HG11	1.98	0.45
3:AC:38:GLY:HA3	24:AC:511:CLA:C2D	2.46	0.45
20:AZ:9:LEU:HD13	20:AZ:54:VAL:HG11	1.97	0.45
4:BD:5337:GLU:O	4:BD:5338:ASN:C	2.55	0.45
15:BU:5066:ILE:CG1	15:BU:5072:TYR:CD1	3.00	0.45
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.17	0.45
1:BA:5013:LEU:CA	1:BA:5016:ARG:HH11	2.30	0.45
13:BO:5126:GLY:O	13:BO:5128:ASP:N	2.50	0.45
8:AI:14:PHE:CE2	8:AI:18:LEU:HD11	2.52	0.45
16:BV:5124:ALA:HB1	16:BV:5131:ARG:CG	2.47	0.45
1:BA:5295:PHE:O	3:BC:5424:SER:OG	2.31	0.45
1:AA:103:ASP:OD1	31:AA:417:LMG:H342	2.16	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
4:AD:277:THR:HG22	35:AD:405:PL9:H272	1.98	0.45
2:BB:5229:LEU:O	2:BB:5231:MET:N	2.50	0.45
24:BB:5612:CLA:HBA1	30:BB:5625:SQD:H102	1.98	0.45
3:BC:5095:LEU:HD21	24:BC:5501:CLA:OBD	2.16	0.45
3:BC:5239:TRP:CE3	3:BC:5243:ILE:HD11	2.27	0.45
7:BH:5055:LEU:HB2	7:BH:5058:VAL:CG1	2.46	0.45
2:BB:5357:ARG:NH2	4:BD:5337:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:AO:147:THR:O	13:AO:172:PHE:CE2	2.70	0.45
3:AC:249:ILE:O	3:AC:253:LEU:HG	2.17	0.45
4:BD:5067:TYR:CE1	4:BD:5076:VAL:HG11	2.51	0.45
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.28	0.45
3:AC:472:LEU:HG	4:AD:251:ARG:HH12	1.80	0.45
6:AF:37:ILE:HG22	9:AJ:28:PHE:CE1	2.52	0.45
2:BB:5088:PRO:HD2	28:BB:5602:DGD:O4D	2.17	0.45
13:AO:91:PHE:CD1	13:AO:260:LYS:HB2	2.51	0.45
13:AO:71:LEU:HD23	13:AO:265:PHE:CB	2.47	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
13:BO:5056:TYR:O	13:BO:5161:SER:HA	2.17	0.45
1:BA:5235:TYR:C	1:BA:5237:TYR:H	2.20	0.45
1:AA:176:ILE:HD12	24:AA:405:CLA:HED3	1.98	0.45
1:AA:179:THR:HG22	1:AA:183:MET:CE	2.47	0.45
2:AB:112:CYS:HA	27:AB:617:BCR:H282	1.98	0.45
2:AB:69:LEU:HD21	24:AB:603:CLA:OBD	2.17	0.45
8:AI:19:PHE:CE1	8:AI:23:PHE:CE2	3.00	0.45
2:BB:5008:VAL:HG22	24:BB:5615:CLA:O1A	2.17	0.45
24:BB:5620:CLA:HHC	24:BB:5620:CLA:HBB1	1.99	0.45
3:BC:5256:PRO:HG2	3:BC:5266:TRP:CH2	2.51	0.45
24:AC:511:CLA:H2	24:AC:511:CLA:H61	1.86	0.45
3:BC:5328:VAL:HG23	3:BC:5329:GLY:N	2.31	0.45
2:AB:345:VAL:HG21	2:AB:402:TYR:HE2	1.82	0.45
13:AO:168:PHE:O	13:AO:224:SER:HA	2.17	0.45
3:AC:347:GLY:CA	13:AO:43:ASN:HB2	2.45	0.45
18:AX:24:LEU:HA	18:AX:24:LEU:HD12	1.69	0.45
18:BX:5043:ILE:O	18:BX:5043:ILE:CG2	2.64	0.45
12:AM:5:GLN:HE22	32:AM:102:LMT:H3'	1.82	0.45
7:AH:18:TYR:CD1	7:AH:18:TYR:C	2.89	0.45
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.31	0.45
24:AB:611:CLA:H52	24:AB:614:CLA:HBC2	1.99	0.45
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CGA	2.47	0.45
3:BC:5164:HIS:HA	3:BC:5167:VAL:HG23	1.98	0.45
24:BD:5405:CLA:H41	18:BX:5023:LEU:CD1	2.42	0.45
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.45
24:BC:5511:CLA:H151	20:BZ:5024:PRO:CG	2.45	0.45
2:AB:476:ARG:CZ	2:AB:476:ARG:HB3	2.46	0.45
20:BZ:5030:PRO:HB3	20:BZ:5033:TRP:CZ3	2.51	0.45
31:BM:5102:LMG:O9	31:BM:5102:LMG:O8	2.35	0.45
3:BC:5472:LEU:O	3:BC:5473:ASP:O	2.35	0.45
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.32	0.45
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:453:ALA:C	8:AI:34:ARG:HB2	2.38	0.45
2:BB:5073:GLY:O	2:BB:5093:PHE:CD1	2.70	0.45
1:AA:224:ILE:H	1:AA:224:ILE:HG13	1.55	0.45
4:AD:70:GLY:O	9:AJ:37:GLY:CA	2.64	0.44
1:AA:93:PHE:CE2	24:AA:407:CLA:HBA1	2.52	0.44
2:AB:223:GLN:HG3	2:AB:227:LYS:CE	2.41	0.44
31:AB:620:LMG:C19	11:AL:22:LEU:HG	2.46	0.44
18:AX:12:ILE:CD1	18:AX:16:LEU:HD12	2.47	0.44
30:BB:5625:SQD:H281	32:BB:5627:LMT:H82	1.98	0.44
3:BC:5437:PHE:HZ	24:BC:5510:CLA:HMB3	1.82	0.44
2:AB:193:TYR:CD1	2:AB:260:SER:HA	2.52	0.44
13:BO:5155:THR:HG23	13:BO:5168:PHE:CD2	2.52	0.44
4:BD:5052:THR:HG22	4:BD:5067:TYR:CZ	2.53	0.44
4:BD:5053:THR:CB	4:BD:5067:TYR:HD2	2.30	0.44
6:AF:31:ILE:HG12	36:AF:101:HEM:HMC2	1.99	0.44
1:BA:5271:LEU:CD1	25:BA:5409:MST:H162	2.45	0.44
16:BV:5092:ARG:HG3	16:BV:5092:ARG:NH1	2.31	0.44
5:BE:5051:ARG:O	5:BE:5054:SER:N	2.50	0.44
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.44
2:BB:5435:GLU:O	2:BB:5436:THR:C	2.56	0.44
1:AA:187:GLN:HG2	4:AD:183:LEU:HD21	2.00	0.44
2:BB:5035:GLY:O	2:BB:5038:ALA:HB3	2.16	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
4:AD:87:HIS:HD2	4:AD:166:SER:HA	1.74	0.44
1:BA:5032:TRP:CZ2	8:BI:5022:GLY:HA2	2.52	0.44
4:BD:5261:PHE:CG	4:BD:5267:LEU:HD12	2.53	0.44
24:BC:5511:CLA:C14	20:BZ:5024:PRO:HG2	2.47	0.44
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CD2	2.53	0.44
2:BB:5173:GLY:N	2:BB:5265:ILE:HD11	2.33	0.44
1:BA:5011:ALA:O	1:BA:5012:ASN:HB3	2.17	0.44
6:AF:15:ILE:HG23	36:AF:101:HEM:HAA1	1.98	0.44
1:BA:5343:LEU:O	1:BA:5344:ALA:CB	2.64	0.44
13:BO:5184:ASP:OD2	13:BO:5188:ARG:HB2	2.17	0.44
16:AV:121:LEU:CD2	16:AV:138:LEU:HD11	2.47	0.44
2:BB:5399:VAL:HG12	2:BB:5417:VAL:HG22	1.99	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.21	0.44
2:AB:248:ALA:CA	24:AB:603:CLA:H42	2.32	0.44
3:AC:437:PHE:CD2	24:AC:508:CLA:HMC2	2.52	0.44
31:AD:408:LMG:HC71	11:AL:15:THR:HG23	1.98	0.44
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.91	0.44
18:AX:12:ILE:H	27:AX:101:BCR:C29	2.30	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5042:LEU:HD23	1:BA:5042:LEU:HA	1.76	0.44
24:BC:5507:CLA:O1D	24:BC:5509:CLA:H101	2.17	0.44
8:BI:5030:ARG:O	8:BI:5031:ASN:HB3	2.17	0.44
31:BI:5101:LMG:H132	32:BI:5102:LMT:H42	1.98	0.44
13:BO:5055:ALA:HA	13:BO:5230:VAL:HG11	1.99	0.44
31:AA:414:LMG:H142	29:AA:415:LHG:H102	1.99	0.44
5:BE:5009:PRO:O	5:BE:5010:PHE:C	2.55	0.44
5:BE:5078:THR:O	5:BE:5082:GLN:OE1	2.36	0.44
12:BM:5001:MET:CG	12:BM:5002:GLU:N	2.81	0.44
12:AM:28:GLN:HB3	12:BM:5027:VAL:HG12	1.99	0.44
9:AJ:24:ILE:HG23	9:AJ:25:VAL:N	2.32	0.44
1:BA:5051:ALA:HA	27:BA:5411:BCR:H381	1.99	0.44
2:BB:5485:GLU:HG2	2:BB:5486:LEU:N	2.31	0.44
3:BC:5056:HIS:C	3:BC:5058:GLY:N	2.70	0.44
2:BB:5045:PHE:HE2	2:BB:5047:PRO:HB3	1.83	0.44
4:AD:78:VAL:HG11	4:AD:114:ILE:HD12	1.98	0.44
18:BX:5030:LEU:HD23	18:BX:5030:LEU:HA	1.87	0.44
4:AD:127:LEU:HD23	4:AD:127:LEU:HA	1.80	0.44
11:AL:24:ILE:HG21	12:AM:19:SER:OG	2.17	0.44
1:BA:5153:SER:CB	24:BA:5405:CLA:H11	2.47	0.44
13:BO:5080:GLU:O	13:BO:5089:ALA:CB	2.65	0.44
5:BE:5015:THR:CG2	9:BJ:5006:GLY:HA2	2.47	0.44
1:BA:5261:GLN:CD	2:BB:5489:GLU:HG3	2.36	0.44
7:BH:5019:GLY:O	7:BH:5021:VAL:CG1	2.66	0.44
5:BE:5026:THR:HB	36:BF:5101:HEM:C3B	2.53	0.44
3:BC:5166:ILE:HG13	3:BC:5248:GLY:HA3	1.99	0.44
4:BD:5291:LEU:O	4:BD:5292:ASN:HB2	2.17	0.44
6:BF:5030:THR:HG22	6:BF:5034:LEU:HD12	1.99	0.44
4:BD:5126:MET:HE1	4:BD:5147:SER:HA	2.00	0.44
3:BC:5205:ASP:OD1	3:BC:5207:ARG:HB3	2.17	0.44
13:BO:5109:GLY:HA3	13:BO:5122:VAL:O	2.16	0.44
2:BB:5334:ASP:HB3	13:BO:5202:GLN:HG3	2.00	0.44
3:AC:414:ILE:HD11	16:AV:163:TYR:CG	2.53	0.44
1:AA:91:LEU:HD11	1:AA:163:ILE:HA	1.99	0.44
2:AB:139:PHE:HZ	24:AB:609:CLA:HMB3	1.83	0.44
2:AB:252:VAL:HG12	24:AB:603:CLA:O1A	2.17	0.44
3:AC:165:LEU:HD11	24:AC:506:CLA:CHC	2.47	0.44
3:AC:438:LEU:HD23	28:AC:517:DGD:HAW2	1.99	0.44
11:AL:17:LEU:HD12	12:AM:22:LEU:HB3	2.00	0.44
1:BA:5215:HIS:O	1:BA:5216:GLY:C	2.56	0.44
2:BB:5222:PRO:HG3	7:BH:5027:THR:N	2.30	0.44
24:BD:5402:CLA:H2	34:BD:5404:PHO:HBB1	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:BL:5016:SER:HA	11:BL:5019:LEU:CD1	2.48	0.44
18:BX:5012:ILE:HD13	18:BX:5016:LEU:HD12	1.98	0.44
15:BU:5058:ASN:OD1	15:BU:5084:PRO:CA	2.65	0.44
3:AC:42:LEU:HD21	24:AC:511:CLA:H2A	1.98	0.44
2:BB:5413:ASP:O	2:BB:5414:PRO:C	2.55	0.44
1:AA:11:ALA:O	1:AA:12:ASN:HB3	2.18	0.44
1:AA:59:ASP:OD2	1:AA:62:GLY:HA2	2.17	0.44
3:BC:5452:ALA:C	3:BC:5454:GLY:N	2.68	0.44
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.44
3:BC:5081:MET:HE2	3:BC:5090:PRO:HD3	2.00	0.44
13:AO:210:ARG:HA	15:AU:39:LEU:HD13	1.99	0.44
4:AD:195:PRO:HD3	11:AL:34:TYR:CE1	2.52	0.44
2:AB:11:VAL:HG23	11:AL:6:ASN:O	2.18	0.44
1:AA:113:GLN:HB3	1:AA:117:PHE:CE2	2.52	0.44
15:AU:56:ASP:OD2	15:AU:115:THR:OG1	2.36	0.44
24:AB:606:CLA:H52	27:AB:619:BCR:H321	2.00	0.44
4:AD:122:LEU:HB3	4:AD:150:ILE:HD11	1.99	0.44
1:AA:214:MET:CE	4:AD:142:ASN:OD1	2.65	0.44
4:AD:186:GLN:HB2	24:AD:401:CLA:HBC1	2.00	0.44
2:BB:5466:HIS:HE1	24:BB:5612:CLA:C4D	2.30	0.44
24:BB:5607:CLA:H2	24:BB:5609:CLA:H91	2.00	0.44
3:BC:5057:ALA:CB	24:BC:5512:CLA:HED2	2.48	0.44
4:BD:5221:THR:O	4:BD:5221:THR:HG23	2.16	0.44
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.18	0.44
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.18	0.44
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.17	0.44
3:AC:344:SER:HB2	3:AC:345:PRO:CD	2.48	0.44
12:AM:20:VAL:HG11	12:BM:5020:VAL:HG22	2.00	0.44
6:AF:17:THR:O	6:AF:21:VAL:HG23	2.18	0.44
28:BB:5602:DGD:C6E	32:BB:5626:LMT:H2'	2.47	0.44
18:AX:22:GLY:HA2	18:AX:25:SER:OG	2.18	0.44
2:BB:5054:PRO:HD2	2:BB:5057:ARG:HG3	2.00	0.44
3:BC:5176:VAL:O	3:BC:5180:MET:HG3	2.17	0.44
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.44
1:AA:41:LEU:HD21	1:AA:122:GLY:HA3	2.00	0.44
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.18	0.44
13:AO:184:ASP:HB2	13:AO:185:PRO:HD2	1.99	0.44
1:BA:5210:LEU:C	1:BA:5210:LEU:HD23	2.38	0.44
3:AC:217:PRO:O	28:AC:517:DGD:HB21	2.17	0.44
1:BA:5135:TYR:HD2	1:BA:5136:ARG:HH11	1.64	0.44
3:BC:5053:HIS:HB3	24:BC:5512:CLA:OBD	2.17	0.44
3:BC:5053:HIS:ND1	24:BC:5509:CLA:H141	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5116:VAL:CG2	3:BC:5117:VAL:N	2.81	0.44
8:BI:5028:PRO:O	8:BI:5031:ASN:ND2	2.51	0.44
8:BI:5011:VAL:CG2	32:BI:5102:LMT:H101	2.46	0.44
31:BD:5410:LMG:HC71	11:BL:5015:THR:HG23	1.99	0.44
10:BK:5025:LEU:HB2	10:BK:5026:PRO:HD3	2.00	0.44
4:BD:5145:ALA:HB2	4:BD:5272:LEU:CD2	2.47	0.44
13:BO:5036:ILE:HG23	13:BO:5041:LEU:HB2	2.00	0.44
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	2.18	0.44
20:BZ:5002:THR:O	20:BZ:5005:PHE:HB3	2.18	0.44
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.53	0.44
10:AK:12:PRO:CB	20:AZ:62:VAL:HG11	2.48	0.44
13:AO:94:THR:HB	13:AO:135:GLN:O	2.18	0.44
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.44
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.32	0.44
1:AA:292:THR:HB	28:AC:518:DGD:HAH2	1.99	0.44
1:BA:5210:LEU:C	1:BA:5210:LEU:CD2	2.86	0.44
1:BA:5304:HIS:CD2	1:BA:5313:VAL:HG11	2.52	0.44
24:AB:614:CLA:H162	31:AB:620:LMG:H422	1.98	0.44
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.44
4:AD:14:TRP:CG	4:AD:15:PHE:N	2.85	0.44
11:AL:16:SER:O	11:AL:19:LEU:HD12	2.17	0.44
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.18	0.44
3:BC:5264:PHE:CE1	27:BC:5516:BCR:H321	2.49	0.44
35:BD:5406:PL9:H103	35:BD:5406:PL9:HC72	1.77	0.44
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG11	2.53	0.44
10:BK:5044:GLY:O	10:BK:5045:PHE:C	2.56	0.44
1:BA:5059:ASP:OD1	1:BA:5064:ARG:N	2.50	0.44
2:BB:5144:PHE:CE1	2:BB:5210:ILE:CG2	3.01	0.44
2:BB:5363:PHE:CD1	4:BD:5326:ARG:HD2	2.52	0.44
4:AD:161:PRO:CB	4:AD:170:ALA:HB2	2.47	0.44
13:AO:141:ARG:HH11	13:AO:141:ARG:HG2	1.83	0.44
4:BD:5126:MET:HE2	4:BD:5146:PHE:HB3	2.00	0.44
2:BB:5326:ARG:HD3	2:BB:5442:ILE:HG22	1.98	0.44
3:BC:5416:SER:CA	28:BC:5519:DGD:O3E	2.66	0.44
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.44
2:AB:153:PHE:CZ	2:AB:158:LEU:HD21	2.53	0.44
2:AB:12:LEU:HB2	24:AB:612:CLA:HMC2	1.98	0.44
2:AB:7:ARG:HG2	24:AB:611:CLA:HED1	1.99	0.44
28:AA:411:DGD:HA82	3:AC:223:TRP:CH2	2.53	0.44
24:BA:5406:CLA:H72	31:BL:5101:LMG:C25	2.47	0.44
4:BD:5279:LEU:CD2	24:BD:5402:CLA:HMA2	2.48	0.44
3:BC:5028:GLN:HB2	24:BC:5511:CLA:HED1	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5029:GLU:CB	10:BK:5046:ARG:NH1	2.79	0.44
7:AH:19:GLY:O	7:AH:21:VAL:CG1	2.66	0.44
1:BA:5131:TRP:HZ3	1:BA:5132:GLU:HG3	1.83	0.44
4:AD:253:TRP:HA	4:AD:256:ILE:CG2	2.48	0.44
1:BA:5107:TYR:CD1	13:BO:5141:ARG:NH1	2.86	0.44
2:BB:5049:ASP:HA	2:BB:5050:PRO:HD2	1.81	0.44
3:BC:5080:PRO:HB3	3:BC:5082:TYR:CE1	2.53	0.44
1:BA:5276:ALA:HB2	4:BD:5215:GLY:HA3	2.00	0.44
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA1	2.00	0.43
1:BA:5214:MET:O	1:BA:5215:HIS:C	2.54	0.43
2:BB:5226:TYR:HA	2:BB:5231:MET:CE	2.48	0.43
24:BB:5607:CLA:CGA	24:BB:5607:CLA:H3A	2.48	0.43
2:BB:5091:TRP:CE3	24:BB:5610:CLA:O1A	2.71	0.43
4:BD:5039:PRO:HB3	24:BD:5405:CLA:HMC3	2.00	0.43
24:AB:607:CLA:HMD3	27:BT:5101:BCR:H271	2.00	0.43
3:AC:311:GLN:OE1	3:AC:355:THR:CG2	2.66	0.43
4:AD:128:ARG:CG	4:AD:129:GLN:N	2.81	0.43
2:BB:5137:LYS:HG3	2:BB:5220:ARG:NH2	2.32	0.43
3:BC:5347:GLY:CA	13:BO:5043:ASN:HB2	2.47	0.43
30:AB:627:SQD:H45	14:BT:5023:PHE:CD1	2.52	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:CB	2.47	0.43
2:AB:246:PHE:CD2	2:AB:463:PHE:HA	2.53	0.43
4:BD:5253:TRP:HB2	4:BD:5260:ALA:CB	2.48	0.43
2:AB:169:SER:O	7:AH:65:LEU:HG	2.18	0.43
13:AO:51:THR:OG1	13:AO:52:ALA:N	2.50	0.43
13:BO:5190:LEU:HB2	13:BO:5214:LYS:HB2	2.00	0.43
2:AB:433:ASP:OD1	2:AB:433:ASP:C	2.55	0.43
4:BD:5183:LEU:HD23	4:BD:5183:LEU:HA	1.87	0.43
1:AA:157:VAL:HG21	24:AA:405:CLA:HMC1	2.00	0.43
24:AB:608:CLA:HBA1	30:AB:622:SQD:H102	2.00	0.43
4:AD:266:TRP:HE1	31:AD:408:LMG:HC72	1.82	0.43
2:AB:250:PHE:HB3	28:AH:101:DGD:HB82	2.00	0.43
14:AT:23:PHE:CD1	30:BB:5601:SQD:H45	2.53	0.43
1:BA:5093:PHE:CE2	24:BA:5408:CLA:HBA1	2.52	0.43
24:BB:5614:CLA:H2	24:BB:5614:CLA:H61	1.88	0.43
24:BB:5616:CLA:H13	24:BB:5617:CLA:CBB	2.47	0.43
9:AJ:3:SER:CA	9:AJ:7:ARG:HH22	2.32	0.43
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.81	0.43
1:AA:309:ALA:HB3	16:AV:27:ALA:O	2.17	0.43
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.40	0.43
2:AB:137:LYS:HG3	2:AB:220:ARG:NH2	2.33	0.43
11:AL:9:PRO:HB3	31:BM:5102:LMG:O2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5081:PRO:HB2	4:BD:5085:MET:HG3	1.99	0.43
5:BE:5008:ARG:NH2	9:BJ:5004:GLU:HB2	2.34	0.43
3:AC:143:TYR:O	3:AC:144:SER:CB	2.65	0.43
4:BD:5190:ASN:HB2	4:BD:5296:TYR:CE1	2.53	0.43
2:AB:247:PHE:O	2:AB:251:VAL:HG23	2.19	0.43
24:AA:405:CLA:H61	34:AD:402:PHO:HMB3	2.00	0.43
18:AX:20:PHE:HZ	27:AX:101:BCR:H371	1.84	0.43
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CA	2.30	0.43
2:BB:5222:PRO:O	2:BB:5223:GLN:C	2.56	0.43
31:AM:101:LMG:H132	24:BB:5618:CLA:H12	2.00	0.43
3:BC:5224:ILE:HG22	3:BC:5289:PHE:CZ	2.53	0.43
2:BB:5222:PRO:CG	7:BH:5027:THR:H	2.26	0.43
12:BM:5021:PHE:CD2	12:BM:5022:LEU:HD23	2.53	0.43
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.43
3:BC:5161:LEU:HD23	3:BC:5251:HIS:HD2	1.84	0.43
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.73	0.43
3:AC:166:ILE:HG13	3:AC:248:GLY:HA3	2.01	0.43
1:BA:5010:SER:C	1:BA:5012:ASN:N	2.71	0.43
13:BO:5155:THR:HG22	13:BO:5167:ASP:O	2.18	0.43
1:BA:5193:LEU:CD1	4:BD:5179:PHE:HB3	2.47	0.43
16:AV:54:GLU:O	16:AV:58:LEU:HG	2.18	0.43
3:AC:185:LEU:HD12	3:AC:230:LEU:HD12	2.00	0.43
2:BB:5024:LEU:HD13	2:BB:5111:ALA:N	2.34	0.43
3:BC:5407:VAL:HA	28:BC:5519:DGD:O2E	2.18	0.43
3:AC:438:LEU:HD12	3:AC:438:LEU:O	2.18	0.43
31:AI:101:LMG:H132	32:AI:102:LMT:H42	2.00	0.43
27:AT:101:BCR:H271	24:BB:5611:CLA:HMD3	2.01	0.43
2:BB:5260:SER:HG	2:BB:5262:THR:HG22	1.77	0.43
2:BB:5476:ARG:CZ	2:BB:5476:ARG:HB3	2.44	0.43
2:BB:5179:GLN:NE2	2:BB:5179:GLN:HA	2.22	0.43
5:BE:5007:GLU:O	5:BE:5009:PRO:HD3	2.17	0.43
13:BO:5168:PHE:O	13:BO:5224:SER:HA	2.18	0.43
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.43
1:BA:5309:ALA:HB3	5:BE:5053:ASP:HA	2.01	0.43
2:BB:5356:VAL:HG22	2:BB:5370:LEU:CD2	2.48	0.43
2:BB:5075:TRP:CZ3	28:BB:5602:DGD:HB32	2.54	0.43
13:BO:5135:GLN:HE21	13:BO:5135:GLN:HB3	1.53	0.43
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.17	0.43
2:BB:5343:HIS:O	2:BB:5401:PHE:HA	2.18	0.43
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:CD1	2.48	0.43
14:AT:18:PHE:CD1	27:AT:101:BCR:HC8	2.54	0.43
24:BB:5607:CLA:HMB1	24:BB:5607:CLA:HAB	1.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5266:TRP:HB3	3:BC:5271:TYR:OH	2.17	0.43
3:AC:29:GLU:CD	3:AC:29:GLU:N	2.72	0.43
4:AD:17:ILE:CG2	18:AX:42:GLN:HG2	2.42	0.43
27:AC:514:BCR:H11C	27:AK:102:BCR:H322	2.00	0.43
1:AA:271:LEU:HD21	25:AA:408:MST:H83	2.00	0.43
2:BB:5348:ASN:O	2:BB:5349:LYS:C	2.56	0.43
2:AB:37:MET:O	2:AB:41:GLU:HG3	2.18	0.43
16:AV:148:GLU:N	16:AV:149:PRO:HD2	2.34	0.43
4:BD:5078:VAL:HG11	4:BD:5114:ILE:HD12	2.01	0.43
1:AA:281:VAL:HG13	1:AA:282:GLY:N	2.33	0.43
2:AB:230:ARG:HD2	2:AB:230:ARG:H	1.84	0.43
2:AB:5:TRP:CZ2	31:AB:620:LMG:H291	2.53	0.43
2:AB:68:ARG:NH1	24:AB:604:CLA:HED1	2.30	0.43
2:AB:90:PHE:HE2	2:AB:91:TRP:CZ3	2.35	0.43
24:AC:510:CLA:H122	24:AC:510:CLA:H161	1.85	0.43
1:BA:5078:ILE:O	1:BA:5176:ILE:HB	2.18	0.43
1:BA:5149:ALA:HB1	1:BA:5283:VAL:HG12	2.00	0.43
24:BC:5502:CLA:HBB1	24:BC:5502:CLA:HHC	2.01	0.43
24:BC:5505:CLA:HAA2	24:BC:5505:CLA:HBD	2.00	0.43
24:BC:5507:CLA:O1A	24:BC:5509:CLA:H2	2.19	0.43
7:BH:5043:LEU:O	7:BH:5047:GLU:HG3	2.17	0.43
19:BY:5023:UNK:O	19:BY:5024:UNK:C	2.67	0.43
14:AT:31:LYS:O	14:AT:32:LYS:HB2	2.18	0.43
3:AC:380:ILE:CA	3:AC:384:ILE:HD11	2.40	0.43
2:BB:5159:THR:OG1	2:BB:5161:LEU:HD13	2.19	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
5:BE:5082:GLN:O	5:BE:5083:LEU:C	2.56	0.43
3:AC:377:LEU:CD2	13:AO:126:GLY:HA2	2.48	0.43
1:BA:5013:LEU:HA	1:BA:5016:ARG:NH1	2.33	0.43
6:AF:15:ILE:HG22	6:AF:16:PHE:CD1	2.50	0.43
3:BC:5466:VAL:HA	3:BC:5469:MET:CE	2.48	0.43
13:AO:180:ALA:HB2	15:AU:120:ALA:O	2.18	0.43
3:BC:5203:THR:O	3:BC:5235:GLY:HA3	2.19	0.43
24:AA:405:CLA:HED2	4:AD:198:MET:SD	2.58	0.43
27:AA:410:BCR:H312	8:AI:15:PHE:CE1	2.54	0.43
2:AB:12:LEU:CD1	2:AB:19:LEU:HA	2.36	0.43
30:AB:622:SQD:H281	32:AB:624:LMT:H82	2.00	0.43
3:AC:95:LEU:HD21	24:AC:501:CLA:OBD	2.18	0.43
24:AC:505:CLA:HMD2	27:AC:516:BCR:H343	2.01	0.43
2:BB:5098:LEU:O	2:BB:5102:VAL:HG23	2.18	0.43
2:BB:5457:VAL:HG12	2:BB:5458:PHE:N	2.33	0.43
1:BA:5214:MET:CE	4:BD:5142:ASN:OD1	2.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5261:PHE:HE1	4:BD:5266:TRP:CD1	2.37	0.43
8:BI:5027:ASP:N	8:BI:5028:PRO:HD3	2.33	0.43
24:AC:511:CLA:H141	20:AZ:20:VAL:O	2.18	0.43
3:AC:315:MET:HE2	3:AC:365:TRP:HZ3	1.83	0.43
15:AU:66:ILE:HG12	15:AU:72:TYR:CD1	2.54	0.43
3:BC:5452:ALA:O	3:BC:5453:ALA:C	2.57	0.43
11:BL:5024:ILE:HG22	11:BL:5025:LEU:N	2.33	0.43
4:AD:52:THR:HG22	4:AD:67:TYR:CZ	2.53	0.43
14:BT:5029:ILE:O	14:BT:5031:LYS:N	2.52	0.43
3:BC:5404:LEU:HD12	3:BC:5404:LEU:HA	1.73	0.43
1:AA:228:THR:CG2	1:AA:229:GLU:N	2.81	0.43
3:BC:5324:LEU:HB3	15:BU:5062:ILE:HD13	2.01	0.43
4:AD:253:TRP:HB2	4:AD:260:ALA:CB	2.49	0.43
1:BA:5342:ASP:HB2	4:BD:5352:LEU:HD21	1.99	0.43
2:AB:358:ARG:O	2:AB:360:PRO:HD3	2.18	0.43
3:BC:5071:GLU:OE2	3:BC:5088:LEU:HG	2.19	0.43
13:AO:127:ILE:H	13:AO:127:ILE:HG12	1.64	0.43
1:AA:281:VAL:HG11	28:AC:519:DGD:CIA	2.49	0.43
2:AB:249:ALA:O	2:AB:252:VAL:HG22	2.19	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
2:BB:5229:LEU:O	2:BB:5230:ARG:C	2.56	0.43
24:BB:5616:CLA:H12	24:BB:5619:CLA:HAA2	2.01	0.43
1:AA:325:ASN:HA	1:AA:328:MET:CE	2.31	0.43
16:BV:5063:CYS:O	16:BV:5064:ALA:C	2.56	0.43
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.43
5:AE:15:THR:CG2	9:AJ:6:GLY:HA2	2.49	0.43
1:BA:5013:LEU:HD12	1:BA:5016:ARG:NH1	2.33	0.43
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE1	2.53	0.43
2:BB:5011:VAL:CG2	11:BL:5007:ARG:HA	2.49	0.43
2:AB:271:THR:N	2:AB:274:GLN:OE1	2.47	0.43
1:AA:248:ILE:HG12	1:AA:248:ILE:O	2.18	0.43
2:BB:5024:LEU:HB3	2:BB:5111:ALA:HB2	2.00	0.43
1:BA:5299:GLY:O	3:BC:5403:SER:HB2	2.18	0.43
5:BE:5057:ALA:H	5:BE:5060:GLN:NE2	2.17	0.43
6:AF:30:THR:HG22	6:AF:34:LEU:CD1	2.48	0.43
4:AD:43:LEU:HD23	4:AD:117:HIS:CE1	2.53	0.43
1:BA:5065:GLU:N	1:BA:5066:PRO:HD3	2.34	0.43
24:AC:504:CLA:H141	28:AC:518:DGD:HBT1	2.01	0.43
3:BC:5415:ASN:O	3:BC:5416:SER:CB	2.63	0.43
1:AA:51:ALA:HA	27:AA:410:BCR:H381	2.01	0.43
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:68:ARG:NH2	24:AB:604:CLA:HED1	2.29	0.43
2:AB:102:VAL:HG13	27:AB:618:BCR:H401	2.00	0.43
1:BA:5176:ILE:HD12	24:BA:5406:CLA:HED3	2.01	0.43
3:BC:5438:LEU:HD12	3:BC:5438:LEU:O	2.19	0.43
3:BC:5062:PHE:HZ	10:BK:5028:ILE:CD1	2.29	0.43
3:BC:5313:GLN:HB2	3:BC:5313:GLN:HE21	1.54	0.43
5:AE:16:SER:HB2	9:AJ:3:SER:O	2.18	0.43
24:AC:512:CLA:H122	24:AC:512:CLA:H162	1.87	0.43
2:AB:354:LEU:HD21	2:AB:378:LYS:CB	2.49	0.43
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.73	0.43
4:AD:217:THR:O	4:AD:221:THR:HB	2.18	0.43
27:BC:5514:BCR:H11C	27:BK:5102:BCR:H322	2.00	0.43
13:BO:5147:THR:O	13:BO:5172:PHE:CE2	2.71	0.43
13:AO:120:THR:HA	13:AO:153:ALA:O	2.19	0.43
3:AC:466:VAL:HA	3:AC:469:MET:CE	2.48	0.43
16:AV:130:MET:SD	16:AV:133:LEU:HD22	2.58	0.43
16:BV:5071:ILE:CD1	16:BV:5072:THR:N	2.81	0.43
2:BB:5011:VAL:HG23	11:BL:5007:ARG:HA	2.01	0.43
15:BU:5130:ASN:O	15:BU:5132:LEU:HD23	2.18	0.43
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.43
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.43
1:BA:5113:GLN:HB3	1:BA:5117:PHE:CE2	2.54	0.43
1:BA:5207:GLY:HA3	1:BA:5278:TRP:HE1	1.84	0.43
1:AA:18:CYS:O	1:AA:22:THR:CG2	2.65	0.43
1:AA:286:THR:HG23	24:AA:404:CLA:HED3	2.01	0.43
2:AB:222:PRO:HB3	7:AH:26:GLY:N	2.34	0.43
24:AB:603:CLA:H3A	24:AB:603:CLA:CGA	2.49	0.43
4:AD:39:PRO:HB3	24:AD:404:CLA:HMC3	2.00	0.43
11:AL:16:SER:HA	11:AL:19:LEU:CG	2.45	0.43
1:BA:5157:VAL:HG21	24:BA:5406:CLA:HMC1	2.00	0.43
24:BB:5609:CLA:H143	24:BB:5614:CLA:HBA1	2.01	0.43
1:BA:5032:TRP:HB2	8:BI:5023:PHE:CZ	2.54	0.43
19:BY:5023:UNK:O	19:BY:5025:UNK:N	2.52	0.43
4:BD:5272:LEU:O	4:BD:5276:VAL:HG23	2.19	0.43
13:AO:32:THR:OG1	13:AO:33:TYR:N	2.52	0.43
2:AB:345:VAL:HG21	2:AB:402:TYR:CE2	2.53	0.43
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.68	0.43
20:AZ:31:GLN:HG3	20:AZ:32:ASP:OD2	2.19	0.43
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	2.00	0.43
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.49	0.43
1:BA:5239:PHE:HB3	14:BT:5028:ARG:O	2.18	0.43
4:AD:171:PRO:HG3	4:AD:181:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:BE:5008:ARG:HB2	6:BF:5013:TYR:HB3	2.00	0.43
3:BC:5366:LEU:HD21	3:BC:5370:ARG:NH2	2.34	0.43
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.18	0.43
1:AA:295:PHE:HD2	3:AC:291:TRP:CD2	2.37	0.43
2:BB:5037:MET:O	2:BB:5041:GLU:HG3	2.19	0.43
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:HG12	2.00	0.43
3:AC:417:VAL:O	3:AC:417:VAL:HG13	2.19	0.43
3:AC:232:ASP:OD2	3:AC:232:ASP:N	2.52	0.43
5:BE:5035:TRP:C	5:BE:5035:TRP:CD1	2.92	0.43
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.43
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CHA	2.48	0.42
2:AB:250:PHE:HD1	28:AH:101:DGD:HB92	1.83	0.42
2:AB:102:VAL:HB	24:AB:606:CLA:H91	2.00	0.42
24:AD:404:CLA:H41	18:AX:23:LEU:CD1	2.43	0.42
2:BB:5135:LEU:HD21	2:BB:5234:ILE:HD13	2.01	0.42
24:BB:5609:CLA:H41	24:BB:5609:CLA:H61	1.83	0.42
3:BC:5239:TRP:O	3:BC:5243:ILE:HD12	2.19	0.42
3:BC:5437:PHE:CD2	24:BC:5508:CLA:HMC2	2.54	0.42
19:BY:5021:UNK:O	19:BY:5022:UNK:C	2.66	0.42
3:BC:5042:LEU:CD1	24:BC:5511:CLA:HMA3	2.50	0.42
13:BO:5069:LEU:HD12	13:BO:5070:CYS:N	2.33	0.42
6:BF:5025:THR:O	6:BF:5029:PRO:HG2	2.18	0.42
3:BC:5466:VAL:HA	3:BC:5469:MET:HE1	2.01	0.42
2:AB:490:GLN:O	2:AB:491:VAL:O	2.37	0.42
2:AB:144:PHE:HE1	2:AB:210:ILE:CG2	2.31	0.42
16:AV:92:ARG:HG3	16:AV:92:ARG:NH1	2.33	0.42
3:AC:404:LEU:HA	3:AC:404:LEU:HD12	1.69	0.42
2:BB:5437:LEU:N	2:BB:5437:LEU:HD12	2.34	0.42
16:BV:5121:LEU:HD21	16:BV:5138:LEU:HD11	2.01	0.42
7:BH:5040:VAL:O	7:BH:5044:ILE:HG13	2.19	0.42
2:BB:5169:SER:O	7:BH:5065:LEU:HG	2.19	0.42
23:AA:403[A]:CL:CL	4:AD:317:LYS:HD3	2.56	0.42
13:BO:5127:ILE:H	13:BO:5127:ILE:HG12	1.65	0.42
1:AA:303:ASN:O	1:AA:304:HIS:HB2	2.20	0.42
28:BC:5518:DGD:HBT2	27:BJ:5101:BCR:H342	2.01	0.42
1:AA:96:ILE:HD12	24:AA:407:CLA:HMD1	2.00	0.42
4:AD:266:TRP:NE1	31:AD:408:LMG:HC72	2.34	0.42
2:BB:5015:ASP:N	2:BB:5016:PRO:CD	2.81	0.42
3:BC:5165:LEU:HD11	24:BC:5506:CLA:CHC	2.48	0.42
3:BC:5243:ILE:O	24:BC:5506:CLA:HMC1	2.19	0.42
4:BD:5210:LEU:HD21	35:BD:5406:PL9:H13	2.00	0.42
1:BA:5259:ILE:N	1:BA:5259:ILE:CD1	2.69	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:BU:5072:TYR:CG	15:BU:5073:PRO:N	2.84	0.42
2:BB:5137:LYS:HE2	7:BH:5017:GLU:CG	2.49	0.42
10:AK:14:ALA:HB2	20:AZ:61:VAL:HG12	2.01	0.42
16:AV:90:PRO:O	16:AV:92:ARG:CD	2.67	0.42
29:BA:5413:LHG:HC62	3:BC:5443:TRP:HH2	1.85	0.42
2:BB:5358:ARG:O	2:BB:5360:PRO:HD3	2.19	0.42
13:BO:5075:THR:HG21	13:BO:5077:LEU:HD21	2.01	0.42
13:BO:5051:THR:OG1	13:BO:5052:ALA:N	2.52	0.42
3:BC:5426:LEU:HA	3:BC:5426:LEU:HD23	1.86	0.42
3:AC:415:ASN:CB	9:AJ:39:SER:OG	2.67	0.42
1:AA:20:TRP:O	1:AA:23:SER:HB3	2.18	0.42
24:AB:614:CLA:HMB1	24:AB:614:CLA:HAB	1.89	0.42
31:AM:101:LMG:O8	31:AM:101:LMG:O9	2.37	0.42
2:BB:5234:ILE:C	2:BB:5236:THR:H	2.23	0.42
24:BB:5607:CLA:H203	24:BB:5613:CLA:H92	2.00	0.42
4:BD:5122:LEU:HD21	24:BD:5402:CLA:C9	2.41	0.42
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	2.01	0.42
3:AC:385:GLN:O	3:AC:388:GLN:HB2	2.19	0.42
2:AB:297:THR:OG1	2:AB:298:LEU:N	2.52	0.42
2:BB:5345:VAL:HG21	2:BB:5402:TYR:CE2	2.54	0.42
1:AA:288:LEU:CD1	3:AC:432:VAL:HG23	2.44	0.42
2:BB:5141:ILE:O	2:BB:5144:PHE:HB3	2.20	0.42
30:AB:627:SQD:H45	14:BT:5023:PHE:HD1	1.85	0.42
3:AC:304:PRO:HB3	3:AC:395:TYR:CG	2.54	0.42
4:AD:181:PHE:CZ	4:AD:185:PHE:CE1	3.07	0.42
3:BC:5321:ASP:OD2	15:BU:5129:ASN:HB2	2.19	0.42
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	2.00	0.42
4:BD:5155:SER:HA	4:BD:5159:ILE:HG13	2.01	0.42
4:BD:5164:GLN:NE2	4:BD:5290:ALA:O	2.53	0.42
2:BB:5477:ASP:OD2	2:BB:5478:VAL:HG13	2.19	0.42
28:AC:518:DGD:HBT2	27:AJ:101:BCR:H342	2.02	0.42
2:AB:162:PHE:O	24:AB:606:CLA:HMD3	2.19	0.42
2:AB:466:HIS:CE1	24:AB:608:CLA:ND	2.87	0.42
24:AB:613:CLA:H41	24:AB:613:CLA:H61	1.63	0.42
27:AC:516:BCR:HC41	8:AI:20:VAL:CG1	2.48	0.42
1:BA:5042:LEU:HA	1:BA:5045:THR:HG22	2.01	0.42
2:BB:5230:ARG:HD2	2:BB:5230:ARG:H	1.84	0.42
24:BB:5618:CLA:HAA2	24:BB:5618:CLA:HBD	2.01	0.42
10:BK:5018:PHE:O	10:BK:5019:ASP:C	2.57	0.42
9:AJ:3:SER:CB	9:AJ:7:ARG:HH22	2.32	0.42
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CE1	2.54	0.42
13:BO:5178:ARG:HG3	13:BO:5178:ARG:NH1	2.28	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BB:5144:PHE:HE1	2:BB:5210:ILE:CG2	2.33	0.42
32:BC:5522:LMT:H41	8:BI:5021:PHE:HE1	1.84	0.42
1:BA:5131:TRP:CZ3	1:BA:5132:GLU:HG3	2.53	0.42
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.19	0.42
13:BO:5141:ARG:HH11	13:BO:5141:ARG:HG2	1.83	0.42
15:BU:5056:ASP:HB3	15:BU:5060:THR:H	1.84	0.42
13:AO:57:PRO:HA	13:AO:161:SER:OG	2.19	0.42
2:AB:12:LEU:HD13	2:AB:19:LEU:CA	2.38	0.42
3:AC:229:ASN:O	3:AC:233:VAL:HG23	2.18	0.42
1:BA:5217:SER:HB2	4:BD:5141:TYR:O	2.19	0.42
3:BC:5217:PRO:O	28:BC:5517:DGD:HB21	2.20	0.42
5:BE:5069:ARG:CG	5:BE:5070:PHE:N	2.82	0.42
19:BY:5018:UNK:O	19:BY:5022:UNK:N	2.52	0.42
13:BO:5081:GLU:HA	13:BO:5082:PRO:HD3	1.88	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.19	0.42
16:BV:5062:ALA:O	36:BV:5201:HEM:HAB	2.20	0.42
13:AO:70:CYS:SG	13:AO:105:ASP:OD1	2.77	0.42
2:AB:357:ARG:NH2	4:AD:337:GLU:OE1	2.53	0.42
2:BB:5274:GLN:HG2	2:BB:5279:TYR:CD2	2.54	0.42
20:BZ:5030:PRO:C	20:BZ:5032:ASP:N	2.72	0.42
2:AB:124:ARG:NH1	2:AB:124:ARG:HG3	2.33	0.42
1:AA:257:ARG:NH1	2:AB:489:GLU:OE2	2.52	0.42
13:BO:5091:PHE:CD1	13:BO:5260:LYS:HB2	2.55	0.42
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.85	0.42
13:AO:73:PRO:HG3	13:AO:146:PHE:CE2	2.54	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HG21	2.50	0.42
2:AB:466:HIS:HE1	24:AB:608:CLA:C4D	2.31	0.42
2:AB:450:TRP:NE1	24:AB:607:CLA:HBA2	2.34	0.42
2:AB:224:ARG:CZ	32:AB:624:LMT:H2'	2.50	0.42
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.20	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
14:AT:14:ILE:HD13	14:AT:17:PHE:CD2	2.55	0.42
2:BB:5112:CYS:HA	27:BB:5621:BCR:H282	2.01	0.42
2:BB:5238:LEU:CD2	2:BB:5469:HIS:CD2	3.03	0.42
3:BC:5272:LEU:CA	24:BC:5509:CLA:HMD3	2.50	0.42
8:BI:5019:PHE:CE1	8:BI:5023:PHE:CE2	3.02	0.42
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.20	0.42
6:AF:27:ALA:CB	36:AF:101:HEM:HBC2	2.46	0.42
8:AI:21:PHE:HA	8:AI:21:PHE:HD1	1.76	0.42
3:AC:337:LEU:HA	13:AO:131:PRO:HG3	2.01	0.42
2:BB:5246:PHE:CD2	2:BB:5463:PHE:HA	2.54	0.42
1:BA:5069:GLY:HA2	1:BA:5075:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:BO:5094:THR:HB	13:BO:5135:GLN:O	2.20	0.42
4:AD:164:GLN:NE2	4:AD:290:ALA:O	2.53	0.42
1:BA:5207:GLY:O	1:BA:5210:LEU:HB3	2.19	0.42
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.42
2:AB:91:TRP:CE3	24:AB:606:CLA:O1A	2.73	0.42
24:AB:607:CLA:HAB	24:AB:607:CLA:HMB1	1.88	0.42
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.19	0.42
24:AA:405:CLA:H62	34:AD:402:PHO:HMA1	2.01	0.42
1:BA:5118:HIS:HE1	24:BA:5408:CLA:C1A	2.32	0.42
1:BA:5157:VAL:HG13	1:BA:5172:MET:HB2	2.00	0.42
2:BB:5188:ASP:HA	7:BH:5058:VAL:HG23	2.02	0.42
3:BC:5223:TRP:CH2	3:BC:5224:ILE:HD11	2.54	0.42
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.19	0.42
1:AA:259:ILE:N	1:AA:259:ILE:CD1	2.71	0.42
3:AC:324:LEU:HB3	15:AU:62:ILE:HD13	2.01	0.42
4:AD:79:SER:HA	4:AD:172:SER:HB3	2.02	0.42
3:BC:5142:GLU:C	3:BC:5144:SER:H	2.22	0.42
13:BO:5059:ASP:O	13:BO:5061:SER:N	2.53	0.42
13:AO:56:TYR:CD1	13:AO:235:GLY:HA2	2.55	0.42
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	2.02	0.42
28:AC:518:DGD:O1B	28:AC:518:DGD:C1G	2.68	0.42
3:BC:5418:ASN:HB2	28:BC:5519:DGD:O4E	2.20	0.42
1:AA:149:ALA:HB1	1:AA:283:VAL:CG1	2.49	0.42
3:AC:276:LEU:HA	3:AC:276:LEU:HD23	1.76	0.42
2:BB:5238:LEU:CA	24:BB:5616:CLA:HMD3	2.50	0.42
4:BD:5014:TRP:CG	4:BD:5015:PHE:N	2.88	0.42
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.42
3:BC:5318:LEU:C	3:BC:5318:LEU:HD23	2.40	0.42
1:AA:262:TYR:HE1	31:AA:414:LMG:HO5	1.66	0.42
1:AA:288:LEU:CD2	3:AC:432:VAL:HG23	2.49	0.42
7:BH:5019:GLY:O	7:BH:5021:VAL:HG13	2.20	0.42
6:AF:20:TRP:NE1	6:AF:24:HIS:CE1	2.88	0.42
6:BF:5023:VAL:O	6:BF:5027:ALA:HB2	2.20	0.42
1:BA:5240:GLY:HA3	14:BT:5029:ILE:CG2	2.48	0.42
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.51	0.42
9:BJ:5021:VAL:HA	9:BJ:5024:ILE:HG22	2.02	0.42
4:AD:68:LEU:HB2	6:AF:40:MET:HE1	2.02	0.42
3:AC:366:LEU:HD23	3:AC:366:LEU:O	2.20	0.42
13:AO:141:ARG:NH1	13:AO:141:ARG:HG2	2.35	0.42
2:BB:5475:PHE:HB3	2:BB:5478:VAL:HG22	2.02	0.42
1:BA:5225:ARG:CA	2:BB:5481:GLY:HA3	2.50	0.42
1:AA:292:THR:HB	28:AC:518:DGD:CDA	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BA:5200:LEU:HD12	1:BA:5285:PHE:CG	2.54	0.42
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.42
2:AB:19:LEU:HA	2:AB:19:LEU:HD12	1.80	0.42
18:AX:16:LEU:HD13	18:AX:16:LEU:C	2.39	0.42
1:BA:5286:THR:HG23	24:BA:5405:CLA:HED3	2.02	0.42
2:BB:5162:PHE:O	24:BB:5610:CLA:HMD3	2.20	0.42
4:BD:5203:GLY:O	4:BD:5207:GLY:N	2.51	0.42
4:BD:5274:VAL:CB	4:BD:5275:PRO:HD3	2.47	0.42
24:BA:5405:CLA:H111	34:BD:5403:PHO:H3A	2.00	0.42
8:BI:5027:ASP:O	8:BI:5028:PRO:C	2.56	0.42
32:BB:5603:LMT:H5'	32:BB:5603:LMT:H1B	1.79	0.42
20:BZ:5031:GLN:HG3	20:BZ:5032:ASP:OD2	2.18	0.42
20:AZ:30:PRO:HB3	20:AZ:33:TRP:CZ3	2.54	0.42
4:AD:128:ARG:HE	4:AD:128:ARG:HB2	1.66	0.42
1:AA:254:TYR:OH	4:AD:129:GLN:HB3	2.20	0.42
2:AB:356:VAL:HG21	2:AB:424:ALA:CB	2.50	0.42
4:BD:5161:PRO:HG3	4:BD:5170:ALA:HB2	2.02	0.42
4:AD:303:ILE:HG21	12:AM:2:GLU:HG2	2.02	0.42
6:AF:30:THR:HG22	6:AF:34:LEU:HD12	2.01	0.42
2:AB:264:PRO:HG2	2:AB:267:LEU:HB2	2.02	0.42
1:AA:281:VAL:HG11	28:AC:519:DGD:HAG3	2.01	0.42
2:AB:450:TRP:CZ3	24:AB:607:CLA:H2	2.55	0.42
3:AC:243:ILE:O	24:AC:506:CLA:HAC1	2.20	0.42
14:AT:14:ILE:HD13	14:AT:14:ILE:HA	1.88	0.42
1:BA:5183:MET:HG3	24:BA:5406:CLA:CBC	2.50	0.42
2:BB:5135:LEU:HB2	2:BB:5136:PRO:CD	2.41	0.42
2:BB:5237:VAL:HB	24:BB:5616:CLA:CMD	2.50	0.42
2:BB:5450:TRP:NE1	24:BB:5611:CLA:HBA2	2.35	0.42
2:BB:5224:ARG:NH1	32:BB:5627:LMT:H2'	2.35	0.42
3:BC:5128:GLY:HA3	24:BC:5513:CLA:C3C	2.50	0.42
3:BC:5160:ILE:HA	3:BC:5163:PHE:CD2	2.54	0.42
24:BC:5509:CLA:HHC	24:BC:5509:CLA:HBB1	2.02	0.42
5:BE:5015:THR:O	9:BJ:5008:ILE:HD13	2.19	0.42
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.20	0.42
1:BA:5133:LEU:HD23	4:BD:5252:PHE:HD1	1.81	0.42
20:AZ:38:GLN:O	20:AZ:42:LEU:HG	2.19	0.42
1:AA:13:LEU:CA	1:AA:16:ARG:HH11	2.33	0.42
3:AC:335:THR:HA	13:AO:178:ARG:HD3	2.02	0.42
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.42
5:AE:78:THR:HA	5:AE:81:GLU:CG	2.49	0.42
3:BC:5269:GLU:OE1	3:BC:5447:ARG:HD3	2.20	0.42
3:BC:5141:GLU:HA	3:BC:5148:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
1:BA:5147:TYR:CG	1:BA:5147:TYR:O	2.73	0.42
1:AA:220:THR:HG23	4:AD:141:TYR:CD1	2.54	0.41
2:AB:187:PRO:HG2	2:AB:188:ASP:N	2.35	0.41
24:AB:616:CLA:HHC	24:AB:616:CLA:HBB1	2.01	0.41
1:BA:5032:TRP:CB	8:BI:5023:PHE:CZ	3.03	0.41
2:BB:5152:GLY:C	24:BB:5610:CLA:HMC3	2.40	0.41
24:BB:5606:CLA:H93	7:BH:5046:LEU:HD13	2.02	0.41
2:BB:5466:HIS:CE1	24:BB:5612:CLA:ND	2.87	0.41
24:BB:5615:CLA:H52	24:BB:5618:CLA:HBC2	2.01	0.41
3:BC:5229:ASN:O	3:BC:5233:VAL:HG23	2.19	0.41
3:BC:5307:PRO:O	3:BC:5311:GLN:HG2	2.20	0.41
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.55	0.41
32:AB:629:LMT:H51	14:BT:5004:ILE:CG1	2.42	0.41
2:BB:5324:LEU:HD13	4:BD:5293:LEU:CD2	2.50	0.41
20:BZ:5005:PHE:HA	20:BZ:5057:LEU:CD2	2.50	0.41
2:AB:390:TYR:HD2	4:AD:344:GLU:OE1	2.02	0.41
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.85	0.41
16:BV:5090:PRO:O	16:BV:5092:ARG:CD	2.67	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
1:BA:5191:ASN:ND2	1:BA:5194:MET:HB2	2.35	0.41
4:BD:5318:ASN:O	4:BD:5321:LEU:HB2	2.20	0.41
27:BA:5411:BCR:H312	8:BI:5015:PHE:CE1	2.54	0.41
1:AA:232:SER:HB3	1:AA:235:TYR:CD2	2.55	0.41
13:BO:5065:ARG:CB	13:BO:5065:ARG:HH11	2.33	0.41
13:BO:5141:ARG:HG2	13:BO:5141:ARG:NH1	2.35	0.41
2:AB:363:PHE:CD1	4:AD:326:ARG:HD2	2.55	0.41
15:AU:89:GLU:N	15:AU:89:GLU:CD	2.74	0.41
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.41
9:AJ:32:ALA:HA	31:AJ:102:LMG:O3	2.20	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
2:AB:198:VAL:HG11	24:AB:603:CLA:HED2	2.02	0.41
24:AB:603:CLA:H203	24:AB:609:CLA:H92	2.02	0.41
3:AC:225:VAL:O	3:AC:225:VAL:HG12	2.20	0.41
24:AC:502:CLA:HAA2	24:AC:502:CLA:HBD	2.01	0.41
31:AM:101:LMG:H132	24:BB:5618:CLA:C1	2.51	0.41
12:AM:17:VAL:HG12	12:AM:18:PRO:N	2.34	0.41
2:BB:5225:LEU:O	2:BB:5226:TYR:C	2.59	0.41
2:BB:5185:TRP:HD1	24:BB:5606:CLA:HBB2	1.85	0.41
24:BB:5618:CLA:H162	31:BL:5101:LMG:C42	2.50	0.41
3:BC:5215:LYS:HZ3	3:BC:5226:SER:CB	2.32	0.41
12:BM:5018:PRO:O	12:BM:5021:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5062:PHE:CD2	10:BK:5029:PRO:HG3	2.50	0.41
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.21	0.41
24:AC:511:CLA:H143	20:AZ:24:PRO:HG2	2.02	0.41
16:BV:5062:ALA:O	36:BV:5201:HEM:CAB	2.68	0.41
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.20	0.41
3:AC:441:HIS:HD2	3:AC:442:LEU:HD12	1.85	0.41
7:BH:5018:TYR:CD1	7:BH:5018:TYR:C	2.94	0.41
13:AO:114:ASN:HD21	13:AO:120:THR:CG2	2.29	0.41
3:BC:5337:LEU:HD23	3:BC:5342:MET:HE1	2.01	0.41
3:BC:5337:LEU:HA	13:BO:5131:PRO:HG3	2.02	0.41
7:BH:5017:GLU:CD	7:BH:5017:GLU:N	2.72	0.41
4:AD:53:THR:HA	4:AD:67:TYR:CD2	2.56	0.41
1:BA:5239:PHE:O	14:BT:5030:THR:N	2.53	0.41
1:BA:5243:GLU:HA	4:BD:5240:ALA:O	2.20	0.41
1:AA:306:VAL:HG22	1:AA:314:ILE:HB	2.03	0.41
2:AB:348:ASN:O	2:AB:349:LYS:C	2.58	0.41
1:AA:140:ARG:HB2	4:AD:220:ASN:HA	2.01	0.41
13:AO:46:PRO:HB2	13:AO:266:TYR:CD2	2.55	0.41
4:BD:5161:PRO:CB	4:BD:5170:ALA:HB2	2.50	0.41
13:BO:5106:GLN:HE21	13:BO:5106:GLN:HB3	1.68	0.41
28:BC:5519:DGD:HD3	9:BJ:5032:ALA:O	2.20	0.41
2:AB:238:LEU:CA	24:AB:612:CLA:HMD3	2.50	0.41
24:AB:614:CLA:HAA2	24:AB:614:CLA:HBD	2.01	0.41
24:AB:615:CLA:HHC	24:AB:615:CLA:HBB1	2.02	0.41
4:AD:199:MET:HG2	35:AD:405:PL9:H312	2.03	0.41
1:BA:5096:ILE:C	1:BA:5098:GLU:H	2.24	0.41
24:BA:5406:CLA:H72	31:BL:5101:LMG:H241	2.02	0.41
14:AT:23:PHE:HD1	30:BB:5601:SQD:H45	1.85	0.41
2:BB:5224:ARG:CZ	32:BB:5627:LMT:H2'	2.50	0.41
1:BA:5135:TYR:CE1	3:BC:5449:ARG:HB3	2.55	0.41
7:BH:5035:MET:SD	27:BX:5101:BCR:H322	2.61	0.41
1:BA:5321:ILE:HG22	1:BA:5325:ASN:ND2	2.35	0.41
20:BZ:5022:GLY:O	20:BZ:5023:VAL:C	2.58	0.41
5:AE:8:ARG:NH2	9:AJ:4:GLU:HB2	2.35	0.41
9:BJ:5003:SER:CB	9:BJ:5007:ARG:NH2	2.83	0.41
3:BC:5466:VAL:HG21	4:BD:5248:THR:OG1	2.20	0.41
1:BA:5048:PHE:HA	1:BA:5115:ILE:CD1	2.48	0.41
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	2.02	0.41
3:AC:204:LEU:HA	3:AC:204:LEU:HD23	1.79	0.41
2:AB:373:LYS:HG3	2:AB:374:ASN:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:BV:5069:GLY:O	16:BV:5156:TRP:O	2.38	0.41
4:BD:5019:ASP:O	4:BD:5020:ASP:C	2.57	0.41
3:BC:5417:VAL:HG13	3:BC:5417:VAL:O	2.19	0.41
13:AO:156:GLN:OE1	13:AO:156:GLN:HA	2.20	0.41
28:AC:519:DGD:HD3	9:AJ:32:ALA:O	2.20	0.41
1:BA:5278:TRP:HB3	1:BA:5279:PRO:CD	2.42	0.41
12:AM:21:PHE:CD2	12:AM:22:LEU:HD23	2.55	0.41
1:BA:5119:PHE:CZ	24:BA:5405:CLA:H101	2.52	0.41
2:BB:5034:ALA:HB2	24:BB:5609:CLA:C2D	2.51	0.41
5:BE:5069:ARG:HG3	5:BE:5070:PHE:CD1	2.55	0.41
7:BH:5063:LYS:O	7:BH:5064:ALA:HB3	2.20	0.41
13:BO:5120:THR:HG22	13:BO:5154:SER:CB	2.50	0.41
1:AA:57:PRO:HA	1:AA:68:SER:HA	2.03	0.41
6:BF:5024:HIS:NE2	36:BF:5101:HEM:NB	2.67	0.41
4:AD:53:THR:CB	4:AD:67:TYR:HD2	2.34	0.41
1:BA:5306:VAL:HG22	1:BA:5314:ILE:HB	2.02	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HD13	2.02	0.41
3:AC:367:GLU:OE1	3:AC:367:GLU:HA	2.18	0.41
1:BA:5138:GLY:CA	8:BI:5032:PRO:HG2	2.51	0.41
15:BU:5077:LYS:O	15:BU:5081:LYS:HB2	2.21	0.41
1:AA:36:ILE:HD13	1:AA:36:ILE:HA	1.89	0.41
1:AA:200:LEU:HD21	28:AC:519:DGD:CCA	2.50	0.41
1:BA:5292:THR:HB	28:BC:5518:DGD:CDA	2.50	0.41
9:BJ:5038:SER:OG	9:BJ:5039:SER:N	2.53	0.41
2:AB:252:VAL:HG23	2:AB:253:ALA:N	2.35	0.41
3:AC:244:CYS:HA	24:AC:506:CLA:CMC	2.51	0.41
3:AC:449:ARG:HE	24:AC:505:CLA:HED1	1.86	0.41
4:AD:259:ILE:HD13	14:AT:21:ILE:HG12	2.02	0.41
7:AH:42:LEU:HA	7:AH:42:LEU:HD12	1.83	0.41
18:AX:12:ILE:CA	27:AX:101:BCR:H401	2.48	0.41
1:BA:5172:MET:HA	1:BA:5173:PRO:HD3	1.97	0.41
2:BB:5026:HIS:HB2	24:BB:5616:CLA:HMB2	2.01	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:CZ2	2.38	0.41
3:BC:5244:CYS:HA	24:BC:5506:CLA:CMC	2.51	0.41
3:AC:62:PHE:CD2	10:AK:29:PRO:HG3	2.50	0.41
19:BY:5025:UNK:C	19:BY:5027:UNK:N	2.82	0.41
3:AC:42:LEU:CD1	24:AC:511:CLA:HMA3	2.50	0.41
4:BD:5272:LEU:HD22	4:BD:5276:VAL:HG21	2.03	0.41
2:BB:5271:THR:N	2:BB:5274:GLN:OE1	2.45	0.41
2:AB:483:ASP:CB	2:AB:484:PRO:CD	2.94	0.41
2:BB:5298:LEU:HD12	2:BB:5298:LEU:HA	1.89	0.41
4:AD:218:VAL:HG22	4:AD:244:TYR:CD2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:AK:21:LEU:HD11	27:AK:102:BCR:HC42	2.03	0.41
7:BH:5016:SER:C	7:BH:5018:TYR:H	2.23	0.41
1:BA:5340:PRO:HG3	15:BU:5133:TYR:CD1	2.55	0.41
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.41
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.24	0.41
1:AA:184:ILE:CD1	4:AD:186:GLN:HG2	2.51	0.41
24:AA:405:CLA:H72	31:AB:620:LMG:H241	2.01	0.41
24:AB:605:CLA:H143	24:AB:610:CLA:HBA1	2.02	0.41
2:AB:4:PRO:CG	2:AB:7:ARG:HD2	2.42	0.41
24:AC:505:CLA:HAA2	24:AC:505:CLA:HBD	2.02	0.41
3:AC:437:PHE:CD2	24:AC:508:CLA:CMC	3.04	0.41
4:AD:202:ALA:HB3	35:AD:405:PL9:C30	2.49	0.41
1:BA:5020:TRP:O	1:BA:5023:SER:HB3	2.19	0.41
1:BA:5044:ALA:HB1	34:BD:5403:PHO:H91	2.02	0.41
2:BB:5112:CYS:CB	27:BB:5623:BCR:H393	2.51	0.41
2:BB:5135:LEU:HD23	2:BB:5138:MET:CE	2.50	0.41
24:BB:5615:CLA:HBB1	24:BB:5615:CLA:HHC	2.03	0.41
2:BB:5193:TYR:CE1	2:BB:5260:SER:HA	2.55	0.41
3:AC:149:TYR:HB3	3:AC:156:LYS:HD3	2.02	0.41
20:BZ:5032:ASP:HA	20:BZ:5034:ASP:OD2	2.21	0.41
15:BU:5072:TYR:CB	15:BU:5073:PRO:CD	2.98	0.41
2:BB:5489:GLU:CB	5:BE:5003:GLY:N	2.76	0.41
3:AC:459:ILE:HG21	3:AC:464:GLU:HG3	2.02	0.41
13:AO:168:PHE:HB2	13:AO:225:LEU:HB2	2.03	0.41
3:AC:466:VAL:HG13	4:AD:251:ARG:CD	2.50	0.41
2:AB:278:SER:HB3	2:AB:281:GLN:NE2	2.32	0.41
3:AC:71:GLU:OE2	3:AC:88:LEU:HG	2.21	0.41
4:AD:84:SER:HB3	5:AE:68:ASP:HA	2.03	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.20	0.41
1:AA:278:TRP:CD2	28:AC:519:DGD:CIA	2.96	0.41
27:AJ:101:BCR:H20C	27:AJ:101:BCR:H361	1.91	0.41
1:AA:119:PHE:CZ	24:AA:404:CLA:H101	2.53	0.41
2:AB:12:LEU:HD13	2:AB:19:LEU:HD12	2.03	0.41
24:AB:612:CLA:H12	24:AB:615:CLA:HAA2	2.03	0.41
3:AC:229:ASN:ND2	3:AC:231:GLU:HB2	2.36	0.41
3:AC:243:ILE:O	24:AC:506:CLA:HMC1	2.20	0.41
29:AA:412:LHG:C1	3:AC:447:ARG:HE	2.34	0.41
4:AD:261:PHE:CG	4:AD:267:LEU:HD12	2.56	0.41
10:BK:5019:ASP:N	10:BK:5020:PRO:CD	2.81	0.41
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.60	0.41
3:BC:5038:GLY:HA3	24:BC:5511:CLA:CMD	2.51	0.41
3:BC:5311:GLN:OE1	3:BC:5355:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BC:5384:ILE:H	3:BC:5384:ILE:HG12	1.75	0.41
3:AC:48:LYS:HE2	3:AC:138:GLU:OE2	2.20	0.41
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.41
6:BF:5015:ILE:HG23	36:BF:5101:HEM:HAA1	2.03	0.41
1:BA:5129:ARG:NH2	4:BD:5256:ILE:O	2.54	0.41
2:AB:369:ILE:HD13	4:AD:340:VAL:O	2.21	0.41
18:BX:5044:ASP:C	18:BX:5045:LYS:HD3	2.41	0.41
7:AH:40:VAL:O	7:AH:44:ILE:HG13	2.21	0.41
4:BD:5030:VAL:HG12	4:BD:5031:GLY:N	2.35	0.41
1:BA:5224:ILE:H	1:BA:5224:ILE:HG13	1.57	0.41
24:AA:404:CLA:H111	34:AD:402:PHO:H3A	2.02	0.41
28:BA:5412:DGD:HA82	3:BC:5223:TRP:CH2	2.56	0.41
2:BB:5103:LEU:O	2:BB:5107:LEU:HG	2.20	0.41
24:BC:5513:CLA:NB	27:BC:5515:BCR:H383	2.36	0.41
24:BC:5505:CLA:HMD2	27:BC:5516:BCR:H343	2.01	0.41
4:BD:5162:LEU:HD21	4:BD:5167:TRP:CH2	2.56	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
10:BK:5030:VAL:CG1	10:BK:5031:LEU:N	2.84	0.41
4:AD:272:LEU:O	4:AD:276:VAL:HG23	2.21	0.41
27:AC:515:BCR:H331	27:AC:515:BCR:H342	2.02	0.41
5:AE:10:PHE:N	5:AE:10:PHE:CD2	2.89	0.41
4:BD:5128:ARG:O	4:BD:5129:GLN:C	2.59	0.41
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.41
7:BH:5018:TYR:CG	7:BH:5019:GLY:N	2.89	0.41
3:BC:5466:VAL:HG13	4:BD:5251:ARG:CD	2.51	0.41
2:AB:324:LEU:HA	4:AD:293:LEU:HD21	1.99	0.41
2:AB:113:TRP:NE1	2:AB:117:TYR:CD1	2.89	0.41
4:BD:5056:THR:OG1	4:BD:5057:SER:N	2.53	0.41
13:AO:86:ARG:O	13:AO:86:ARG:CG	2.69	0.41
3:AC:332:GLN:HG3	13:AO:129:PHE:CE2	2.56	0.41
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.41
2:AB:73:GLY:O	2:AB:93:PHE:CD1	2.74	0.41
4:AD:168:PHE:CD2	4:AD:168:PHE:O	2.74	0.41
1:BA:5289:GLY:HA2	1:BA:5292:THR:CG2	2.51	0.41
1:BA:5278:TRP:HA	28:BC:5519:DGD:CIA	2.51	0.41
9:BJ:5036:LEU:C	9:BJ:5038:SER:H	2.22	0.41
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.20	0.41
3:AC:272:LEU:CA	24:AC:509:CLA:HMD3	2.51	0.41
4:AD:162:LEU:HD22	28:AH:101:DGD:O1A	2.21	0.41
14:BT:5018:PHE:CD1	27:BT:5101:BCR:HC8	2.56	0.41
1:AA:151:LEU:HD21	1:AA:155:PHE:HE2	1.85	0.41
2:AB:329:PRO:CD	24:AB:607:CLA:HED1	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:26:HIS:HB2	24:AB:612:CLA:HMB2	2.03	0.41
2:AB:224:ARG:NH1	32:AB:624:LMT:H2'	2.35	0.41
24:AB:611:CLA:HMD1	31:AD:407:LMG:HC92	2.02	0.41
24:AB:602:CLA:C9	7:AH:46:LEU:HD22	2.51	0.41
11:AL:24:ILE:HG22	11:AL:25:LEU:N	2.35	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:HZ2	1.68	0.41
1:BA:5205:VAL:HG21	24:BA:5405:CLA:HMA2	2.03	0.41
2:BB:5150:CYS:HB2	24:BB:5607:CLA:CMC	2.47	0.41
27:AT:101:BCR:H372	27:BB:5621:BCR:H353	2.03	0.41
4:BD:5214:HIS:HA	35:BD:5406:PL9:O2	2.21	0.41
24:AB:607:CLA:HAC2	27:BT:5101:BCR:H393	2.02	0.41
19:BY:5021:UNK:HA	19:BY:5024:UNK:CB	2.51	0.41
13:BO:5162:ILE:O	13:BO:5230:VAL:HG11	2.20	0.41
3:AC:114:VAL:CG2	31:AC:521:LMG:H141	2.50	0.41
4:BD:5145:ALA:CB	4:BD:5272:LEU:HD21	2.51	0.41
10:BK:5043:VAL:CG2	10:BK:5046:ARG:HE	2.34	0.41
2:BB:5137:LYS:HE3	7:BH:5014:LEU:O	2.21	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41
2:AB:173:GLY:N	2:AB:265:ILE:HD11	2.36	0.41
13:BO:5078:VAL:HG22	13:BO:5259:VAL:HG22	2.03	0.41
4:BD:5179:PHE:HA	4:BD:5182:LEU:HD12	2.03	0.41
27:BD:5407:BCR:H392	9:BJ:5025:VAL:HG21	2.03	0.41
6:AF:40:MET:O	6:AF:43:ILE:HG13	2.21	0.41
16:BV:5148:GLU:N	16:BV:5149:PRO:HD2	2.36	0.41
3:BC:5455:PHE:C	3:BC:5457:LYS:H	2.24	0.41
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:CG1	2.51	0.41
16:BV:5039:ASN:HD21	16:BV:5043:LYS:HB3	1.86	0.41
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.20	0.41
24:AC:504:CLA:H2	28:AC:518:DGD:C2A	2.51	0.41
28:BC:5518:DGD:C1G	28:BC:5518:DGD:O1B	2.69	0.41
4:BD:5070:GLY:O	9:BJ:5037:GLY:CA	2.69	0.41
2:AB:222:PRO:O	2:AB:223:GLN:C	2.58	0.41
3:AC:266:TRP:HZ3	24:AC:507:CLA:HBC2	1.86	0.41
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.33	0.41
2:BB:5005:TRP:CE3	24:BB:5615:CLA:H42	2.56	0.41
2:BB:5187:PRO:C	2:BB:5189:GLY:H	2.24	0.41
2:BB:5328:GLY:O	24:BB:5611:CLA:HBA1	2.21	0.41
24:BB:5606:CLA:H161	28:BH:5101:DGD:HAW1	2.02	0.41
32:BB:5627:LMT:H92	7:BH:5035:MET:HE1	2.03	0.41
4:BD:5202:ALA:HB3	35:BD:5406:PL9:C30	2.51	0.41
10:AK:30:VAL:CG1	10:AK:31:LEU:N	2.84	0.41
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:AO:55:ALA:HA	13:AO:230:VAL:HG11	2.03	0.41
3:BC:5305:THR:HG23	3:BC:5307:PRO:HG2	2.03	0.41
29:BA:5415:LHG:H272	10:BK:5045:PHE:CE2	2.56	0.41
1:BA:5258:LEU:HD12	4:BD:5128:ARG:CG	2.51	0.41
2:BB:5297:THR:OG1	2:BB:5298:LEU:N	2.54	0.41
2:BB:5377:VAL:HG11	4:BD:5342:PRO:CG	2.51	0.41
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.56	0.41
6:BF:5024:HIS:HA	6:BF:5027:ALA:HB3	2.03	0.41
3:BC:5472:LEU:HD11	4:BD:5255:GLN:CD	2.40	0.41
8:AI:25:SER:HA	32:AI:103:LMT:H6D	2.02	0.41
2:BB:5348:ASN:O	2:BB:5350:GLU:N	2.54	0.41
32:BM:5101:LMT:H5'	32:BM:5101:LMT:H1B	1.97	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
4:AD:126:MET:HE2	4:AD:146:PHE:HB3	2.02	0.41
13:BO:5056:TYR:CD1	13:BO:5235:GLY:HA2	2.55	0.41
3:BC:5172:ALA:O	3:BC:5176:VAL:HG23	2.21	0.41
3:AC:390:ARG:NE	16:AV:126:ILE:CG2	2.84	0.41
2:AB:447:PRO:O	2:AB:448:ARG:C	2.60	0.41
2:AB:45:PHE:HE2	2:AB:47:PRO:HB3	1.86	0.41
3:AC:282:MET:SD	24:AC:503:CLA:H142	2.61	0.40
3:AC:269:GLU:OE1	3:AC:447:ARG:HD3	2.21	0.40
24:AC:509:CLA:HBB1	24:AC:509:CLA:HHC	2.03	0.40
24:AB:602:CLA:H93	7:AH:46:LEU:HD22	2.02	0.40
8:AI:11:VAL:O	8:AI:15:PHE:HD2	2.04	0.40
1:BA:5184:ILE:CD1	4:BD:5186:GLN:HG2	2.51	0.40
2:BB:5004:PRO:HB2	2:BB:5006:TYR:CE1	2.56	0.40
2:BB:5238:LEU:CD2	2:BB:5469:HIS:HD2	2.34	0.40
2:BB:5328:GLY:N	24:BB:5611:CLA:O1A	2.49	0.40
4:BD:5263:ASN:O	4:BD:5265:ARG:N	2.54	0.40
2:AB:431:GLU:OE2	13:BO:5084:ASN:ND2	2.54	0.40
2:BB:5172:TYR:O	2:BB:5174:LEU:HG	2.21	0.40
6:AF:29:PRO:O	6:AF:32:PHE:HB3	2.21	0.40
1:BA:5012:ASN:O	1:BA:5015:GLU:HB3	2.22	0.40
16:AV:71:ILE:CD1	16:AV:72:THR:N	2.82	0.40
1:AA:333:GLU:HB2	1:AA:337:HIS:CE1	2.53	0.40
1:AA:340:PRO:HG3	15:AU:133:TYR:CD1	2.56	0.40
7:AH:63:LYS:C	7:AH:65:LEU:N	2.73	0.40
1:BA:5295:PHE:HD2	3:BC:5291:TRP:CD2	2.39	0.40
1:AA:76:ASN:ND2	11:AL:33:SER:HB3	2.37	0.40
9:AJ:10:LEU:HD12	9:AJ:10:LEU:HA	1.86	0.40
1:BA:5206:PHE:HD2	1:BA:5206:PHE:HA	1.77	0.40
1:AA:278:TRP:HA	28:AC:519:DGD:HAG1	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:BD:5277:THR:HG22	35:BD:5406:PL9:H272	2.02	0.40
11:BL:5008:GLN:H	11:BL:5008:GLN:HE21	1.68	0.40
14:AT:29:ILE:HG22	14:AT:30:THR:H	1.86	0.40
9:BJ:5008:ILE:HD12	9:BJ:5008:ILE:H	1.85	0.40
3:AC:113:VAL:CG1	31:AC:521:LMG:H132	2.49	0.40
13:BO:5032:THR:OG1	13:BO:5033:TYR:N	2.54	0.40
2:AB:121:GLU:CG	7:AH:4:ARG:CA	2.94	0.40
2:BB:5161:LEU:N	2:BB:5161:LEU:CD1	2.84	0.40
1:BA:5029:TYR:HD2	1:BA:5133:LEU:HB2	1.87	0.40
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.89	0.40
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.29	0.40
6:AF:15:ILE:CG2	6:AF:16:PHE:HD1	2.33	0.40
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.40
28:BB:5602:DGD:HE61	32:BB:5626:LMT:H2'	2.02	0.40
27:AD:406:BCR:H392	9:AJ:25:VAL:HG21	2.03	0.40
16:AV:121:LEU:HD21	16:AV:138:LEU:HD11	2.02	0.40
10:AK:15:TYR:OH	20:AZ:58:ASN:ND2	2.52	0.40
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.51	0.40
15:AU:75:LEU:HA	15:AU:75:LEU:HD23	1.85	0.40
1:BA:5200:LEU:HD11	28:BC:5519:DGD:CCA	2.27	0.40
1:AA:217:SER:O	1:AA:220:THR:HG22	2.22	0.40
2:AB:238:LEU:CD2	2:AB:469:HIS:CD2	3.05	0.40
24:AB:603:CLA:HMB1	24:AB:603:CLA:HAB	1.80	0.40
35:AD:405:PL9:H103	35:AD:405:PL9:HC72	1.74	0.40
5:AE:69:ARG:CG	5:AE:70:PHE:N	2.83	0.40
24:BC:5502:CLA:HAA2	24:BC:5502:CLA:HBD	2.03	0.40
24:BC:5505:CLA:C2	24:BC:5505:CLA:HAA1	2.51	0.40
24:BC:5507:CLA:H122	27:BC:5516:BCR:H362	2.03	0.40
3:AC:161:LEU:HD23	3:AC:251:HIS:HD2	1.85	0.40
10:AK:46:ARG:HB2	10:AK:46:ARG:NH1	2.36	0.40
4:BD:5148:ALA:HB3	4:BD:5149:PRO:CD	2.41	0.40
32:AB:629:LMT:H5'	32:AB:629:LMT:H1B	1.80	0.40
15:BU:5072:TYR:CD2	15:BU:5073:PRO:N	2.90	0.40
4:AD:180:ARG:NH1	4:AD:333:ASP:OD1	2.54	0.40
1:BA:5069:GLY:CA	1:BA:5075:ASN:ND2	2.84	0.40
2:BB:5385:ARG:O	2:BB:5386:ALA:C	2.60	0.40
2:BB:5151:PHE:CE1	2:BB:5203:ILE:HG23	2.57	0.40
1:AA:200:LEU:CD2	28:AC:519:DGD:CCA	2.99	0.40
1:AA:278:TRP:HE3	28:AC:519:DGD:HAG1	1.83	0.40
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.17	0.40
1:AA:39:PRO:HG3	27:AA:410:BCR:HC8	2.04	0.40
24:AC:502:CLA:HBB1	24:AC:502:CLA:HHC	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:210:LEU:HD21	35:AD:405:PL9:H13	2.03	0.40
4:AD:262:SER:N	31:AD:408:LMG:O3	2.55	0.40
27:AT:101:BCR:H393	24:BB:5611:CLA:HAC2	2.03	0.40
24:BB:5615:CLA:HMD1	31:BD:5409:LMG:HC92	2.03	0.40
3:BC:5278:ALA:HB1	24:BC:5501:CLA:H142	2.03	0.40
13:BO:5081:GLU:C	13:BO:5083:LYS:H	2.25	0.40
14:AT:30:THR:HB	14:AT:31:LYS:NZ	2.35	0.40
3:AC:134:ILE:HD11	24:AC:511:CLA:C9	2.49	0.40
3:AC:38:GLY:HA3	24:AC:511:CLA:CMD	2.50	0.40
27:BK:5102:BCR:H332	20:BZ:5017:PHE:CD1	2.56	0.40
8:BI:5007:THR:O	8:BI:5008:VAL:C	2.59	0.40
3:BC:5447:ARG:HG2	3:BC:5447:ARG:HH11	1.86	0.40
4:AD:313:THR:H	4:AD:316:THR:HG23	1.86	0.40
15:AU:51:TYR:HE1	15:AU:60:THR:HG1	1.66	0.40
1:BA:5238:LYS:O	1:BA:5241:GLN:HG3	2.21	0.40
2:AB:285:ASN:N	2:AB:285:ASN:HD22	2.18	0.40
18:AX:30:LEU:HD23	18:AX:30:LEU:HA	1.88	0.40
2:AB:243:ALA:O	24:AB:608:CLA:HBC3	2.22	0.40
7:AH:41:PHE:O	7:AH:45:ILE:HG12	2.21	0.40
24:BA:5406:CLA:H62	34:BD:5403:PHO:HMA1	2.02	0.40
24:BB:5607:CLA:HMB2	24:BB:5607:CLA:H52	2.02	0.40
24:BB:5619:CLA:HBB1	24:BB:5619:CLA:HHC	2.03	0.40
4:BD:5261:PHE:HB2	35:BD:5406:PL9:H522	2.03	0.40
4:BD:5262:SER:N	31:BD:5410:LMG:O3	2.54	0.40
24:AC:511:CLA:H151	20:AZ:24:PRO:CG	2.50	0.40
3:AC:307:PRO:O	3:AC:311:GLN:HG2	2.21	0.40
13:BO:5132:VAL:HG12	13:BO:5133:THR:N	2.37	0.40
1:BA:5011:ALA:HB1	1:BA:5015:GLU:OE1	2.21	0.40
6:BF:5029:PRO:O	6:BF:5032:PHE:HB3	2.22	0.40
6:AF:21:VAL:HG21	30:AF:102:SQD:H101	2.02	0.40
6:BF:5020:TRP:NE1	6:BF:5024:HIS:CE1	2.89	0.40
1:AA:271:LEU:CD1	25:AA:408:MST:H162	2.48	0.40
1:BA:5296:ASN:HB3	3:BC:5401:LEU:HD13	2.04	0.40
2:BB:5170:ASP:CB	2:BB:5171:PRO:CD	2.97	0.40
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.02	0.40
13:BO:5065:ARG:CB	13:BO:5065:ARG:NH1	2.85	0.40
4:AD:24:ARG:NH2	18:AX:44:ASP:O	2.55	0.40
2:AB:283:GLU:O	2:AB:287:ARG:HG3	2.21	0.40
4:BD:5095:PRO:HG3	18:BX:5015:SER:HB3	2.03	0.40
5:AE:38:VAL:HG21	6:AF:36:ALA:O	2.21	0.40
12:BM:5016:LEU:HA	12:BM:5016:LEU:HD23	1.78	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%)	284 (85%)	42 (13%)	7 (2%)	11	55
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	55
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	6	38
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	7	41
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	5	36
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	5	34
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	8	46
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	9	51
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	5	34
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	5	34
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	42
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	42
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	11
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	18
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	19
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	19
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	9
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	9
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	22
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	22
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%)	24 (75%)	8 (25%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	4	28
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	6	38
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	38
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	3	24
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	31
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	30	80
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	30	80
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	1	4
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	1	4
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	1	4
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	26
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	26
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	5	36

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO
2	AB	490	GLN
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
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA

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Mol	Chain	Res	Type
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	5012	ASN
1	BA	5141	PRO
1	BA	5142	TRP
2	BB	5176	GLY
2	BB	5230	ARG
2	BB	5484	PRO
2	BB	5488	PRO
3	BC	5144	SER
3	BC	5257	PHE
3	BC	5416	SER
3	BC	5452	ALA
4	BD	5239	GLN
4	BD	5240	ALA
4	BD	5262	SER
7	BH	5018	TYR
8	BI	5025	SER
9	BJ	5035	GLY
13	BO	5052	ALA
14	BT	5030	THR
15	BU	5072	TYR
15	BU	5083	ALA
17	By	5043	ARG
18	BX	5045	LYS
20	BZ	5032	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

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Mol	Chain	Res	Type
15	AU	39	LEU
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	5349	LYS
2	BB	5436	THR
3	BC	5136	GLY
3	BC	5141	GLU
3	BC	5194	GLY
4	BD	5234	ALA
7	BH	5026	GLY
9	BJ	5038	SER
13	BO	5158	ASN
13	BO	5231	ASP
15	BU	5073	PRO
16	BV	5075	ASN
18	BX	5043	ILE
2	AB	13	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
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	5013	ILE
2	BB	5127	ARG
2	BB	5183	PRO
2	BB	5414	PRO
3	BC	5032	GLY
3	BC	5046	SER

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Mol	Chain	Res	Type
3	BC	5209	ILE
3	BC	5375	LEU
3	BC	5411	ALA
3	BC	5456	GLU
4	BD	5263	ASN
4	BD	5264	LYS
5	BE	5009	PRO
7	BH	5016	SER
10	BK	5013	GLU
10	BK	5045	PHE
13	BO	5165	SER
17	By	5025	ILE
20	BZ	5024	PRO
20	BZ	5028	ALA
2	AB	173	GLY
2	AB	231	MET
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	5235	GLU
5	BE	5010	PHE
13	BO	5060	SER
13	BO	5082	PRO
1	AA	97	TRP
2	AB	235	GLU
3	AC	462	GLU
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
2	BB	5435	GLU
2	BB	5490	GLN
3	BC	5453	ALA
3	BC	5462	GLU
4	BD	5252	PHE
6	BF	5041	GLN
7	BH	5006	TRP
13	BO	5085	LYS
13	BO	5088	GLU

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Mol	Chain	Res	Type
15	BU	5042	VAL
17	By	5024	MET
18	BX	5044	ASP
1	AA	334	ARG
2	AB	435	GLU
4	AD	351	ALA
13	AO	88	GLU
18	AX	12	ILE
1	BA	5097	TRP
1	BA	5334	ARG
2	BB	5173	GLY
3	BC	5382	ASN
4	BD	5351	ALA
5	BE	5052	PRO
13	BO	5051	THR
13	BO	5159	VAL
18	BX	5012	ILE
1	AA	21	VAL
2	AB	16	PRO
9	AJ	5	GLY
13	AO	159	VAL
1	BA	5021	VAL
3	AC	201	ASN
17	Ay	35	ILE
3	BC	5201	ASN
5	AE	52	PRO
7	AH	60	VAL
8	AI	32	PRO
13	AO	232	GLY
2	BB	5016	PRO
8	BI	5032	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	5039	PRO
13	AO	152	VAL
9	BJ	5005	GLY
13	BO	5152	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%)	250 (92%)	21 (8%)	18	59
1	BA	271/280 (97%)	253 (93%)	18 (7%)	24	67
2	AB	390/407 (96%)	372 (95%)	18 (5%)	37	80
2	BB	390/407 (96%)	374 (96%)	16 (4%)	41	82
3	AC	347/362 (96%)	326 (94%)	21 (6%)	26	71
3	BC	347/362 (96%)	325 (94%)	22 (6%)	25	69
4	AD	275/283 (97%)	249 (90%)	26 (10%)	12	45
4	BD	275/283 (97%)	249 (90%)	26 (10%)	12	45
5	AE	72/73 (99%)	66 (92%)	6 (8%)	16	55
5	BE	72/73 (99%)	66 (92%)	6 (8%)	16	55
6	AF	29/39 (74%)	27 (93%)	2 (7%)	22	65
6	BF	29/39 (74%)	28 (97%)	1 (3%)	49	86
7	AH	53/55 (96%)	42 (79%)	11 (21%)	2	8
7	BH	53/55 (96%)	43 (81%)	10 (19%)	2	11
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	42	83
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	42	83
10	AK	30/30 (100%)	29 (97%)	1 (3%)	50	87
10	BK	30/30 (100%)	29 (97%)	1 (3%)	50	87
11	AL	35/35 (100%)	33 (94%)	2 (6%)	29	74
11	BL	35/35 (100%)	32 (91%)	3 (9%)	15	52
12	AM	31/33 (94%)	30 (97%)	1 (3%)	51	87
12	BM	31/33 (94%)	29 (94%)	2 (6%)	24	68
13	AO	202/208 (97%)	187 (93%)	15 (7%)	20	62
13	BO	202/208 (97%)	187 (93%)	15 (7%)	20	62
14	AT	29/29 (100%)	28 (97%)	1 (3%)	49	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	BT	29/29 (100%)	27 (93%)	2 (7%)	22	65
15	AU	84/89 (94%)	76 (90%)	8 (10%)	12	45
15	BU	84/89 (94%)	76 (90%)	8 (10%)	12	45
16	AV	116/117 (99%)	111 (96%)	5 (4%)	40	81
16	BV	116/117 (99%)	110 (95%)	6 (5%)	32	76
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	1	3
17	By	20/37 (54%)	15 (75%)	5 (25%)	1	3
18	AX	30/34 (88%)	29 (97%)	1 (3%)	50	87
18	BX	30/34 (88%)	29 (97%)	1 (3%)	50	87
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	28	73
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	18	59
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	21	64

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	13	LEU
1	AA	30	VAL
1	AA	32	TRP
1	AA	56	PRO
1	AA	121	LEU
1	AA	129	ARG
1	AA	145	VAL
1	AA	170	ASP
1	AA	202	VAL
1	AA	206	PHE
1	AA	210	LEU
1	AA	218	LEU
1	AA	226	GLU
1	AA	243	GLU
1	AA	245	THR
1	AA	247	ASN
1	AA	259	ILE
1	AA	266	ASN
1	AA	286	THR
1	AA	298	ASN
1	AA	335	ASN
2	AB	16	PRO

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Mol	Chain	Res	Type
2	AB	18	ARG
2	AB	62	VAL
2	AB	79	SER
2	AB	121	GLU
2	AB	161	LEU
2	AB	179	GLN
2	AB	245	VAL
2	AB	246	PHE
2	AB	297	THR
2	AB	311	PHE
2	AB	433	ASP
2	AB	439	SER
2	AB	467	ILE
2	AB	484	PRO
2	AB	485	GLU
2	AB	488	PRO
2	AB	490	GLN
3	AC	27	ASP
3	AC	29	GLU
3	AC	78	GLU
3	AC	97	TRP
3	AC	121	SER
3	AC	165	LEU
3	AC	188	THR
3	AC	228	ASN
3	AC	244	CYS
3	AC	259	TRP
3	AC	289	PHE
3	AC	295	THR
3	AC	318	LEU
3	AC	321	ASP
3	AC	324	LEU
3	AC	355	THR
3	AC	424	SER
3	AC	430	HIS
3	AC	456	GLU
3	AC	461	ARG
3	AC	473	ASP
4	AD	14	TRP
4	AD	43	LEU
4	AD	84	SER
4	AD	91	LEU

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Mol	Chain	Res	Type
4	AD	110	LEU
4	AD	112	THR
4	AD	130	PHE
4	AD	166	SER
4	AD	180	ARG
4	AD	201	VAL
4	AD	205	LEU
4	AD	242	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	262	SER
4	AD	264	LYS
4	AD	272	LEU
4	AD	279	LEU
4	AD	282	SER
4	AD	291	LEU
4	AD	293	LEU
4	AD	316	THR
4	AD	323	GLU
4	AD	331	PRO
4	AD	345	VAL
4	AD	346	LEU
5	AE	9	PRO
5	AE	10	PHE
5	AE	52	PRO
5	AE	60	GLN
5	AE	68	ASP
5	AE	84	LYS
6	AF	18	VAL
6	AF	19	ARG
7	AH	12	ARG
7	AH	14	LEU
7	AH	21	VAL
7	AH	25	TRP
7	AH	27	THR
7	AH	42	LEU
7	AH	43	LEU
7	AH	45	ILE
7	AH	49	TYR
7	AH	56	ASP
7	AH	60	VAL
9	AJ	7	ARG

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Mol	Chain	Res	Type
10	AK	19	ASP
11	AL	8	GLN
11	AL	15	THR
12	AM	25	LEU
13	AO	31	LEU
13	AO	41	LEU
13	AO	60	SER
13	AO	65	ARG
13	AO	84	ASN
13	AO	86	ARG
13	AO	97	VAL
13	AO	106	GLN
13	AO	141	ARG
13	AO	152	VAL
13	AO	158	ASN
13	AO	165	SER
13	AO	171	GLU
13	AO	207	GLU
13	AO	224	SER
14	AT	29	ILE
15	AU	44	ASP
15	AU	53	GLU
15	AU	61	ASN
15	AU	98	THR
15	AU	103	GLN
15	AU	114	VAL
15	AU	119	THR
15	AU	132	LEU
16	AV	32	GLU
16	AV	40	SER
16	AV	68	VAL
16	AV	89	THR
16	AV	92	ARG
17	Ay	21	GLN
17	Ay	28	ILE
17	Ay	34	MET
17	Ay	35	ILE
17	Ay	36	ILE
18	AX	45	LYS
20	AZ	33	TRP
20	AZ	58	ASN
20	AZ	62	VAL

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Mol	Chain	Res	Type
1	BA	5013	LEU
1	BA	5030	VAL
1	BA	5032	TRP
1	BA	5121	LEU
1	BA	5129	ARG
1	BA	5145	VAL
1	BA	5202	VAL
1	BA	5206	PHE
1	BA	5210	LEU
1	BA	5218	LEU
1	BA	5226	GLU
1	BA	5243	GLU
1	BA	5245	THR
1	BA	5247	ASN
1	BA	5259	ILE
1	BA	5286	THR
1	BA	5298	ASN
1	BA	5335	ASN
2	BB	5016	PRO
2	BB	5018	ARG
2	BB	5062	VAL
2	BB	5121	GLU
2	BB	5161	LEU
2	BB	5179	GLN
2	BB	5246	PHE
2	BB	5297	THR
2	BB	5311	PHE
2	BB	5433	ASP
2	BB	5439	SER
2	BB	5467	ILE
2	BB	5484	PRO
2	BB	5485	GLU
2	BB	5488	PRO
2	BB	5490	GLN
3	BC	5027	ASP
3	BC	5029	GLU
3	BC	5078	GLU
3	BC	5097	TRP
3	BC	5121	SER
3	BC	5165	LEU
3	BC	5188	THR
3	BC	5228	ASN

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Mol	Chain	Res	Type
3	BC	5244	CYS
3	BC	5259	TRP
3	BC	5289	PHE
3	BC	5295	THR
3	BC	5318	LEU
3	BC	5321	ASP
3	BC	5324	LEU
3	BC	5355	THR
3	BC	5424	SER
3	BC	5430	HIS
3	BC	5432	VAL
3	BC	5456	GLU
3	BC	5461	ARG
3	BC	5473	ASP
4	BD	5014	TRP
4	BD	5043	LEU
4	BD	5084	SER
4	BD	5091	LEU
4	BD	5110	LEU
4	BD	5112	THR
4	BD	5128	ARG
4	BD	5130	PHE
4	BD	5166	SER
4	BD	5180	ARG
4	BD	5201	VAL
4	BD	5205	LEU
4	BD	5242	GLU
4	BD	5259	ILE
4	BD	5262	SER
4	BD	5264	LYS
4	BD	5272	LEU
4	BD	5279	LEU
4	BD	5282	SER
4	BD	5291	LEU
4	BD	5293	LEU
4	BD	5316	THR
4	BD	5323	GLU
4	BD	5331	PRO
4	BD	5345	VAL
4	BD	5346	LEU
5	BE	5009	PRO
5	BE	5010	PHE

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Mol	Chain	Res	Type
5	BE	5052	PRO
5	BE	5060	GLN
5	BE	5068	ASP
5	BE	5084	LYS
6	BF	5018	VAL
7	BH	5012	ARG
7	BH	5021	VAL
7	BH	5025	TRP
7	BH	5027	THR
7	BH	5042	LEU
7	BH	5043	LEU
7	BH	5045	ILE
7	BH	5049	TYR
7	BH	5056	ASP
7	BH	5060	VAL
8	BI	5032	PRO
9	BJ	5007	ARG
10	BK	5023	ASP
11	BL	5008	GLN
11	BL	5009	PRO
11	BL	5015	THR
12	BM	5025	LEU
12	BM	5034	LYS
13	BO	5031	LEU
13	BO	5041	LEU
13	BO	5060	SER
13	BO	5065	ARG
13	BO	5084	ASN
13	BO	5086	ARG
13	BO	5097	VAL
13	BO	5106	GLN
13	BO	5141	ARG
13	BO	5152	VAL
13	BO	5158	ASN
13	BO	5165	SER
13	BO	5171	GLU
13	BO	5207	GLU
13	BO	5224	SER
14	BT	5029	ILE
14	BT	5032	LYS
15	BU	5044	ASP
15	BU	5053	GLU

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Mol	Chain	Res	Type
15	BU	5061	ASN
15	BU	5098	THR
15	BU	5103	GLN
15	BU	5114	VAL
15	BU	5119	THR
15	BU	5132	LEU
16	BV	5032	GLU
16	BV	5040	SER
16	BV	5068	VAL
16	BV	5089	THR
16	BV	5092	ARG
16	BV	5125	ASP
17	By	5021	GLN
17	By	5028	ILE
17	By	5034	MET
17	By	5035	ILE
17	By	5036	ILE
18	BX	5045	LYS
20	BZ	5025	VAL
20	BZ	5033	TRP
20	BZ	5058	ASN
20	BZ	5062	VAL

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

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	75	ASN
1	AA	92	HIS
1	AA	118	HIS
1	AA	199	GLN
1	AA	234	ASN
1	AA	241	GLN
1	AA	247	ASN
1	AA	272	HIS
1	AA	315	ASN
1	AA	337	HIS
1	AA	338	ASN
2	AB	53	ASN
2	AB	157	HIS
2	AB	179	GLN

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Mol	Chain	Res	Type
2	AB	201	HIS
2	AB	216	HIS
2	AB	281	GLN
2	AB	282	GLN
2	AB	285	ASN
2	AB	331	ASN
2	AB	490	GLN
3	AC	155	ASN
3	AC	201	ASN
3	AC	228	ASN
3	AC	322	GLN
3	AC	388	GLN
3	AC	398	HIS
4	AD	83	ASN
4	AD	129	GLN
4	AD	332	GLN
5	AE	60	GLN
5	AE	75	GLN
6	AF	41	GLN
11	AL	8	GLN
11	AL	37	ASN
12	AM	5	GLN
12	AM	32	GLN
13	AO	62	GLN
13	AO	84	ASN
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	181	ASN
13	AO	202	GLN
13	AO	222	GLN
18	AX	47	GLN
20	AZ	58	ASN
1	BA	5012	ASN
1	BA	5019	ASN
1	BA	5075	ASN
1	BA	5092	HIS
1	BA	5118	HIS
1	BA	5199	GLN

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Mol	Chain	Res	Type
1	BA	5234	ASN
1	BA	5241	GLN
1	BA	5247	ASN
1	BA	5272	HIS
1	BA	5312	ASN
1	BA	5315	ASN
1	BA	5337	HIS
1	BA	5338	ASN
2	BB	5053	ASN
2	BB	5157	HIS
2	BB	5179	GLN
2	BB	5201	HIS
2	BB	5216	HIS
2	BB	5281	GLN
2	BB	5282	GLN
2	BB	5285	ASN
2	BB	5331	ASN
2	BB	5338	GLN
2	BB	5469	HIS
2	BB	5490	GLN
3	BC	5155	ASN
3	BC	5201	ASN
3	BC	5228	ASN
3	BC	5322	GLN
3	BC	5388	GLN
3	BC	5398	HIS
3	BC	5418	ASN
4	BD	5083	ASN
4	BD	5129	GLN
4	BD	5250	ASN
4	BD	5332	GLN
5	BE	5060	GLN
5	BE	5075	GLN
6	BF	5041	GLN
11	BL	5008	GLN
11	BL	5037	ASN
12	BM	5005	GLN
12	BM	5028	GLN
12	BM	5032	GLN
13	BO	5062	GLN
13	BO	5084	ASN
13	BO	5087	GLN

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Mol	Chain	Res	Type
13	BO	5106	GLN
13	BO	5114	ASN
13	BO	5135	GLN
13	BO	5150	ASN
13	BO	5173	ASN
13	BO	5181	ASN
13	BO	5202	GLN
13	BO	5222	GLN
16	BV	5060	GLN
18	BX	5042	GLN
18	BX	5047	GLN
20	BZ	5058	ASN

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 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 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	BCT	AA	402	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	AA	404	-	73,73,73	2.53	21 (28%)	96,113,113	1.93	22 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AA	405	-	73,73,73	2.57	26 (35%)	96,113,113	2.28	31 (32%)
24	CLA	AA	406	-	73,73,73	2.56	22 (30%)	96,113,113	2.16	27 (28%)
24	CLA	AA	407	-	73,73,73	2.57	22 (30%)	96,113,113	2.04	26 (27%)
25	MST	AA	408	-	16,16,16	0.52	0	22,22,22	3.87	8 (36%)
26	OEC	AA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	AA	410	-	41,41,41	1.60	7 (17%)	56,56,56	2.04	21 (37%)
28	DGD	AA	411	-	57,57,67	1.84	15 (26%)	71,71,81	3.79	25 (35%)
29	LHG	AA	412	-	38,38,48	1.95	6 (15%)	44,44,54	1.40	4 (9%)
30	SQD	AA	413	-	51,51,54	7.21	28 (54%)	62,62,65	3.42	23 (37%)
31	LMG	AA	414	-	44,44,55	1.41	3 (6%)	52,52,63	1.68	8 (15%)
29	LHG	AA	415	-	36,36,48	1.72	4 (11%)	42,42,54	1.10	3 (7%)
30	SQD	AA	416	-	54,54,54	2.69	29 (53%)	65,65,65	3.22	22 (33%)
31	LMG	AA	417	-	42,42,55	1.62	7 (16%)	50,50,63	2.41	12 (24%)
24	CLA	AB	601	-	73,73,73	2.93	25 (34%)	96,113,113	1.79	18 (18%)
24	CLA	AB	602	-	73,73,73	2.58	23 (31%)	96,113,113	1.89	22 (22%)
24	CLA	AB	603	-	73,73,73	2.71	21 (28%)	96,113,113	2.23	29 (30%)
24	CLA	AB	604	-	73,73,73	2.59	25 (34%)	96,113,113	1.91	23 (23%)
24	CLA	AB	605	-	73,73,73	2.79	25 (34%)	96,113,113	2.00	27 (28%)
24	CLA	AB	606	-	73,73,73	2.69	24 (32%)	96,113,113	1.97	26 (27%)
24	CLA	AB	607	-	73,73,73	2.56	26 (35%)	96,113,113	2.24	29 (30%)
24	CLA	AB	608	-	73,73,73	2.77	25 (34%)	96,113,113	2.24	29 (30%)
24	CLA	AB	609	-	73,73,73	2.70	23 (31%)	96,113,113	1.90	23 (23%)
24	CLA	AB	610	-	73,73,73	2.51	20 (27%)	96,113,113	1.84	23 (23%)
24	CLA	AB	611	-	73,73,73	2.60	22 (30%)	96,113,113	2.08	31 (32%)
24	CLA	AB	612	-	73,73,73	2.68	22 (30%)	96,113,113	1.94	26 (27%)
24	CLA	AB	613	-	73,73,73	2.43	19 (26%)	96,113,113	1.87	23 (23%)
24	CLA	AB	614	-	73,73,73	2.98	24 (32%)	96,113,113	2.10	23 (23%)
24	CLA	AB	615	-	73,73,73	2.65	23 (31%)	96,113,113	1.91	20 (20%)
24	CLA	AB	616	-	73,73,73	2.67	21 (28%)	96,113,113	1.80	20 (20%)
27	BCR	AB	617	-	41,41,41	1.57	6 (14%)	56,56,56	2.09	21 (37%)
27	BCR	AB	618	-	41,41,41	1.91	7 (17%)	56,56,56	2.05	16 (28%)
27	BCR	AB	619	-	41,41,41	1.82	8 (19%)	56,56,56	1.94	18 (32%)
31	LMG	AB	620	-	51,51,55	5.72	5 (9%)	59,59,63	2.03	15 (25%)
31	LMG	AB	621	-	49,49,55	1.41	3 (6%)	57,57,63	1.90	14 (24%)
30	SQD	AB	622	-	43,43,54	7.89	23 (53%)	54,54,65	3.49	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	AB	623	-	36,36,36	1.73	7 (19%)	47,47,47	0.99	2 (4%)
32	LMT	AB	624	-	36,36,36	1.61	6 (16%)	47,47,47	0.93	2 (4%)
33	DMS	AB	625	-	3,3,3	0.71	0	3,3,3	1.36	0
33	DMS	AB	626	-	3,3,3	0.66	0	3,3,3	0.99	0
30	SQD	AB	627	-	47,47,54	3.10	25 (53%)	58,58,65	3.31	15 (25%)
28	DGD	AB	628	-	53,53,67	1.47	6 (11%)	67,67,81	2.15	15 (22%)
32	LMT	AB	629	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	6 (12%)
32	LMT	AB	630	-	36,36,36	1.70	8 (22%)	47,47,47	1.00	1 (2%)
24	CLA	AC	501	-	73,73,73	2.68	23 (31%)	96,113,113	2.03	24 (25%)
24	CLA	AC	502	-	73,73,73	2.59	22 (30%)	96,113,113	1.91	22 (22%)
24	CLA	AC	503	-	73,73,73	2.64	24 (32%)	96,113,113	2.06	27 (28%)
24	CLA	AC	504	-	73,73,73	2.54	24 (32%)	96,113,113	2.09	24 (25%)
24	CLA	AC	505	-	73,73,73	2.89	26 (35%)	96,113,113	2.06	23 (23%)
24	CLA	AC	506	-	73,73,73	2.79	24 (32%)	96,113,113	1.96	24 (25%)
24	CLA	AC	507	-	73,73,73	2.43	23 (31%)	96,113,113	1.82	20 (20%)
24	CLA	AC	508	-	73,73,73	2.62	23 (31%)	96,113,113	2.08	27 (28%)
24	CLA	AC	509	-	73,73,73	2.69	21 (28%)	96,113,113	1.93	22 (22%)
24	CLA	AC	510	-	73,73,73	2.60	22 (30%)	96,113,113	1.83	21 (21%)
24	CLA	AC	511	3	73,73,73	2.87	21 (28%)	96,113,113	2.05	25 (26%)
24	CLA	AC	512	-	73,73,73	2.76	23 (31%)	96,113,113	1.88	22 (22%)
24	CLA	AC	513	-	73,73,73	2.87	21 (28%)	96,113,113	1.89	21 (21%)
27	BCR	AC	514	-	41,41,41	1.60	7 (17%)	56,56,56	2.13	23 (41%)
27	BCR	AC	515	-	41,41,41	1.74	7 (17%)	56,56,56	2.22	21 (37%)
27	BCR	AC	516	-	41,41,41	1.63	8 (19%)	56,56,56	2.23	21 (37%)
28	DGD	AC	517	-	54,54,67	1.73	9 (16%)	68,68,81	2.88	23 (33%)
28	DGD	AC	518	-	63,63,67	1.30	7 (11%)	77,77,81	2.95	25 (32%)
28	DGD	AC	519	-	67,67,67	1.45	10 (14%)	81,81,81	3.46	29 (35%)
31	LMG	AC	520	-	48,48,55	1.83	7 (14%)	56,56,63	1.94	18 (32%)
31	LMG	AC	521	-	45,45,55	1.40	4 (8%)	53,53,63	2.05	15 (28%)
24	CLA	AD	401	-	73,73,73	2.54	24 (32%)	96,113,113	1.95	24 (25%)
34	PHO	AD	402	-	69,69,69	2.89	17 (24%)	92,99,99	1.75	19 (20%)
34	PHO	AD	403	-	69,69,69	3.08	19 (27%)	92,99,99	1.81	22 (23%)
24	CLA	AD	404	-	73,73,73	2.66	25 (34%)	96,113,113	1.97	22 (22%)
35	PL9	AD	405	-	55,55,55	4.31	18 (32%)	69,69,69	3.01	24 (34%)
27	BCR	AD	406	-	41,41,41	1.64	7 (17%)	56,56,56	2.33	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	AD	407	-	49,49,55	5.81	3 (6%)	57,57,63	2.72	21 (36%)
31	LMG	AD	408	-	48,48,55	5.81	6 (12%)	56,56,63	2.17	13 (23%)
32	LMT	AD	409	-	32,32,36	1.77	8 (25%)	43,43,47	1.31	2 (4%)
28	DGD	AE	101	-	64,64,67	1.60	13 (20%)	78,78,81	1.50	11 (14%)
36	HEM	AF	101	5,6	50,50,50	3.49	25 (50%)	46,82,82	3.17	18 (39%)
30	SQD	AF	102	-	45,45,54	10.56	25 (55%)	56,56,65	3.67	20 (35%)
28	DGD	AH	101	-	59,59,67	1.55	12 (20%)	73,73,81	2.13	18 (24%)
31	LMG	AI	101	-	43,43,55	1.67	4 (9%)	51,51,63	1.77	7 (13%)
32	LMT	AI	102	-	36,36,36	1.58	8 (22%)	47,47,47	1.00	1 (2%)
32	LMT	AI	103	-	36,36,36	1.41	6 (16%)	47,47,47	1.76	8 (17%)
27	BCR	AJ	101	-	41,41,41	2.46	12 (29%)	56,56,56	3.15	25 (44%)
31	LMG	AJ	102	-	46,46,55	1.21	5 (10%)	54,54,63	2.65	16 (29%)
27	BCR	AK	102	-	41,41,41	1.76	6 (14%)	56,56,56	2.45	26 (46%)
31	LMG	AM	101	-	42,42,55	1.18	5 (11%)	50,50,63	1.73	8 (16%)
32	LMT	AM	102	-	36,36,36	1.71	9 (25%)	47,47,47	0.91	2 (4%)
27	BCR	AT	101	-	41,41,41	1.62	6 (14%)	56,56,56	2.22	24 (42%)
33	DMS	AU	201	-	3,3,3	0.90	0	3,3,3	1.06	0
36	HEM	AV	201	16	50,50,50	3.38	26 (52%)	46,82,82	3.10	13 (28%)
33	DMS	AV	202	-	3,3,3	0.74	0	3,3,3	1.00	0
27	BCR	AX	101	-	41,41,41	1.84	8 (19%)	56,56,56	2.19	21 (37%)
30	SQD	BA	5401	-	54,54,54	2.69	29 (53%)	65,65,65	3.20	22 (33%)
31	LMG	BA	5402	-	42,42,55	1.50	5 (11%)	50,50,63	2.43	13 (26%)
22	BCT	BA	5403	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	BA	5405	-	73,73,73	2.51	23 (31%)	96,113,113	1.91	24 (25%)
24	CLA	BA	5406	-	73,73,73	2.66	24 (32%)	96,113,113	2.32	27 (28%)
24	CLA	BA	5407	-	73,73,73	2.68	27 (36%)	96,113,113	2.15	24 (25%)
24	CLA	BA	5408	-	73,73,73	2.66	23 (31%)	96,113,113	2.02	25 (26%)
25	MST	BA	5409	-	16,16,16	0.48	0	22,22,22	3.78	8 (36%)
26	OEC	BA	5410	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	BA	5411	-	41,41,41	1.66	8 (19%)	56,56,56	2.06	21 (37%)
28	DGD	BA	5412	-	57,57,67	1.84	13 (22%)	71,71,81	3.81	24 (33%)
29	LHG	BA	5413	-	38,38,48	1.89	5 (13%)	44,44,54	1.38	4 (9%)
30	SQD	BA	5414	-	51,51,54	7.20	28 (54%)	62,62,65	3.39	24 (38%)
29	LHG	BA	5415	-	36,36,48	1.70	4 (11%)	42,42,54	1.10	3 (7%)
30	SQD	BB	5601	-	47,47,54	3.11	26 (55%)	58,58,65	3.29	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	BB	5602	-	53,53,67	1.58	7 (13%)	67,67,81	2.17	14 (20%)
32	LMT	BB	5603	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	5 (10%)
32	LMT	BB	5604	-	36,36,36	1.68	9 (25%)	47,47,47	1.00	1 (2%)
24	CLA	BB	5605	-	73,73,73	2.94	23 (31%)	96,113,113	1.79	17 (17%)
24	CLA	BB	5606	-	73,73,73	2.56	23 (31%)	96,113,113	1.91	21 (21%)
24	CLA	BB	5607	-	73,73,73	2.66	19 (26%)	96,113,113	2.23	29 (30%)
24	CLA	BB	5608	-	73,73,73	2.59	24 (32%)	96,113,113	1.94	26 (27%)
24	CLA	BB	5609	-	73,73,73	2.70	23 (31%)	96,113,113	1.99	27 (28%)
24	CLA	BB	5610	-	73,73,73	2.74	25 (34%)	96,113,113	1.98	26 (27%)
24	CLA	BB	5611	-	73,73,73	2.54	24 (32%)	96,113,113	2.24	30 (31%)
24	CLA	BB	5612	-	73,73,73	2.78	24 (32%)	96,113,113	2.24	27 (28%)
24	CLA	BB	5613	-	73,73,73	2.68	22 (30%)	96,113,113	1.92	26 (27%)
24	CLA	BB	5614	-	73,73,73	2.52	21 (28%)	96,113,113	1.82	20 (20%)
24	CLA	BB	5615	-	73,73,73	2.64	22 (30%)	96,113,113	2.09	31 (32%)
24	CLA	BB	5616	-	73,73,73	2.72	22 (30%)	96,113,113	1.97	24 (25%)
24	CLA	BB	5617	-	73,73,73	2.43	24 (32%)	96,113,113	1.87	20 (20%)
24	CLA	BB	5618	-	73,73,73	2.91	22 (30%)	96,113,113	2.08	23 (23%)
24	CLA	BB	5619	-	73,73,73	2.63	22 (30%)	96,113,113	1.92	23 (23%)
24	CLA	BB	5620	-	73,73,73	2.68	21 (28%)	96,113,113	1.81	20 (20%)
27	BCR	BB	5621	-	41,41,41	1.50	7 (17%)	56,56,56	2.08	19 (33%)
27	BCR	BB	5622	-	41,41,41	1.86	7 (17%)	56,56,56	2.04	17 (30%)
27	BCR	BB	5623	-	41,41,41	1.69	8 (19%)	56,56,56	1.92	17 (30%)
31	LMG	BB	5624	-	49,49,55	1.52	3 (6%)	57,57,63	1.90	14 (24%)
30	SQD	BB	5625	-	43,43,54	7.88	23 (53%)	54,54,65	3.52	18 (33%)
32	LMT	BB	5626	-	36,36,36	1.73	8 (22%)	47,47,47	1.01	2 (4%)
32	LMT	BB	5627	-	36,36,36	1.58	7 (19%)	47,47,47	0.92	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.69	0	3,3,3	1.07	0
33	DMS	BB	5629	-	3,3,3	0.67	0	3,3,3	1.14	0
24	CLA	BC	5501	-	73,73,73	2.75	24 (32%)	96,113,113	2.03	24 (25%)
24	CLA	BC	5502	-	73,73,73	2.64	23 (31%)	96,113,113	1.96	22 (22%)
24	CLA	BC	5503	-	73,73,73	2.71	24 (32%)	96,113,113	2.02	27 (28%)
24	CLA	BC	5504	-	73,73,73	2.64	25 (34%)	96,113,113	2.08	24 (25%)
24	CLA	BC	5505	-	73,73,73	2.93	26 (35%)	96,113,113	2.06	21 (21%)
24	CLA	BC	5506	-	73,73,73	2.79	24 (32%)	96,113,113	1.97	25 (26%)
24	CLA	BC	5507	-	73,73,73	2.52	23 (31%)	96,113,113	1.83	21 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BC	5508	-	73,73,73	2.69	22 (30%)	96,113,113	2.10	28 (29%)
24	CLA	BC	5509	-	73,73,73	2.89	22 (30%)	96,113,113	1.90	20 (20%)
24	CLA	BC	5510	-	73,73,73	2.65	22 (30%)	96,113,113	1.85	20 (20%)
24	CLA	BC	5511	3	73,73,73	3.00	24 (32%)	96,113,113	2.04	21 (21%)
24	CLA	BC	5512	-	73,73,73	2.81	23 (31%)	96,113,113	1.87	21 (21%)
24	CLA	BC	5513	-	73,73,73	2.97	22 (30%)	96,113,113	1.88	21 (21%)
27	BCR	BC	5514	-	41,41,41	1.78	6 (14%)	56,56,56	2.09	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.88	7 (17%)	56,56,56	2.21	22 (39%)
27	BCR	BC	5516	-	41,41,41	1.77	7 (17%)	56,56,56	2.19	20 (35%)
28	DGD	BC	5517	-	54,54,67	1.66	10 (18%)	68,68,81	2.88	22 (32%)
28	DGD	BC	5518	-	63,63,67	1.38	7 (11%)	77,77,81	2.93	24 (31%)
28	DGD	BC	5519	-	67,67,67	1.49	11 (16%)	81,81,81	3.46	30 (37%)
31	LMG	BC	5520	-	48,48,55	1.93	5 (10%)	56,56,63	1.92	17 (30%)
31	LMG	BC	5521	-	45,45,55	1.32	4 (8%)	53,53,63	2.04	14 (26%)
32	LMT	BC	5522	-	36,36,36	1.48	7 (19%)	47,47,47	1.76	8 (17%)
24	CLA	BD	5402	-	73,73,73	2.59	24 (32%)	96,113,113	1.96	24 (25%)
34	PHO	BD	5403	-	69,69,69	2.99	18 (26%)	92,99,99	1.77	21 (22%)
34	PHO	BD	5404	-	69,69,69	3.17	21 (30%)	92,99,99	1.82	22 (23%)
24	CLA	BD	5405	-	73,73,73	2.67	24 (32%)	96,113,113	1.95	23 (23%)
35	PL9	BD	5406	-	55,55,55	4.43	20 (36%)	69,69,69	3.00	24 (34%)
27	BCR	BD	5407	-	41,41,41	1.81	9 (21%)	56,56,56	2.31	24 (42%)
31	LMG	BD	5408	-	46,46,55	1.16	5 (10%)	54,54,63	2.64	17 (31%)
31	LMG	BD	5409	-	49,49,55	5.79	2 (4%)	57,57,63	2.73	22 (38%)
31	LMG	BD	5410	-	48,48,55	5.79	3 (6%)	56,56,63	2.17	13 (23%)
32	LMT	BD	5411	-	32,32,36	1.71	7 (21%)	43,43,47	1.31	3 (6%)
31	LMG	BE	5101	-	44,44,55	1.45	4 (9%)	52,52,63	1.69	8 (15%)
28	DGD	BE	5102	-	64,64,67	1.58	12 (18%)	78,78,81	1.49	9 (11%)
36	HEM	BF	5101	5,6	50,50,50	3.62	26 (52%)	46,82,82	3.19	18 (39%)
30	SQD	BF	5102	-	45,45,54	10.56	26 (57%)	56,56,65	3.68	21 (37%)
28	DGD	BH	5101	-	59,59,67	1.50	10 (16%)	73,73,81	2.13	19 (26%)
31	LMG	BI	5101	-	43,43,55	1.77	4 (9%)	51,51,63	1.76	7 (13%)
32	LMT	BI	5102	-	36,36,36	1.62	7 (19%)	47,47,47	0.99	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.40	13 (31%)	56,56,56	3.13	25 (44%)
27	BCR	BK	5102	-	41,41,41	1.90	8 (19%)	56,56,56	2.41	24 (42%)
31	LMG	BL	5101	-	51,51,55	5.70	5 (9%)	59,59,63	2.02	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BM	5101	-	36,36,36	1.72	8 (22%)	47,47,47	0.90	2 (4%)
31	LMG	BM	5102	-	42,42,55	1.26	5 (11%)	50,50,63	1.73	8 (16%)
27	BCR	BT	5101	-	41,41,41	1.76	6 (14%)	56,56,56	2.22	24 (42%)
36	HEM	BV	5201	16	50,50,50	3.41	27 (54%)	46,82,82	3.13	13 (28%)
33	DMS	BV	5202	-	3,3,3	0.84	0	3,3,3	0.93	0
33	DMS	BV	5203	-	3,3,3	0.82	0	3,3,3	1.12	0
27	BCR	BX	5101	-	41,41,41	1.87	9 (21%)	56,56,56	2.22	22 (39%)

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	BCT	AA	402	21	-	0/0/0/0	0/0/0/0
24	CLA	AA	404	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	405	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	406	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	407	-	1/1/20/25	0/37/135/135	0/0/9/9
25	MST	AA	408	-	-	0/10/10/10	0/1/1/1
26	OEC	AA	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	AA	410	-	-	0/29/63/63	0/2/2/2
28	DGD	AA	411	-	-	0/45/85/95	0/2/2/2
29	LHG	AA	412	-	-	0/43/43/53	0/0/0/0
30	SQD	AA	413	-	-	0/46/66/69	0/1/1/1
31	LMG	AA	414	-	-	0/39/59/70	0/1/1/1
29	LHG	AA	415	-	-	0/41/41/53	0/0/0/0
30	SQD	AA	416	-	-	0/49/69/69	0/1/1/1
31	LMG	AA	417	-	-	0/37/57/70	0/1/1/1
24	CLA	AB	601	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	602	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	603	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	604	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	605	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	606	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	610	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	612	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	613	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	614	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	615	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	616	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
31	LMG	AB	620	-	-	0/46/66/70	0/1/1/1
31	LMG	AB	621	-	-	0/44/64/70	0/1/1/1
30	SQD	AB	622	-	-	0/38/58/69	0/1/1/1
32	LMT	AB	623	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
33	DMS	AB	625	-	-	0/0/0/0	0/0/0/0
33	DMS	AB	626	-	-	0/0/0/0	0/0/0/0
30	SQD	AB	627	-	-	0/42/62/69	0/1/1/1
28	DGD	AB	628	-	-	0/41/81/95	0/2/2/2
32	LMT	AB	629	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	630	-	-	0/21/61/61	0/2/2/2
24	CLA	AC	501	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	504	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	508	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	509	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	510	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	511	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	512	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	513	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	516	-	-	0/29/63/63	0/2/2/2
28	DGD	AC	517	-	-	0/42/82/95	0/2/2/2
28	DGD	AC	518	-	1/1/13/13	0/51/91/95	0/2/2/2
28	DGD	AC	519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	AC	520	-	-	0/43/63/70	0/1/1/1
31	LMG	AC	521	-	-	0/40/60/70	0/1/1/1
24	CLA	AD	401	-	1/1/20/25	0/37/135/135	0/0/9/9
34	PHO	AD	402	-	2/2/17/22	0/49/103/103	0/1/6/6
34	PHO	AD	403	-	2/2/17/22	0/49/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AD	404	-	1/1/20/25	0/37/135/135	0/0/9/9
35	PL9	AD	405	-	-	2/53/73/73	0/1/1/1
27	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
31	LMG	AD	407	-	-	0/44/64/70	0/1/1/1
31	LMG	AD	408	-	-	0/43/63/70	0/1/1/1
32	LMT	AD	409	-	-	0/17/57/61	0/2/2/2
28	DGD	AE	101	-	-	0/52/92/95	0/2/2/2
36	HEM	AF	101	5,6	-	0/14/114/114	0/0/8/8
30	SQD	AF	102	-	-	0/40/60/69	0/1/1/1
28	DGD	AH	101	-	-	0/47/87/95	0/2/2/2
31	LMG	AI	101	-	-	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AI	103	-	-	0/21/61/61	0/2/2/2
27	BCR	AJ	101	-	-	0/29/63/63	0/2/2/2
31	LMG	AJ	102	-	-	0/41/61/70	0/1/1/1
27	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
31	LMG	AM	101	-	-	0/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
27	BCR	AT	101	-	-	0/29/63/63	0/2/2/2
33	DMS	AU	201	-	-	0/0/0/0	0/0/0/0
36	HEM	AV	201	16	-	0/14/114/114	0/0/8/8
33	DMS	AV	202	-	-	0/0/0/0	0/0/0/0
27	BCR	AX	101	-	-	0/29/63/63	0/2/2/2
30	SQD	BA	5401	-	-	0/49/69/69	0/1/1/1
31	LMG	BA	5402	-	-	0/37/57/70	0/1/1/1
22	BCT	BA	5403	21	-	0/0/0/0	0/0/0/0
24	CLA	BA	5405	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5406	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5407	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5408	-	1/1/20/25	0/37/135/135	0/0/9/9
25	MST	BA	5409	-	-	0/10/10/10	0/1/1/1
26	OEC	BA	5410	1,3	-	0/0/0/54	0/0/0/5
27	BCR	BA	5411	-	-	0/29/63/63	0/2/2/2
28	DGD	BA	5412	-	-	0/45/85/95	0/2/2/2
29	LHG	BA	5413	-	-	0/43/43/53	0/0/0/0
30	SQD	BA	5414	-	-	0/46/66/69	0/1/1/1
29	LHG	BA	5415	-	-	0/41/41/53	0/0/0/0
30	SQD	BB	5601	-	-	0/42/62/69	0/1/1/1
28	DGD	BB	5602	-	-	0/41/81/95	0/2/2/2
32	LMT	BB	5603	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5604	-	-	0/21/61/61	0/2/2/2
24	CLA	BB	5605	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BB	5606	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5610	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5613	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5614	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5615	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5616	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5617	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5618	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5619	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5620	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	BB	5621	-	-	0/29/63/63	0/2/2/2
27	BCR	BB	5622	-	-	0/29/63/63	0/2/2/2
27	BCR	BB	5623	-	-	0/29/63/63	0/2/2/2
31	LMG	BB	5624	-	-	0/44/64/70	0/1/1/1
30	SQD	BB	5625	-	-	0/38/58/69	0/1/1/1
32	LMT	BB	5626	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5627	-	-	0/21/61/61	0/2/2/2
33	DMS	BB	5628	-	-	0/0/0/0	0/0/0/0
33	DMS	BB	5629	-	-	0/0/0/0	0/0/0/0
24	CLA	BC	5501	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5504	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5508	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5509	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5510	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5511	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5512	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5513	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	BC	5514	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5516	-	-	0/29/63/63	0/2/2/2
28	DGD	BC	5517	-	-	0/42/82/95	0/2/2/2
28	DGD	BC	5518	-	1/1/13/13	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	BC	5519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	BC	5520	-	-	0/43/63/70	0/1/1/1
31	LMG	BC	5521	-	-	0/40/60/70	0/1/1/1
32	LMT	BC	5522	-	-	0/21/61/61	0/2/2/2
24	CLA	BD	5402	-	1/1/20/25	0/37/135/135	0/0/9/9
34	PHO	BD	5403	-	2/2/17/22	0/49/103/103	0/1/6/6
34	PHO	BD	5404	-	2/2/17/22	0/49/103/103	0/1/6/6
24	CLA	BD	5405	-	1/1/20/25	0/37/135/135	0/0/9/9
35	PL9	BD	5406	-	-	1/53/73/73	0/1/1/1
27	BCR	BD	5407	-	-	0/29/63/63	0/2/2/2
31	LMG	BD	5408	-	-	0/41/61/70	0/1/1/1
31	LMG	BD	5409	-	-	0/44/64/70	0/1/1/1
31	LMG	BD	5410	-	-	0/43/63/70	0/1/1/1
32	LMT	BD	5411	-	-	0/17/57/61	0/2/2/2
31	LMG	BE	5101	-	-	0/39/59/70	0/1/1/1
28	DGD	BE	5102	-	-	0/52/92/95	0/2/2/2
36	HEM	BF	5101	5,6	-	0/14/114/114	0/0/8/8
30	SQD	BF	5102	-	-	0/40/60/69	0/1/1/1
28	DGD	BH	5101	-	-	0/47/87/95	0/2/2/2
31	LMG	BI	5101	-	-	0/38/58/70	0/1/1/1
32	LMT	BI	5102	-	-	0/21/61/61	0/2/2/2
27	BCR	BJ	5101	-	-	0/29/63/63	0/2/2/2
27	BCR	BK	5102	-	-	0/29/63/63	0/2/2/2
31	LMG	BL	5101	-	-	0/46/66/70	0/1/1/1
32	LMT	BM	5101	-	-	0/21/61/61	0/2/2/2
31	LMG	BM	5102	-	-	0/37/57/70	0/1/1/1
27	BCR	BT	5101	-	-	0/29/63/63	0/2/2/2
36	HEM	BV	5201	16	-	0/14/114/114	0/0/8/8
33	DMS	BV	5202	-	-	0/0/0/0	0/0/0/0
33	DMS	BV	5203	-	-	0/0/0/0	0/0/0/0
27	BCR	BX	5101	-	-	0/29/63/63	0/2/2/2

All (2655) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BF	5102	SQD	C19-C18	-48.56	1.35	1.55
30	AF	102	SQD	C32-C31	-48.38	1.35	1.55
30	AF	102	SQD	C19-C18	-48.33	1.35	1.55
30	BF	5102	SQD	C32-C31	-48.02	1.36	1.55
30	AA	413	SQD	C35-C34	-47.92	1.36	1.55
30	BA	5414	SQD	C35-C34	-47.74	1.36	1.55
30	BB	5625	SQD	C18-C17	-46.43	1.36	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	622	SQD	C18-C17	-46.17	1.36	1.55
31	AD	407	LMG	C25-C24	-39.98	1.39	1.55
31	BD	5409	LMG	C25-C24	-39.76	1.39	1.55
31	AB	620	LMG	C25-C24	-39.70	1.39	1.55
31	AD	408	LMG	C25-C24	-39.67	1.39	1.55
31	BD	5410	LMG	C25-C24	-39.56	1.39	1.55
31	BL	5101	LMG	C25-C24	-39.41	1.39	1.55
30	AB	622	SQD	C31-C30	13.19	1.60	1.55
24	AB	608	CLA	C2-C3	12.64	1.58	1.32
24	BB	5612	CLA	C2-C3	12.63	1.58	1.32
24	AB	606	CLA	C2-C3	12.63	1.58	1.32
24	BB	5610	CLA	C2-C3	12.61	1.58	1.32
24	AB	607	CLA	C2-C3	12.26	1.57	1.32
24	BB	5620	CLA	C2-C3	12.26	1.57	1.32
24	BC	5511	CLA	C2-C3	12.23	1.57	1.32
30	BB	5625	SQD	C31-C30	12.11	1.60	1.55
34	BD	5404	PHO	CHC-C1C	12.08	1.43	1.35
24	AB	614	CLA	C2-C3	12.00	1.56	1.32
24	BB	5613	CLA	C2-C3	12.00	1.56	1.32
24	AC	511	CLA	C2-C3	11.99	1.56	1.32
24	AB	616	CLA	C2-C3	11.99	1.56	1.32
24	AB	603	CLA	C2-C3	11.92	1.56	1.32
34	AD	403	PHO	CHC-C1C	11.82	1.43	1.35
24	BC	5505	CLA	C2-C3	11.79	1.56	1.32
35	AD	405	PL9	C28-C29	11.76	1.56	1.32
24	AB	609	CLA	C2-C3	11.75	1.56	1.32
24	BC	5506	CLA	C2-C3	11.71	1.56	1.32
24	BB	5607	CLA	C2-C3	11.71	1.56	1.32
35	BD	5406	PL9	C13-C14	11.67	1.56	1.32
34	AD	403	PHO	C2-C3	11.63	1.56	1.32
24	AC	506	CLA	C2-C3	11.60	1.56	1.32
24	BB	5615	CLA	C2-C3	11.60	1.56	1.32
24	BB	5611	CLA	C2-C3	11.59	1.56	1.32
24	BB	5605	CLA	C2-C3	11.59	1.56	1.32
35	BD	5406	PL9	C28-C29	11.58	1.56	1.32
24	BB	5618	CLA	C2-C3	11.57	1.56	1.32
35	BD	5406	PL9	C23-C24	11.55	1.56	1.32
35	AD	405	PL9	C13-C14	11.53	1.55	1.32
34	BD	5404	PHO	C2-C3	11.52	1.55	1.32
24	AC	505	CLA	C2-C3	11.51	1.55	1.32
34	BD	5403	PHO	C2-C3	11.51	1.55	1.32
24	AB	605	CLA	C2-C3	11.47	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	513	CLA	C2-C3	11.46	1.55	1.32
24	BC	5513	CLA	C2-C3	11.44	1.55	1.32
24	AC	501	CLA	C2-C3	11.43	1.55	1.32
35	BD	5406	PL9	C33-C34	11.41	1.55	1.32
24	BD	5405	CLA	C2-C3	11.40	1.55	1.32
24	AC	502	CLA	C2-C3	11.38	1.55	1.32
24	BB	5609	CLA	C2-C3	11.37	1.55	1.32
24	AB	601	CLA	C2-C3	11.35	1.55	1.32
24	BC	5501	CLA	C2-C3	11.33	1.55	1.32
24	BA	5408	CLA	C2-C3	11.27	1.55	1.32
24	BC	5509	CLA	C2-C3	11.25	1.55	1.32
24	BC	5508	CLA	C2-C3	11.23	1.55	1.32
24	AA	405	CLA	C2-C3	11.22	1.55	1.32
24	AB	611	CLA	C2-C3	11.18	1.55	1.32
24	BA	5406	CLA	C2-C3	11.18	1.55	1.32
34	AD	402	PHO	C2-C3	11.18	1.55	1.32
35	BD	5406	PL9	C43-C44	11.13	1.55	1.32
24	AC	508	CLA	C2-C3	11.07	1.55	1.32
35	AD	405	PL9	C33-C34	11.06	1.55	1.32
24	AA	406	CLA	C2-C3	11.06	1.55	1.32
24	BC	5502	CLA	C2-C3	11.06	1.55	1.32
24	AB	612	CLA	C2-C3	11.04	1.55	1.32
36	AV	201	HEM	C3D-C4D	11.04	1.53	1.45
24	BC	5504	CLA	C2-C3	10.98	1.54	1.32
24	BB	5606	CLA	C2-C3	10.96	1.54	1.32
24	AA	407	CLA	C2-C3	10.93	1.54	1.32
24	BC	5503	CLA	C2-C3	10.92	1.54	1.32
35	BD	5406	PL9	C8-C9	10.92	1.54	1.32
24	BB	5616	CLA	C2-C3	10.91	1.54	1.32
24	AC	503	CLA	C2-C3	10.88	1.54	1.32
36	AF	101	HEM	C3D-C4D	10.88	1.53	1.45
24	BD	5402	CLA	C2-C3	10.87	1.54	1.32
24	BC	5507	CLA	C2-C3	10.87	1.54	1.32
24	AD	404	CLA	C2-C3	10.85	1.54	1.32
24	BC	5512	CLA	C2-C3	10.84	1.54	1.32
36	BV	5201	HEM	C3D-C4D	10.83	1.53	1.45
24	BA	5407	CLA	C2-C3	10.83	1.54	1.32
24	AC	510	CLA	C2-C3	10.83	1.54	1.32
35	AD	405	PL9	C8-C9	10.79	1.54	1.32
24	AB	602	CLA	C2-C3	10.79	1.54	1.32
24	AB	604	CLA	C2-C3	10.78	1.54	1.32
24	AC	512	CLA	C2-C3	10.77	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	AD	405	PL9	C43-C44	10.76	1.54	1.32
30	BB	5601	SQD	C31-C30	10.75	1.59	1.55
24	BC	5510	CLA	C2-C3	10.73	1.54	1.32
30	AB	627	SQD	C31-C30	10.70	1.59	1.55
24	BB	5617	CLA	C2-C3	10.68	1.54	1.32
24	AD	401	CLA	C2-C3	10.68	1.54	1.32
24	BB	5608	CLA	C2-C3	10.67	1.54	1.32
36	BF	5101	HEM	C3D-C4D	10.64	1.53	1.45
24	AC	504	CLA	C2-C3	10.63	1.54	1.32
24	AB	613	CLA	C2-C3	10.63	1.54	1.32
24	AA	404	CLA	C2-C3	10.57	1.54	1.32
24	AB	610	CLA	C2-C3	10.55	1.54	1.32
24	AC	509	CLA	C2-C3	10.54	1.54	1.32
24	AC	507	CLA	C2-C3	10.46	1.53	1.32
24	AB	615	CLA	C2-C3	10.41	1.53	1.32
24	BB	5614	CLA	C2-C3	10.39	1.53	1.32
24	BB	5619	CLA	C2-C3	10.33	1.53	1.32
35	AD	405	PL9	C23-C24	10.32	1.53	1.32
24	BB	5605	CLA	C3B-C2B	10.18	1.53	1.40
34	BD	5403	PHO	CHC-C1C	9.88	1.42	1.35
24	BC	5505	CLA	C3B-C2B	9.88	1.52	1.40
30	AA	416	SQD	C6-C5	-9.84	1.40	1.52
34	AD	402	PHO	CHC-C1C	9.82	1.42	1.35
31	BC	5520	LMG	C42-C41	-9.76	1.51	1.55
24	AB	601	CLA	C3B-C2B	9.65	1.52	1.40
24	AC	505	CLA	C3B-C2B	9.56	1.52	1.40
34	BD	5404	PHO	C3B-C2B	9.46	1.52	1.40
24	BA	5405	CLA	C2-C3	9.40	1.51	1.32
24	AB	614	CLA	MG-NA	9.39	2.35	2.07
30	BA	5401	SQD	C6-C5	-9.35	1.41	1.52
24	BC	5513	CLA	MG-NA	9.33	2.34	2.07
24	BA	5406	CLA	C3B-C2B	9.21	1.51	1.40
24	BC	5511	CLA	MG-NA	9.18	2.34	2.07
24	BC	5512	CLA	C3B-C2B	9.14	1.51	1.40
24	BC	5513	CLA	C3B-C2B	9.11	1.51	1.40
31	AC	520	LMG	C42-C41	-9.08	1.51	1.55
24	AC	513	CLA	MG-NA	9.06	2.34	2.07
24	BC	5509	CLA	C3B-C2B	9.04	1.51	1.40
24	AC	511	CLA	MG-NA	9.04	2.34	2.07
24	AC	512	CLA	C3B-C2B	8.92	1.51	1.40
24	AB	605	CLA	C3B-C2B	8.87	1.51	1.40
34	BD	5403	PHO	C3B-C2B	8.84	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5503	CLA	C3B-C2B	8.81	1.51	1.40
24	BB	5618	CLA	MG-NA	8.79	2.33	2.07
24	BC	5501	CLA	C3B-C2B	8.78	1.51	1.40
30	AB	622	SQD	C6-C5	-8.72	1.41	1.52
24	AC	506	CLA	C3B-C2B	8.71	1.51	1.40
24	BB	5609	CLA	C3B-C2B	8.67	1.51	1.40
24	BB	5619	CLA	C3B-C2B	8.65	1.51	1.40
24	BC	5511	CLA	C3B-C2B	8.61	1.51	1.40
24	BB	5613	CLA	C3B-C2B	8.61	1.51	1.40
24	AC	513	CLA	C3B-C2B	8.59	1.51	1.40
24	BA	5407	CLA	C3B-C2B	8.57	1.51	1.40
24	BC	5506	CLA	C3B-C2B	8.57	1.51	1.40
24	AB	609	CLA	C3B-C2B	8.56	1.51	1.40
30	BB	5625	SQD	C6-C5	-8.54	1.42	1.52
31	BI	5101	LMG	C23-C22	-8.52	1.51	1.55
24	BC	5510	CLA	C3B-C2B	8.47	1.51	1.40
24	AB	616	CLA	C3B-C2B	8.47	1.51	1.40
35	BD	5406	PL9	C2-C3	8.40	1.57	1.34
24	BB	5614	CLA	C3B-C2B	8.38	1.50	1.40
24	AC	509	CLA	MG-NA	8.36	2.32	2.07
34	AD	403	PHO	C3B-C2B	8.34	1.50	1.40
24	AB	615	CLA	C3B-C2B	8.32	1.50	1.40
35	AD	405	PL9	C2-C3	8.30	1.57	1.34
24	AC	503	CLA	C3B-C2B	8.28	1.50	1.40
24	BC	5502	CLA	C3B-C2B	8.25	1.50	1.40
34	BD	5404	PHO	C3D-C4D	8.21	1.53	1.40
30	BB	5625	SQD	C4-C3	8.20	1.74	1.52
34	BD	5403	PHO	C3D-C4D	8.19	1.53	1.40
24	AC	511	CLA	C3B-C2B	8.18	1.50	1.40
24	AA	406	CLA	C3B-C2B	8.16	1.50	1.40
34	AD	403	PHO	C3D-C4D	8.13	1.52	1.40
24	AC	510	CLA	C3B-C2B	8.11	1.50	1.40
34	AD	402	PHO	C3D-C4D	8.08	1.52	1.40
24	AB	614	CLA	C3B-C2B	8.05	1.50	1.40
24	AB	604	CLA	C3B-C2B	8.04	1.50	1.40
24	BB	5618	CLA	C3B-C2B	8.03	1.50	1.40
24	BC	5507	CLA	C3B-C2B	8.02	1.50	1.40
24	BB	5615	CLA	C3B-C2B	8.02	1.50	1.40
24	AB	610	CLA	C3B-C2B	8.02	1.50	1.40
30	AB	622	SQD	C4-C3	8.01	1.73	1.52
24	BC	5509	CLA	MG-NA	8.00	2.30	2.07
24	AD	404	CLA	C3B-C2B	7.99	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5608	CLA	C3B-C2B	7.98	1.50	1.40
36	AV	201	HEM	C2B-C1B	-7.98	1.39	1.45
24	BD	5405	CLA	C3B-C2B	7.94	1.50	1.40
36	BF	5101	HEM	C3D-C2D	-7.93	1.36	1.44
36	BF	5101	HEM	C4A-C3A	7.93	1.55	1.43
30	BF	5102	SQD	C6-C5	-7.92	1.42	1.52
24	AC	501	CLA	C3B-C2B	7.90	1.50	1.40
30	AF	102	SQD	C6-C5	-7.87	1.42	1.52
30	AA	413	SQD	C6-C5	-7.85	1.42	1.52
24	BA	5405	CLA	C3B-C2B	7.85	1.50	1.40
24	BB	5620	CLA	C3B-C2B	7.84	1.50	1.40
36	AF	101	HEM	C2B-C1B	-7.82	1.39	1.45
24	AB	612	CLA	C3B-C2B	7.82	1.50	1.40
24	AB	608	CLA	C3B-C2B	7.79	1.50	1.40
24	AB	611	CLA	C3B-C2B	7.78	1.50	1.40
34	AD	402	PHO	C3B-C2B	7.78	1.50	1.40
36	BF	5101	HEM	C2B-C1B	-7.76	1.39	1.45
24	BD	5402	CLA	C3B-C2B	7.76	1.50	1.40
30	BB	5601	SQD	C6-C5	-7.74	1.42	1.52
36	BV	5201	HEM	C2B-C1B	-7.74	1.39	1.45
24	BB	5616	CLA	C3B-C2B	7.71	1.50	1.40
24	BA	5408	CLA	C3B-C2B	7.69	1.50	1.40
24	AC	509	CLA	C3B-C2B	7.67	1.50	1.40
30	AB	627	SQD	C6-C5	-7.67	1.43	1.52
30	AB	627	SQD	C4-C3	7.65	1.72	1.52
24	BB	5606	CLA	C3B-C2B	7.65	1.50	1.40
24	BB	5610	CLA	C3B-C2B	7.63	1.50	1.40
30	BA	5401	SQD	C4-C3	7.59	1.72	1.52
24	BC	5508	CLA	C3B-C2B	7.59	1.49	1.40
24	AA	407	CLA	C3B-C2B	7.56	1.49	1.40
24	AC	502	CLA	C3B-C2B	7.56	1.49	1.40
29	AA	412	LHG	P-O5	7.53	1.79	1.51
30	BA	5414	SQD	C4-C3	7.50	1.72	1.52
24	AC	504	CLA	C3B-C2B	7.49	1.49	1.40
31	AI	101	LMG	C23-C22	-7.49	1.52	1.55
24	AA	404	CLA	C3B-C2B	7.48	1.49	1.40
29	BA	5413	LHG	P-O5	7.46	1.79	1.51
30	BB	5601	SQD	C4-C3	7.44	1.72	1.52
24	BC	5504	CLA	C3B-C2B	7.44	1.49	1.40
30	BA	5414	SQD	C6-C5	-7.44	1.43	1.52
24	AD	401	CLA	C3B-C2B	7.41	1.49	1.40
30	AA	416	SQD	C4-C3	7.40	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	AF	101	HEM	C4A-C3A	7.38	1.55	1.43
31	BB	5624	LMG	C23-C22	-7.34	1.52	1.55
24	AB	602	CLA	C3B-C2B	7.31	1.49	1.40
35	BD	5406	PL9	C48-C49	7.28	1.55	1.32
30	BF	5102	SQD	C4-C3	7.26	1.71	1.52
24	AC	508	CLA	C3B-C2B	7.20	1.49	1.40
24	AC	508	CLA	C3B-C4B	7.21	1.49	1.41
24	BC	5508	CLA	C3B-C4B	7.19	1.49	1.41
24	BB	5612	CLA	C3B-C2B	7.18	1.49	1.40
24	AB	603	CLA	C3B-C4B	7.17	1.49	1.41
30	AF	102	SQD	C4-C3	7.13	1.71	1.52
35	AD	405	PL9	C48-C49	7.10	1.55	1.32
24	AC	507	CLA	C3B-C2B	7.08	1.49	1.40
36	BV	5201	HEM	C3D-C2D	-7.05	1.37	1.44
24	AB	601	CLA	C3C-C2C	7.02	1.51	1.36
24	AA	405	CLA	C3B-C2B	7.01	1.49	1.40
24	BB	5616	CLA	MG-NA	6.97	2.27	2.07
36	AV	201	HEM	C3D-C2D	-6.96	1.37	1.44
24	BB	5612	CLA	C3B-C4B	6.96	1.49	1.41
24	BB	5605	CLA	C3C-C2C	6.94	1.51	1.36
30	AA	413	SQD	C4-C3	6.90	1.70	1.52
24	BB	5607	CLA	MG-NA	6.89	2.27	2.07
24	AC	506	CLA	C3B-C4B	6.88	1.49	1.41
27	AJ	101	BCR	C30-C25	6.84	1.63	1.53
36	AF	101	HEM	O1D-CGD	6.82	1.46	1.22
24	AB	606	CLA	C3B-C2B	6.82	1.48	1.40
24	AD	404	CLA	C3C-C2C	6.82	1.51	1.36
24	BC	5504	CLA	C3C-C2C	6.81	1.51	1.36
36	BF	5101	HEM	O1D-CGD	6.78	1.45	1.22
24	BB	5611	CLA	C3B-C2B	6.77	1.48	1.40
24	BC	5506	CLA	C3B-C4B	6.77	1.49	1.41
24	AB	603	CLA	MG-NA	6.76	2.27	2.07
31	AA	417	LMG	C22-C21	-6.75	1.52	1.55
24	BC	5513	CLA	C3C-C2C	6.72	1.51	1.36
31	AB	621	LMG	C23-C22	-6.71	1.52	1.55
24	AB	603	CLA	C3C-C2C	6.70	1.51	1.36
24	BC	5511	CLA	C3C-C2C	6.68	1.51	1.36
36	AV	201	HEM	C4A-C3A	6.65	1.54	1.43
36	BV	5201	HEM	O1D-CGD	6.62	1.45	1.22
34	BD	5404	PHO	C3C-C2C	6.62	1.51	1.36
35	BD	5406	PL9	O2-C1	6.60	1.43	1.24
24	AC	513	CLA	C3C-C2C	6.60	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BD	5405	CLA	C3C-C2C	6.58	1.50	1.36
35	AD	405	PL9	O2-C1	6.58	1.43	1.24
24	AC	512	CLA	CHB-C4A	6.55	1.42	1.33
24	BB	5607	CLA	C3B-C4B	6.55	1.49	1.41
24	AB	604	CLA	C3C-C2C	6.52	1.50	1.36
36	AF	101	HEM	C3D-C2D	-6.51	1.37	1.44
24	AB	615	CLA	CHB-C4A	6.50	1.42	1.33
24	AB	601	CLA	CHB-C4A	6.50	1.42	1.33
24	BC	5509	CLA	C3C-C2C	6.49	1.50	1.36
24	AC	511	CLA	C3C-C2C	6.49	1.50	1.36
27	BJ	5101	BCR	C30-C25	6.47	1.63	1.53
24	BC	5512	CLA	CHB-C4A	6.45	1.42	1.33
24	BA	5405	CLA	C3C-C2C	6.42	1.50	1.36
24	BC	5512	CLA	C3C-C2C	6.41	1.50	1.36
24	BA	5408	CLA	C3C-C2C	6.40	1.50	1.36
24	AA	404	CLA	C3C-C2C	6.39	1.50	1.36
24	AB	614	CLA	C3B-C4B	6.39	1.48	1.41
24	BB	5612	CLA	C3C-C2C	6.38	1.50	1.36
24	BC	5502	CLA	C3C-C2C	6.38	1.50	1.36
24	BC	5511	CLA	C3B-C4B	6.38	1.48	1.41
24	BB	5616	CLA	C3C-C2C	6.37	1.50	1.36
24	BC	5505	CLA	C3C-C2C	6.35	1.50	1.36
24	AB	612	CLA	MG-NA	6.34	2.26	2.07
24	AC	505	CLA	C3C-C2C	6.33	1.50	1.36
36	AV	201	HEM	O1D-CGD	6.31	1.44	1.22
24	BB	5607	CLA	C3C-C2C	6.26	1.50	1.36
24	AB	605	CLA	C3B-C4B	6.25	1.48	1.41
24	AB	608	CLA	C3B-C4B	6.24	1.48	1.41
24	AD	401	CLA	C3B-C4B	6.24	1.48	1.41
24	AB	615	CLA	C3C-C2C	6.22	1.50	1.36
28	BC	5517	DGD	CEA-CDA	-6.21	1.52	1.55
24	BB	5605	CLA	CHB-C4A	6.21	1.41	1.33
24	AC	505	CLA	CAA-C2A	-6.21	1.42	1.54
24	BC	5506	CLA	C3C-C2C	6.20	1.50	1.36
24	BB	5618	CLA	C3C-C2C	6.20	1.50	1.36
24	AC	504	CLA	C3C-C2C	6.20	1.50	1.36
24	BB	5609	CLA	C3B-C4B	6.19	1.48	1.41
24	BA	5407	CLA	C3B-C4B	6.18	1.48	1.41
24	AB	608	CLA	C3C-C2C	6.18	1.50	1.36
24	AB	612	CLA	C3C-C2C	6.18	1.50	1.36
24	AC	512	CLA	C3B-C4B	6.17	1.48	1.41
24	BD	5402	CLA	C3C-C2C	6.17	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	407	CLA	C3C-C2C	6.15	1.50	1.36
34	AD	403	PHO	C3C-C2C	6.15	1.50	1.36
24	BC	5509	CLA	C3B-C4B	6.15	1.48	1.41
24	BB	5614	CLA	C3C-C2C	6.14	1.50	1.36
24	BA	5407	CLA	C3C-C2C	6.14	1.50	1.36
24	BB	5619	CLA	CHB-C4A	6.14	1.41	1.33
24	BB	5610	CLA	C3C-C2C	6.14	1.50	1.36
24	BC	5501	CLA	C3C-C2C	6.13	1.50	1.36
24	AB	610	CLA	C3C-C2C	6.13	1.50	1.36
24	AC	501	CLA	CHB-C4A	6.13	1.41	1.33
24	BA	5406	CLA	C3B-C4B	6.12	1.48	1.41
24	AB	602	CLA	C3B-C4B	6.12	1.48	1.41
24	BC	5505	CLA	C3B-C4B	6.11	1.48	1.41
28	AC	517	DGD	CEA-CDA	-6.11	1.52	1.55
24	AB	611	CLA	C3B-C4B	6.09	1.48	1.41
24	AA	404	CLA	C3B-C4B	6.08	1.48	1.41
31	BD	5409	LMG	C41-C40	-6.08	1.52	1.55
24	BB	5606	CLA	C3C-C2C	6.07	1.49	1.36
24	AD	401	CLA	C3C-C2C	6.06	1.49	1.36
24	AC	512	CLA	C3C-C2C	6.05	1.49	1.36
24	BC	5510	CLA	CHB-C4A	6.05	1.41	1.33
24	AB	613	CLA	C3B-C2B	6.03	1.47	1.40
24	BC	5503	CLA	C3B-C4B	6.01	1.48	1.41
24	BC	5512	CLA	C3B-C4B	5.99	1.48	1.41
34	AD	402	PHO	C3C-C2C	5.97	1.49	1.36
24	BC	5510	CLA	C3C-C2C	5.97	1.49	1.36
24	AB	602	CLA	C3C-C2C	5.96	1.49	1.36
24	BC	5503	CLA	C3C-C2C	5.95	1.49	1.36
24	AC	509	CLA	C3C-C2C	5.95	1.49	1.36
24	AC	506	CLA	C3C-C2C	5.94	1.49	1.36
31	AA	414	LMG	C22-C21	-5.93	1.52	1.55
24	AB	606	CLA	C3C-C2C	5.92	1.49	1.36
24	AC	503	CLA	C3C-C2C	5.91	1.49	1.36
31	BE	5101	LMG	C22-C21	-5.89	1.52	1.55
24	AA	407	CLA	C3B-C4B	5.89	1.48	1.41
36	BV	5201	HEM	C4A-C3A	5.88	1.52	1.43
29	AA	415	LHG	C18-C17	-5.87	1.52	1.55
24	AC	508	CLA	C3C-C2C	5.87	1.49	1.36
24	AB	614	CLA	C3C-C2C	5.86	1.49	1.36
24	BA	5408	CLA	C3B-C4B	5.85	1.48	1.41
24	AC	511	CLA	C3B-C4B	5.85	1.48	1.41
28	BA	5412	DGD	O5D-C1E	5.84	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	501	CLA	C3C-C2C	5.84	1.49	1.36
24	BA	5406	CLA	C3C-C2C	5.84	1.49	1.36
29	AA	415	LHG	C30-C29	-5.83	1.52	1.55
27	BJ	5101	BCR	C5-C6	5.83	1.43	1.34
24	BB	5608	CLA	C3C-C2C	5.82	1.49	1.36
24	AB	609	CLA	C3B-C4B	5.81	1.48	1.41
24	BB	5608	CLA	C3B-C4B	5.81	1.48	1.41
29	BA	5415	LHG	C30-C29	-5.80	1.52	1.55
24	AC	510	CLA	CHB-C4A	5.79	1.41	1.33
24	AC	504	CLA	C3B-C4B	5.78	1.48	1.41
24	BD	5402	CLA	C3B-C4B	5.78	1.48	1.41
24	BC	5508	CLA	C3C-C2C	5.77	1.49	1.36
34	BD	5403	PHO	C3C-C2C	5.76	1.49	1.36
24	BB	5611	CLA	C3B-C4B	5.76	1.48	1.41
24	AB	607	CLA	C3C-C2C	5.76	1.49	1.36
24	AB	609	CLA	C3C-C2C	5.74	1.49	1.36
24	AA	406	CLA	C3B-C4B	5.73	1.48	1.41
24	AC	505	CLA	CHB-C4A	5.73	1.41	1.33
24	AB	612	CLA	C3B-C4B	5.72	1.48	1.41
24	BB	5615	CLA	C3B-C4B	5.72	1.48	1.41
24	AA	405	CLA	C3B-C4B	5.72	1.48	1.41
24	BB	5616	CLA	C3B-C4B	5.72	1.48	1.41
24	BB	5620	CLA	CHB-C4A	5.71	1.41	1.33
27	AJ	101	BCR	C5-C6	5.70	1.43	1.34
24	BC	5504	CLA	C3B-C4B	5.70	1.48	1.41
24	BB	5619	CLA	C3C-C2C	5.70	1.49	1.36
24	BB	5615	CLA	C3C-C2C	5.68	1.49	1.36
27	BC	5514	BCR	C1-C6	5.68	1.61	1.53
28	AA	411	DGD	O5D-C1E	5.67	1.50	1.40
29	BA	5415	LHG	C18-C17	-5.66	1.52	1.55
31	BL	5101	LMG	O7-C8	-5.66	1.32	1.46
24	BC	5513	CLA	C3B-C4B	5.65	1.48	1.41
34	AD	402	PHO	C1D-CHD	5.64	1.41	1.35
24	BB	5618	CLA	C3B-C4B	5.63	1.48	1.41
24	BC	5505	CLA	CHB-C4A	5.63	1.41	1.33
24	BB	5610	CLA	C3B-C4B	5.61	1.47	1.41
24	AB	601	CLA	O2D-CGD	5.60	1.47	1.33
24	BC	5510	CLA	C3B-C4B	5.59	1.47	1.41
24	AC	510	CLA	C3C-C2C	5.59	1.48	1.36
24	AB	605	CLA	CHB-C4A	5.59	1.40	1.33
24	BB	5617	CLA	C3C-C2C	5.58	1.48	1.36
27	AB	619	BCR	C30-C25	5.58	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AC	517	DGD	C9B-C8B	-5.57	1.52	1.55
34	BD	5404	PHO	C3B-C4B	5.57	1.47	1.41
24	AB	613	CLA	C3B-C4B	5.56	1.47	1.41
24	AB	613	CLA	C3C-C2C	5.55	1.48	1.36
24	AC	503	CLA	C3B-C4B	5.53	1.47	1.41
24	BA	5405	CLA	C3B-C4B	5.53	1.47	1.41
27	BB	5622	BCR	C1-C6	5.52	1.61	1.53
27	BK	5102	BCR	C30-C25	5.52	1.61	1.53
24	AA	406	CLA	C3C-C2C	5.51	1.48	1.36
24	BB	5620	CLA	C3C-C2C	5.50	1.48	1.36
24	BB	5613	CLA	C3C-C2C	5.50	1.48	1.36
34	BD	5403	PHO	C1D-CHD	5.49	1.41	1.35
24	AB	605	CLA	C3C-C2C	5.49	1.48	1.36
24	AC	509	CLA	C3B-C4B	5.48	1.47	1.41
24	BC	5501	CLA	CHB-C4A	5.48	1.40	1.33
24	BB	5605	CLA	MG-NA	5.47	2.23	2.07
24	AB	606	CLA	C3B-C4B	5.47	1.47	1.41
24	AC	502	CLA	C3C-C2C	5.46	1.48	1.36
24	AB	607	CLA	C3B-C4B	5.45	1.47	1.41
24	AD	404	CLA	CHB-C4A	5.45	1.40	1.33
27	BX	5101	BCR	C26-C25	5.44	1.43	1.34
31	BA	5402	LMG	C22-C21	-5.44	1.53	1.55
24	BB	5617	CLA	C3B-C2B	5.43	1.47	1.40
31	BB	5624	LMG	C43-C42	-5.43	1.53	1.55
24	BC	5508	CLA	O2D-CGD	5.42	1.47	1.33
24	AB	607	CLA	C3B-C2B	5.41	1.47	1.40
24	AC	502	CLA	C3B-C4B	5.41	1.47	1.41
24	BB	5605	CLA	O2D-CGD	5.38	1.47	1.33
36	BV	5201	HEM	C3C-CAC	5.38	1.58	1.40
24	AB	611	CLA	C3C-C2C	5.38	1.48	1.36
27	AX	101	BCR	C26-C25	5.38	1.42	1.34
27	BC	5514	BCR	C30-C25	5.37	1.61	1.53
31	BL	5101	LMG	O1-C1	5.37	1.49	1.40
27	AB	618	BCR	C1-C6	5.36	1.61	1.53
24	BB	5606	CLA	C3B-C4B	5.36	1.47	1.41
31	AD	407	LMG	C41-C40	-5.35	1.53	1.55
36	BF	5101	HEM	C3C-C2C	5.35	1.51	1.45
24	BB	5613	CLA	C3B-C4B	5.34	1.47	1.41
24	AC	507	CLA	C3C-C2C	5.34	1.48	1.36
27	BT	5101	BCR	C1-C6	5.33	1.61	1.53
24	AC	503	CLA	CHB-C4A	5.32	1.40	1.33
31	BC	5520	LMG	C23-C22	-5.31	1.53	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5404	PHO	C1D-CHD	5.30	1.41	1.35
27	BC	5515	BCR	C30-C25	5.29	1.61	1.53
24	AB	616	CLA	CHB-C4A	5.28	1.40	1.33
31	AB	620	LMG	O7-C8	-5.28	1.33	1.46
27	AK	102	BCR	C30-C25	5.28	1.61	1.53
24	BC	5507	CLA	C3C-C2C	5.28	1.48	1.36
24	BB	5609	CLA	C3C-C2C	5.26	1.48	1.36
27	BD	5407	BCR	C30-C25	5.25	1.61	1.53
24	BB	5619	CLA	C3B-C4B	5.24	1.47	1.41
27	AB	619	BCR	C1-C6	5.24	1.61	1.53
24	AB	616	CLA	C3C-C2C	5.23	1.48	1.36
24	AB	615	CLA	C3B-C4B	5.22	1.47	1.41
24	AC	505	CLA	C3B-C4B	5.22	1.47	1.41
27	AC	515	BCR	C30-C25	5.21	1.61	1.53
31	AB	620	LMG	O1-C1	5.19	1.49	1.40
24	AA	405	CLA	C3C-C2C	5.19	1.47	1.36
24	BC	5501	CLA	C3B-C4B	5.19	1.47	1.41
24	BC	5505	CLA	CAA-C2A	-5.19	1.44	1.54
24	AB	605	CLA	O2D-CGD	5.19	1.46	1.33
24	BC	5513	CLA	O2D-CGD	5.18	1.46	1.33
31	AC	520	LMG	C23-C22	-5.17	1.53	1.55
24	AC	510	CLA	C3B-C4B	5.16	1.47	1.41
28	BC	5518	DGD	CEA-CDA	-5.13	1.53	1.55
36	AF	101	HEM	C3C-CAC	5.13	1.57	1.40
24	BB	5607	CLA	C3B-C2B	5.12	1.46	1.40
27	BA	5411	BCR	C1-C6	5.10	1.61	1.53
27	AJ	101	BCR	C1-C6	5.09	1.61	1.53
31	AC	521	LMG	C40-C39	-5.08	1.53	1.55
27	BD	5407	BCR	C26-C25	5.07	1.42	1.34
27	BC	5515	BCR	C1-C6	5.05	1.61	1.53
34	AD	403	PHO	C3B-C4B	5.05	1.47	1.41
27	BK	5102	BCR	C5-C6	5.05	1.42	1.34
36	BF	5101	HEM	C3C-CAC	5.05	1.56	1.40
27	BX	5101	BCR	C30-C25	5.03	1.61	1.53
24	BC	5506	CLA	O2D-CGD	5.02	1.46	1.33
24	BC	5502	CLA	C3B-C4B	5.02	1.47	1.41
24	AB	601	CLA	MG-NA	5.01	2.22	2.07
28	BA	5412	DGD	O6D-C1D	4.99	1.54	1.41
24	AC	506	CLA	O2D-CGD	4.97	1.46	1.33
24	BC	5509	CLA	CHB-C4A	4.97	1.40	1.33
24	AC	509	CLA	O2D-CGD	4.97	1.46	1.33
27	AB	618	BCR	C26-C25	4.97	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	513	CLA	O2D-CGD	4.96	1.46	1.33
27	AC	514	BCR	C30-C25	4.94	1.60	1.53
36	AV	201	HEM	C3C-CAC	4.94	1.56	1.40
36	BF	5101	HEM	C3B-C2B	4.94	1.51	1.45
24	BC	5503	CLA	CHB-C4A	4.92	1.40	1.33
27	BT	5101	BCR	C5-C6	4.91	1.42	1.34
24	AB	616	CLA	C3B-C4B	4.91	1.47	1.41
28	AC	519	DGD	O6D-C1D	4.90	1.54	1.41
31	AB	621	LMG	C43-C42	-4.89	1.53	1.55
24	BD	5405	CLA	CHB-C4A	4.89	1.40	1.33
27	AB	618	BCR	C30-C25	4.88	1.60	1.53
24	AB	609	CLA	CHB-C4A	4.87	1.40	1.33
24	AB	603	CLA	C3B-C2B	4.87	1.46	1.40
27	BB	5622	BCR	C30-C25	4.87	1.60	1.53
24	AC	513	CLA	C3B-C4B	4.86	1.47	1.41
27	BB	5623	BCR	C1-C6	4.85	1.60	1.53
24	BA	5408	CLA	CHB-C4A	4.85	1.39	1.33
24	BB	5618	CLA	O2D-CGD	4.84	1.45	1.33
24	BB	5617	CLA	C3B-C4B	4.83	1.47	1.41
24	BB	5611	CLA	C3C-C2C	4.83	1.47	1.36
24	AB	613	CLA	CHB-C4A	4.83	1.39	1.33
27	AD	406	BCR	C26-C25	4.82	1.42	1.34
24	BB	5609	CLA	O2D-CGD	4.81	1.45	1.33
28	BC	5519	DGD	O6D-C1D	4.81	1.54	1.41
27	AJ	101	BCR	C14-C13	4.81	1.42	1.35
24	BB	5620	CLA	O2D-CGD	4.81	1.45	1.33
27	BJ	5101	BCR	C1-C6	4.81	1.60	1.53
27	BC	5516	BCR	C5-C6	4.80	1.42	1.34
27	AX	101	BCR	C30-C25	4.79	1.60	1.53
24	BC	5507	CLA	O2D-CGD	4.78	1.45	1.33
24	AB	604	CLA	C3B-C4B	4.79	1.46	1.41
24	AB	614	CLA	CHB-C4A	4.78	1.39	1.33
24	AC	501	CLA	C3B-C4B	4.77	1.46	1.41
24	AB	606	CLA	O2D-CGD	4.77	1.45	1.33
27	BC	5516	BCR	C1-C6	4.76	1.60	1.53
24	AB	602	CLA	CHB-C4A	4.76	1.39	1.33
24	AA	404	CLA	O2D-CGD	4.75	1.45	1.33
28	BB	5602	DGD	O5D-C1E	4.75	1.48	1.40
36	AV	201	HEM	C2C-C1C	4.74	1.53	1.45
28	BH	5101	DGD	CFA-CEA	-4.72	1.53	1.55
34	BD	5403	PHO	O2D-CGD	4.72	1.45	1.33
28	BC	5517	DGD	O5D-C1E	4.71	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	610	CLA	O2D-CGD	4.71	1.45	1.33
24	BC	5511	CLA	C1B-NB	4.71	1.42	1.34
36	AF	101	HEM	C2C-C1C	4.71	1.53	1.45
24	AB	609	CLA	O2D-CGD	4.71	1.45	1.33
24	BB	5608	CLA	CHB-C4A	4.70	1.39	1.33
24	BB	5617	CLA	CHB-C4A	4.70	1.39	1.33
27	AT	101	BCR	C1-C6	4.69	1.60	1.53
28	BC	5518	DGD	O6D-C1D	4.69	1.53	1.41
36	BF	5101	HEM	C2C-C1C	4.68	1.53	1.45
34	AD	403	PHO	C1D-CHD	4.67	1.40	1.35
24	AC	507	CLA	C4C-C3C	4.67	1.53	1.45
24	AB	616	CLA	O2D-CGD	4.67	1.45	1.33
24	BB	5612	CLA	O2A-CGA	4.66	1.47	1.33
24	BC	5501	CLA	O2D-CGD	4.66	1.45	1.33
28	BC	5517	DGD	O6D-C1D	4.64	1.53	1.41
24	BB	5609	CLA	CHB-C4A	4.64	1.39	1.33
24	BB	5607	CLA	O2D-CGD	4.64	1.45	1.33
24	BB	5613	CLA	O2D-CGD	4.64	1.45	1.33
24	AB	608	CLA	O2A-CGA	4.63	1.47	1.33
30	AB	622	SQD	O8-S	4.63	1.58	1.46
27	AA	410	BCR	C1-C6	4.63	1.60	1.53
28	AH	101	DGD	CFA-CEA	-4.60	1.53	1.55
36	BV	5201	HEM	C2C-C1C	4.60	1.53	1.45
24	BC	5502	CLA	C1B-NB	4.59	1.41	1.34
24	BB	5615	CLA	O2D-CGD	4.58	1.45	1.33
24	AC	506	CLA	C1B-NB	4.58	1.41	1.34
24	AB	610	CLA	CHB-C4A	4.58	1.39	1.33
24	AB	614	CLA	O2D-CGD	4.57	1.45	1.33
24	BC	5502	CLA	O2D-CGD	4.55	1.45	1.33
28	BB	5602	DGD	CDB-CCB	-4.54	1.53	1.55
27	AX	101	BCR	C1-C6	4.54	1.60	1.53
35	BD	5406	PL9	C6-C1	-4.53	1.39	1.48
31	BC	5521	LMG	C40-C39	-4.53	1.53	1.55
28	AH	101	DGD	CDB-CCB	-4.53	1.53	1.55
24	BB	5610	CLA	O2D-CGD	4.52	1.44	1.33
24	BC	5510	CLA	O2D-CGD	4.52	1.44	1.33
27	AJ	101	BCR	C26-C25	4.52	1.41	1.34
24	BB	5614	CLA	C4C-C3C	4.52	1.53	1.45
24	AB	615	CLA	C1A-NA	4.52	1.42	1.32
24	BC	5509	CLA	O2D-CGD	4.52	1.44	1.33
24	AB	606	CLA	C4D-C3D	4.51	1.53	1.42
24	BC	5510	CLA	C4D-C3D	4.51	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5612	CLA	CHB-C4A	4.51	1.39	1.33
24	BC	5511	CLA	O2D-CGD	4.51	1.44	1.33
24	BC	5503	CLA	C4D-C3D	4.51	1.53	1.42
24	BD	5402	CLA	C1C-C2C	4.50	1.53	1.44
27	BJ	5101	BCR	C26-C25	4.51	1.41	1.34
24	BB	5615	CLA	C4D-C3D	4.50	1.53	1.42
24	AC	512	CLA	C4D-C3D	4.50	1.53	1.42
24	AB	601	CLA	C4D-C3D	4.50	1.53	1.42
24	BB	5605	CLA	C1B-NB	4.50	1.41	1.34
36	AF	101	HEM	C3B-C2B	4.49	1.50	1.45
24	BB	5618	CLA	C4D-C3D	4.49	1.53	1.42
24	AA	407	CLA	C4D-C3D	4.49	1.53	1.42
24	BC	5512	CLA	C4D-C3D	4.49	1.53	1.42
24	BC	5509	CLA	C4D-C3D	4.49	1.53	1.42
30	BB	5625	SQD	O8-S	4.49	1.58	1.46
24	AC	513	CLA	C4D-C3D	4.48	1.53	1.42
24	BB	5605	CLA	C4D-C3D	4.48	1.53	1.42
24	BB	5606	CLA	C4D-C3D	4.48	1.53	1.42
24	BB	5619	CLA	C1A-NA	4.48	1.42	1.32
24	BB	5610	CLA	C4D-C3D	4.48	1.53	1.42
24	AC	509	CLA	CHB-C4A	4.48	1.39	1.33
24	AC	502	CLA	C4D-C3D	4.48	1.53	1.42
24	BD	5405	CLA	O2D-CGD	4.47	1.44	1.33
24	AD	401	CLA	C1C-C2C	4.47	1.53	1.44
28	AC	518	DGD	O6D-C1D	4.47	1.53	1.41
24	AC	508	CLA	C4D-C3D	4.47	1.53	1.42
24	BC	5513	CLA	C4D-C3D	4.47	1.53	1.42
24	AC	506	CLA	C4D-C3D	4.47	1.53	1.42
24	AB	614	CLA	C4D-C3D	4.47	1.53	1.42
24	AB	602	CLA	C4D-C3D	4.47	1.53	1.42
24	AB	616	CLA	C4D-C3D	4.46	1.53	1.42
35	AD	405	PL9	C6-C1	-4.47	1.39	1.48
24	AC	507	CLA	C4D-C3D	4.46	1.53	1.42
24	AB	608	CLA	C4D-C3D	4.46	1.53	1.42
29	BA	5413	LHG	P-O3	4.46	1.79	1.59
24	AC	504	CLA	C4D-C3D	4.46	1.53	1.42
24	BB	5614	CLA	C4D-C3D	4.46	1.53	1.42
24	BC	5507	CLA	C4D-C3D	4.46	1.53	1.42
24	BD	5405	CLA	C4D-C3D	4.46	1.53	1.42
24	AC	511	CLA	C4D-C3D	4.45	1.53	1.42
24	AB	607	CLA	C4D-C3D	4.46	1.53	1.42
36	AV	201	HEM	CBC-CAC	4.45	1.54	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AD	404	CLA	C4D-C3D	4.45	1.52	1.42
24	BA	5405	CLA	C4D-C3D	4.45	1.52	1.42
24	AC	505	CLA	C1C-C2C	4.45	1.53	1.44
24	BC	5505	CLA	C4D-C3D	4.45	1.52	1.42
24	BB	5605	CLA	C1A-NA	4.45	1.42	1.32
24	AB	605	CLA	C4D-C3D	4.45	1.52	1.42
24	AB	612	CLA	C4D-C3D	4.45	1.52	1.42
34	AD	403	PHO	O2D-CGD	4.45	1.44	1.33
36	BV	5201	HEM	CBC-CAC	4.45	1.54	1.29
24	BA	5405	CLA	C1C-C2C	4.45	1.53	1.44
24	BB	5618	CLA	CHB-C4A	4.45	1.39	1.33
24	BC	5511	CLA	C4D-C3D	4.45	1.52	1.42
24	BB	5617	CLA	C4D-C3D	4.45	1.52	1.42
24	AA	404	CLA	C4D-C3D	4.45	1.52	1.42
31	AI	101	LMG	C37-C36	-4.45	1.53	1.55
24	BB	5618	CLA	C1C-C2C	4.45	1.53	1.44
24	AC	509	CLA	C4D-C3D	4.45	1.52	1.42
24	AB	615	CLA	C4D-C3D	4.44	1.52	1.42
24	AC	505	CLA	C4D-C3D	4.44	1.52	1.42
24	BC	5508	CLA	C4D-C3D	4.44	1.52	1.42
24	BB	5612	CLA	C4D-C3D	4.44	1.52	1.42
24	AB	610	CLA	C4D-C3D	4.44	1.52	1.42
24	BC	5501	CLA	C1A-NA	4.44	1.42	1.32
24	BB	5619	CLA	C4D-C3D	4.44	1.52	1.42
24	BB	5611	CLA	C4D-C3D	4.44	1.52	1.42
24	AC	506	CLA	CHB-C4A	4.44	1.39	1.33
24	BB	5608	CLA	C4D-C3D	4.43	1.52	1.42
31	BM	5102	LMG	C37-C36	-4.43	1.53	1.55
24	BB	5609	CLA	C4D-C3D	4.43	1.52	1.42
24	BA	5405	CLA	O2D-CGD	4.43	1.44	1.33
24	AB	603	CLA	C4D-C3D	4.43	1.52	1.42
24	AC	510	CLA	C4D-C3D	4.43	1.52	1.42
24	BA	5408	CLA	C4D-C3D	4.43	1.52	1.42
24	BA	5406	CLA	C1C-C2C	4.43	1.53	1.44
24	AB	614	CLA	C1C-C2C	4.43	1.53	1.44
24	AB	611	CLA	C4D-C3D	4.43	1.52	1.42
24	AC	508	CLA	O2D-CGD	4.43	1.44	1.33
24	BC	5513	CLA	C1C-C2C	4.43	1.53	1.44
27	BC	5515	BCR	C26-C25	4.43	1.41	1.34
28	BE	5102	DGD	O3G-C1D	4.43	1.48	1.40
24	AC	505	CLA	MG-NA	4.43	2.20	2.07
24	BA	5408	CLA	C1C-C2C	4.43	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5512	CLA	C4C-C3C	4.42	1.53	1.45
24	AD	404	CLA	C3B-C4B	4.42	1.46	1.41
24	BC	5504	CLA	C4D-C3D	4.42	1.52	1.42
24	BC	5506	CLA	C4D-C3D	4.42	1.52	1.42
24	BB	5613	CLA	C4D-C3D	4.42	1.52	1.42
24	BB	5620	CLA	C3B-C4B	4.42	1.46	1.41
24	BC	5506	CLA	C1C-C2C	4.42	1.53	1.44
30	BB	5625	SQD	O47-C7	4.42	1.47	1.34
24	AC	503	CLA	C4D-C3D	4.42	1.52	1.42
24	BB	5606	CLA	CHB-C4A	4.42	1.39	1.33
24	BA	5406	CLA	C4D-C3D	4.42	1.52	1.42
24	AC	506	CLA	C1C-C2C	4.42	1.53	1.44
24	BB	5620	CLA	C4D-C3D	4.42	1.52	1.42
24	BC	5502	CLA	C4D-C3D	4.41	1.52	1.42
24	AB	613	CLA	C4D-C3D	4.41	1.52	1.42
30	BF	5102	SQD	O5-C5	4.41	1.55	1.44
24	AA	405	CLA	C1C-C2C	4.41	1.53	1.44
24	BD	5405	CLA	C3B-C4B	4.41	1.46	1.41
24	BB	5616	CLA	C4D-C3D	4.41	1.52	1.42
24	AC	501	CLA	C4D-C3D	4.41	1.52	1.42
24	BC	5509	CLA	C1B-NB	4.41	1.41	1.34
24	BC	5505	CLA	C1C-C2C	4.40	1.53	1.44
24	BC	5501	CLA	C4D-C3D	4.40	1.52	1.42
24	BD	5402	CLA	C4D-C3D	4.40	1.52	1.42
24	BC	5510	CLA	C1C-C2C	4.40	1.53	1.44
24	AB	604	CLA	C1C-C2C	4.40	1.53	1.44
24	BB	5607	CLA	C4D-C3D	4.40	1.52	1.42
24	BC	5511	CLA	C1C-C2C	4.39	1.53	1.44
24	AC	513	CLA	C1C-C2C	4.39	1.53	1.44
36	BV	5201	HEM	C3B-C2B	4.39	1.50	1.45
24	AB	609	CLA	C4D-C3D	4.39	1.52	1.42
27	AC	515	BCR	C26-C25	4.39	1.41	1.34
24	BB	5611	CLA	C1C-C2C	4.39	1.53	1.44
30	BA	5401	SQD	O5-C5	4.38	1.55	1.44
24	AC	509	CLA	C1C-C2C	4.38	1.53	1.44
24	AA	406	CLA	C4D-C3D	4.38	1.52	1.42
24	AB	608	CLA	C1C-C2C	4.38	1.53	1.44
24	AB	604	CLA	C4D-C3D	4.38	1.52	1.42
24	AB	607	CLA	C1C-C2C	4.38	1.53	1.44
36	BF	5101	HEM	CBB-CAB	4.38	1.53	1.29
24	BA	5407	CLA	C4D-C3D	4.38	1.52	1.42
24	BC	5504	CLA	C1C-C2C	4.38	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BI	5101	LMG	C37-C36	-4.38	1.53	1.55
24	AB	608	CLA	CHB-C4A	4.38	1.39	1.33
24	AB	605	CLA	C1B-NB	4.38	1.41	1.34
24	AA	404	CLA	C1C-C2C	4.37	1.53	1.44
24	AA	407	CLA	C1C-C2C	4.37	1.53	1.44
30	AF	102	SQD	O5-C5	4.37	1.55	1.44
24	AC	501	CLA	C1A-NA	4.37	1.41	1.32
27	AK	102	BCR	C5-C6	4.37	1.41	1.34
24	AA	405	CLA	C4D-C3D	4.37	1.52	1.42
24	AC	511	CLA	C1C-C2C	4.37	1.53	1.44
24	BC	5508	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	605	CLA	C1C-C2C	4.36	1.53	1.44
24	AD	404	CLA	C1C-C2C	4.36	1.53	1.44
24	AC	503	CLA	C1C-C2C	4.36	1.53	1.44
28	AA	411	DGD	O6D-C1D	4.36	1.53	1.41
24	BB	5614	CLA	CHB-C4A	4.36	1.39	1.33
24	AB	613	CLA	C1C-C2C	4.36	1.53	1.44
24	BB	5613	CLA	C1C-C2C	4.36	1.53	1.44
24	BC	5502	CLA	C1C-C2C	4.36	1.53	1.44
27	BB	5623	BCR	C30-C25	4.36	1.60	1.53
24	BB	5616	CLA	C1C-C2C	4.36	1.53	1.44
24	AA	406	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	602	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	610	CLA	C4C-C3C	4.36	1.53	1.45
24	AB	603	CLA	C1C-C2C	4.36	1.53	1.44
30	BB	5625	SQD	C16-C17	-4.35	1.35	1.52
24	BB	5612	CLA	C1C-C2C	4.35	1.53	1.44
24	AB	611	CLA	C1C-C2C	4.35	1.53	1.44
24	AB	609	CLA	C1C-C2C	4.35	1.53	1.44
24	AC	508	CLA	C1C-C2C	4.35	1.53	1.44
24	BB	5614	CLA	C3B-C4B	4.35	1.46	1.41
24	BC	5507	CLA	C1C-C2C	4.35	1.53	1.44
24	BA	5405	CLA	C4C-C3C	4.35	1.53	1.45
24	AC	502	CLA	O2D-CGD	4.35	1.44	1.33
24	AD	401	CLA	C4D-C3D	4.35	1.52	1.42
24	BB	5607	CLA	C1C-C2C	4.35	1.53	1.44
36	BF	5101	HEM	CBC-CAC	4.35	1.53	1.29
24	AB	601	CLA	C1B-NB	4.35	1.41	1.34
24	AC	510	CLA	C1C-C2C	4.35	1.53	1.44
27	BC	5515	BCR	C5-C6	4.35	1.41	1.34
27	BA	5411	BCR	C30-C25	4.35	1.60	1.53
24	BC	5509	CLA	C1C-C2C	4.35	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	507	CLA	C1C-C2C	4.34	1.53	1.44
24	AB	612	CLA	C1C-C2C	4.34	1.53	1.44
24	BC	5503	CLA	C1C-C2C	4.34	1.53	1.44
24	AB	601	CLA	C1C-C2C	4.34	1.53	1.44
29	AA	412	LHG	P-O3	4.34	1.78	1.59
31	BA	5402	LMG	C37-C36	-4.34	1.53	1.55
24	AB	610	CLA	C1C-C2C	4.34	1.53	1.44
24	BB	5617	CLA	C1C-C2C	4.34	1.53	1.44
24	BC	5512	CLA	C1C-C2C	4.34	1.53	1.44
24	AB	616	CLA	C1C-C2C	4.34	1.53	1.44
24	AB	602	CLA	C4C-C3C	4.33	1.53	1.45
24	AB	615	CLA	C1C-C2C	4.34	1.53	1.44
24	BD	5402	CLA	C4C-C3C	4.33	1.53	1.45
24	BB	5608	CLA	C1C-C2C	4.33	1.53	1.44
24	BA	5407	CLA	C1C-C2C	4.33	1.53	1.44
30	BB	5601	SQD	O8-S	4.33	1.57	1.46
24	BB	5606	CLA	C1C-C2C	4.33	1.53	1.44
30	AB	622	SQD	C16-C17	-4.33	1.35	1.52
34	BD	5404	PHO	O2D-CGD	4.33	1.44	1.33
24	AC	512	CLA	C1C-C2C	4.33	1.53	1.44
24	AC	501	CLA	C1C-C2C	4.32	1.53	1.44
32	BB	5603	LMT	C1B-C2B	-4.32	1.39	1.52
24	BB	5614	CLA	C1C-C2C	4.32	1.53	1.44
24	BB	5609	CLA	C1C-C2C	4.32	1.53	1.44
24	BB	5616	CLA	C4C-C3C	4.32	1.52	1.45
32	BD	5411	LMT	C1B-C2B	-4.32	1.39	1.52
28	BE	5102	DGD	CFA-CEA	-4.32	1.53	1.55
24	BB	5619	CLA	C1C-C2C	4.32	1.53	1.44
27	BJ	5101	BCR	C14-C13	4.32	1.41	1.35
28	AC	517	DGD	O6D-C1D	4.32	1.52	1.41
32	AB	624	LMT	C1B-C2B	-4.32	1.39	1.52
24	BD	5405	CLA	C1C-C2C	4.31	1.53	1.44
32	AB	629	LMT	C1B-C2B	-4.31	1.39	1.52
24	AC	504	CLA	C1C-C2C	4.31	1.53	1.44
36	AF	101	HEM	CBB-CAB	4.31	1.53	1.29
24	BC	5501	CLA	C1C-C2C	4.31	1.53	1.44
24	BB	5605	CLA	C1C-C2C	4.31	1.53	1.44
27	BB	5622	BCR	C26-C25	4.30	1.41	1.34
32	AD	409	LMT	C1B-C2B	-4.30	1.39	1.52
32	AI	103	LMT	C1B-C2B	-4.30	1.39	1.52
30	AF	102	SQD	C1-C2	4.30	1.65	1.52
24	BC	5506	CLA	C1B-NB	4.30	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	5627	LMT	C1B-C2B	-4.30	1.39	1.52
24	AB	606	CLA	C1C-C2C	4.30	1.53	1.44
36	BV	5201	HEM	CBB-CAB	4.30	1.53	1.29
32	BB	5604	LMT	C1B-C2B	-4.30	1.39	1.52
34	AD	403	PHO	C4C-C3C	4.30	1.53	1.45
24	BC	5504	CLA	O2D-CGD	4.30	1.44	1.33
24	AB	603	CLA	O2A-CGA	4.30	1.46	1.33
24	AB	604	CLA	C1A-NA	4.30	1.41	1.32
30	BF	5102	SQD	O47-C7	4.29	1.47	1.34
24	BC	5510	CLA	C1B-NB	4.29	1.41	1.34
24	BB	5615	CLA	C1C-C2C	4.29	1.53	1.44
24	BB	5610	CLA	C1C-C2C	4.29	1.53	1.44
32	BM	5101	LMT	C1B-C2B	-4.29	1.39	1.52
32	AI	102	LMT	C1B-C2B	-4.29	1.39	1.52
32	AB	630	LMT	C1B-C2B	-4.28	1.39	1.52
30	BA	5414	SQD	O47-C7	4.28	1.47	1.34
32	BI	5102	LMT	C1B-C2B	-4.28	1.39	1.52
24	BB	5606	CLA	O2D-CGD	4.28	1.44	1.33
31	AA	417	LMG	C37-C36	-4.27	1.53	1.55
32	AM	102	LMT	C1B-C2B	-4.27	1.39	1.52
24	BD	5402	CLA	O2D-CGD	4.27	1.44	1.33
24	AC	502	CLA	C1C-C2C	4.27	1.53	1.44
27	AT	101	BCR	C5-C6	4.27	1.41	1.34
32	BB	5626	LMT	C1B-C2B	-4.27	1.39	1.52
24	BC	5513	CLA	C1B-NB	4.27	1.41	1.34
24	BB	5620	CLA	C1C-C2C	4.26	1.53	1.44
32	BC	5522	LMT	C1B-C2B	-4.26	1.39	1.52
27	AC	514	BCR	C1-C6	4.26	1.59	1.53
34	BD	5403	PHO	C4D-CHA	-4.25	1.37	1.44
32	AB	623	LMT	C1B-C2B	-4.25	1.39	1.52
24	AB	614	CLA	C1B-NB	4.24	1.41	1.34
24	BB	5610	CLA	C4C-C3C	4.24	1.52	1.45
24	BC	5505	CLA	O2D-CGD	4.24	1.44	1.33
24	AB	601	CLA	C4C-C3C	4.24	1.52	1.45
24	BB	5615	CLA	CHB-C4A	4.23	1.39	1.33
24	BC	5512	CLA	O2D-CGD	4.23	1.44	1.33
24	AC	507	CLA	O2D-CGD	4.23	1.44	1.33
24	BC	5507	CLA	C4C-C3C	4.23	1.52	1.45
24	AC	510	CLA	O2D-CGD	4.23	1.44	1.33
24	BC	5511	CLA	CHB-C4A	4.22	1.39	1.33
24	BD	5402	CLA	CHB-C4A	4.23	1.39	1.33
28	AE	101	DGD	CFA-CEA	-4.22	1.53	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	AM	101	LMG	C37-C36	-4.22	1.53	1.55
24	AB	602	CLA	O2D-CGD	4.22	1.44	1.33
24	AC	512	CLA	C4C-C3C	4.22	1.52	1.45
24	AB	606	CLA	C4C-C3C	4.21	1.52	1.45
24	BC	5503	CLA	O2D-CGD	4.21	1.44	1.33
31	AJ	102	LMG	C22-C21	-4.21	1.53	1.55
36	AF	101	HEM	C3C-C2C	4.21	1.50	1.45
30	BA	5401	SQD	O47-C7	4.21	1.47	1.34
27	BT	5101	BCR	C30-C25	4.21	1.59	1.53
27	BX	5101	BCR	C1-C6	4.21	1.59	1.53
24	BB	5618	CLA	C4C-C3C	4.20	1.52	1.45
30	AA	413	SQD	O8-S	4.20	1.57	1.46
24	AB	611	CLA	O2D-CGD	4.20	1.44	1.33
27	AD	406	BCR	C30-C25	4.20	1.59	1.53
24	AC	510	CLA	C4C-C3C	4.20	1.52	1.45
36	AF	101	HEM	CBC-CAC	4.20	1.52	1.29
30	AB	627	SQD	O8-S	4.20	1.57	1.46
30	BA	5414	SQD	O8-S	4.20	1.57	1.46
24	BC	5513	CLA	C4C-C3C	4.19	1.52	1.45
24	AB	616	CLA	C1A-NA	4.19	1.41	1.32
24	BB	5609	CLA	C1B-NB	4.19	1.41	1.34
24	BB	5613	CLA	C1B-NB	4.18	1.41	1.34
24	BC	5505	CLA	C1B-NB	4.18	1.41	1.34
24	AC	512	CLA	O2D-CGD	4.17	1.44	1.33
24	AD	401	CLA	CHB-C4A	4.17	1.39	1.33
27	BK	5102	BCR	C26-C25	4.17	1.41	1.34
27	AB	617	BCR	C26-C25	4.17	1.41	1.34
28	AC	518	DGD	CEA-CDA	-4.17	1.53	1.55
30	BB	5625	SQD	O5-C5	4.16	1.54	1.44
24	BB	5620	CLA	C1A-NA	4.16	1.41	1.32
24	BB	5608	CLA	O2D-CGD	4.15	1.43	1.33
30	AB	622	SQD	O5-C5	4.15	1.54	1.44
30	AA	413	SQD	O47-C7	4.15	1.46	1.34
24	AC	502	CLA	C1B-NB	4.15	1.41	1.34
24	AC	511	CLA	O2D-CGD	4.14	1.43	1.33
24	AC	507	CLA	CHB-C4A	4.14	1.39	1.33
24	BC	5507	CLA	CHB-C4A	4.14	1.39	1.33
24	AC	509	CLA	C1A-NA	4.14	1.41	1.32
24	BB	5619	CLA	MG-NA	4.13	2.19	2.07
24	AB	603	CLA	O2D-CGD	4.13	1.43	1.33
34	BD	5403	PHO	C4C-C3C	4.13	1.52	1.45
30	AA	416	SQD	O5-C5	4.13	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AA	415	LHG	O8-C23	4.12	1.45	1.33
27	AK	102	BCR	C26-C25	4.12	1.40	1.34
24	AB	613	CLA	C4C-C3C	4.12	1.52	1.45
24	AC	512	CLA	C1A-NA	4.12	1.41	1.32
27	AA	410	BCR	C30-C25	4.11	1.59	1.53
30	BB	5601	SQD	C6-S	4.11	1.84	1.77
24	BB	5619	CLA	O2D-CGD	4.11	1.43	1.33
24	AA	407	CLA	O2D-CGD	4.11	1.43	1.33
24	AB	614	CLA	C4C-C3C	4.11	1.52	1.45
30	BB	5601	SQD	O5-C5	4.11	1.54	1.44
24	BC	5508	CLA	C1B-NB	4.10	1.41	1.34
24	BB	5607	CLA	O2A-CGA	4.10	1.45	1.33
24	AB	606	CLA	CHB-C4A	4.10	1.38	1.33
24	BB	5616	CLA	O2D-CGD	4.10	1.43	1.33
30	BB	5625	SQD	C1-C2	4.09	1.64	1.52
30	BF	5102	SQD	O8-S	4.09	1.57	1.46
24	BB	5606	CLA	C4C-C3C	4.10	1.52	1.45
29	BA	5415	LHG	O8-C23	4.09	1.45	1.33
24	BA	5408	CLA	O2D-CGD	4.09	1.43	1.33
24	AB	611	CLA	CHB-C4A	4.09	1.38	1.33
24	AC	506	CLA	C4C-C3C	4.08	1.52	1.45
24	AB	604	CLA	CHB-C4A	4.08	1.38	1.33
24	BC	5512	CLA	C1B-NB	4.08	1.41	1.34
24	AC	501	CLA	O2D-CGD	4.08	1.43	1.33
24	AB	615	CLA	O2D-CGD	4.06	1.43	1.33
27	AC	516	BCR	C5-C6	4.06	1.40	1.34
36	AV	201	HEM	C3C-C2C	4.06	1.50	1.45
30	BA	5414	SQD	C33-C34	-4.06	1.36	1.52
24	AA	404	CLA	C4C-C3C	4.06	1.52	1.45
28	AC	519	DGD	O5D-C6D	-4.05	1.36	1.43
24	AB	601	CLA	C1A-NA	4.04	1.41	1.32
28	AA	411	DGD	O6E-C1E	4.04	1.52	1.41
24	AC	513	CLA	C4C-C3C	4.04	1.52	1.45
34	AD	402	PHO	O2D-CGD	4.03	1.43	1.33
36	BV	5201	HEM	CHC-C1C	4.03	1.42	1.36
27	BB	5621	BCR	C26-C25	4.03	1.40	1.34
24	BB	5620	CLA	C4C-C3C	4.03	1.52	1.45
30	AB	622	SQD	O47-C7	4.03	1.46	1.34
24	AC	511	CLA	C1B-NB	4.03	1.41	1.34
36	AV	201	HEM	CBB-CAB	4.03	1.51	1.29
24	AB	613	CLA	C1A-NA	4.02	1.41	1.32
30	BF	5102	SQD	C1-C2	4.02	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	623	LMT	O5B-C1B	4.02	1.52	1.41
24	AC	510	CLA	C1A-NA	4.02	1.41	1.32
30	AF	102	SQD	O48-C23	4.01	1.45	1.33
24	AC	505	CLA	O2A-CGA	4.01	1.45	1.33
30	BB	5601	SQD	C1-C2	4.00	1.64	1.52
24	AC	512	CLA	C1B-NB	4.00	1.41	1.34
29	AA	412	LHG	P-O6	4.00	1.77	1.59
24	BC	5501	CLA	C4C-C3C	3.99	1.52	1.45
24	AD	404	CLA	C4C-C3C	3.99	1.52	1.45
30	AF	102	SQD	C6-S	3.99	1.83	1.77
24	BB	5605	CLA	C3B-C4B	3.99	1.45	1.41
30	AA	413	SQD	C33-C34	-3.99	1.36	1.52
30	AB	622	SQD	C1-C2	3.99	1.64	1.52
24	BB	5605	CLA	C4C-C3C	3.99	1.52	1.45
24	AC	503	CLA	C1B-NB	3.98	1.41	1.34
24	BB	5610	CLA	CHB-C4A	3.98	1.38	1.33
28	BH	5101	DGD	O5D-C1E	3.98	1.47	1.40
24	AC	507	CLA	C1A-NA	3.98	1.41	1.32
24	AC	508	CLA	CHB-C4A	3.98	1.38	1.33
30	AA	416	SQD	O47-C7	3.97	1.46	1.34
30	AF	102	SQD	O47-C7	3.97	1.46	1.34
24	BC	5512	CLA	C1A-NA	3.96	1.41	1.32
24	AB	614	CLA	C4B-NB	3.96	1.40	1.34
36	BV	5201	HEM	C3C-C2C	3.96	1.50	1.45
24	AD	401	CLA	C4C-C3C	3.95	1.52	1.45
36	BF	5101	HEM	O2D-CGD	3.95	1.44	1.30
30	AB	627	SQD	C6-S	3.95	1.83	1.77
30	AB	622	SQD	C6-S	3.95	1.83	1.77
30	AA	416	SQD	O8-S	3.95	1.56	1.46
30	AB	627	SQD	C1-C2	3.95	1.64	1.52
30	AB	627	SQD	O5-C5	3.95	1.54	1.44
24	BC	5503	CLA	C4C-C3C	3.95	1.52	1.45
34	BD	5404	PHO	C4C-C3C	3.95	1.52	1.45
32	AB	630	LMT	O5B-C1B	3.94	1.51	1.41
30	AB	622	SQD	O48-C23	3.94	1.45	1.33
24	AC	503	CLA	O2D-CGD	3.94	1.43	1.33
27	AT	101	BCR	C30-C25	3.94	1.59	1.53
24	BC	5508	CLA	MG-NB	3.94	2.13	2.05
28	AE	101	DGD	O3G-C1D	3.94	1.47	1.40
36	BF	5101	HEM	CHC-C1C	3.93	1.42	1.36
34	AD	402	PHO	C4D-CHA	-3.93	1.37	1.44
30	BB	5625	SQD	C6-S	3.93	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	612	CLA	C1A-NA	3.93	1.40	1.32
30	BF	5102	SQD	C6-S	3.93	1.83	1.77
24	BB	5618	CLA	C4B-NB	3.92	1.40	1.34
24	BC	5501	CLA	C1B-NB	3.92	1.40	1.34
24	BC	5509	CLA	C1A-NA	3.92	1.40	1.32
24	BA	5406	CLA	C1A-NA	3.92	1.40	1.32
24	BC	5511	CLA	C4B-NB	3.92	1.40	1.34
24	AB	609	CLA	C1B-NB	3.92	1.40	1.34
24	BC	5509	CLA	C4C-C3C	3.92	1.52	1.45
24	AC	508	CLA	C1B-NB	3.91	1.40	1.34
24	AB	608	CLA	C1A-NA	3.91	1.40	1.32
24	AC	504	CLA	O2D-CGD	3.91	1.43	1.33
36	AV	201	HEM	C3B-C2B	3.91	1.50	1.45
24	AD	404	CLA	O2D-CGD	3.91	1.43	1.33
24	BB	5618	CLA	C1B-NB	3.91	1.40	1.34
24	BB	5617	CLA	O2D-CGD	3.90	1.43	1.33
24	BC	5503	CLA	C1A-NA	3.90	1.40	1.32
24	BB	5616	CLA	C1A-NA	3.90	1.40	1.32
24	BC	5502	CLA	CHB-C4A	3.90	1.38	1.33
27	AC	515	BCR	C1-C6	3.89	1.59	1.53
24	AC	512	CLA	MG-NA	3.89	2.18	2.07
24	AD	401	CLA	O2D-CGD	3.88	1.43	1.33
24	AB	616	CLA	C4C-C3C	3.87	1.52	1.45
27	AA	410	BCR	C26-C25	3.87	1.40	1.34
24	BC	5504	CLA	C4C-C3C	3.87	1.52	1.45
27	BK	5102	BCR	C1-C6	3.87	1.59	1.53
24	BC	5505	CLA	O2A-CGA	3.87	1.45	1.33
24	AB	610	CLA	C3B-C4B	3.87	1.45	1.41
24	BB	5613	CLA	CHB-C4A	3.87	1.38	1.33
24	AB	604	CLA	C4C-C3C	3.87	1.52	1.45
24	BB	5613	CLA	C4C-C3C	3.87	1.52	1.45
24	AC	505	CLA	C1A-NA	3.86	1.40	1.32
27	AB	617	BCR	C5-C6	3.86	1.40	1.34
24	AB	615	CLA	C4C-C3C	3.86	1.52	1.45
29	BA	5415	LHG	O7-C7	3.86	1.45	1.34
28	AH	101	DGD	O5D-C1E	3.85	1.47	1.40
24	AC	503	CLA	C4C-C3C	3.85	1.52	1.45
24	AA	404	CLA	MG-NA	3.85	2.18	2.07
30	BF	5102	SQD	C17-C18	-3.85	1.37	1.52
24	BC	5505	CLA	C1A-NA	3.85	1.40	1.32
24	BC	5506	CLA	C4C-C3C	3.84	1.52	1.45
24	BC	5503	CLA	C1B-NB	3.84	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	505	CLA	O2D-CGD	3.84	1.43	1.33
30	BA	5414	SQD	O5-C5	3.84	1.54	1.44
24	BB	5612	CLA	C1A-NA	3.84	1.40	1.32
24	BC	5507	CLA	C1A-NA	3.84	1.40	1.32
35	BD	5406	PL9	C37-C38	-3.84	1.39	1.50
27	BC	5516	BCR	C30-C25	3.84	1.59	1.53
28	BA	5412	DGD	O6E-C1E	3.84	1.51	1.41
24	BD	5405	CLA	C4C-C3C	3.83	1.52	1.45
30	BB	5601	SQD	O7-S	3.83	1.57	1.45
24	BC	5506	CLA	CHB-C4A	3.83	1.38	1.33
30	BA	5414	SQD	O7-S	3.83	1.57	1.45
28	AE	101	DGD	O5D-C1E	3.83	1.47	1.40
27	AJ	101	BCR	C29-C30	3.82	1.63	1.54
27	AJ	101	BCR	C10-C9	3.82	1.40	1.35
24	BB	5614	CLA	C1A-NA	3.82	1.40	1.32
24	AA	405	CLA	O2D-CGD	3.82	1.43	1.33
30	AF	102	SQD	O6-C1	3.82	1.47	1.40
24	BA	5406	CLA	C1B-NB	3.82	1.40	1.34
24	BC	5510	CLA	C4C-C3C	3.82	1.52	1.45
28	AB	628	DGD	O5D-C1E	3.82	1.47	1.40
24	BB	5614	CLA	O2D-CGD	3.81	1.43	1.33
24	AB	601	CLA	C3B-C4B	3.81	1.45	1.41
30	BF	5102	SQD	O48-C23	3.81	1.44	1.33
24	BB	5611	CLA	C4C-C3C	3.81	1.52	1.45
29	AA	415	LHG	O7-C7	3.81	1.45	1.34
24	BC	5508	CLA	CHB-C4A	3.80	1.38	1.33
24	AA	407	CLA	C1A-NA	3.80	1.40	1.32
24	BB	5607	CLA	C1A-NA	3.80	1.40	1.32
32	BB	5626	LMT	O5B-C1B	3.80	1.51	1.41
30	AB	622	SQD	O7-S	3.80	1.57	1.45
24	AC	511	CLA	C4B-NB	3.79	1.40	1.34
35	BD	5406	PL9	C32-C33	-3.79	1.39	1.50
36	BV	5201	HEM	O2D-CGD	3.79	1.44	1.30
24	AA	405	CLA	CHB-C4A	3.79	1.38	1.33
24	AB	608	CLA	O2D-CGD	3.78	1.43	1.33
24	AB	612	CLA	O2D-CGD	3.78	1.43	1.33
30	BA	5401	SQD	O8-S	3.77	1.56	1.46
35	AD	405	PL9	C32-C33	-3.77	1.39	1.50
36	AF	101	HEM	C3C-C4C	3.77	1.52	1.45
28	AB	628	DGD	O3G-C1D	3.77	1.47	1.40
30	BA	5414	SQD	C6-S	3.77	1.83	1.77
28	AC	518	DGD	C2A-C1A	-3.77	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	507	CLA	C3B-C4B	3.76	1.45	1.41
24	AB	609	CLA	C4C-C3C	3.76	1.51	1.45
24	AB	603	CLA	C4C-C3C	3.76	1.51	1.45
28	BC	5518	DGD	C2A-C1A	-3.76	1.39	1.50
27	AX	101	BCR	C29-C30	3.75	1.63	1.54
24	AB	605	CLA	MG-NB	3.75	2.13	2.05
24	BC	5510	CLA	C1A-NA	3.75	1.40	1.32
28	AA	411	DGD	CDB-CCB	-3.74	1.53	1.55
24	AB	607	CLA	C1A-NA	3.74	1.40	1.32
24	BB	5617	CLA	C1A-NA	3.74	1.40	1.32
30	AA	416	SQD	C1-C2	3.74	1.63	1.52
24	BC	5511	CLA	C4C-C3C	3.74	1.51	1.45
30	AF	102	SQD	C17-C18	-3.74	1.37	1.52
30	BB	5625	SQD	O48-C23	3.73	1.44	1.33
30	AB	627	SQD	O7-S	3.73	1.56	1.45
24	BB	5611	CLA	C1A-NA	3.73	1.40	1.32
24	AB	607	CLA	O2D-CGD	3.73	1.42	1.33
24	BA	5407	CLA	C1B-NB	3.73	1.40	1.34
24	AB	612	CLA	C4C-C3C	3.73	1.51	1.45
30	BF	5102	SQD	O6-C1	3.73	1.46	1.40
24	BD	5405	CLA	MG-NA	3.72	2.18	2.07
24	BB	5615	CLA	C1B-NB	3.72	1.40	1.34
36	AF	101	HEM	O2D-CGD	3.72	1.43	1.30
24	BC	5509	CLA	C4B-NB	3.72	1.40	1.34
24	BC	5507	CLA	C3B-C4B	3.71	1.45	1.41
28	BC	5517	DGD	C2A-C1A	-3.71	1.39	1.50
24	AC	510	CLA	C1B-NB	3.71	1.40	1.34
24	BB	5610	CLA	C1A-NA	3.71	1.40	1.32
24	AA	406	CLA	C4C-C3C	3.71	1.51	1.45
27	AC	515	BCR	C5-C6	3.70	1.40	1.34
28	AC	519	DGD	C2A-C1A	-3.71	1.39	1.50
28	AC	517	DGD	O5D-C1E	3.70	1.46	1.40
24	BA	5408	CLA	MG-NB	3.70	2.13	2.05
24	BC	5502	CLA	MG-NA	3.70	2.18	2.07
24	AC	509	CLA	C4C-C3C	3.70	1.51	1.45
28	BH	5101	DGD	C2A-C1A	-3.70	1.39	1.50
27	BJ	5101	BCR	C29-C30	3.70	1.63	1.54
30	BA	5401	SQD	C1-C2	3.69	1.63	1.52
36	AF	101	HEM	CHC-C1C	3.69	1.41	1.36
24	AB	601	CLA	O1D-CGD	3.69	1.30	1.21
24	AA	407	CLA	CHB-C4A	3.69	1.38	1.33
24	AD	401	CLA	C1A-NA	3.69	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BF	5101	HEM	C3C-C4C	3.68	1.52	1.45
24	BD	5405	CLA	C1A-NA	3.68	1.40	1.32
28	AC	517	DGD	C2A-C1A	-3.68	1.39	1.50
32	AI	102	LMT	O5B-C1B	3.68	1.51	1.41
28	BC	5519	DGD	C2A-C1A	-3.67	1.39	1.50
24	AB	611	CLA	C1B-NB	3.66	1.40	1.34
30	BA	5414	SQD	C1-C2	3.66	1.63	1.52
32	AB	623	LMT	O1'-C1'	3.66	1.46	1.40
24	AB	616	CLA	C1B-NB	3.66	1.40	1.34
27	AC	516	BCR	C1-C6	3.66	1.59	1.53
24	AB	613	CLA	O2D-CGD	3.66	1.42	1.33
28	AB	628	DGD	C2A-C1A	-3.66	1.39	1.50
36	BF	5101	HEM	C4D-ND	-3.66	1.32	1.39
24	AC	511	CLA	CHB-C4A	3.65	1.38	1.33
28	AH	101	DGD	C2A-C1A	-3.65	1.39	1.50
29	AA	412	LHG	O8-C23	3.65	1.44	1.33
24	BB	5612	CLA	O2D-CGD	3.65	1.42	1.33
24	BC	5508	CLA	C1A-NA	3.65	1.40	1.32
24	AC	505	CLA	C1B-NB	3.65	1.40	1.34
35	AD	405	PL9	C37-C38	-3.65	1.40	1.50
24	BC	5513	CLA	C4B-NB	3.65	1.40	1.34
34	AD	402	PHO	C1B-CHB	3.65	1.39	1.35
24	BC	5506	CLA	C1A-NA	3.65	1.40	1.32
24	BB	5608	CLA	C4C-C3C	3.65	1.51	1.45
24	AB	604	CLA	O2D-CGD	3.64	1.42	1.33
24	AC	501	CLA	C4C-C3C	3.63	1.51	1.45
28	AE	101	DGD	C2A-C1A	-3.63	1.39	1.50
32	AD	409	LMT	O5B-C1B	3.63	1.51	1.41
28	BC	5519	DGD	C3E-C2E	3.63	1.62	1.52
24	AB	614	CLA	O2A-CGA	3.63	1.44	1.33
24	AB	605	CLA	C1A-NA	3.63	1.40	1.32
24	AD	404	CLA	MG-NA	3.63	2.18	2.07
24	AC	513	CLA	C4B-NB	3.62	1.40	1.34
28	BB	5602	DGD	C2A-C1A	-3.62	1.39	1.50
24	BB	5607	CLA	C4C-C3C	3.62	1.51	1.45
27	AB	618	BCR	C5-C6	3.61	1.40	1.34
28	BE	5102	DGD	O5D-C1E	3.61	1.46	1.40
24	BB	5613	CLA	C1A-NA	3.61	1.40	1.32
28	BE	5102	DGD	C2A-C1A	-3.61	1.39	1.50
28	AA	411	DGD	C2A-C1A	-3.61	1.39	1.50
28	BH	5101	DGD	CDB-CCB	-3.61	1.53	1.55
24	BC	5504	CLA	C1A-NA	3.61	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	508	CLA	MG-NB	3.61	2.13	2.05
30	AB	627	SQD	O48-C23	3.60	1.44	1.33
32	BB	5604	LMT	O5B-C1B	3.60	1.51	1.41
27	BX	5101	BCR	C29-C30	3.60	1.63	1.54
24	BB	5609	CLA	C1A-NA	3.60	1.40	1.32
27	BD	5407	BCR	C29-C30	3.60	1.63	1.54
24	BB	5612	CLA	C1B-NB	3.59	1.40	1.34
27	BA	5411	BCR	C26-C25	3.59	1.40	1.34
24	BA	5407	CLA	C4C-C3C	3.59	1.51	1.45
24	BC	5513	CLA	CHB-C4A	3.59	1.38	1.33
28	AB	628	DGD	O6D-C1D	3.59	1.51	1.41
28	BA	5412	DGD	C2A-C1A	-3.58	1.39	1.50
24	AA	404	CLA	CHB-C4A	3.58	1.38	1.33
24	BB	5615	CLA	C1A-NA	3.58	1.40	1.32
24	AC	511	CLA	C4C-C3C	3.58	1.51	1.45
24	AB	601	CLA	C4B-NB	3.58	1.40	1.34
36	AV	201	HEM	O2D-CGD	3.58	1.43	1.30
32	BM	5101	LMT	O5B-C1B	3.57	1.50	1.41
24	AB	613	CLA	MG-NA	3.57	2.17	2.07
24	BA	5407	CLA	MG-NB	3.57	2.12	2.05
30	BA	5401	SQD	O48-C23	3.57	1.44	1.33
24	AB	602	CLA	C1A-NA	3.57	1.40	1.32
28	BB	5602	DGD	O6D-C1D	3.56	1.50	1.41
27	AB	619	BCR	C5-C6	3.56	1.40	1.34
24	AC	508	CLA	C1A-NA	3.56	1.40	1.32
28	BA	5412	DGD	CDB-CCB	-3.56	1.53	1.55
24	AC	502	CLA	O2A-CGA	3.56	1.44	1.33
24	AB	607	CLA	C4C-C3C	3.56	1.51	1.45
24	BB	5615	CLA	C4C-NC	3.56	1.44	1.37
32	BI	5102	LMT	O5B-C1B	3.56	1.50	1.41
24	AC	513	CLA	C1A-NA	3.55	1.40	1.32
29	BA	5413	LHG	O7-C7	3.55	1.45	1.34
24	AC	513	CLA	C1B-NB	3.55	1.40	1.34
30	AA	413	SQD	C1-C2	3.54	1.63	1.52
24	BC	5512	CLA	MG-NA	3.54	2.17	2.07
24	AC	505	CLA	C4C-C3C	3.54	1.51	1.45
24	BC	5512	CLA	C4B-NB	3.54	1.40	1.34
24	AB	610	CLA	C1A-NA	3.54	1.40	1.32
27	BB	5621	BCR	C5-C6	3.53	1.39	1.34
24	BB	5619	CLA	C1B-NB	3.53	1.40	1.34
27	AC	514	BCR	C26-C25	3.53	1.39	1.34
24	BC	5513	CLA	C1A-NA	3.53	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5611	CLA	O2D-CGD	3.53	1.42	1.33
24	BB	5618	CLA	O2A-CGA	3.53	1.44	1.33
24	AC	513	CLA	CHB-C4A	3.53	1.38	1.33
24	AB	611	CLA	MG-NB	3.52	2.12	2.05
29	BA	5413	LHG	P-O6	3.52	1.75	1.59
24	BA	5405	CLA	CHB-C4A	3.52	1.38	1.33
24	BA	5407	CLA	O1D-CGD	3.51	1.30	1.21
24	BA	5408	CLA	C4C-C3C	3.51	1.51	1.45
24	BB	5610	CLA	MG-NB	3.51	2.12	2.05
27	BJ	5101	BCR	C10-C9	3.51	1.40	1.35
24	BC	5504	CLA	C1B-NB	3.51	1.40	1.34
24	AB	606	CLA	C1A-NA	3.50	1.40	1.32
30	AA	413	SQD	O5-C5	3.50	1.53	1.44
24	AD	404	CLA	C1B-NB	3.50	1.40	1.34
24	AC	504	CLA	C1A-NA	3.50	1.40	1.32
34	AD	403	PHO	C1C-C2C	3.50	1.53	1.45
32	AM	102	LMT	C6B-C5B	-3.50	1.39	1.52
28	AC	518	DGD	O5D-C1E	3.49	1.46	1.40
24	BB	5605	CLA	O1D-CGD	3.49	1.30	1.21
24	BB	5617	CLA	C4C-C3C	3.49	1.51	1.45
32	AB	629	LMT	O5B-C1B	3.49	1.50	1.41
24	AC	502	CLA	CHB-C4A	3.49	1.38	1.33
27	BB	5622	BCR	C2-C1	3.49	1.62	1.54
32	AD	409	LMT	C6B-C5B	-3.49	1.39	1.52
30	AF	102	SQD	O8-S	3.48	1.55	1.46
32	BD	5411	LMT	C6B-C5B	-3.48	1.39	1.52
28	BC	5518	DGD	O5D-C1E	3.48	1.46	1.40
32	AB	623	LMT	C6B-C5B	-3.48	1.39	1.52
24	AA	406	CLA	C1A-NA	3.48	1.39	1.32
32	BB	5604	LMT	C6B-C5B	-3.48	1.39	1.52
24	AC	509	CLA	C1B-NB	3.47	1.40	1.34
31	BC	5521	LMG	C22-C21	-3.48	1.53	1.55
32	AI	103	LMT	C6B-C5B	-3.47	1.39	1.52
30	AF	102	SQD	O7-S	3.47	1.56	1.45
30	BB	5625	SQD	O7-S	3.47	1.56	1.45
31	AJ	102	LMG	O1-C1	3.47	1.46	1.40
32	AB	624	LMT	C6B-C5B	-3.47	1.39	1.52
30	AB	627	SQD	O47-C7	3.46	1.44	1.34
32	AI	102	LMT	C6B-C5B	-3.46	1.39	1.52
31	BD	5408	LMG	C41-C40	-3.46	1.53	1.55
32	BC	5522	LMT	C6B-C5B	-3.46	1.39	1.52
32	BB	5603	LMT	C6B-C5B	-3.46	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	606	CLA	C1D-C2D	3.46	1.51	1.42
34	BD	5403	PHO	C1C-C2C	3.46	1.53	1.45
34	BD	5404	PHO	C1C-C2C	3.46	1.53	1.45
32	BB	5627	LMT	C6B-C5B	-3.46	1.39	1.52
30	BA	5401	SQD	O7-S	3.46	1.56	1.45
32	BM	5101	LMT	C6B-C5B	-3.46	1.39	1.52
32	AB	630	LMT	C6B-C5B	-3.46	1.39	1.52
24	BB	5609	CLA	MG-NB	3.46	2.12	2.05
32	BC	5522	LMT	O5B-C1B	3.46	1.50	1.41
32	BI	5102	LMT	C6B-C5B	-3.45	1.39	1.52
32	BB	5626	LMT	C6B-C5B	-3.45	1.39	1.52
24	BC	5505	CLA	CMC-C2C	3.45	1.58	1.50
30	BB	5601	SQD	O47-C7	3.45	1.44	1.34
24	BB	5605	CLA	O2A-CGA	3.45	1.43	1.33
24	BA	5408	CLA	C1B-NB	3.45	1.40	1.34
24	BA	5407	CLA	O2D-CGD	3.45	1.42	1.33
24	AB	612	CLA	C2A-C1A	-3.44	1.46	1.52
24	BB	5616	CLA	C2A-C1A	-3.44	1.46	1.52
27	BC	5516	BCR	C2-C1	3.44	1.62	1.54
32	AB	629	LMT	C6B-C5B	-3.44	1.39	1.52
30	AF	102	SQD	O5-C1	3.44	1.50	1.41
24	BC	5504	CLA	MG-NB	3.43	2.12	2.05
24	BB	5607	CLA	C4B-NB	3.43	1.40	1.34
24	AD	404	CLA	CMC-C2C	3.43	1.58	1.50
24	AB	611	CLA	C4C-C3C	3.43	1.51	1.45
24	AB	602	CLA	MG-NB	3.43	2.12	2.05
36	AF	101	HEM	C4D-ND	-3.42	1.32	1.39
24	AA	406	CLA	C1B-NB	3.42	1.40	1.34
32	BB	5603	LMT	O5B-C1B	3.42	1.50	1.41
24	AC	509	CLA	O1D-CGD	3.42	1.29	1.21
31	AC	521	LMG	C22-C21	-3.42	1.53	1.55
32	BB	5626	LMT	O1'-C1'	3.41	1.46	1.40
24	BB	5608	CLA	C1A-NA	3.41	1.39	1.32
34	AD	402	PHO	C1C-C2C	3.41	1.53	1.45
28	AH	101	DGD	O2G-C2G	3.41	1.55	1.46
24	BD	5405	CLA	C1B-NB	3.41	1.40	1.34
24	AC	503	CLA	C1A-NA	3.41	1.39	1.32
24	BB	5615	CLA	MG-NB	3.41	2.12	2.05
32	BD	5411	LMT	O5B-C1B	3.41	1.50	1.41
24	BD	5405	CLA	C1D-C2D	3.40	1.51	1.42
24	BB	5614	CLA	C1B-NB	3.40	1.40	1.34
24	BD	5402	CLA	C1A-NA	3.40	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AA	411	DGD	O2G-C1B	3.40	1.44	1.34
24	AB	602	CLA	C1B-NB	3.40	1.40	1.34
24	BA	5406	CLA	O2D-CGD	3.40	1.42	1.33
30	AB	622	SQD	O6-C1	3.40	1.46	1.40
24	BC	5505	CLA	CBB-CAB	3.40	1.54	1.28
24	AC	504	CLA	CHB-C4A	3.40	1.38	1.33
31	BL	5101	LMG	C43-C42	-3.40	1.53	1.55
36	AV	201	HEM	CHC-C1C	3.40	1.41	1.36
24	AC	505	CLA	CBB-CAB	3.39	1.54	1.28
24	BA	5406	CLA	CBA-CGA	3.39	1.60	1.50
24	BC	5506	CLA	O2A-CGA	3.39	1.43	1.33
24	BC	5502	CLA	C4C-C3C	3.39	1.51	1.45
24	AB	610	CLA	MG-NA	3.39	2.17	2.07
24	AC	504	CLA	MG-NB	3.38	2.12	2.05
24	AB	601	CLA	CBB-CAB	3.38	1.54	1.28
24	AA	405	CLA	MG-NB	3.38	2.12	2.05
28	BA	5412	DGD	O2G-C1B	3.38	1.44	1.34
24	AA	407	CLA	C1B-NB	3.38	1.40	1.34
30	AA	413	SQD	C6-S	3.38	1.82	1.77
27	AK	102	BCR	C29-C30	3.38	1.62	1.54
27	BX	5101	BCR	C5-C6	3.38	1.39	1.34
27	BB	5623	BCR	C5-C6	3.38	1.39	1.34
24	AA	407	CLA	C1D-C2D	3.37	1.51	1.42
28	BH	5101	DGD	O2G-C2G	3.37	1.55	1.46
35	BD	5406	PL9	C38-C39	3.37	1.39	1.32
24	AD	404	CLA	C1A-NA	3.37	1.39	1.32
24	BC	5504	CLA	CHB-C4A	3.37	1.37	1.33
32	AM	102	LMT	O5B-C1B	3.37	1.50	1.41
30	AA	416	SQD	O48-C23	3.36	1.43	1.33
24	BC	5511	CLA	O1D-CGD	3.36	1.29	1.21
24	AC	506	CLA	C4C-NC	3.36	1.43	1.37
30	BF	5102	SQD	O7-S	3.36	1.55	1.45
27	AB	618	BCR	C2-C1	3.36	1.62	1.54
24	BB	5610	CLA	C1D-C2D	3.35	1.51	1.42
24	AC	504	CLA	C4C-C3C	3.35	1.51	1.45
27	AK	102	BCR	C1-C6	3.34	1.58	1.53
34	AD	402	PHO	C3B-C4B	3.34	1.45	1.41
24	AA	405	CLA	CBB-CAB	3.34	1.54	1.28
24	BB	5610	CLA	C1B-NB	3.34	1.39	1.34
24	AC	501	CLA	C1B-NB	3.34	1.39	1.34
34	BD	5403	PHO	C3B-C4B	3.34	1.45	1.41
24	BB	5606	CLA	C1A-NA	3.34	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AD	404	CLA	C1D-C2D	3.34	1.51	1.42
24	AB	611	CLA	C4C-NC	3.34	1.43	1.37
24	AB	601	CLA	O2A-CGA	3.34	1.43	1.33
24	BA	5408	CLA	C1A-NA	3.34	1.39	1.32
24	BD	5402	CLA	C1C-NC	3.33	1.44	1.37
24	BC	5508	CLA	C4C-NC	3.33	1.43	1.37
32	BM	5101	LMT	O1B-C4'	3.33	1.52	1.43
24	BC	5501	CLA	CBB-CAB	3.33	1.54	1.28
24	BB	5620	CLA	O1D-CGD	3.33	1.29	1.21
24	AA	405	CLA	C1A-NA	3.33	1.39	1.32
30	BB	5625	SQD	O3-C3	3.33	1.51	1.43
24	AB	609	CLA	C1A-NA	3.33	1.39	1.32
27	AB	619	BCR	C26-C25	3.33	1.39	1.34
32	BB	5604	LMT	O1B-C4'	3.32	1.52	1.43
24	AB	605	CLA	CBB-CAB	3.32	1.54	1.28
24	AB	604	CLA	C4B-NB	3.32	1.39	1.34
24	BC	5503	CLA	C1D-C2D	3.32	1.50	1.42
30	BA	5401	SQD	O6-C1	3.32	1.46	1.40
24	BB	5605	CLA	CBB-CAB	3.32	1.53	1.28
24	BA	5405	CLA	C1A-NA	3.31	1.39	1.32
24	BC	5506	CLA	MG-NB	3.31	2.12	2.05
24	AC	505	CLA	CMC-C2C	3.31	1.58	1.50
24	BB	5617	CLA	C4B-NB	3.31	1.39	1.34
24	AA	405	CLA	CBA-CGA	3.31	1.60	1.50
35	BD	5406	PL9	C18-C19	3.31	1.39	1.32
24	BC	5506	CLA	C4C-NC	3.30	1.43	1.37
24	BA	5407	CLA	MG-NA	3.31	2.17	2.07
28	BB	5602	DGD	O3G-C1D	3.30	1.46	1.40
24	BB	5609	CLA	CBB-CAB	3.30	1.53	1.28
24	BC	5505	CLA	C4C-C3C	3.30	1.51	1.45
24	AB	614	CLA	CHC-C1C	3.30	1.46	1.35
24	BB	5613	CLA	CBB-CAB	3.30	1.53	1.28
30	BA	5414	SQD	O48-C23	3.30	1.43	1.33
24	BC	5511	CLA	C1A-NA	3.30	1.39	1.32
36	AF	101	HEM	FE-NC	3.30	2.08	1.95
24	AB	616	CLA	O1D-CGD	3.30	1.29	1.21
24	AC	506	CLA	C1A-NA	3.29	1.39	1.32
35	AD	405	PL9	C18-C19	3.29	1.39	1.32
30	BB	5601	SQD	O48-C23	3.29	1.43	1.33
24	AB	604	CLA	CBB-CAB	3.29	1.53	1.28
24	BB	5620	CLA	C1B-NB	3.29	1.39	1.34
24	AB	603	CLA	C1A-NA	3.29	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5605	CLA	C4B-NB	3.29	1.39	1.34
24	BA	5407	CLA	CBB-CAB	3.28	1.53	1.28
24	AB	609	CLA	O2A-CGA	3.28	1.43	1.33
24	BC	5513	CLA	O1D-CGD	3.28	1.29	1.21
24	AC	504	CLA	C1B-NB	3.28	1.39	1.34
32	BB	5603	LMT	O1B-C1B	3.28	1.50	1.41
24	AB	611	CLA	C1A-NA	3.28	1.39	1.32
24	BB	5618	CLA	CHC-C1C	3.28	1.46	1.35
27	BC	5515	BCR	C29-C30	3.27	1.62	1.54
24	AC	501	CLA	CBB-CAB	3.27	1.53	1.28
30	AA	416	SQD	O6-C1	3.27	1.46	1.40
24	AB	606	CLA	MG-NB	3.27	2.12	2.05
24	BC	5505	CLA	MG-NA	3.27	2.16	2.07
32	AI	103	LMT	O5B-C1B	3.27	1.50	1.41
27	BC	5516	BCR	C26-C25	3.26	1.39	1.34
27	BB	5623	BCR	C2-C1	3.26	1.62	1.54
24	BB	5619	CLA	CBB-CAB	3.26	1.53	1.28
24	AB	612	CLA	C4B-NB	3.26	1.39	1.34
24	AA	406	CLA	O2D-CGD	3.26	1.41	1.33
24	AB	605	CLA	O2A-CGA	3.26	1.43	1.33
24	AB	612	CLA	C1B-NB	3.26	1.39	1.34
24	BC	5501	CLA	O2A-CGA	3.26	1.43	1.33
24	AC	502	CLA	C1A-NA	3.26	1.39	1.32
24	BC	5511	CLA	MG-NB	3.25	2.12	2.05
31	AC	521	LMG	O6-C1	3.25	1.50	1.41
24	BB	5615	CLA	C2A-C1A	-3.25	1.46	1.52
24	AB	601	CLA	C4C-NC	3.25	1.43	1.37
27	AJ	101	BCR	C21-C22	3.25	1.40	1.35
24	BA	5406	CLA	OBD-CAD	3.25	1.27	1.22
24	BB	5611	CLA	MG-NA	3.25	2.16	2.07
30	BF	5102	SQD	O5-C1	3.25	1.50	1.41
24	AB	615	CLA	C1B-NB	3.25	1.39	1.34
24	AB	615	CLA	CBB-CAB	3.25	1.53	1.28
34	BD	5404	PHO	C1B-CHB	3.25	1.38	1.35
32	AM	102	LMT	O1B-C4'	3.25	1.51	1.43
24	BB	5619	CLA	C4C-C3C	3.25	1.51	1.45
24	BC	5504	CLA	C4B-NB	3.25	1.39	1.34
35	AD	405	PL9	C38-C39	3.25	1.39	1.32
27	BC	5514	BCR	C26-C25	3.25	1.39	1.34
24	BC	5513	CLA	CBB-CAB	3.25	1.53	1.28
24	BA	5406	CLA	CBB-CAB	3.25	1.53	1.28
34	BD	5404	PHO	CBB-CAB	3.24	1.53	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AC	516	BCR	C30-C25	3.24	1.58	1.53
27	AB	619	BCR	C29-C30	3.24	1.62	1.54
32	AB	629	LMT	O1B-C1B	3.24	1.50	1.41
24	AA	404	CLA	C1A-NA	3.24	1.39	1.32
30	AB	622	SQD	O3-C3	3.24	1.50	1.43
24	BA	5407	CLA	C1A-NA	3.24	1.39	1.32
30	AA	416	SQD	O7-S	3.23	1.55	1.45
24	BA	5407	CLA	CBA-CGA	3.24	1.60	1.50
24	BB	5608	CLA	MG-NB	3.23	2.12	2.05
24	AD	401	CLA	CMC-C2C	3.23	1.57	1.50
24	AB	614	CLA	MG-NB	3.23	2.12	2.05
27	BD	5407	BCR	C5-C6	3.23	1.39	1.34
34	AD	402	PHO	C4C-C3C	3.23	1.51	1.45
24	BC	5512	CLA	MG-NB	3.23	2.12	2.05
34	AD	403	PHO	C4D-CHA	-3.23	1.38	1.44
24	AB	616	CLA	CBB-CAB	3.23	1.53	1.28
24	AA	406	CLA	MG-NB	3.23	2.12	2.05
24	AA	406	CLA	CBB-CAB	3.23	1.53	1.28
24	BB	5612	CLA	CBB-CAB	3.23	1.53	1.28
24	AB	607	CLA	CHB-C4A	3.23	1.37	1.33
34	BD	5403	PHO	O1D-CGD	3.22	1.29	1.21
24	BC	5503	CLA	C4C-NC	3.22	1.43	1.37
27	AB	618	BCR	C29-C30	3.22	1.62	1.54
24	BB	5609	CLA	O2A-CGA	3.22	1.43	1.33
24	BA	5407	CLA	C4B-NB	3.22	1.39	1.34
24	AB	604	CLA	C1B-NB	3.21	1.39	1.34
24	AB	602	CLA	CBB-CAB	3.21	1.53	1.28
27	BA	5411	BCR	C5-C6	3.21	1.39	1.34
24	BA	5408	CLA	C1C-NC	3.21	1.43	1.37
24	AB	605	CLA	C4C-C3C	3.20	1.50	1.45
24	AC	506	CLA	O2A-CGA	3.20	1.43	1.33
24	BC	5503	CLA	C4B-NB	3.20	1.39	1.34
24	AC	511	CLA	C1A-NA	3.20	1.39	1.32
27	AD	406	BCR	C29-C30	3.20	1.62	1.54
30	BA	5401	SQD	O5-C1	3.20	1.50	1.41
24	BC	5503	CLA	CBB-CAB	3.20	1.53	1.28
24	AC	513	CLA	CBB-CAB	3.20	1.53	1.28
24	BC	5505	CLA	O1D-CGD	3.19	1.29	1.21
24	AB	608	CLA	C1B-NB	3.19	1.39	1.34
27	BT	5101	BCR	C2-C1	3.19	1.62	1.54
24	AA	406	CLA	MG-NA	3.19	2.16	2.07
24	AB	608	CLA	CBB-CAB	3.19	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5616	CLA	O1D-CGD	3.19	1.29	1.21
27	BB	5623	BCR	C29-C30	3.18	1.62	1.54
24	AB	609	CLA	CBB-CAB	3.18	1.52	1.28
32	AB	624	LMT	O1'-C1'	3.18	1.45	1.40
27	AC	516	BCR	C26-C25	3.18	1.39	1.34
24	BA	5405	CLA	C4C-NC	3.18	1.43	1.37
27	AB	619	BCR	C2-C1	3.18	1.62	1.54
24	BC	5502	CLA	O2A-CGA	3.18	1.43	1.33
24	BC	5502	CLA	CBB-CAB	3.18	1.52	1.28
24	AC	506	CLA	CBB-CAB	3.18	1.52	1.28
34	BD	5403	PHO	CBB-CAB	3.18	1.52	1.28
34	AD	402	PHO	CBB-CAB	3.18	1.52	1.28
24	BB	5613	CLA	MG-NA	3.18	2.16	2.07
27	BJ	5101	BCR	C21-C22	3.18	1.39	1.35
24	BB	5618	CLA	C1A-NA	3.17	1.39	1.32
24	BA	5406	CLA	C1D-C2D	3.17	1.50	1.42
24	BC	5506	CLA	CBB-CAB	3.17	1.52	1.28
24	BA	5408	CLA	C1D-C2D	3.17	1.50	1.42
24	BB	5608	CLA	CBB-CAB	3.17	1.52	1.28
24	BD	5402	CLA	C4B-NB	3.17	1.39	1.34
24	BA	5408	CLA	C4B-NB	3.17	1.39	1.34
27	BB	5621	BCR	C2-C1	3.17	1.62	1.54
24	AC	510	CLA	CBB-CAB	3.17	1.52	1.28
24	BC	5510	CLA	CBB-CAB	3.16	1.52	1.28
34	AD	403	PHO	CBB-CAB	3.16	1.52	1.28
24	BC	5512	CLA	CBB-CAB	3.16	1.52	1.28
24	BB	5606	CLA	CBB-CAB	3.16	1.52	1.28
24	AB	603	CLA	C1B-C2B	-3.16	1.39	1.43
24	AC	512	CLA	CBB-CAB	3.16	1.52	1.28
24	BB	5608	CLA	C1B-NB	3.16	1.39	1.34
24	BD	5405	CLA	O1D-CGD	3.16	1.29	1.21
24	BD	5405	CLA	CMC-C2C	3.16	1.57	1.50
24	AC	503	CLA	MG-NB	3.16	2.12	2.05
24	AB	607	CLA	O2A-CGA	3.16	1.42	1.33
24	BB	5609	CLA	C4C-C3C	3.16	1.50	1.45
30	AA	413	SQD	O48-C23	3.15	1.42	1.33
31	AC	521	LMG	O1-C1	3.15	1.45	1.40
24	BC	5502	CLA	C4C-NC	3.15	1.43	1.37
24	AB	612	CLA	C1D-C2D	3.15	1.50	1.42
24	BA	5405	CLA	CBB-CAB	3.15	1.52	1.28
24	AC	506	CLA	MG-NB	3.15	2.12	2.05
24	BB	5620	CLA	CBB-CAB	3.14	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5618	CLA	MG-NB	3.14	2.12	2.05
27	AJ	101	BCR	C2-C1	3.14	1.62	1.54
24	AB	612	CLA	CHB-C4A	3.14	1.37	1.33
24	AA	405	CLA	CMC-C2C	3.14	1.57	1.50
24	BB	5614	CLA	CBB-CAB	3.14	1.52	1.28
24	BA	5407	CLA	C1D-C2D	3.14	1.50	1.42
24	BC	5503	CLA	O2A-CGA	3.13	1.42	1.33
24	AA	406	CLA	CBA-CGA	3.13	1.60	1.50
24	AC	507	CLA	CBB-CAB	3.13	1.52	1.28
24	BB	5617	CLA	C1D-C2D	3.12	1.50	1.42
24	AD	401	CLA	CBB-CAB	3.13	1.52	1.28
27	BC	5514	BCR	C29-C30	3.13	1.61	1.54
24	BC	5507	CLA	CBB-CAB	3.12	1.52	1.28
24	AC	501	CLA	MG-NA	3.12	2.16	2.07
27	AT	101	BCR	C29-C30	3.12	1.61	1.54
27	BB	5622	BCR	C29-C30	3.12	1.61	1.54
24	BA	5406	CLA	CMC-C2C	3.12	1.57	1.50
24	AB	610	CLA	CBB-CAB	3.12	1.52	1.28
24	BC	5512	CLA	C4C-NC	3.12	1.43	1.37
24	AA	405	CLA	C1B-C2B	-3.12	1.39	1.43
24	BC	5512	CLA	O1D-CGD	3.12	1.29	1.21
24	AB	606	CLA	CBB-CAB	3.11	1.52	1.28
27	AB	617	BCR	C2-C1	3.11	1.61	1.54
24	BC	5502	CLA	C1A-NA	3.11	1.39	1.32
36	BF	5101	HEM	CMC-C2C	3.11	1.57	1.47
27	BX	5101	BCR	C2-C1	3.11	1.61	1.54
31	BL	5101	LMG	O6-C1	3.10	1.49	1.41
24	BC	5509	CLA	O1D-CGD	3.10	1.29	1.21
24	BC	5504	CLA	C4C-NC	3.10	1.43	1.37
24	AD	404	CLA	C1B-C2B	-3.10	1.39	1.43
29	BA	5413	LHG	O8-C23	3.10	1.42	1.33
24	AB	604	CLA	MG-NB	3.10	2.11	2.05
28	BB	5602	DGD	O6E-C1E	3.10	1.49	1.41
24	AC	502	CLA	C1D-C2D	3.10	1.50	1.42
30	AA	416	SQD	O3-C3	3.10	1.50	1.43
31	AB	620	LMG	C43-C42	-3.09	1.53	1.55
24	AC	503	CLA	CBB-CAB	3.09	1.52	1.28
30	BB	5625	SQD	O6-C1	3.09	1.45	1.40
24	AA	404	CLA	CMC-C2C	3.09	1.57	1.50
24	BB	5620	CLA	MG-NB	3.09	2.11	2.05
34	AD	403	PHO	C1B-CHB	3.09	1.38	1.35
27	BJ	5101	BCR	C2-C1	3.09	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BK	5102	BCR	C29-C30	3.09	1.61	1.54
24	BC	5506	CLA	C4B-NB	3.08	1.39	1.34
24	AC	508	CLA	CBB-CAB	3.08	1.52	1.28
24	AB	609	CLA	MG-NA	3.08	2.16	2.07
24	AB	615	CLA	MG-NA	3.08	2.16	2.07
24	BC	5507	CLA	C1D-C2D	3.08	1.50	1.42
24	BB	5606	CLA	C4C-NC	3.08	1.43	1.37
24	AC	502	CLA	MG-NB	3.08	2.11	2.05
24	BA	5407	CLA	CHB-C4A	3.08	1.37	1.33
24	AA	404	CLA	C1B-C2B	-3.08	1.39	1.43
36	BV	5201	HEM	C3C-C4C	3.08	1.51	1.45
27	AC	515	BCR	C29-C30	3.08	1.61	1.54
24	AC	503	CLA	O2A-CGA	3.08	1.42	1.33
24	AC	509	CLA	CBB-CAB	3.08	1.52	1.28
24	AB	603	CLA	C4B-NB	3.08	1.39	1.34
31	AA	414	LMG	O1-C1	3.08	1.45	1.40
24	BB	5612	CLA	C4C-C3C	3.08	1.50	1.45
24	AC	512	CLA	MG-NB	3.08	2.11	2.05
24	BB	5605	CLA	C4C-NC	3.08	1.43	1.37
30	AA	413	SQD	O7-S	3.07	1.54	1.45
24	AC	502	CLA	CBB-CAB	3.07	1.52	1.28
24	BB	5607	CLA	C1B-C2B	-3.07	1.39	1.43
28	AB	628	DGD	O6E-C1E	3.07	1.49	1.41
30	AA	416	SQD	O5-C1	3.07	1.49	1.41
27	BB	5622	BCR	C5-C6	3.07	1.39	1.34
30	BA	5414	SQD	O5-C1	3.07	1.49	1.41
24	BB	5610	CLA	CBB-CAB	3.07	1.52	1.28
24	AA	407	CLA	C4C-C3C	3.07	1.50	1.45
24	AB	607	CLA	C1B-C2B	-3.07	1.39	1.43
24	BC	5508	CLA	C4B-NB	3.07	1.39	1.34
24	BC	5501	CLA	C4B-NB	3.07	1.39	1.34
24	BC	5504	CLA	C1B-C2B	-3.07	1.39	1.43
24	BB	5611	CLA	C1D-C2D	3.07	1.50	1.42
24	AA	406	CLA	C1B-C2B	-3.06	1.39	1.43
24	AB	607	CLA	MG-NA	3.06	2.16	2.07
24	AB	605	CLA	O1D-CGD	3.06	1.28	1.21
24	BD	5402	CLA	CBB-CAB	3.06	1.51	1.28
24	BB	5615	CLA	C1B-C2B	-3.06	1.39	1.43
24	AC	510	CLA	C4B-NB	3.06	1.39	1.34
27	AB	617	BCR	C30-C25	3.06	1.58	1.53
36	AV	201	HEM	C3C-C4C	3.06	1.51	1.45
30	AA	413	SQD	O6-C44	-3.06	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5507	CLA	C1B-NB	3.06	1.39	1.34
36	BF	5101	HEM	FE-NC	3.06	2.08	1.95
24	AC	512	CLA	C4B-NB	3.06	1.39	1.34
24	AA	404	CLA	CBB-CAB	3.06	1.51	1.28
24	BA	5408	CLA	C1B-C2B	-3.06	1.39	1.43
24	AC	501	CLA	C1D-C2D	3.06	1.50	1.42
24	BB	5608	CLA	C4B-NB	3.05	1.39	1.34
36	BV	5201	HEM	CMC-C2C	3.05	1.57	1.47
24	AB	604	CLA	CMC-C2C	3.05	1.57	1.50
29	AA	412	LHG	C12-C11	-3.05	1.53	1.55
24	BC	5513	CLA	O2A-CGA	3.05	1.42	1.33
28	AA	411	DGD	O1G-C1A	3.05	1.42	1.33
24	AC	501	CLA	O2A-CGA	3.05	1.42	1.33
24	AB	615	CLA	C4B-NB	3.05	1.39	1.34
24	AB	610	CLA	C1B-NB	3.05	1.39	1.34
24	AA	407	CLA	C4B-NB	3.05	1.39	1.34
24	AB	606	CLA	O1D-CGD	3.05	1.28	1.21
24	BB	5620	CLA	C4C-NC	3.05	1.43	1.37
24	BB	5612	CLA	C1B-C2B	-3.04	1.39	1.43
24	BB	5616	CLA	O2A-CGA	3.04	1.42	1.33
24	BA	5408	CLA	CMC-C2C	3.04	1.57	1.50
24	BC	5501	CLA	O1D-CGD	3.04	1.28	1.21
24	BB	5614	CLA	CMC-C2C	3.04	1.57	1.50
24	BC	5508	CLA	CBB-CAB	3.04	1.51	1.28
24	AB	609	CLA	O1D-CGD	3.04	1.28	1.21
31	BD	5408	LMG	O1-C1	3.04	1.45	1.40
27	AC	516	BCR	C2-C1	3.04	1.61	1.54
24	BC	5502	CLA	C1D-C2D	3.03	1.50	1.42
32	BB	5627	LMT	O5B-C1B	3.04	1.49	1.41
24	AB	614	CLA	C1A-NA	3.03	1.38	1.32
24	AB	613	CLA	C1B-C2B	-3.03	1.39	1.43
24	BB	5611	CLA	O2A-CGA	3.03	1.42	1.33
24	AB	608	CLA	C4C-C3C	3.03	1.50	1.45
34	BD	5403	PHO	C1B-CHB	3.03	1.38	1.35
24	AC	504	CLA	C4B-NB	3.03	1.39	1.34
36	BV	5201	HEM	FE-NC	3.03	2.07	1.95
24	BB	5619	CLA	MG-NB	3.03	2.11	2.05
24	AC	513	CLA	C1D-C2D	3.03	1.50	1.42
24	BB	5613	CLA	C1B-C2B	-3.03	1.39	1.43
24	AD	401	CLA	C1B-C2B	-3.02	1.39	1.43
36	BF	5101	HEM	FE-NB	3.02	2.08	1.96
24	BB	5617	CLA	C1B-C2B	-3.02	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	611	CLA	C2A-C1A	-3.02	1.46	1.52
24	AB	608	CLA	C1D-C2D	3.02	1.50	1.42
29	AA	412	LHG	O7-C7	3.02	1.43	1.34
24	AC	507	CLA	C1B-C2B	-3.02	1.39	1.43
24	BB	5615	CLA	CBB-CAB	3.02	1.51	1.28
24	BD	5405	CLA	CBB-CAB	3.02	1.51	1.28
24	AD	404	CLA	C4C-NC	3.02	1.43	1.37
24	AA	404	CLA	O1D-CGD	3.02	1.28	1.21
27	BD	5407	BCR	C1-C6	3.02	1.58	1.53
24	BB	5612	CLA	C1D-C2D	3.02	1.50	1.42
24	AB	602	CLA	C1D-C2D	3.02	1.50	1.42
31	AJ	102	LMG	C41-C40	-3.02	1.54	1.55
24	BB	5613	CLA	O2A-CGA	3.02	1.42	1.33
24	AD	404	CLA	CBB-CAB	3.01	1.51	1.28
27	BT	5101	BCR	C29-C30	3.01	1.61	1.54
24	AC	502	CLA	C4C-NC	3.01	1.43	1.37
24	AB	610	CLA	C1B-C2B	-3.01	1.39	1.43
24	AB	605	CLA	C1D-C2D	3.01	1.50	1.42
24	AD	401	CLA	C4B-NB	3.01	1.39	1.34
24	BB	5617	CLA	O1D-CGD	3.01	1.28	1.21
24	AB	613	CLA	C1D-C2D	3.00	1.50	1.42
24	AC	501	CLA	CMC-C2C	3.00	1.57	1.50
24	BB	5616	CLA	CBB-CAB	3.00	1.51	1.28
27	BC	5514	BCR	C2-C1	3.01	1.61	1.54
24	BB	5613	CLA	MG-NB	3.00	2.11	2.05
24	BB	5618	CLA	C1B-C2B	-3.00	1.39	1.43
24	BB	5610	CLA	MG-NA	3.00	2.16	2.07
24	AB	606	CLA	C1B-C2B	-3.00	1.39	1.43
24	BC	5510	CLA	C4C-NC	3.00	1.43	1.37
24	AA	406	CLA	C1D-C2D	3.00	1.50	1.42
24	BC	5509	CLA	CBB-CAB	3.00	1.51	1.28
24	BC	5508	CLA	C1B-C2B	-3.00	1.39	1.43
34	AD	402	PHO	O1D-CGD	3.00	1.28	1.21
28	AH	101	DGD	O6D-C1D	3.00	1.49	1.41
27	BT	5101	BCR	C26-C25	2.99	1.39	1.34
32	AD	409	LMT	O1'-C1'	2.99	1.45	1.40
27	AC	514	BCR	C29-C30	2.99	1.61	1.54
27	BD	5407	BCR	C2-C1	2.99	1.61	1.54
24	AC	504	CLA	C1D-C2D	2.99	1.50	1.42
24	BD	5402	CLA	C1B-C2B	-2.99	1.39	1.43
24	BB	5615	CLA	O1D-CGD	2.99	1.28	1.21
24	BC	5502	CLA	MG-NB	2.99	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	615	CLA	MG-NB	2.99	2.11	2.05
24	AB	607	CLA	C5-C3	2.99	1.58	1.51
24	BB	5611	CLA	C1B-C2B	-2.99	1.39	1.43
27	AT	101	BCR	C2-C1	2.99	1.61	1.54
24	AC	513	CLA	O1D-CGD	2.99	1.28	1.21
24	AB	610	CLA	CMC-C2C	2.98	1.57	1.50
24	AB	614	CLA	C1B-C2B	-2.98	1.39	1.43
32	AB	630	LMT	O1B-C4'	2.99	1.51	1.43
31	AA	414	LMG	O6-C1	2.98	1.49	1.41
24	BC	5513	CLA	C1D-C2D	2.98	1.50	1.42
24	AB	616	CLA	MG-NA	2.98	2.16	2.07
24	AB	612	CLA	C1B-C2B	-2.98	1.39	1.43
30	AA	413	SQD	O3-C3	2.98	1.50	1.43
24	BB	5610	CLA	C1B-C2B	-2.98	1.39	1.43
24	BC	5510	CLA	O1D-CGD	2.98	1.28	1.21
24	BB	5615	CLA	C4B-NB	2.98	1.39	1.34
24	BB	5613	CLA	O1D-CGD	2.98	1.28	1.21
32	BB	5627	LMT	O1'-C1'	2.98	1.45	1.40
24	AB	603	CLA	CBB-CAB	2.98	1.51	1.28
24	BC	5511	CLA	O2A-CGA	2.97	1.42	1.33
24	AB	606	CLA	MG-NA	2.97	2.16	2.07
27	AC	515	BCR	C2-C1	2.97	1.61	1.54
24	AB	605	CLA	C4B-NB	2.97	1.39	1.34
24	AC	503	CLA	C1B-C2B	-2.97	1.39	1.43
31	AD	408	LMG	C40-C39	-2.97	1.54	1.55
24	BC	5506	CLA	C1B-C2B	-2.97	1.39	1.43
31	BE	5101	LMG	O6-C1	2.97	1.49	1.41
30	BA	5401	SQD	O3-C3	2.97	1.50	1.43
24	BB	5609	CLA	C1B-C2B	-2.97	1.39	1.43
24	AC	508	CLA	C4C-NC	2.97	1.43	1.37
34	BD	5404	PHO	C4D-CHA	-2.97	1.39	1.44
24	BD	5405	CLA	C1B-C2B	-2.96	1.39	1.43
24	BC	5507	CLA	C1B-C2B	-2.96	1.39	1.43
24	AC	505	CLA	C1B-C2B	-2.96	1.39	1.43
24	BC	5511	CLA	CHC-C1C	2.96	1.45	1.35
24	AB	605	CLA	C1B-C2B	-2.96	1.39	1.43
34	AD	402	PHO	CMC-C2C	2.96	1.57	1.50
31	BD	5408	LMG	C22-C21	-2.96	1.54	1.55
24	AC	509	CLA	C1B-C2B	-2.96	1.39	1.43
24	AC	505	CLA	CAA-CBA	-2.96	1.42	1.52
24	AC	502	CLA	C4C-C3C	2.96	1.50	1.45
27	BB	5623	BCR	C26-C25	2.96	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	624	LMT	O5B-C1B	2.96	1.49	1.41
28	BA	5412	DGD	O1G-C1A	2.95	1.42	1.33
24	AC	504	CLA	C1B-C2B	-2.95	1.39	1.43
24	AC	511	CLA	O2A-CGA	2.95	1.42	1.33
24	AB	611	CLA	CBB-CAB	2.95	1.51	1.28
32	BM	5101	LMT	O1'-C1'	2.95	1.45	1.40
24	AA	407	CLA	C1B-C2B	-2.95	1.39	1.43
24	BC	5505	CLA	C1B-C2B	-2.95	1.39	1.43
24	BA	5407	CLA	C1B-C2B	-2.95	1.39	1.43
24	BB	5611	CLA	CHB-C4A	2.95	1.37	1.33
24	BB	5619	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	612	CLA	CBB-CAB	2.95	1.51	1.28
24	AC	511	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	611	CLA	C1B-C2B	-2.95	1.39	1.43
24	BA	5405	CLA	MG-NA	2.95	2.16	2.07
27	BK	5102	BCR	C2-C1	2.95	1.61	1.54
24	AC	510	CLA	MG-NB	2.95	2.11	2.05
24	BC	5502	CLA	O1D-CGD	2.95	1.28	1.21
24	AC	513	CLA	O2A-CGA	2.95	1.42	1.33
24	BC	5505	CLA	C4B-NB	2.95	1.39	1.34
24	BB	5608	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	615	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	609	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	601	CLA	C1B-C2B	-2.95	1.39	1.43
24	AB	608	CLA	C2A-C1A	-2.95	1.47	1.52
24	BA	5406	CLA	C1B-C2B	-2.95	1.39	1.43
24	BB	5612	CLA	MG-NB	2.94	2.11	2.05
24	BB	5620	CLA	C4B-NB	2.94	1.39	1.34
24	BB	5614	CLA	C1B-C2B	-2.94	1.39	1.43
24	AB	602	CLA	C1B-C2B	-2.94	1.39	1.43
24	AC	501	CLA	C1B-C2B	-2.94	1.39	1.43
24	BC	5512	CLA	MG-NC	2.94	2.15	2.07
24	BA	5405	CLA	C4B-NB	2.94	1.39	1.34
32	AM	102	LMT	O1'-C1'	2.94	1.45	1.40
34	AD	403	PHO	C3D-CAD	-2.94	1.41	1.47
24	AA	406	CLA	C4B-NB	2.94	1.39	1.34
24	BB	5616	CLA	CHB-C4A	2.94	1.37	1.33
24	BA	5405	CLA	C1B-C2B	-2.94	1.39	1.43
24	AC	513	CLA	C1B-C2B	-2.94	1.39	1.43
24	BB	5605	CLA	C1B-C2B	-2.94	1.39	1.43
24	AC	508	CLA	C1B-C2B	-2.93	1.39	1.43
24	BC	5512	CLA	CMC-C2C	2.93	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	617	BCR	C29-C30	2.93	1.61	1.54
28	BC	5519	DGD	C4E-C3E	2.93	1.60	1.52
24	AB	604	CLA	C1B-C2B	-2.93	1.39	1.43
24	BB	5606	CLA	C1B-C2B	-2.93	1.39	1.43
24	BB	5612	CLA	CMC-C2C	2.93	1.57	1.50
24	AC	510	CLA	C1B-C2B	-2.93	1.39	1.43
24	AB	602	CLA	C4C-NC	2.92	1.43	1.37
24	BA	5405	CLA	O1D-CGD	2.92	1.28	1.21
24	AB	608	CLA	C1B-C2B	-2.92	1.39	1.43
32	BB	5603	LMT	O5'-C1'	2.92	1.49	1.41
24	AB	606	CLA	O2A-CGA	2.92	1.42	1.33
24	AC	511	CLA	CHC-C1C	2.92	1.45	1.35
36	BV	5201	HEM	O2A-CGA	-2.92	1.20	1.30
24	BB	5616	CLA	C1B-C2B	-2.92	1.39	1.43
28	BC	5519	DGD	O5D-C6D	-2.92	1.38	1.43
24	BC	5508	CLA	C4C-C3C	2.92	1.50	1.45
24	BC	5504	CLA	CBB-CAB	2.91	1.50	1.28
24	BC	5502	CLA	C1B-C2B	-2.91	1.39	1.43
24	BB	5619	CLA	C4B-NB	2.91	1.39	1.34
28	AE	101	DGD	O6E-C1E	2.91	1.49	1.41
30	AA	413	SQD	O5-C1	2.91	1.49	1.41
24	BC	5513	CLA	C1B-C2B	-2.91	1.39	1.43
24	BC	5507	CLA	O2A-CGA	2.91	1.42	1.33
30	AB	627	SQD	O3-C3	2.91	1.50	1.43
24	AC	503	CLA	C1D-C2D	2.91	1.49	1.42
30	BA	5414	SQD	O3-C3	2.91	1.50	1.43
24	AB	616	CLA	O2A-CGA	2.91	1.42	1.33
24	BC	5509	CLA	C1B-C2B	-2.91	1.39	1.43
24	AC	502	CLA	O1D-CGD	2.91	1.28	1.21
28	BH	5101	DGD	O6D-C1D	2.91	1.49	1.41
24	AC	506	CLA	C1B-C2B	-2.91	1.39	1.43
24	AC	503	CLA	C4C-NC	2.91	1.43	1.37
24	AB	616	CLA	C1B-C2B	-2.91	1.39	1.43
24	BC	5504	CLA	O2A-CGA	2.90	1.42	1.33
24	BC	5511	CLA	C1B-C2B	-2.90	1.39	1.43
24	AC	504	CLA	CBB-CAB	2.90	1.50	1.28
24	BD	5402	CLA	CMC-C2C	2.90	1.57	1.50
24	BC	5504	CLA	C1D-C2D	2.90	1.49	1.42
24	BB	5608	CLA	MG-NA	2.90	2.15	2.07
31	BC	5521	LMG	O1-C1	2.90	1.45	1.40
24	AC	504	CLA	MG-NA	2.90	2.15	2.07
24	AD	404	CLA	O1D-CGD	2.90	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BE	5102	DGD	C3G-C2G	2.90	1.58	1.50
24	AC	508	CLA	C4C-C3C	2.90	1.50	1.45
24	BB	5609	CLA	MG-NA	2.90	2.15	2.07
24	BB	5609	CLA	C4B-NB	2.90	1.39	1.34
24	BC	5501	CLA	CMC-C2C	2.89	1.57	1.50
31	AJ	102	LMG	O7-C8	-2.89	1.39	1.46
36	AF	101	HEM	CMC-C2C	2.89	1.56	1.47
24	BB	5620	CLA	C1B-C2B	-2.89	1.39	1.43
24	BA	5408	CLA	CBB-CAB	2.89	1.50	1.28
24	BB	5611	CLA	C4B-NB	2.89	1.39	1.34
27	AX	101	BCR	C5-C6	2.89	1.38	1.34
27	BA	5411	BCR	C29-C30	2.89	1.61	1.54
24	BC	5510	CLA	C1B-C2B	-2.89	1.39	1.43
27	AD	406	BCR	C2-C1	2.89	1.61	1.54
34	BD	5403	PHO	C1D-C2D	2.88	1.49	1.42
31	BD	5408	LMG	O7-C8	-2.88	1.39	1.46
24	BD	5402	CLA	C1B-NB	2.88	1.39	1.34
24	AB	612	CLA	MG-NB	2.88	2.11	2.05
28	BA	5412	DGD	O5D-C6D	-2.88	1.38	1.43
24	BB	5606	CLA	MG-NB	2.88	2.11	2.05
24	BA	5407	CLA	CMC-C2C	2.88	1.57	1.50
32	AM	102	LMT	C4'-C5'	2.88	1.60	1.52
24	BC	5509	CLA	MG-NB	2.88	2.11	2.05
24	BB	5607	CLA	C1D-C2D	2.88	1.49	1.42
27	AA	410	BCR	C29-C30	2.88	1.61	1.54
31	AB	620	LMG	O6-C1	2.87	1.49	1.41
24	AA	405	CLA	O1D-CGD	2.87	1.28	1.21
24	AB	610	CLA	C1D-C2D	2.87	1.49	1.42
24	BC	5503	CLA	C1B-C2B	-2.87	1.39	1.43
24	BB	5613	CLA	C1D-C2D	2.87	1.49	1.42
24	BC	5512	CLA	C1B-C2B	-2.87	1.39	1.43
24	AC	509	CLA	CMC-C2C	2.87	1.57	1.50
24	AC	512	CLA	C4C-NC	2.87	1.43	1.37
24	AB	611	CLA	O2A-CGA	2.87	1.42	1.33
24	BB	5616	CLA	C4B-NB	2.87	1.39	1.34
24	AB	604	CLA	C4C-NC	2.87	1.43	1.37
24	BB	5618	CLA	CBB-CAB	2.87	1.50	1.28
24	BC	5511	CLA	CBB-CAB	2.87	1.50	1.28
24	AC	503	CLA	CMC-C2C	2.87	1.57	1.50
24	BA	5405	CLA	CMC-C2C	2.87	1.57	1.50
24	BC	5509	CLA	CMC-C2C	2.87	1.57	1.50
24	AB	601	CLA	MG-NB	2.87	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5506	CLA	O1D-CGD	2.87	1.28	1.21
24	BB	5607	CLA	CBB-CAB	2.87	1.50	1.28
24	AC	507	CLA	O2A-CGA	2.87	1.42	1.33
24	AC	507	CLA	C1B-NB	2.86	1.39	1.34
24	BB	5614	CLA	MG-NA	2.86	2.15	2.07
24	AA	405	CLA	C4C-C3C	2.86	1.50	1.45
24	BB	5611	CLA	C5-C3	2.86	1.58	1.51
24	AC	506	CLA	O1D-CGD	2.86	1.28	1.21
24	BC	5512	CLA	C1D-C2D	2.86	1.49	1.42
24	BB	5610	CLA	C4B-NB	2.86	1.39	1.34
24	AC	510	CLA	O1D-CGD	2.86	1.28	1.21
36	AV	201	HEM	O2A-CGA	-2.86	1.20	1.30
36	AV	201	HEM	FE-NC	2.86	2.07	1.95
24	AB	613	CLA	C4B-NB	2.85	1.39	1.34
24	BB	5606	CLA	CMC-C2C	2.85	1.57	1.50
24	AC	502	CLA	C4B-NB	2.85	1.39	1.34
30	AF	102	SQD	O3-C3	2.85	1.49	1.43
27	AD	406	BCR	C1-C6	2.85	1.57	1.53
31	BC	5521	LMG	O6-C1	2.85	1.49	1.41
24	BC	5510	CLA	C1D-C2D	2.85	1.49	1.42
24	BD	5405	CLA	C4C-NC	2.85	1.42	1.37
24	AA	407	CLA	CBB-CAB	2.85	1.50	1.28
24	AC	502	CLA	C1B-C2B	-2.85	1.39	1.43
24	BB	5606	CLA	C1B-NB	2.85	1.39	1.34
24	BB	5606	CLA	C1D-C2D	2.85	1.49	1.42
24	AA	407	CLA	MG-NB	2.85	2.11	2.05
24	AD	404	CLA	C4B-NB	2.85	1.39	1.34
24	BC	5501	CLA	C1B-C2B	-2.84	1.39	1.43
24	AB	614	CLA	CBB-CAB	2.84	1.50	1.28
24	AC	512	CLA	C1B-C2B	-2.84	1.39	1.43
24	AC	506	CLA	C1D-C2D	2.84	1.49	1.42
24	AB	608	CLA	C4C-NC	2.84	1.42	1.37
24	AC	511	CLA	O1D-CGD	2.84	1.28	1.21
36	AF	101	HEM	CHD-C4C	2.84	1.40	1.36
27	BB	5621	BCR	C29-C30	2.84	1.61	1.54
24	BB	5609	CLA	O1D-CGD	2.84	1.28	1.21
24	AB	611	CLA	C4B-NB	2.84	1.39	1.34
34	BD	5404	PHO	C3D-CAD	-2.84	1.41	1.47
24	AC	501	CLA	MG-NB	2.84	2.11	2.05
24	BB	5616	CLA	C1B-NB	2.84	1.39	1.34
24	AB	608	CLA	MG-NB	2.84	2.11	2.05
24	BC	5511	CLA	C1D-C2D	2.83	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AA	411	DGD	C3G-C2G	2.83	1.58	1.50
24	BB	5615	CLA	C4C-C3C	2.83	1.50	1.45
24	AC	511	CLA	CBB-CAB	2.83	1.50	1.28
24	AB	601	CLA	MG-NC	2.83	2.15	2.07
27	AA	410	BCR	C2-C1	2.83	1.61	1.54
24	AC	511	CLA	MG-NB	2.83	2.11	2.05
24	BB	5609	CLA	C1D-C2D	2.83	1.49	1.42
24	BC	5506	CLA	CMC-C2C	2.82	1.57	1.50
24	AC	510	CLA	C1D-C2D	2.82	1.49	1.42
24	BB	5610	CLA	O1D-CGD	2.82	1.28	1.21
31	BA	5402	LMG	O6-C1	2.82	1.49	1.41
24	AB	606	CLA	C1B-NB	2.82	1.39	1.34
24	AA	405	CLA	C3D-C2D	-2.82	1.33	1.40
24	AB	605	CLA	CMC-C2C	2.81	1.56	1.50
28	BH	5101	DGD	C1G-C2G	2.81	1.58	1.50
24	AC	503	CLA	MG-NA	2.81	2.15	2.07
24	AB	609	CLA	C1D-C2D	2.81	1.49	1.42
31	BC	5520	LMG	O6-C1	2.81	1.49	1.41
24	BB	5615	CLA	C1D-C2D	2.81	1.49	1.42
24	AA	405	CLA	O2A-CGA	2.81	1.41	1.33
28	BE	5102	DGD	O6E-C1E	2.80	1.49	1.41
24	BC	5503	CLA	MG-NC	2.81	2.15	2.07
24	BC	5501	CLA	MG-NB	2.80	2.11	2.05
24	AC	506	CLA	C4B-NB	2.80	1.39	1.34
24	AB	603	CLA	O1D-CGD	2.80	1.28	1.21
24	AB	609	CLA	MG-NB	2.79	2.11	2.05
27	BB	5622	BCR	C14-C13	2.79	1.39	1.35
32	BB	5604	LMT	O1B-C1B	2.79	1.49	1.41
34	AD	402	PHO	O2A-CGA	2.78	1.41	1.33
24	AB	613	CLA	CBB-CAB	2.78	1.49	1.28
24	BB	5608	CLA	C2A-C1A	-2.78	1.47	1.52
24	BB	5619	CLA	O2A-CGA	2.78	1.41	1.33
24	BB	5606	CLA	C4B-NB	2.78	1.39	1.34
28	AA	411	DGD	O5D-C6D	-2.78	1.38	1.43
28	AE	101	DGD	C3G-C2G	2.78	1.58	1.50
24	BB	5608	CLA	C1D-C2D	2.78	1.49	1.42
24	BB	5607	CLA	O1D-CGD	2.78	1.28	1.21
24	BA	5408	CLA	C4C-NC	2.78	1.42	1.37
24	BB	5619	CLA	O1D-CGD	2.77	1.28	1.21
24	BB	5608	CLA	O1D-CGD	2.77	1.28	1.21
24	AA	406	CLA	CHB-C4A	2.77	1.37	1.33
24	AC	502	CLA	MG-NA	2.77	2.15	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5607	CLA	CBA-CGA	2.77	1.59	1.50
32	AD	409	LMT	C8-C7	-2.77	1.54	1.55
24	AC	505	CLA	C4B-NB	2.77	1.39	1.34
32	BD	5411	LMT	O1'-C1'	2.77	1.45	1.40
24	AC	511	CLA	C1D-C2D	2.77	1.49	1.42
24	BC	5503	CLA	O1D-CGD	2.77	1.28	1.21
32	AB	629	LMT	O5'-C1'	2.77	1.48	1.41
24	BC	5506	CLA	C1D-C2D	2.77	1.49	1.42
32	AD	409	LMT	O1B-C1B	2.77	1.49	1.41
24	BC	5512	CLA	C1C-NC	2.77	1.43	1.37
28	BC	5519	DGD	O6E-C1E	2.77	1.48	1.41
30	BF	5102	SQD	O3-C3	2.76	1.49	1.43
24	BC	5507	CLA	MG-NC	2.76	2.15	2.07
24	BA	5406	CLA	C4B-NB	2.76	1.39	1.34
24	AB	611	CLA	C1D-C2D	2.76	1.49	1.42
24	AD	404	CLA	MG-NB	2.76	2.11	2.05
30	BB	5601	SQD	O6-C1	2.76	1.45	1.40
24	BB	5617	CLA	CBB-CAB	2.76	1.49	1.28
24	BC	5504	CLA	CMC-C2C	2.76	1.56	1.50
24	AB	608	CLA	CMC-C2C	2.76	1.56	1.50
24	BA	5408	CLA	O1D-CGD	2.76	1.28	1.21
24	AB	603	CLA	CBA-CGA	2.76	1.58	1.50
24	AB	609	CLA	C4B-NB	2.75	1.39	1.34
24	AC	512	CLA	O1D-CGD	2.75	1.28	1.21
31	AA	417	LMG	O6-C1	2.75	1.48	1.41
28	AB	628	DGD	CDB-CCB	-2.75	1.54	1.55
24	BB	5617	CLA	C1C-NC	2.75	1.43	1.37
35	BD	5406	PL9	C27-C28	2.75	1.58	1.50
24	AD	401	CLA	C1B-NB	2.74	1.39	1.34
24	BC	5503	CLA	MG-NB	2.74	2.11	2.05
36	AF	101	HEM	CAA-C2A	2.74	1.56	1.52
24	AC	512	CLA	CMC-C2C	2.74	1.56	1.50
24	AB	615	CLA	CMC-C2C	2.74	1.56	1.50
27	BC	5515	BCR	C2-C1	2.74	1.61	1.54
24	AB	614	CLA	C1D-C2D	2.74	1.49	1.42
28	AH	101	DGD	C1G-C2G	2.74	1.58	1.50
31	BI	5101	LMG	O6-C1	2.74	1.48	1.41
27	BA	5411	BCR	C2-C1	2.73	1.60	1.54
24	BC	5505	CLA	CAA-CBA	-2.73	1.43	1.52
24	BA	5406	CLA	C3D-C2D	-2.73	1.33	1.40
32	BM	5101	LMT	C4'-C5'	2.73	1.60	1.52
27	BC	5516	BCR	C29-C30	2.73	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5414	SQD	O6-C44	-2.73	1.38	1.43
24	AA	407	CLA	O1D-CGD	2.73	1.28	1.21
24	BC	5503	CLA	CMC-C2C	2.73	1.56	1.50
34	AD	402	PHO	C1D-C2D	2.73	1.49	1.42
24	AA	405	CLA	C4D-ND	-2.72	1.31	1.38
28	AA	411	DGD	O6D-C5D	2.73	1.51	1.44
30	AB	622	SQD	C44-C45	2.72	1.58	1.50
24	BC	5509	CLA	O2A-CGA	2.72	1.41	1.33
24	AC	512	CLA	C1D-C2D	2.72	1.49	1.42
24	AB	609	CLA	C4C-NC	2.72	1.42	1.37
24	BB	5607	CLA	CHC-C1C	2.72	1.44	1.35
24	AB	608	CLA	CAA-C2A	-2.72	1.49	1.54
24	BB	5613	CLA	C4B-NB	2.72	1.39	1.34
30	AA	413	SQD	C8-C7	2.72	1.58	1.50
24	AB	613	CLA	O1D-CGD	2.72	1.28	1.21
24	BB	5611	CLA	CBB-CAB	2.72	1.49	1.28
28	BC	5519	DGD	O5D-C1E	2.71	1.45	1.40
24	BC	5501	CLA	C1D-C2D	2.71	1.49	1.42
24	AD	401	CLA	C4C-NC	2.71	1.42	1.37
28	BA	5412	DGD	C3G-C2G	2.71	1.58	1.50
27	AX	101	BCR	C2-C1	2.71	1.60	1.54
24	AB	602	CLA	CMC-C2C	2.71	1.56	1.50
24	BC	5501	CLA	MG-NA	2.71	2.15	2.07
30	BB	5625	SQD	C12-C11	-2.71	1.35	1.51
24	AB	608	CLA	CBA-CGA	2.71	1.58	1.50
24	BB	5618	CLA	CMC-C2C	2.71	1.56	1.50
32	AB	630	LMT	O1B-C1B	2.71	1.49	1.41
30	BB	5601	SQD	O3-C3	2.71	1.49	1.43
24	AB	615	CLA	O2A-CGA	2.70	1.41	1.33
27	AC	514	BCR	C2-C1	2.70	1.60	1.54
28	BE	5102	DGD	O6D-C1D	2.70	1.48	1.41
24	AB	605	CLA	MG-NA	2.70	2.15	2.07
36	AV	201	HEM	CMC-C2C	2.70	1.56	1.47
31	BA	5402	LMG	O1-C1	2.70	1.45	1.40
31	BB	5624	LMG	O6-C1	2.70	1.48	1.41
24	BB	5605	CLA	CMC-C2C	2.70	1.56	1.50
27	AD	406	BCR	C5-C6	2.70	1.38	1.34
24	AD	401	CLA	C1C-NC	2.69	1.42	1.37
32	BI	5102	LMT	O1'-C1'	2.69	1.45	1.40
24	AB	603	CLA	C1D-C2D	2.69	1.49	1.42
24	BB	5618	CLA	C1D-C2D	2.69	1.49	1.42
24	BB	5620	CLA	O2A-CGA	2.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5606	CLA	MG-NC	2.69	2.15	2.07
32	BI	5102	LMT	O1B-C1B	2.69	1.49	1.41
24	BB	5612	CLA	CBA-CGA	2.68	1.58	1.50
27	BB	5621	BCR	C1-C6	2.68	1.57	1.53
35	BD	5406	PL9	C3-C4	2.68	1.54	1.49
34	BD	5403	PHO	CMC-C2C	2.68	1.56	1.50
24	BB	5612	CLA	C2A-C1A	-2.68	1.47	1.52
24	AB	607	CLA	CBB-CAB	2.68	1.49	1.28
24	AC	501	CLA	C4B-NB	2.68	1.38	1.34
24	BC	5508	CLA	C1D-C2D	2.68	1.49	1.42
24	BB	5615	CLA	O2A-CGA	2.68	1.41	1.33
31	BE	5101	LMG	C39-C38	-2.68	1.54	1.55
32	AB	623	LMT	O5'-C1'	2.68	1.48	1.41
27	AC	514	BCR	C5-C6	2.68	1.38	1.34
28	AE	101	DGD	O6D-C1D	2.68	1.48	1.41
24	BC	5505	CLA	MG-NC	2.68	2.15	2.07
24	AB	601	CLA	CMC-C2C	2.68	1.56	1.50
24	BD	5405	CLA	O2A-CGA	2.68	1.41	1.33
24	AB	616	CLA	C4C-NC	2.68	1.42	1.37
24	AB	604	CLA	C1D-C2D	2.67	1.49	1.42
30	AB	622	SQD	C12-C11	-2.67	1.35	1.51
24	AC	508	CLA	C4B-NB	2.67	1.38	1.34
24	AA	405	CLA	C1D-C2D	2.67	1.49	1.42
24	BB	5608	CLA	C4C-NC	2.67	1.42	1.37
35	AD	405	PL9	C27-C28	2.67	1.58	1.50
24	BC	5509	CLA	C1D-C2D	2.67	1.49	1.42
24	AC	507	CLA	C1D-C2D	2.66	1.49	1.42
24	BB	5616	CLA	C1D-C2D	2.66	1.49	1.42
31	AI	101	LMG	O6-C1	2.66	1.48	1.41
24	AC	513	CLA	CHC-C1C	2.66	1.44	1.35
31	BD	5410	LMG	O6-C1	2.66	1.48	1.41
27	BB	5621	BCR	C30-C25	2.66	1.57	1.53
24	BA	5405	CLA	C1C-NC	2.66	1.42	1.37
24	BD	5405	CLA	MG-NB	2.66	2.10	2.05
24	BD	5405	CLA	C4B-NB	2.66	1.38	1.34
32	BM	5101	LMT	O1B-C1B	2.66	1.48	1.41
24	AB	612	CLA	CMC-C2C	2.66	1.56	1.50
27	AK	102	BCR	C2-C1	2.66	1.60	1.54
24	BB	5612	CLA	O1D-CGD	2.66	1.27	1.21
24	AC	509	CLA	C4B-NB	2.65	1.38	1.34
36	BF	5101	HEM	C1C-NC	2.66	1.41	1.38
24	AB	604	CLA	O2A-CGA	2.65	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	617	BCR	C1-C6	2.65	1.57	1.53
31	BE	5101	LMG	O1-C1	2.65	1.44	1.40
28	AE	101	DGD	O6E-C5E	2.65	1.51	1.44
30	BB	5625	SQD	O5-C1	2.65	1.48	1.41
30	AA	413	SQD	C17-C16	-2.65	1.35	1.51
24	AC	504	CLA	C4C-NC	2.65	1.42	1.37
24	BC	5506	CLA	MG-NC	2.65	2.15	2.07
24	BB	5619	CLA	C1D-C2D	2.65	1.49	1.42
32	AB	624	LMT	O5'-C1'	2.65	1.48	1.41
24	BC	5501	CLA	CBA-CGA	2.65	1.58	1.50
30	BB	5625	SQD	C11-C10	-2.64	1.35	1.51
24	AB	611	CLA	O1D-CGD	2.64	1.27	1.21
24	BB	5618	CLA	O1D-CGD	2.65	1.27	1.21
30	BB	5601	SQD	C12-C11	-2.64	1.35	1.51
24	AB	607	CLA	CBA-CGA	2.64	1.58	1.50
24	AC	508	CLA	C1D-C2D	2.64	1.49	1.42
28	AC	517	DGD	O3G-C3G	-2.64	1.38	1.43
24	BA	5406	CLA	O1D-CGD	2.64	1.27	1.21
30	AB	622	SQD	O5-C1	2.64	1.48	1.41
24	AB	606	CLA	OBD-CAD	2.64	1.26	1.22
36	AF	101	HEM	FE-NB	2.63	2.06	1.96
24	AC	512	CLA	MG-NC	2.63	2.15	2.07
24	AB	612	CLA	O2A-CGA	2.63	1.41	1.33
24	BC	5513	CLA	MG-NB	2.63	2.10	2.05
24	BC	5510	CLA	C4B-NB	2.63	1.38	1.34
28	BE	5102	DGD	C1G-C2G	2.62	1.58	1.50
24	BA	5405	CLA	C1D-C2D	2.62	1.49	1.42
24	AC	510	CLA	C4C-NC	2.62	1.42	1.37
27	BC	5514	BCR	C5-C6	2.62	1.38	1.34
24	AA	404	CLA	C4B-NB	2.62	1.38	1.34
24	BD	5402	CLA	MG-NB	2.62	2.10	2.05
24	BA	5406	CLA	C4C-C3C	2.62	1.49	1.45
30	AB	627	SQD	C15-C14	-2.62	1.35	1.51
32	BD	5411	LMT	O1B-C1B	2.62	1.48	1.41
24	AA	407	CLA	CMC-C2C	2.62	1.56	1.50
24	BC	5510	CLA	CMC-C2C	2.62	1.56	1.50
24	AC	513	CLA	MG-NB	2.61	2.10	2.05
32	AB	630	LMT	O1'-C1'	2.61	1.44	1.40
24	BB	5619	CLA	CMC-C2C	2.61	1.56	1.50
28	AC	517	DGD	O6D-C5D	2.61	1.50	1.44
27	BB	5621	BCR	C23-C22	-2.61	1.40	1.45
24	BB	5614	CLA	MG-NB	2.61	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BB	5601	SQD	C15-C14	-2.61	1.35	1.51
24	BA	5406	CLA	C4C-NC	2.61	1.42	1.37
24	AB	612	CLA	CHC-C1C	2.61	1.44	1.35
24	BB	5609	CLA	CMC-C2C	2.61	1.56	1.50
24	BD	5402	CLA	C4C-NC	2.61	1.42	1.37
24	BC	5508	CLA	O1D-CGD	2.60	1.27	1.21
24	AB	615	CLA	O1D-CGD	2.60	1.27	1.21
31	AD	408	LMG	O1-C1	2.60	1.44	1.40
34	BD	5404	PHO	CMC-C2C	2.61	1.56	1.50
27	BC	5516	BCR	C19-C18	-2.60	1.40	1.45
24	AB	612	CLA	O1D-CGD	2.60	1.27	1.21
24	AC	503	CLA	O1D-CGD	2.60	1.27	1.21
24	BC	5510	CLA	MG-NA	2.60	2.14	2.07
36	AV	201	HEM	C1A-NA	2.60	1.40	1.36
32	BB	5603	LMT	O1B-C4'	2.60	1.50	1.43
30	AB	627	SQD	C20-C19	-2.60	1.35	1.51
30	AB	627	SQD	O5-C1	2.60	1.48	1.41
24	AB	616	CLA	C4B-NB	2.60	1.38	1.34
30	BB	5601	SQD	C16-C15	-2.60	1.35	1.51
30	BA	5414	SQD	C17-C16	-2.60	1.35	1.51
30	AA	413	SQD	C15-C14	-2.59	1.35	1.51
31	AB	621	LMG	O6-C1	2.59	1.48	1.41
28	AH	101	DGD	O6E-C1E	2.59	1.48	1.41
36	BV	5201	HEM	FE-NB	2.59	2.06	1.96
32	BB	5604	LMT	O1'-C1'	2.59	1.44	1.40
24	BB	5612	CLA	CAA-C2A	-2.59	1.49	1.54
24	BB	5611	CLA	CBA-CGA	2.59	1.58	1.50
27	AJ	101	BCR	C24-C23	2.59	1.40	1.32
36	BV	5201	HEM	C4D-ND	-2.59	1.34	1.39
30	AB	622	SQD	C11-C10	-2.59	1.35	1.51
36	AF	101	HEM	O2A-CGA	-2.59	1.21	1.30
30	AB	627	SQD	C16-C15	-2.59	1.36	1.51
24	AC	503	CLA	C4B-NB	2.58	1.38	1.34
24	AC	506	CLA	MG-NC	2.58	2.14	2.07
24	AA	405	CLA	C1B-NB	2.58	1.38	1.34
30	AB	627	SQD	C12-C11	-2.58	1.36	1.51
24	AB	616	CLA	MG-NB	2.58	2.10	2.05
24	AB	608	CLA	O1D-CGD	2.58	1.27	1.21
30	BB	5601	SQD	O5-C1	2.58	1.48	1.41
24	AD	401	CLA	O1D-CGD	2.58	1.27	1.21
28	AC	519	DGD	O3G-C3G	2.58	1.48	1.43
32	AB	630	LMT	O5'-C1'	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	603	CLA	CHC-C1C	2.58	1.43	1.35
27	BJ	5101	BCR	C24-C23	2.58	1.40	1.32
31	AD	408	LMG	O6-C1	2.57	1.48	1.41
30	BF	5102	SQD	C17-C16	-2.57	1.36	1.51
28	BA	5412	DGD	O6D-C5D	2.57	1.50	1.44
24	BB	5620	CLA	MG-NA	2.57	2.14	2.07
28	AE	101	DGD	C1G-C2G	2.57	1.57	1.50
30	BA	5414	SQD	C33-C32	-2.57	1.36	1.51
24	BB	5617	CLA	MG-NB	2.57	2.10	2.05
24	BB	5608	CLA	O2A-CGA	2.57	1.41	1.33
24	AB	607	CLA	O1D-CGD	2.57	1.27	1.21
30	BA	5414	SQD	C15-C14	-2.57	1.36	1.51
31	BC	5520	LMG	O1-C1	2.57	1.44	1.40
24	AB	608	CLA	C4B-NB	2.57	1.38	1.34
24	BB	5620	CLA	MG-NC	2.57	2.14	2.07
24	BC	5507	CLA	O1D-CGD	2.56	1.27	1.21
24	BD	5402	CLA	O2A-CGA	2.56	1.41	1.33
30	BB	5601	SQD	C20-C19	-2.56	1.36	1.51
24	AB	610	CLA	C4C-NC	2.56	1.42	1.37
24	BC	5508	CLA	CHC-C1C	2.56	1.43	1.35
27	AT	101	BCR	C26-C25	2.56	1.38	1.34
24	AA	407	CLA	C1C-NC	2.56	1.42	1.37
24	BB	5616	CLA	MG-NB	2.55	2.10	2.05
32	BB	5626	LMT	O5'-C1'	2.55	1.48	1.41
30	AB	627	SQD	C19-C18	-2.55	1.36	1.51
24	BC	5513	CLA	CHC-C1C	2.55	1.43	1.35
24	BB	5614	CLA	C4C-NC	2.55	1.42	1.37
30	AB	627	SQD	C14-C13	-2.55	1.36	1.51
36	BF	5101	HEM	O2A-CGA	-2.55	1.21	1.30
24	AC	505	CLA	C2A-C1A	-2.55	1.47	1.52
30	BB	5601	SQD	C11-C10	-2.55	1.36	1.51
30	AA	413	SQD	C16-C15	-2.54	1.36	1.51
28	AE	101	DGD	O6D-C5D	2.54	1.50	1.44
24	BB	5613	CLA	CMC-C2C	2.54	1.56	1.50
36	AV	201	HEM	CHD-C4C	2.54	1.40	1.36
24	AC	509	CLA	C1D-C2D	2.54	1.49	1.42
28	BH	5101	DGD	O6E-C1E	2.54	1.48	1.41
24	AB	602	CLA	O1D-CGD	2.54	1.27	1.21
24	BB	5610	CLA	O2A-CGA	2.54	1.41	1.33
24	BB	5606	CLA	O2A-CGA	2.54	1.41	1.33
30	BB	5601	SQD	C14-C13	-2.53	1.36	1.51
24	AB	610	CLA	MG-NB	2.53	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5614	CLA	C4B-NB	2.53	1.38	1.34
30	BA	5414	SQD	C16-C15	-2.53	1.36	1.51
30	AA	413	SQD	C33-C32	-2.53	1.36	1.51
24	AA	405	CLA	OBD-CAD	2.53	1.26	1.22
36	BF	5101	HEM	CAA-C2A	2.53	1.56	1.52
24	BD	5402	CLA	C1D-C2D	2.52	1.48	1.42
27	AA	410	BCR	C5-C6	2.52	1.38	1.34
24	BB	5614	CLA	C1D-C2D	2.52	1.48	1.42
24	AA	406	CLA	CHC-C1C	2.52	1.43	1.35
24	BB	5610	CLA	CMC-C2C	2.52	1.56	1.50
24	AB	613	CLA	C1B-NB	2.52	1.38	1.34
24	AA	407	CLA	MG-NA	2.52	2.14	2.07
24	AB	607	CLA	C1D-C2D	2.52	1.48	1.42
24	BA	5405	CLA	MG-NB	2.52	2.10	2.05
30	BF	5102	SQD	C11-C10	-2.51	1.36	1.51
36	BF	5101	HEM	CBA-CGA	2.51	1.56	1.50
24	BC	5502	CLA	CMC-C2C	2.51	1.56	1.50
24	AB	606	CLA	C4C-NC	2.51	1.42	1.37
24	BC	5507	CLA	C4B-NB	2.51	1.38	1.34
24	AC	501	CLA	O1D-CGD	2.51	1.27	1.21
32	AB	623	LMT	O1B-C1B	2.51	1.48	1.41
30	BF	5102	SQD	C16-C15	-2.51	1.36	1.51
30	AB	627	SQD	C11-C10	-2.51	1.36	1.51
30	BB	5601	SQD	C17-C16	-2.51	1.36	1.51
24	AD	404	CLA	C2A-C1A	-2.51	1.47	1.52
31	AC	520	LMG	O6-C1	2.51	1.48	1.41
24	BD	5402	CLA	O1D-CGD	2.50	1.27	1.21
24	BC	5504	CLA	O1D-CGD	2.50	1.27	1.21
24	AB	602	CLA	C4B-NB	2.50	1.38	1.34
24	BB	5611	CLA	MG-NB	2.50	2.10	2.05
24	BC	5502	CLA	C2A-C1A	-2.50	1.47	1.52
24	AC	504	CLA	O2A-CGA	2.50	1.40	1.33
30	BA	5401	SQD	C8-C7	2.50	1.58	1.50
24	AD	401	CLA	MG-NA	2.49	2.14	2.07
24	BB	5607	CLA	CMC-C2C	2.49	1.56	1.50
28	AE	101	DGD	O2G-C2G	2.49	1.52	1.46
24	AC	507	CLA	C4C-NC	2.49	1.42	1.37
24	BC	5512	CLA	O2A-CGA	2.49	1.40	1.33
30	AB	627	SQD	C13-C12	-2.49	1.36	1.51
30	AF	102	SQD	C17-C16	-2.49	1.36	1.51
30	BB	5601	SQD	C19-C18	-2.49	1.36	1.51
36	BV	5201	HEM	C1A-NA	2.49	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AF	102	SQD	C11-C10	-2.49	1.36	1.51
24	BB	5612	CLA	C4C-NC	2.48	1.42	1.37
24	BB	5608	CLA	CMC-C2C	2.48	1.56	1.50
31	BM	5102	LMG	C22-C21	-2.48	1.54	1.55
24	AB	603	CLA	CMC-C2C	2.48	1.56	1.50
30	BA	5414	SQD	C11-C10	-2.48	1.36	1.51
31	BD	5408	LMG	O6-C1	2.48	1.48	1.41
35	AD	405	PL9	C3-C4	2.48	1.53	1.49
24	AB	615	CLA	C1C-NC	2.48	1.42	1.37
24	BC	5508	CLA	MG-NC	2.48	2.14	2.07
34	AD	403	PHO	CMC-C2C	2.48	1.56	1.50
30	AA	416	SQD	C17-C16	-2.48	1.36	1.51
24	AB	615	CLA	C1D-C2D	2.48	1.48	1.42
24	BA	5406	CLA	O2A-CGA	2.48	1.40	1.33
32	BD	5411	LMT	C4'-C5'	2.48	1.59	1.52
24	AB	606	CLA	C4B-NB	2.48	1.38	1.34
24	BC	5504	CLA	CHC-C1C	2.48	1.43	1.35
24	AB	607	CLA	C4B-NB	2.48	1.38	1.34
31	BM	5102	LMG	O1-C1	2.48	1.44	1.40
34	BD	5404	PHO	C1D-C2D	2.48	1.48	1.42
24	AC	504	CLA	CMC-C2C	2.47	1.56	1.50
27	AC	516	BCR	C29-C30	2.47	1.60	1.54
24	AD	404	CLA	O2A-CGA	2.47	1.40	1.33
27	AC	516	BCR	C19-C18	-2.47	1.40	1.45
30	BB	5601	SQD	C13-C12	-2.47	1.36	1.51
24	AB	602	CLA	C1C-NC	2.47	1.42	1.37
24	BB	5617	CLA	CMC-C2C	2.47	1.56	1.50
32	AI	102	LMT	O1'-C1'	2.47	1.44	1.40
24	AB	607	CLA	CMC-C2C	2.47	1.56	1.50
24	BA	5407	CLA	O2A-CGA	2.47	1.40	1.33
30	BA	5414	SQD	C12-C11	-2.47	1.36	1.51
24	AA	404	CLA	C1D-C2D	2.47	1.48	1.42
24	AB	614	CLA	O1D-CGD	2.47	1.27	1.21
30	BA	5414	SQD	C8-C7	2.47	1.58	1.50
30	AB	627	SQD	O6-C1	2.47	1.44	1.40
24	BC	5504	CLA	C1C-NC	2.47	1.42	1.37
24	BC	5501	CLA	C4C-NC	2.46	1.42	1.37
27	BJ	5101	BCR	C17-C18	2.46	1.39	1.35
24	BC	5505	CLA	MG-NB	2.46	2.10	2.05
31	AM	101	LMG	O1-C1	2.46	1.44	1.40
30	BA	5414	SQD	C19-C18	-2.46	1.36	1.51
24	AC	506	CLA	CMC-C2C	2.46	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	AF	101	HEM	CMD-C2D	2.46	1.55	1.47
24	AB	615	CLA	C4C-NC	2.46	1.42	1.37
24	BD	5402	CLA	MG-NA	2.45	2.14	2.07
24	AB	610	CLA	O1D-CGD	2.45	1.27	1.21
24	BC	5505	CLA	C2A-C1A	-2.45	1.47	1.52
30	BF	5102	SQD	C15-C14	-2.45	1.36	1.51
24	BB	5610	CLA	OBD-CAD	2.45	1.25	1.22
27	AB	619	BCR	C23-C22	-2.45	1.40	1.45
24	AC	508	CLA	O2A-CGA	2.45	1.40	1.33
36	BV	5201	HEM	CAD-CBD	2.45	1.59	1.52
30	AB	627	SQD	C17-C16	-2.45	1.36	1.51
24	AB	601	CLA	C1C-NC	2.45	1.42	1.37
27	BX	5101	BCR	C14-C13	2.45	1.39	1.35
24	AC	507	CLA	MG-NC	2.44	2.14	2.07
36	AV	201	HEM	C4D-ND	-2.44	1.34	1.39
28	BE	5102	DGD	O2G-C2G	2.44	1.52	1.46
30	AA	413	SQD	C19-C18	-2.44	1.36	1.51
32	BB	5626	LMT	C4'-C5'	2.44	1.59	1.52
30	BB	5625	SQD	C16-C15	-2.44	1.36	1.51
24	BB	5617	CLA	O2A-CGA	2.44	1.40	1.33
24	AC	507	CLA	O1D-CGD	2.44	1.27	1.21
24	BC	5507	CLA	CMC-C2C	2.44	1.56	1.50
36	BV	5201	HEM	CHA-C4D	2.44	1.39	1.35
24	AB	604	CLA	O1D-CGD	2.44	1.27	1.21
30	BF	5102	SQD	C12-C11	-2.43	1.36	1.51
30	AF	102	SQD	C12-C11	-2.43	1.36	1.51
30	AA	416	SQD	C16-C15	-2.43	1.36	1.51
35	BD	5406	PL9	C7-C3	2.43	1.53	1.51
24	BA	5405	CLA	C1B-NB	2.43	1.38	1.34
24	AB	607	CLA	MG-NB	2.43	2.10	2.05
24	AC	513	CLA	CMC-C2C	2.43	1.56	1.50
27	BC	5515	BCR	C19-C18	-2.43	1.40	1.45
24	BA	5405	CLA	C2A-C1A	-2.43	1.47	1.52
30	BA	5401	SQD	C36-C35	-2.43	1.36	1.51
24	BB	5616	CLA	CMC-C2C	2.43	1.56	1.50
36	AV	201	HEM	C4C-NC	2.43	1.41	1.38
30	AA	413	SQD	C12-C11	-2.43	1.36	1.51
36	BV	5201	HEM	CMD-C2D	2.43	1.55	1.47
32	BC	5522	LMT	C4'-C5'	2.43	1.59	1.52
30	BA	5401	SQD	C6-S	2.43	1.81	1.77
24	AD	401	CLA	CHC-C1C	2.43	1.43	1.35
24	AB	614	CLA	CMC-C2C	2.43	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	5627	LMT	C4'-C5'	2.42	1.59	1.52
30	BB	5625	SQD	C44-C45	2.42	1.57	1.50
24	AD	401	CLA	MG-NB	2.42	2.10	2.05
24	AB	602	CLA	O2A-CGA	2.42	1.40	1.33
24	BB	5606	CLA	O1D-CGD	2.42	1.27	1.21
24	AB	607	CLA	C1C-NC	2.42	1.42	1.37
36	AV	201	HEM	FE-ND	2.42	2.05	1.96
32	BI	5102	LMT	O5'-C1'	2.42	1.48	1.41
34	AD	403	PHO	C1D-C2D	2.42	1.48	1.42
36	BV	5201	HEM	FE-ND	2.41	2.05	1.96
30	AB	622	SQD	C16-C15	-2.41	1.37	1.51
24	AC	510	CLA	MG-NC	2.41	2.14	2.07
27	BK	5102	BCR	C14-C13	2.41	1.38	1.35
36	AF	101	HEM	C4C-NC	2.41	1.41	1.38
30	AA	416	SQD	C19-C18	-2.41	1.37	1.51
30	BF	5102	SQD	C24-C23	2.40	1.57	1.50
30	AA	416	SQD	C12-C11	-2.40	1.37	1.51
24	BB	5611	CLA	CMC-C2C	2.40	1.56	1.50
24	BB	5605	CLA	MG-NB	2.40	2.10	2.05
34	BD	5404	PHO	C4B-NB	2.40	1.40	1.36
24	AB	602	CLA	MG-NC	2.40	2.14	2.07
35	AD	405	PL9	C7-C3	2.40	1.53	1.51
34	AD	403	PHO	O1D-CGD	2.40	1.27	1.21
24	AC	510	CLA	C1C-NC	2.40	1.42	1.37
30	AF	102	SQD	C15-C14	-2.39	1.37	1.51
30	BA	5401	SQD	C12-C11	-2.39	1.37	1.51
24	AA	407	CLA	C4C-NC	2.39	1.42	1.37
30	AF	102	SQD	C24-C23	2.39	1.57	1.50
30	AA	413	SQD	C32-C31	-2.39	1.37	1.51
24	BD	5402	CLA	CHC-C1C	2.39	1.43	1.35
24	BB	5610	CLA	C4C-NC	2.39	1.42	1.37
24	BC	5503	CLA	OBD-CAD	2.39	1.25	1.22
36	AF	101	HEM	FE-ND	2.38	2.05	1.96
28	AA	411	DGD	C4E-C3E	2.38	1.58	1.52
30	AB	622	SQD	C13-C12	-2.38	1.37	1.51
30	AF	102	SQD	C16-C15	-2.38	1.37	1.51
30	AA	416	SQD	C8-C7	2.38	1.57	1.50
24	AC	508	CLA	CHC-C1C	2.38	1.43	1.35
30	BB	5625	SQD	C13-C12	-2.38	1.37	1.51
30	BA	5401	SQD	C33-C32	-2.38	1.37	1.51
28	BE	5102	DGD	O6E-C5E	2.38	1.50	1.44
30	AA	416	SQD	C36-C35	-2.38	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5505	CLA	C4C-NC	2.38	1.42	1.37
24	AC	510	CLA	CMC-C2C	2.38	1.56	1.50
24	AC	504	CLA	O1D-CGD	2.38	1.27	1.21
24	AC	505	CLA	O1D-CGD	2.37	1.27	1.21
30	BA	5414	SQD	C14-C13	-2.37	1.37	1.51
34	BD	5403	PHO	O2A-CGA	2.37	1.40	1.33
24	AA	405	CLA	C1C-NC	2.37	1.42	1.37
24	BC	5504	CLA	MG-NA	2.37	2.14	2.07
24	BB	5605	CLA	MG-NC	2.37	2.14	2.07
27	AX	101	BCR	C38-C26	2.37	1.55	1.51
24	AB	609	CLA	CMC-C2C	2.37	1.56	1.50
24	BC	5506	CLA	C1C-NC	2.37	1.42	1.37
24	AA	406	CLA	CMC-C2C	2.36	1.56	1.50
24	AA	405	CLA	C4C-NC	2.36	1.42	1.37
30	BA	5401	SQD	C17-C16	-2.36	1.37	1.51
30	BA	5401	SQD	C15-C14	-2.36	1.37	1.51
24	BB	5606	CLA	C1C-NC	2.36	1.42	1.37
36	BF	5101	HEM	CHD-C4C	2.36	1.39	1.36
32	AB	630	LMT	C4'-C5'	2.36	1.59	1.52
24	AC	508	CLA	O1D-CGD	2.36	1.27	1.21
30	AA	413	SQD	C14-C13	-2.36	1.37	1.51
24	AC	510	CLA	MG-NA	2.36	2.14	2.07
30	AA	413	SQD	C11-C10	-2.36	1.37	1.51
24	AB	608	CLA	C1C-NC	2.36	1.42	1.37
24	BB	5606	CLA	MG-NA	2.36	2.14	2.07
24	AC	509	CLA	O2A-CGA	2.35	1.40	1.33
32	BB	5604	LMT	O5'-C1'	2.35	1.47	1.41
28	BC	5517	DGD	C9B-C8B	-2.35	1.54	1.55
24	BB	5611	CLA	C1B-NB	2.35	1.38	1.34
30	BA	5401	SQD	C16-C15	-2.35	1.37	1.51
24	AB	604	CLA	C1C-NC	2.35	1.42	1.37
24	BA	5408	CLA	CHC-C1C	2.35	1.43	1.35
24	AC	506	CLA	CBA-CGA	2.35	1.57	1.50
28	BC	5517	DGD	O3G-C1D	2.35	1.44	1.40
24	BC	5506	CLA	CBA-CGA	2.35	1.57	1.50
24	AC	504	CLA	CHC-C1C	2.35	1.43	1.35
32	AB	624	LMT	C4'-C5'	2.35	1.59	1.52
32	AI	103	LMT	O1B-C1B	2.35	1.48	1.41
36	BF	5101	HEM	CMD-C2D	2.35	1.54	1.47
28	BC	5519	DGD	O3E-C3E	-2.35	1.37	1.43
30	AA	413	SQD	C18-C17	-2.35	1.37	1.51
24	BC	5508	CLA	C2A-C1A	-2.35	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	413	SQD	C20-C19	-2.34	1.37	1.51
28	BA	5412	DGD	C1G-C2G	2.34	1.57	1.50
24	BC	5509	CLA	CHC-C1C	2.34	1.43	1.35
24	BC	5513	CLA	CMC-C2C	2.34	1.55	1.50
24	BC	5511	CLA	CMC-C2C	2.34	1.55	1.50
24	AD	401	CLA	C1D-C2D	2.34	1.48	1.42
24	BB	5613	CLA	C4C-NC	2.34	1.42	1.37
30	BB	5601	SQD	C18-C17	-2.34	1.37	1.51
24	AA	405	CLA	C4B-NB	2.34	1.38	1.34
24	BB	5616	CLA	CHC-C1C	2.34	1.43	1.35
28	AC	519	DGD	C4E-C3E	2.34	1.58	1.52
24	BC	5507	CLA	MG-NB	2.34	2.10	2.05
24	AB	606	CLA	C2A-C1A	-2.34	1.48	1.52
30	BA	5414	SQD	C20-C19	-2.34	1.37	1.51
24	BA	5406	CLA	C1C-NC	2.34	1.42	1.37
24	AC	501	CLA	CBA-CGA	2.33	1.57	1.50
24	BA	5407	CLA	C4C-NC	2.33	1.42	1.37
24	AC	507	CLA	CMC-C2C	2.33	1.55	1.50
24	AB	605	CLA	CHC-C1C	2.33	1.43	1.35
24	BB	5612	CLA	C4B-NB	2.33	1.38	1.34
28	BC	5518	DGD	O2G-C1B	2.33	1.41	1.34
24	BA	5406	CLA	C4D-ND	-2.33	1.32	1.38
32	BB	5604	LMT	C4'-C5'	2.33	1.59	1.52
30	AA	416	SQD	C15-C14	-2.33	1.37	1.51
24	AB	607	CLA	C4C-NC	2.33	1.42	1.37
30	AA	416	SQD	C33-C32	-2.32	1.37	1.51
24	AB	607	CLA	CHC-C1C	2.32	1.43	1.35
31	BM	5102	LMG	O7-C10	2.32	1.41	1.34
34	BD	5404	PHO	O1D-CGD	2.32	1.27	1.21
30	BA	5414	SQD	C32-C31	-2.32	1.37	1.51
32	BB	5627	LMT	O5'-C1'	2.32	1.47	1.41
30	AA	416	SQD	C6-S	2.32	1.81	1.77
24	AC	501	CLA	C5-C3	2.32	1.56	1.51
24	BC	5507	CLA	MG-NA	2.31	2.14	2.07
24	BC	5507	CLA	C4C-NC	2.31	1.42	1.37
32	BB	5626	LMT	O1B-C1B	2.31	1.48	1.41
24	BC	5508	CLA	O2A-CGA	2.31	1.40	1.33
24	AA	407	CLA	O2A-CGA	2.31	1.40	1.33
30	BB	5625	SQD	C15-C14	-2.31	1.37	1.51
24	AC	504	CLA	C2A-C1A	-2.31	1.48	1.52
32	AD	409	LMT	C4'-C5'	2.31	1.59	1.52
24	BA	5407	CLA	C3D-C2D	-2.31	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	605	CLA	C1C-NC	2.31	1.42	1.37
30	BA	5401	SQD	C13-C12	-2.31	1.37	1.51
30	AB	622	SQD	C15-C14	-2.31	1.37	1.51
24	AB	614	CLA	C2A-C1A	-2.31	1.48	1.52
31	AA	417	LMG	O7-C8	-2.31	1.40	1.46
31	AA	417	LMG	O1-C1	2.30	1.44	1.40
24	AC	505	CLA	MG-NB	2.30	2.10	2.05
24	AB	604	CLA	C2A-C1A	-2.30	1.48	1.52
32	AB	629	LMT	O1B-C4'	2.30	1.49	1.43
27	BB	5623	BCR	C23-C22	-2.30	1.40	1.45
30	BA	5401	SQD	C32-C31	-2.30	1.37	1.51
24	BC	5501	CLA	MG-NC	2.30	2.14	2.07
24	AC	505	CLA	C4C-NC	2.30	1.41	1.37
31	AC	520	LMG	O1-C1	2.29	1.44	1.40
32	AM	102	LMT	O1B-C1B	2.29	1.47	1.41
36	AV	201	HEM	FE-NB	2.29	2.05	1.96
24	AC	507	CLA	MG-NB	2.29	2.10	2.05
24	BA	5407	CLA	CHC-C1C	2.29	1.42	1.35
28	BA	5412	DGD	O3G-C1D	2.29	1.44	1.40
31	BM	5102	LMG	O6-C1	2.29	1.47	1.41
30	BB	5625	SQD	C14-C13	-2.29	1.37	1.51
30	BA	5414	SQD	C13-C12	-2.29	1.37	1.51
30	BA	5414	SQD	C18-C17	-2.28	1.37	1.51
24	AB	607	CLA	C3B-CAB	-2.28	1.42	1.47
30	AB	627	SQD	C18-C17	-2.28	1.37	1.51
30	AA	416	SQD	C11-C10	-2.28	1.37	1.51
24	AC	512	CLA	C1C-NC	2.28	1.42	1.37
24	AB	605	CLA	C4C-NC	2.28	1.41	1.37
32	AI	102	LMT	O5'-C1'	2.27	1.47	1.41
24	AC	512	CLA	O2A-CGA	2.27	1.40	1.33
24	BA	5408	CLA	O2A-CGA	2.27	1.40	1.33
24	BB	5617	CLA	MG-NA	2.26	2.13	2.07
28	BH	5101	DGD	O3G-C1D	2.26	1.44	1.40
36	BV	5201	HEM	C1C-NC	2.26	1.41	1.38
30	AF	102	SQD	C14-C13	-2.27	1.37	1.51
30	BA	5401	SQD	C34-C33	-2.26	1.37	1.51
27	BB	5623	BCR	C33-C5	2.26	1.54	1.51
28	BC	5517	DGD	C3G-C2G	2.26	1.57	1.50
28	AC	519	DGD	C1E-C2E	-2.26	1.45	1.52
24	BD	5402	CLA	MG-NC	2.26	2.13	2.07
30	AB	622	SQD	C14-C13	-2.26	1.37	1.51
30	BA	5401	SQD	C14-C13	-2.26	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	509	CLA	MG-NB	2.26	2.10	2.05
30	AA	416	SQD	C20-C19	-2.26	1.37	1.51
24	BB	5609	CLA	C2A-C1A	-2.26	1.48	1.52
24	BA	5406	CLA	MG-NB	2.26	2.10	2.05
24	AC	503	CLA	C2A-C1A	-2.25	1.48	1.52
30	AA	413	SQD	C13-C12	-2.25	1.38	1.51
28	BC	5517	DGD	O6D-C5D	2.25	1.50	1.44
24	AB	602	CLA	MG-NA	2.25	2.13	2.07
32	AI	102	LMT	O1B-C1B	2.25	1.47	1.41
30	AF	102	SQD	C44-C45	2.25	1.57	1.50
30	AA	416	SQD	C32-C31	-2.25	1.38	1.51
36	AV	201	HEM	CMD-C2D	2.25	1.54	1.47
24	AA	404	CLA	MG-NB	2.25	2.10	2.05
36	BF	5101	HEM	C4C-NC	2.25	1.41	1.38
31	BI	5101	LMG	O1-C1	2.25	1.44	1.40
24	BB	5614	CLA	O1D-CGD	2.24	1.26	1.21
24	AD	404	CLA	C1C-NC	2.25	1.42	1.37
34	AD	403	PHO	O2A-CGA	2.25	1.40	1.33
30	AF	102	SQD	C13-C12	-2.25	1.38	1.51
32	BD	5411	LMT	O5'-C1'	2.25	1.47	1.41
27	AJ	101	BCR	C17-C18	2.24	1.38	1.35
30	BA	5401	SQD	C35-C34	-2.24	1.38	1.51
28	AH	101	DGD	O3G-C1D	2.24	1.44	1.40
32	BC	5522	LMT	O1B-C1B	2.24	1.47	1.41
30	BF	5102	SQD	C8-C7	2.24	1.57	1.50
30	BB	5601	SQD	C24-C23	2.24	1.57	1.50
24	AB	616	CLA	C1D-C2D	2.24	1.48	1.42
24	AB	604	CLA	CHC-C1C	2.24	1.42	1.35
24	BD	5405	CLA	C2A-C1A	-2.23	1.48	1.52
31	AD	407	LMG	O7-C8	-2.23	1.41	1.46
24	AB	603	CLA	C2A-C1A	-2.23	1.48	1.52
24	BA	5407	CLA	C4D-ND	-2.23	1.32	1.38
30	AA	416	SQD	C13-C12	-2.23	1.38	1.51
24	BB	5619	CLA	C4C-NC	2.23	1.41	1.37
24	BA	5405	CLA	CHC-C1C	2.23	1.42	1.35
24	BB	5611	CLA	O1D-CGD	2.23	1.26	1.21
28	AA	411	DGD	CDA-CCA	-2.23	1.54	1.55
24	BC	5503	CLA	C1C-NC	2.23	1.42	1.37
24	AB	603	CLA	C4C-NC	2.23	1.41	1.37
24	AC	507	CLA	MG-NA	2.22	2.13	2.07
24	BB	5617	CLA	MG-NC	2.22	2.13	2.07
27	AX	101	BCR	C14-C13	2.22	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5610	CLA	C2A-C1A	-2.22	1.48	1.52
24	AB	610	CLA	C4B-NB	2.22	1.38	1.34
28	AC	519	DGD	O5D-C1E	2.22	1.44	1.40
32	AM	102	LMT	O5'-C1'	2.22	1.47	1.41
30	BF	5102	SQD	C14-C13	-2.21	1.38	1.51
24	AC	511	CLA	CMC-C2C	2.21	1.55	1.50
30	AA	413	SQD	O6-C1	2.21	1.44	1.40
30	BA	5401	SQD	C19-C18	-2.21	1.38	1.51
30	BA	5401	SQD	C20-C19	-2.21	1.38	1.51
31	AJ	102	LMG	O6-C1	2.21	1.47	1.41
30	AA	416	SQD	C35-C34	-2.21	1.38	1.51
24	AA	406	CLA	O1D-CGD	2.21	1.26	1.21
24	AC	508	CLA	MG-NC	2.21	2.13	2.07
34	BD	5404	PHO	C4C-NC	2.21	1.42	1.37
27	BK	5102	BCR	C38-C26	2.21	1.54	1.51
36	BV	5201	HEM	CAA-C2A	2.20	1.55	1.52
31	AA	417	LMG	O8-C9	2.20	1.50	1.45
28	AC	519	DGD	C6E-C5E	2.20	1.59	1.52
30	BF	5102	SQD	C13-C12	-2.20	1.38	1.51
32	AB	623	LMT	C4'-C5'	2.20	1.59	1.52
24	AC	502	CLA	MG-NC	2.20	2.13	2.07
24	BA	5408	CLA	MG-NC	2.20	2.13	2.07
32	BI	5102	LMT	O1B-C4'	2.20	1.49	1.43
24	BC	5509	CLA	OBD-CAD	2.19	1.25	1.22
32	BC	5522	LMT	O1'-C1'	2.19	1.44	1.40
27	BD	5407	BCR	C38-C26	2.19	1.54	1.51
30	BA	5401	SQD	C11-C10	-2.19	1.38	1.51
24	AB	606	CLA	CMC-C2C	2.19	1.55	1.50
31	BA	5402	LMG	O7-C8	-2.19	1.41	1.46
24	AB	606	CLA	C1C-NC	2.19	1.42	1.37
24	AA	404	CLA	CHC-C1C	2.19	1.42	1.35
24	AB	616	CLA	MG-NC	2.19	2.13	2.07
24	BB	5620	CLA	C1D-C2D	2.18	1.48	1.42
24	AC	502	CLA	C2A-C1A	-2.18	1.48	1.52
34	BD	5403	PHO	C4B-NB	2.18	1.39	1.36
30	AA	416	SQD	C34-C33	-2.18	1.38	1.51
24	BB	5613	CLA	CBA-CGA	2.18	1.57	1.50
28	AA	411	DGD	C1G-C2G	2.18	1.56	1.50
31	AD	408	LMG	O7-C8	-2.18	1.41	1.46
36	BV	5201	HEM	C2A-C3A	2.18	1.44	1.37
30	AA	416	SQD	C14-C13	-2.18	1.38	1.51
30	AA	416	SQD	C18-C17	-2.18	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5404	PHO	CHA-C1A	2.18	1.42	1.37
24	BB	5615	CLA	MG-NC	2.18	2.13	2.07
24	AA	405	CLA	CHC-C1C	2.17	1.42	1.35
36	AF	101	HEM	CBA-CGA	2.17	1.55	1.50
24	AC	508	CLA	C2A-C1A	-2.17	1.48	1.52
27	AD	406	BCR	C38-C26	2.17	1.54	1.51
27	BX	5101	BCR	C38-C26	2.17	1.54	1.51
28	AC	519	DGD	O4D-C4D	2.17	1.48	1.43
34	BD	5404	PHO	C4A-NA	2.16	1.40	1.34
31	AI	101	LMG	O1-C1	2.16	1.44	1.40
24	BB	5617	CLA	C4C-NC	2.16	1.41	1.37
36	BF	5101	HEM	FE-ND	2.16	2.04	1.96
24	BA	5407	CLA	C1C-NC	2.16	1.41	1.37
27	AC	514	BCR	C23-C22	-2.15	1.41	1.45
24	BC	5510	CLA	MG-NB	2.15	2.09	2.05
24	AD	401	CLA	MG-NC	2.15	2.13	2.07
24	BC	5510	CLA	MG-NC	2.15	2.13	2.07
24	BC	5505	CLA	C1D-C2D	2.15	1.48	1.42
28	BC	5519	DGD	C6E-C5E	2.15	1.59	1.52
24	BB	5614	CLA	MG-NC	2.15	2.13	2.07
31	AA	417	LMG	C4-C5	2.15	1.57	1.53
24	BB	5612	CLA	C1C-NC	2.14	1.41	1.37
31	AD	408	LMG	O3-C3	-2.14	1.37	1.43
24	AB	611	CLA	CHC-C1C	2.14	1.42	1.35
24	AB	613	CLA	C1C-NC	2.14	1.41	1.37
36	AV	201	HEM	CAA-C2A	2.14	1.55	1.52
35	BD	5406	PL9	C47-C48	2.14	1.56	1.50
28	AC	517	DGD	C3G-C2G	2.13	1.56	1.50
24	AC	506	CLA	C1C-NC	2.13	1.41	1.37
31	BC	5520	LMG	O7-C8	2.13	1.51	1.46
24	AC	508	CLA	C4D-ND	-2.13	1.32	1.38
24	BC	5502	CLA	C4B-NB	2.13	1.38	1.34
34	AD	403	PHO	C4A-NA	2.13	1.40	1.34
24	BA	5407	CLA	C2A-C1A	-2.13	1.48	1.52
24	AB	613	CLA	CMC-C2C	2.13	1.55	1.50
24	BB	5605	CLA	C1D-C2D	2.13	1.48	1.42
28	AC	518	DGD	O2G-C1B	2.12	1.40	1.34
27	AC	515	BCR	C19-C18	-2.12	1.41	1.45
24	BC	5504	CLA	C2A-C1A	-2.12	1.48	1.52
30	AF	102	SQD	C8-C7	2.12	1.57	1.50
32	AI	103	LMT	C4'-C5'	2.12	1.58	1.52
24	BC	5503	CLA	C2A-C1A	-2.12	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5609	CLA	C4C-NC	2.12	1.41	1.37
24	AA	406	CLA	O2A-CGA	2.12	1.39	1.33
27	BD	5407	BCR	C14-C13	2.12	1.38	1.35
28	BE	5102	DGD	O6D-C5D	2.12	1.49	1.44
32	BB	5627	LMT	O1B-C4'	2.11	1.49	1.43
24	AB	605	CLA	C2A-C1A	-2.11	1.48	1.52
31	AC	520	LMG	O7-C8	2.11	1.51	1.46
24	AC	507	CLA	C4B-NB	2.11	1.38	1.34
24	BB	5608	CLA	CHC-C1C	2.11	1.42	1.35
24	AB	608	CLA	CHC-C1C	2.10	1.42	1.35
28	BC	5517	DGD	O6E-C1E	2.10	1.47	1.41
24	BC	5506	CLA	CHC-C1C	2.10	1.42	1.35
24	BB	5611	CLA	C2A-C1A	-2.10	1.48	1.52
24	AA	404	CLA	C2A-C1A	-2.10	1.48	1.52
30	AA	416	SQD	O6-C44	-2.10	1.39	1.43
30	AB	627	SQD	C24-C23	2.10	1.56	1.50
24	AB	614	CLA	CAA-C2A	-2.10	1.50	1.54
27	AJ	101	BCR	C7-C6	2.09	1.53	1.45
24	AD	404	CLA	CAC-C3C	2.09	1.57	1.51
24	BB	5617	CLA	CHC-C1C	2.09	1.42	1.35
24	BC	5510	CLA	C1C-NC	2.09	1.41	1.37
27	BJ	5101	BCR	C7-C6	2.09	1.53	1.45
24	AB	604	CLA	MG-NA	2.09	2.13	2.07
24	BB	5610	CLA	C1C-NC	2.09	1.41	1.37
24	AA	404	CLA	C1B-NB	2.09	1.38	1.34
24	AB	614	CLA	C1C-NC	2.09	1.41	1.37
24	AB	607	CLA	C2A-C1A	-2.09	1.48	1.52
30	BA	5414	SQD	O6-C1	2.08	1.43	1.40
24	BB	5618	CLA	C2A-C1A	-2.08	1.48	1.52
24	BC	5511	CLA	C4C-NC	2.08	1.41	1.37
32	BM	5101	LMT	O5'-C1'	2.08	1.47	1.41
24	BB	5609	CLA	CAA-C2A	-2.08	1.50	1.54
31	AM	101	LMG	O7-C10	2.08	1.40	1.34
27	AA	410	BCR	C19-C18	-2.08	1.41	1.45
24	AC	501	CLA	C3D-CAD	-2.08	1.39	1.45
27	AB	618	BCR	C33-C5	2.08	1.54	1.51
24	AC	503	CLA	C1C-NC	2.08	1.41	1.37
24	AC	509	CLA	CHC-C1C	2.08	1.42	1.35
24	AD	401	CLA	O2A-CGA	2.07	1.39	1.33
24	AC	505	CLA	C1D-C2D	2.07	1.47	1.42
24	BB	5611	CLA	CHC-C1C	2.07	1.42	1.35
35	AD	405	PL9	C47-C48	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	619	BCR	C33-C5	2.07	1.54	1.51
35	BD	5406	PL9	C11-C9	2.07	1.56	1.51
31	BD	5410	LMG	O7-C8	-2.07	1.41	1.46
24	AB	615	CLA	MG-NC	2.07	2.13	2.07
36	AV	201	HEM	C1C-NC	2.07	1.41	1.38
24	AC	505	CLA	MG-NC	2.07	2.13	2.07
24	BB	5617	CLA	C1B-NB	2.06	1.37	1.34
24	AC	505	CLA	CHC-C1C	2.06	1.42	1.35
24	BB	5605	CLA	CAC-C3C	2.06	1.56	1.51
30	BF	5102	SQD	C44-C45	2.06	1.56	1.50
28	AH	101	DGD	O6D-C5D	2.06	1.49	1.44
24	BC	5504	CLA	C5-C3	2.06	1.56	1.51
24	AB	601	CLA	CBA-CGA	2.06	1.56	1.50
24	BB	5610	CLA	CBA-CGA	2.06	1.56	1.50
24	BC	5513	CLA	C4C-NC	2.06	1.41	1.37
28	AH	101	DGD	C3G-C2G	2.06	1.56	1.50
28	BB	5602	DGD	C3E-C2E	2.05	1.57	1.52
28	AE	101	DGD	C4E-C5E	2.05	1.57	1.53
27	AC	516	BCR	C33-C5	2.05	1.54	1.51
31	AM	101	LMG	C22-C21	-2.05	1.54	1.55
24	BD	5405	CLA	C1C-NC	2.05	1.41	1.37
24	BB	5615	CLA	CHC-C1C	2.05	1.42	1.35
27	BX	5101	BCR	C24-C23	2.05	1.38	1.32
24	AC	504	CLA	C5-C3	2.05	1.56	1.51
24	AB	611	CLA	MG-NC	2.05	2.13	2.07
24	AB	601	CLA	CAC-C3C	2.05	1.56	1.51
32	AD	409	LMT	O5'-C1'	2.05	1.47	1.41
24	BC	5502	CLA	CHC-C1C	2.05	1.42	1.35
24	BC	5507	CLA	C1C-NC	2.04	1.41	1.37
24	AC	503	CLA	MG-NC	2.04	2.13	2.07
24	AB	604	CLA	MG-NC	2.04	2.13	2.07
24	BD	5405	CLA	MG-NC	2.04	2.13	2.07
24	AB	601	CLA	C1D-C2D	2.04	1.47	1.42
30	BF	5102	SQD	C30-C31	2.03	1.60	1.52
24	BC	5501	CLA	C1C-NC	2.03	1.41	1.37
24	BC	5511	CLA	CBA-CGA	2.03	1.56	1.50
24	BC	5505	CLA	CHC-C1C	2.03	1.42	1.35
24	AC	506	CLA	MG-NA	2.03	2.13	2.07
27	BJ	5101	BCR	C4-C5	2.02	1.55	1.51
24	AB	609	CLA	MG-NC	2.02	2.13	2.07
28	AC	519	DGD	C6A-C5A	-2.02	1.39	1.51
28	BC	5519	DGD	C6A-C5A	-2.03	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	627	SQD	C21-C20	-2.02	1.35	1.51
30	BA	5401	SQD	C18-C17	-2.02	1.39	1.51
27	BD	5407	BCR	C23-C22	-2.02	1.41	1.45
24	AB	605	CLA	CAA-C2A	-2.02	1.50	1.54
24	AD	404	CLA	CBA-CGA	2.02	1.56	1.50
32	AI	102	LMT	O1B-C4'	2.02	1.48	1.43
27	BA	5411	BCR	C19-C18	-2.02	1.41	1.45
24	BC	5511	CLA	C4B-CHC	2.02	1.45	1.39
24	AB	609	CLA	CBA-CGA	2.02	1.56	1.50
32	BB	5603	LMT	C10-C9	-2.02	1.39	1.51
24	BB	5608	CLA	MG-NC	2.02	2.13	2.07
30	BB	5625	SQD	C24-C23	2.02	1.56	1.50
28	AC	518	DGD	C6A-C5A	-2.02	1.39	1.51
35	BD	5406	PL9	C10-C9	2.01	1.55	1.50
32	BB	5604	LMT	C10-C9	-2.01	1.39	1.51
30	BB	5601	SQD	C44-C45	2.01	1.56	1.50
28	BC	5518	DGD	C6A-C5A	-2.02	1.39	1.51
30	AB	622	SQD	C24-C23	2.01	1.56	1.50
27	BA	5411	BCR	C24-C23	2.01	1.38	1.32
32	AB	629	LMT	C10-C9	-2.01	1.39	1.51
32	AI	102	LMT	C10-C9	-2.01	1.39	1.51
30	BA	5401	SQD	O6-C44	-2.01	1.39	1.43
31	AC	520	LMG	C4-C5	2.01	1.57	1.53
32	AM	102	LMT	O5'-C5'	2.01	1.49	1.44
28	BC	5518	DGD	CEB-CDB	-2.01	1.39	1.51
24	BB	5619	CLA	C3D-CAD	-2.01	1.40	1.45
28	AH	101	DGD	C6A-C5A	-2.01	1.39	1.51
28	AA	411	DGD	C6A-C5A	-2.01	1.39	1.51
28	BE	5102	DGD	C4D-C5D	2.01	1.57	1.53
28	AC	518	DGD	CEB-CDB	-2.01	1.39	1.51
31	AC	520	LMG	O7-C10	2.01	1.40	1.34
24	AC	507	CLA	C3B-CAB	-2.01	1.43	1.47
28	BC	5517	DGD	C6A-C5A	-2.00	1.39	1.51
28	BA	5412	DGD	C6A-C5A	-2.01	1.39	1.51
32	AI	103	LMT	C10-C9	-2.00	1.39	1.51
32	BC	5522	LMT	C10-C9	-2.00	1.39	1.51
28	AA	411	DGD	C4D-C3D	-2.00	1.47	1.52
32	BB	5626	LMT	O5B-C5B	2.00	1.49	1.44
28	AE	101	DGD	CEB-CDB	-2.00	1.39	1.51
28	AC	517	DGD	C6A-C5A	-2.00	1.39	1.51
31	AM	101	LMG	O6-C1	2.00	1.46	1.41
30	BB	5601	SQD	C21-C20	-2.00	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BH	5101	DGD	C6A-C5A	-2.00	1.39	1.51
28	BC	5519	DGD	O4D-C4D	2.00	1.47	1.43

All (3253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	518	DGD	O5D-C1E-C2E	13.73	125.75	108.15
28	BC	5518	DGD	O5D-C1E-C2E	13.49	125.43	108.15
28	AC	519	DGD	O5D-C6D-C5D	12.96	131.44	108.96
28	BC	5519	DGD	O5D-C6D-C5D	12.87	131.30	108.96
30	BF	5102	SQD	O7-S-C6	12.72	118.07	106.83
30	AF	102	SQD	O7-S-C6	12.65	118.01	106.83
30	BA	5414	SQD	C5-C6-S	11.88	131.01	114.40
30	AA	413	SQD	C5-C6-S	11.83	130.94	114.40
30	AA	413	SQD	O7-S-C6	11.74	117.20	106.83
28	AA	411	DGD	O5D-C6D-C5D	11.66	129.19	108.96
28	BA	5412	DGD	O5D-C6D-C5D	11.62	129.13	108.96
30	BB	5625	SQD	O7-S-C6	11.50	116.99	106.83
30	BA	5414	SQD	O7-S-C6	11.40	116.91	106.83
28	BC	5519	DGD	O5D-C1E-C2E	11.35	122.70	108.15
30	AA	416	SQD	O7-S-C6	11.30	116.82	106.83
28	AC	519	DGD	O5D-C1E-C2E	11.17	122.46	108.15
30	BA	5401	SQD	O7-S-C6	11.03	116.58	106.83
30	AB	622	SQD	O7-S-C6	10.95	116.51	106.83
30	AB	627	SQD	O7-S-C6	10.64	116.23	106.83
28	BA	5412	DGD	O5D-C1E-C2E	10.60	121.73	108.15
28	AA	411	DGD	O5D-C1E-C2E	10.37	121.44	108.15
28	AC	519	DGD	C3G-O3G-C1D	-10.24	93.25	113.80
30	BB	5601	SQD	O7-S-C6	10.19	115.83	106.83
28	BC	5519	DGD	C3G-O3G-C1D	-10.06	93.61	113.80
30	AF	102	SQD	C5-C6-S	9.97	128.34	114.40
28	BB	5602	DGD	C2G-O2G-C1B	9.95	141.23	117.86
28	BA	5412	DGD	O1G-C1G-C2G	9.95	134.96	108.80
28	AA	411	DGD	O1G-C1G-C2G	9.94	134.92	108.80
30	BF	5102	SQD	C5-C6-S	9.89	128.23	114.40
31	AJ	102	LMG	C8-O7-C10	9.85	140.99	117.86
27	BJ	5101	BCR	C32-C1-C6	-9.80	94.11	110.33
28	BA	5412	DGD	O3G-C1D-C2D	-9.74	95.67	108.15
27	AJ	101	BCR	C32-C1-C6	-9.74	94.20	110.33
28	AB	628	DGD	C2G-O2G-C1B	9.72	140.68	117.86
25	AA	408	MST	C2-N1-C6	9.65	120.12	113.69
28	AA	411	DGD	O3G-C1D-C2D	-9.64	95.80	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5408	LMG	C8-O7-C10	9.62	140.46	117.86
25	BA	5409	MST	C2-N1-C6	9.55	120.06	113.69
30	AA	416	SQD	C5-C6-S	9.48	127.66	114.40
28	BC	5517	DGD	C2G-O2G-C1B	9.47	140.10	117.86
30	AB	627	SQD	C5-C6-S	9.35	127.48	114.40
30	BA	5401	SQD	C5-C6-S	9.33	127.45	114.40
36	BF	5101	HEM	CMA-C3A-C2A	-9.33	107.34	124.94
30	BB	5601	SQD	O6-C1-C2	9.32	120.09	108.15
24	AC	503	CLA	C1-C2-C3	-9.31	110.08	126.23
30	BB	5625	SQD	O6-C1-C2	9.28	120.05	108.15
30	AB	622	SQD	O6-C1-C2	9.25	120.01	108.15
28	AC	517	DGD	C2G-O2G-C1B	9.24	139.56	117.86
30	AB	627	SQD	O6-C1-C2	9.15	119.87	108.15
35	AD	405	PL9	C7-C3-C4	9.15	124.24	116.92
30	BB	5601	SQD	C5-C6-S	9.15	127.19	114.40
36	AF	101	HEM	CMA-C3A-C2A	-9.14	107.71	124.94
24	BC	5503	CLA	C1-C2-C3	-9.14	110.38	126.23
25	AA	408	MST	C2-N3-C4	9.13	119.78	113.69
30	AA	413	SQD	O5-C1-O6	9.07	131.51	109.93
30	AB	622	SQD	C5-C6-S	9.06	127.07	114.40
30	BF	5102	SQD	O6-C1-C2	9.03	119.72	108.15
30	BB	5625	SQD	C5-C6-S	9.02	127.02	114.40
30	AA	416	SQD	O5-C1-O6	9.02	131.39	109.93
36	AV	201	HEM	CMA-C3A-C2A	-9.00	107.97	124.94
35	BD	5406	PL9	C7-C3-C4	8.98	124.11	116.92
30	BA	5401	SQD	O5-C1-O6	8.97	131.28	109.93
36	BV	5201	HEM	CMA-C3A-C2A	-8.97	108.03	124.94
30	AF	102	SQD	O6-C1-C2	8.97	119.64	108.15
30	BA	5414	SQD	O5-C1-O6	8.95	131.22	109.93
28	AC	518	DGD	O5D-C6D-C5D	8.86	124.33	108.96
25	BA	5409	MST	C2-N3-C4	8.81	119.56	113.69
28	BC	5518	DGD	O5D-C6D-C5D	8.81	124.25	108.96
30	BF	5102	SQD	O5-C1-O6	8.75	130.76	109.93
30	AF	102	SQD	O5-C1-O6	8.71	130.67	109.93
28	AC	519	DGD	O6D-C5D-C6D	8.68	124.01	106.62
24	AB	611	CLA	C1-C2-C3	-8.64	111.24	126.23
24	BB	5615	CLA	C1-C2-C3	-8.63	111.26	126.23
28	BA	5412	DGD	O6D-C5D-C6D	8.62	123.89	106.62
28	AA	411	DGD	O6D-C5D-C6D	8.58	123.81	106.62
28	AA	411	DGD	O3G-C3G-C2G	-8.56	90.62	110.99
28	BA	5412	DGD	O3G-C3G-C2G	-8.56	90.63	110.99
28	AC	519	DGD	C2G-O2G-C1B	8.56	137.95	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BJ	5101	BCR	C32-C1-C31	-8.54	79.64	108.47
35	AD	405	PL9	C7-C8-C9	-8.51	112.38	126.76
27	AJ	101	BCR	C32-C1-C31	-8.50	79.78	108.47
36	BV	5201	HEM	C3B-C4B-NB	-8.47	107.94	114.00
35	BD	5406	PL9	C7-C8-C9	-8.44	112.50	126.76
24	BC	5501	CLA	C1-C2-C3	-8.41	111.64	126.23
36	BF	5101	HEM	CMA-C3A-C4A	8.39	141.36	128.46
24	BB	5619	CLA	C1-C2-C3	-8.39	111.68	126.23
36	AV	201	HEM	C3B-C4B-NB	-8.35	108.02	114.00
24	BA	5405	CLA	C1-C2-C3	-8.35	111.74	126.23
24	AC	501	CLA	C1-C2-C3	-8.33	111.77	126.23
28	BC	5519	DGD	C2G-O2G-C1B	8.33	137.41	117.86
24	AB	615	CLA	C1-C2-C3	-8.30	111.83	126.23
24	BB	5608	CLA	C1-C2-C3	-8.29	111.86	126.23
36	AF	101	HEM	CMA-C3A-C4A	8.27	141.18	128.46
30	AB	622	SQD	O5-C1-O6	8.24	129.55	109.93
24	BA	5406	CLA	CBA-CAA-C2A	8.22	134.05	113.95
30	BA	5401	SQD	O6-C1-C2	8.22	118.68	108.15
24	AB	604	CLA	C1-C2-C3	-8.21	111.99	126.23
30	BB	5601	SQD	O5-C1-O6	8.18	129.41	109.93
24	BB	5614	CLA	C1-C2-C3	-8.18	112.05	126.23
24	BC	5512	CLA	C1-C2-C3	-8.17	112.05	126.23
24	AA	404	CLA	C1-C2-C3	-8.16	112.08	126.23
30	AB	627	SQD	O5-C1-O6	8.15	129.33	109.93
24	BD	5402	CLA	C1-C2-C3	-8.14	112.11	126.23
24	AA	405	CLA	CBA-CAA-C2A	8.13	133.82	113.95
30	BB	5625	SQD	O5-C1-O6	8.12	129.25	109.93
28	BC	5519	DGD	O6D-C5D-C6D	8.09	122.82	106.62
24	AC	512	CLA	C1-C2-C3	-8.06	112.25	126.23
24	AC	508	CLA	C1-C2-C3	-8.05	112.26	126.23
28	AA	411	DGD	C6D-C5D-C4D	-8.05	93.70	111.98
30	AA	416	SQD	O6-C1-C2	8.03	118.44	108.15
34	BD	5403	PHO	C1-C2-C3	-8.01	112.33	126.23
24	AB	610	CLA	C1-C2-C3	-7.98	112.39	126.23
24	BC	5510	CLA	C1-C2-C3	-7.98	112.39	126.23
28	BA	5412	DGD	C6D-C5D-C4D	-7.95	93.92	111.98
24	BC	5508	CLA	C1-C2-C3	-7.94	112.45	126.23
24	AC	509	CLA	C1-C2-C3	-7.94	112.46	126.23
24	AC	510	CLA	C1-C2-C3	-7.93	112.46	126.23
24	AD	401	CLA	C1-C2-C3	-7.92	112.48	126.23
36	AF	101	HEM	C3B-C4B-NB	-7.92	108.33	114.00
31	BA	5402	LMG	C8-O7-C10	7.91	136.44	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	C1-C2-C3	-7.89	112.55	126.23
28	BC	5519	DGD	C6D-O5D-C1E	-7.86	98.02	113.80
34	AD	402	PHO	C1-C2-C3	-7.86	112.60	126.23
24	BA	5408	CLA	C1-C2-C3	-7.85	112.62	126.23
36	AV	201	HEM	CMA-C3A-C4A	7.85	140.52	128.46
24	BC	5504	CLA	C1-C2-C3	-7.84	112.62	126.23
24	BA	5407	CLA	C1-C2-C3	-7.84	112.63	126.23
36	BV	5201	HEM	CMA-C3A-C4A	7.83	140.50	128.46
24	AB	612	CLA	C1-C2-C3	-7.83	112.65	126.23
24	BB	5616	CLA	C1-C2-C3	-7.82	112.67	126.23
24	AA	407	CLA	C1-C2-C3	-7.81	112.67	126.23
24	AC	504	CLA	C1-C2-C3	-7.78	112.73	126.23
24	AC	506	CLA	C1-C2-C3	-7.77	112.75	126.23
36	BF	5101	HEM	C3B-C4B-NB	-7.76	108.44	114.00
34	BD	5404	PHO	C1-C2-C3	-7.76	112.77	126.23
31	AD	407	LMG	C8-O7-C10	7.74	136.04	117.86
30	AA	413	SQD	O6-C1-C2	7.74	118.06	108.15
31	AA	417	LMG	C8-O7-C10	7.72	136.00	117.86
24	BC	5509	CLA	C1-C2-C3	-7.72	112.83	126.23
24	BB	5606	CLA	C1-C2-C3	-7.72	112.84	126.23
24	BB	5609	CLA	C1-C2-C3	-7.69	112.88	126.23
31	BD	5409	LMG	C8-O7-C10	7.68	135.90	117.86
24	AA	406	CLA	C1-C2-C3	-7.68	112.91	126.23
24	BC	5506	CLA	C1-C2-C3	-7.68	112.91	126.23
30	BA	5414	SQD	O6-C1-C2	7.67	117.99	108.15
24	BB	5617	CLA	C1-C2-C3	-7.66	112.94	126.23
24	AB	613	CLA	C1-C2-C3	-7.66	112.94	126.23
24	BC	5502	CLA	C1-C2-C3	-7.66	112.95	126.23
24	AD	404	CLA	C1-C2-C3	-7.65	112.96	126.23
24	BB	5612	CLA	C1-C2-C3	-7.65	112.96	126.23
24	BC	5505	CLA	C1-C2-C3	-7.65	112.96	126.23
24	AB	601	CLA	C1-C2-C3	-7.64	112.97	126.23
24	BC	5513	CLA	C1-C2-C3	-7.62	113.00	126.23
28	AC	518	DGD	O6D-C5D-C6D	7.62	121.89	106.62
24	AB	608	CLA	C1-C2-C3	-7.62	113.01	126.23
24	AC	505	CLA	C1-C2-C3	-7.57	113.09	126.23
24	AB	616	CLA	C1-C2-C3	-7.56	113.11	126.23
24	AB	602	CLA	C1-C2-C3	-7.56	113.11	126.23
24	AA	406	CLA	CBA-CAA-C2A	7.55	132.42	113.95
24	AC	513	CLA	C1-C2-C3	-7.55	113.13	126.23
35	AD	405	PL9	C10-C9-C8	-7.54	108.51	123.52
31	AC	520	LMG	O7-C10-C11	7.54	127.60	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5405	CLA	C1-C2-C3	-7.54	113.15	126.23
24	AB	605	CLA	C1-C2-C3	-7.51	113.19	126.23
36	AF	101	HEM	C4A-C3A-C2A	-7.48	101.79	107.00
24	BB	5605	CLA	C1-C2-C3	-7.48	113.26	126.23
24	BB	5613	CLA	C1-C2-C3	-7.46	113.28	126.23
24	BB	5620	CLA	C1-C2-C3	-7.45	113.31	126.23
24	AB	609	CLA	C1-C2-C3	-7.44	113.32	126.23
24	AA	405	CLA	CAA-C2A-C1A	-7.43	92.81	112.51
24	AA	405	CLA	C1-C2-C3	-7.43	113.34	126.23
24	AB	603	CLA	C4B-C3B-CAB	7.42	142.20	127.18
28	BC	5518	DGD	O6D-C5D-C6D	7.42	121.48	106.62
24	BA	5406	CLA	C1-C2-C3	-7.42	113.36	126.23
24	AC	502	CLA	C1-C2-C3	-7.42	113.36	126.23
24	BA	5406	CLA	CAA-C2A-C1A	-7.40	92.90	112.51
24	BB	5607	CLA	C4B-C3B-CAB	7.39	142.15	127.18
28	AC	519	DGD	C6D-O5D-C1E	-7.38	98.99	113.80
24	AC	507	CLA	C1-C2-C3	-7.35	113.48	126.23
24	BC	5507	CLA	C1-C2-C3	-7.33	113.51	126.23
31	BC	5520	LMG	O7-C10-C11	7.33	127.16	111.54
36	BF	5101	HEM	C4A-C3A-C2A	-7.32	101.90	107.00
31	AD	407	LMG	C19-C18-C17	-7.31	75.76	114.56
31	BD	5409	LMG	C19-C18-C17	-7.28	75.90	114.56
24	BB	5618	CLA	C1-C2-C3	-7.28	113.60	126.23
24	BA	5407	CLA	CBA-CAA-C2A	7.27	131.72	113.95
35	BD	5406	PL9	C10-C9-C8	-7.24	109.11	123.52
24	BB	5607	CLA	C1-C2-C3	-7.24	113.68	126.23
24	AB	614	CLA	C1-C2-C3	-7.22	113.70	126.23
35	BD	5406	PL9	C32-C33-C34	-7.21	112.22	127.81
30	BB	5625	SQD	C31-C30-C29	7.19	133.50	112.94
28	BC	5517	DGD	C1G-O1G-C1A	7.19	137.50	116.99
28	BA	5412	DGD	C6D-O5D-C1E	-7.17	99.41	113.80
24	AB	606	CLA	C1-C2-C3	-7.17	113.79	126.23
24	BB	5610	CLA	C1-C2-C3	-7.15	113.82	126.23
24	AB	603	CLA	C1-C2-C3	-7.15	113.83	126.23
30	AB	622	SQD	C31-C30-C29	7.12	133.28	112.94
31	AD	408	LMG	C8-O7-C10	7.11	134.55	117.86
35	AD	405	PL9	C32-C33-C34	-7.10	112.45	127.81
30	AA	413	SQD	O8-S-C6	-7.09	97.44	105.89
30	AB	627	SQD	C31-C30-C29	7.09	133.21	112.94
30	AA	416	SQD	O8-S-C6	-7.09	97.45	105.89
28	AA	411	DGD	C6D-O5D-C1E	-7.07	99.60	113.80
31	BD	5410	LMG	C8-O7-C10	7.07	134.47	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AD	406	BCR	C38-C26-C25	7.07	132.47	124.50
28	AC	517	DGD	C1G-O1G-C1A	7.06	137.16	116.99
30	BB	5601	SQD	C31-C30-C29	7.06	133.12	112.94
30	AF	102	SQD	O8-S-C6	-7.04	97.50	105.89
31	BL	5101	LMG	C7-O1-C1	-6.99	99.77	113.80
30	BF	5102	SQD	O8-S-C6	-6.96	97.60	105.89
28	AH	101	DGD	O2G-C1B-C2B	6.96	126.36	111.54
27	AJ	101	BCR	C32-C1-C2	-6.95	81.14	108.78
24	BB	5612	CLA	CAA-C2A-C1A	-6.93	94.13	112.51
28	BH	5101	DGD	O2G-C1B-C2B	6.93	126.30	111.54
30	BA	5401	SQD	O8-S-C6	-6.92	97.65	105.89
24	AB	608	CLA	CAA-C2A-C1A	-6.91	94.20	112.51
31	AB	620	LMG	C7-O1-C1	-6.88	99.99	113.80
27	BJ	5101	BCR	C32-C1-C2	-6.83	81.62	108.78
28	AC	517	DGD	O5D-C6D-C5D	6.83	120.81	108.96
28	BC	5517	DGD	O5D-C6D-C5D	6.81	120.78	108.96
27	BD	5407	BCR	C38-C26-C25	6.79	132.16	124.50
31	BM	5102	LMG	O7-C10-C11	6.78	125.98	111.54
31	AA	417	LMG	C7-O1-C1	-6.75	100.25	113.80
24	AB	603	CLA	C2B-C3B-CAB	-6.74	113.53	127.33
31	BD	5408	LMG	C7-O1-C1	-6.72	100.31	113.80
36	BV	5201	HEM	C4A-C3A-C2A	-6.72	102.32	107.00
24	BA	5407	CLA	CAA-C2A-C1A	-6.71	94.72	112.51
28	BA	5412	DGD	C3G-O3G-C1D	6.71	127.27	113.80
31	AM	101	LMG	O7-C10-C11	6.71	125.83	111.54
28	AA	411	DGD	C3G-O3G-C1D	6.69	127.24	113.80
31	AD	408	LMG	C13-C12-C11	-6.69	88.49	113.28
31	AC	521	LMG	C8-O7-C10	6.69	133.57	117.86
31	BD	5410	LMG	C13-C12-C11	-6.69	88.49	113.28
24	BB	5607	CLA	C2B-C3B-CAB	-6.69	113.65	127.33
31	BB	5624	LMG	O7-C10-C11	6.68	125.77	111.54
31	AB	621	LMG	O7-C10-C11	6.65	125.72	111.54
31	BC	5521	LMG	C8-O7-C10	6.62	133.41	117.86
36	AV	201	HEM	C4A-C3A-C2A	-6.60	102.40	107.00
31	BA	5402	LMG	C7-O1-C1	-6.60	100.56	113.80
24	BC	5511	CLA	C1-C2-C3	-6.59	114.80	126.23
24	BB	5611	CLA	C1-C2-C3	-6.57	114.83	126.23
31	AJ	102	LMG	C7-O1-C1	-6.56	100.63	113.80
24	BB	5611	CLA	CAA-C2A-C1A	-6.55	95.14	112.51
28	AC	517	DGD	O6D-C5D-C6D	6.55	119.75	106.62
24	AC	511	CLA	C1-C2-C3	-6.53	114.89	126.23
24	AB	614	CLA	C4B-C3B-CAB	6.53	140.40	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5617	CLA	C4B-C3B-CAB	6.52	140.38	127.18
24	AB	613	CLA	C4B-C3B-CAB	6.51	140.37	127.18
28	AC	517	DGD	O1G-C1G-C2G	-6.51	91.68	108.80
27	AJ	101	BCR	C2-C1-C6	6.51	120.75	110.37
24	AB	607	CLA	C1-C2-C3	-6.50	114.96	126.23
27	AK	102	BCR	C33-C5-C6	6.49	131.82	124.50
24	AB	607	CLA	CAA-C2A-C1A	-6.47	95.36	112.51
27	BJ	5101	BCR	C2-C1-C6	6.44	120.64	110.37
25	AA	408	MST	C10-N9-C4	-6.43	120.93	128.05
24	AA	406	CLA	CAA-C2A-C1A	-6.43	95.48	112.51
31	AJ	102	LMG	C13-C12-C11	-6.40	89.56	113.28
30	AB	627	SQD	O8-S-C6	-6.40	98.26	105.89
24	AB	607	CLA	C4B-C3B-CAB	6.38	140.10	127.18
24	BB	5612	CLA	CBA-CAA-C2A	6.37	129.52	113.95
27	AB	618	BCR	C38-C26-C25	6.37	131.69	124.50
31	AB	620	LMG	C13-C12-C11	-6.36	89.70	113.28
31	BD	5408	LMG	C13-C12-C11	-6.36	89.73	113.28
24	AB	607	CLA	C2B-C3B-CAB	-6.36	114.32	127.33
24	AB	614	CLA	C2B-C3B-CAB	-6.35	114.34	127.33
24	AB	607	CLA	CBA-CAA-C2A	6.34	129.45	113.95
28	BC	5517	DGD	O1G-C1G-C2G	-6.33	92.14	108.80
31	BL	5101	LMG	C13-C12-C11	-6.31	89.90	113.28
24	BB	5618	CLA	C4B-C3B-CAB	6.28	139.90	127.18
24	AA	407	CLA	C4B-C3B-CAB	6.27	139.87	127.18
28	BB	5602	DGD	C3G-O3G-C1D	-6.27	101.22	113.80
28	BC	5517	DGD	O6D-C5D-C6D	6.24	119.12	106.62
27	BK	5102	BCR	C33-C5-C6	6.24	131.54	124.50
28	BC	5517	DGD	C6D-O5D-C1E	-6.23	101.29	113.80
31	BA	5402	LMG	C13-C12-C11	-6.23	90.20	113.28
35	AD	405	PL9	C22-C23-C24	-6.23	114.33	127.81
27	AC	516	BCR	C33-C5-C6	6.23	131.53	124.50
24	AB	608	CLA	CBA-CAA-C2A	6.22	129.16	113.95
24	BB	5611	CLA	C4B-C3B-CAB	6.22	139.77	127.18
24	BB	5617	CLA	C2B-C3B-CAB	-6.21	114.61	127.33
31	AA	417	LMG	C13-C12-C11	-6.21	90.26	113.28
27	BB	5622	BCR	C38-C26-C25	6.21	131.51	124.50
27	BC	5516	BCR	C33-C5-C6	6.21	131.50	124.50
24	AC	504	CLA	C4B-C3B-CAB	6.20	139.73	127.18
28	AB	628	DGD	C3G-O3G-C1D	-6.18	101.39	113.80
24	BB	5618	CLA	C2B-C3B-CAB	-6.18	114.68	127.33
24	AC	508	CLA	C4B-C3B-CAB	6.17	139.66	127.18
24	BA	5408	CLA	C4B-C3B-CAB	6.16	139.65	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	613	CLA	C2B-C3B-CAB	-6.14	114.77	127.33
24	AC	511	CLA	C4B-C3B-CAB	6.14	139.60	127.18
28	BC	5519	DGD	C4B-C3B-C2B	-6.13	90.56	113.28
24	BB	5611	CLA	C2B-C3B-CAB	-6.12	114.80	127.33
30	BA	5414	SQD	O8-S-C6	-6.11	98.61	105.89
28	AC	518	DGD	C4A-C3A-C2A	-6.09	90.70	113.28
24	BB	5611	CLA	CBA-CAA-C2A	6.09	128.83	113.95
27	BX	5101	BCR	C38-C26-C25	6.09	131.37	124.50
32	BC	5522	LMT	C1B-O1B-C4'	-6.08	102.55	118.00
24	BC	5504	CLA	C4B-C3B-CAB	6.08	139.48	127.18
24	BC	5511	CLA	C4B-C3B-CAB	6.07	139.47	127.18
27	BC	5515	BCR	C33-C5-C6	6.07	131.35	124.50
25	BA	5409	MST	C10-N9-C4	-6.07	121.33	128.05
30	AB	622	SQD	O8-S-C6	-6.06	98.66	105.89
24	BC	5508	CLA	C4B-C3B-CAB	6.06	139.44	127.18
28	AC	518	DGD	C3G-O3G-C1D	-6.05	101.66	113.80
28	AA	411	DGD	C1D-O6D-C5D	-6.04	102.04	113.73
27	AJ	101	BCR	C38-C26-C25	6.03	131.31	124.50
30	BB	5601	SQD	C10-C9-C8	6.03	135.62	113.28
35	BD	5406	PL9	C22-C23-C24	-6.03	114.77	127.81
27	AC	515	BCR	C38-C26-C25	6.02	131.29	124.50
30	BA	5401	SQD	C10-C9-C8	6.02	135.57	113.28
28	BC	5518	DGD	C6D-O5D-C1E	-6.02	101.72	113.80
34	BD	5403	PHO	C4D-CHA-C1A	-6.01	122.41	129.57
29	AA	412	LHG	C25-C24-C23	6.00	136.79	113.51
30	AA	413	SQD	C10-C9-C8	5.99	135.49	113.28
24	AD	401	CLA	C4B-C3B-CAB	5.99	139.31	127.18
27	AT	101	BCR	C33-C5-C6	5.98	131.25	124.50
24	BB	5612	CLA	C4B-C3B-CAB	5.98	139.28	127.18
24	AA	407	CLA	C2B-C3B-CAB	-5.97	115.11	127.33
30	AA	416	SQD	C10-C9-C8	5.97	135.38	113.28
24	BB	5606	CLA	C4B-C3B-CAB	5.96	139.25	127.18
28	BC	5518	DGD	C3G-O3G-C1D	-5.96	101.84	113.80
28	AC	519	DGD	C4B-C3B-C2B	-5.95	91.23	113.28
30	BA	5414	SQD	C10-C9-C8	5.95	135.31	113.28
24	AC	511	CLA	C2B-C3B-CAB	-5.95	115.16	127.33
28	BA	5412	DGD	C1D-O6D-C5D	-5.94	102.23	113.73
27	BJ	5101	BCR	C38-C26-C25	5.94	131.21	124.50
28	BC	5518	DGD	O2G-C1B-C2B	5.94	124.20	111.54
24	BC	5511	CLA	C2B-C3B-CAB	-5.94	115.18	127.33
34	AD	402	PHO	C4D-CHA-C1A	-5.94	122.50	129.57
30	BB	5601	SQD	O8-S-C6	-5.94	98.81	105.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BT	5101	BCR	C33-C5-C6	5.93	131.20	124.50
28	AC	518	DGD	O2G-C1B-C2B	5.93	124.18	111.54
27	AC	515	BCR	C33-C5-C6	5.93	131.19	124.50
31	BD	5409	LMG	C13-C12-C11	-5.93	91.32	113.28
28	AC	517	DGD	C6D-O5D-C1E	-5.93	101.91	113.80
24	BD	5402	CLA	C4B-C3B-CAB	5.92	139.17	127.18
28	AC	517	DGD	C4B-C3B-C2B	-5.92	91.35	113.28
24	BB	5608	CLA	C4B-C3B-CAB	5.92	139.16	127.18
28	BC	5518	DGD	C4A-C3A-C2A	-5.91	91.37	113.28
24	BA	5408	CLA	C2B-C3B-CAB	-5.91	115.23	127.33
24	AA	404	CLA	C4B-C3B-CAB	5.91	139.15	127.18
28	BC	5517	DGD	C4B-C3B-C2B	-5.91	91.39	113.28
31	AI	101	LMG	O7-C10-C11	5.91	124.13	111.54
24	AB	608	CLA	C4B-C3B-CAB	5.91	139.14	127.18
28	BA	5412	DGD	O1G-C1A-C2A	5.90	129.97	111.90
30	BF	5102	SQD	C32-C31-C30	5.90	129.81	112.94
27	BC	5515	BCR	C38-C26-C25	5.90	131.16	124.50
30	AB	627	SQD	C10-C9-C8	5.90	135.12	113.28
29	BA	5413	LHG	C25-C24-C23	5.89	136.39	113.51
28	BB	5602	DGD	C1G-O1G-C1A	5.89	133.80	116.99
28	AB	628	DGD	C1G-O1G-C1A	5.89	133.79	116.99
27	AX	101	BCR	C38-C26-C25	5.88	131.14	124.50
27	BB	5621	BCR	C38-C26-C25	5.88	131.14	124.50
32	AI	103	LMT	C1B-O1B-C4'	-5.88	103.06	118.00
28	BA	5412	DGD	O6D-C1D-O3G	5.88	123.91	109.93
30	BB	5625	SQD	C10-C9-C8	5.87	135.04	113.28
24	AB	602	CLA	C4B-C3B-CAB	5.87	139.07	127.18
30	BB	5625	SQD	O8-S-C6	-5.87	98.90	105.89
31	AD	407	LMG	C13-C12-C11	-5.87	91.53	113.28
27	AB	617	BCR	C38-C26-C25	5.87	131.12	124.50
30	AF	102	SQD	C32-C31-C30	5.85	129.67	112.94
24	AC	504	CLA	C2B-C3B-CAB	-5.84	115.37	127.33
24	BC	5506	CLA	C4B-C3B-CAB	5.84	139.01	127.18
28	AA	411	DGD	O1G-C1A-C2A	5.83	129.76	111.90
28	AC	519	DGD	C6D-C5D-C4D	-5.83	98.75	111.98
31	BI	5101	LMG	O7-C10-C11	5.83	123.95	111.54
24	BC	5504	CLA	C2B-C3B-CAB	-5.82	115.41	127.33
30	AF	102	SQD	C10-C9-C8	5.82	134.85	113.28
30	BF	5102	SQD	C10-C9-C8	5.82	134.84	113.28
24	AA	406	CLA	C4B-C3B-CAB	5.82	138.96	127.18
30	AB	622	SQD	C10-C9-C8	5.81	134.82	113.28
24	AB	611	CLA	C4B-C3B-CAB	5.81	138.94	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	612	CLA	C4B-C3B-CAB	5.80	138.92	127.18
24	AC	508	CLA	C2B-C3B-CAB	-5.79	115.47	127.33
24	BB	5616	CLA	C4B-C3B-CAB	5.78	138.88	127.18
24	BD	5405	CLA	C4B-C3B-CAB	5.77	138.85	127.18
28	AA	411	DGD	O6D-C1D-O3G	5.76	123.63	109.93
24	AB	606	CLA	C4B-C3B-CAB	5.76	138.84	127.18
24	BA	5405	CLA	C4B-C3B-CAB	5.75	138.83	127.18
24	AC	506	CLA	C4B-C3B-CAB	5.75	138.82	127.18
24	BA	5406	CLA	C4B-C3B-CAB	5.74	138.79	127.18
24	AD	404	CLA	C4B-C3B-CAB	5.73	138.79	127.18
28	BC	5517	DGD	O5D-C1E-C2E	5.73	115.49	108.15
24	BA	5407	CLA	C4B-C3B-CAB	5.72	138.76	127.18
28	AC	518	DGD	C6D-O5D-C1E	-5.71	102.33	113.80
24	AA	405	CLA	C4B-C3B-CAB	5.70	138.73	127.18
24	BC	5508	CLA	C2B-C3B-CAB	-5.70	115.66	127.33
24	AC	512	CLA	C4B-C3B-CAB	5.68	138.67	127.18
24	BB	5618	CLA	CBA-CAA-C2A	5.67	127.82	113.95
27	AC	516	BCR	C38-C26-C25	5.67	130.90	124.50
24	AC	502	CLA	C4B-C3B-CAB	5.67	138.65	127.18
30	BF	5102	SQD	C25-C24-C23	5.67	135.51	113.51
24	BB	5610	CLA	C4B-C3B-CAB	5.65	138.62	127.18
27	BK	5102	BCR	C38-C26-C25	5.65	130.87	124.50
24	AC	504	CLA	CAA-C2A-C1A	-5.64	97.56	112.51
27	BJ	5101	BCR	C31-C1-C6	5.63	119.65	110.33
28	AC	517	DGD	O5D-C1E-C2E	5.63	115.36	108.15
24	AB	614	CLA	CBA-CAA-C2A	5.63	127.70	113.95
30	AF	102	SQD	C25-C24-C23	5.63	135.35	113.51
27	AK	102	BCR	C38-C26-C25	5.61	130.83	124.50
24	AB	604	CLA	C4B-C3B-CAB	5.61	138.54	127.18
31	AD	407	LMG	O7-C8-C7	5.61	129.26	108.50
24	BB	5612	CLA	C2B-C3B-CAB	-5.60	115.86	127.33
24	BB	5615	CLA	C4B-C3B-CAB	5.59	138.51	127.18
27	BT	5101	BCR	C38-C26-C25	5.59	130.80	124.50
24	AC	503	CLA	C4B-C3B-CAB	5.58	138.49	127.18
35	BD	5406	PL9	C12-C13-C14	-5.58	115.73	127.81
30	BA	5414	SQD	C25-C24-C23	5.58	135.16	113.51
24	AC	509	CLA	C4B-C3B-CAB	5.57	138.46	127.18
24	BC	5513	CLA	C4B-C3B-CAB	5.57	138.46	127.18
24	AC	513	CLA	C4B-C3B-CAB	5.56	138.44	127.18
30	AA	413	SQD	C25-C24-C23	5.55	135.05	113.51
31	BD	5409	LMG	O7-C8-C7	5.55	129.03	108.50
24	BC	5503	CLA	C4B-C3B-CAB	5.54	138.40	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5505	CLA	CBA-CAA-C2A	5.53	127.48	113.95
31	BC	5521	LMG	C9-O8-C28	5.53	132.78	116.99
24	BC	5502	CLA	C4B-C3B-CAB	5.52	138.36	127.18
24	BC	5512	CLA	C4B-C3B-CAB	5.52	138.35	127.18
31	BD	5409	LMG	C17-C16-C15	-5.52	85.27	114.56
24	BC	5504	CLA	CAA-C2A-C1A	-5.51	97.90	112.51
24	AD	401	CLA	C2B-C3B-CAB	-5.51	116.06	127.33
27	AJ	101	BCR	C31-C1-C6	5.50	119.44	110.33
24	AB	602	CLA	C2B-C3B-CAB	-5.50	116.08	127.33
27	AC	514	BCR	C38-C26-C25	5.49	130.70	124.50
32	BD	5411	LMT	C1B-O1B-C4'	-5.49	104.06	118.00
24	AC	506	CLA	C2B-C3B-CAB	-5.48	116.11	127.33
31	AJ	102	LMG	O7-C8-C7	5.48	128.79	108.50
27	BC	5516	BCR	C38-C26-C25	5.47	130.68	124.50
30	BB	5601	SQD	C25-C24-C23	5.47	134.76	113.51
24	AC	501	CLA	C4B-C3B-CAB	5.47	138.25	127.18
24	BC	5509	CLA	C4B-C3B-CAB	5.47	138.25	127.18
24	BD	5402	CLA	C2B-C3B-CAB	-5.47	116.14	127.33
24	BC	5506	CLA	C2B-C3B-CAB	-5.46	116.15	127.33
30	AB	627	SQD	C25-C24-C23	5.45	134.67	113.51
24	AB	608	CLA	C2B-C3B-CAB	-5.45	116.17	127.33
31	BM	5102	LMG	C9-O8-C28	5.45	132.54	116.99
34	AD	403	PHO	C4D-CHA-C1A	-5.44	123.08	129.57
24	BB	5606	CLA	C2B-C3B-CAB	-5.44	116.19	127.33
24	AB	615	CLA	C4B-C3B-CAB	5.44	138.20	127.18
31	AD	407	LMG	C17-C16-C15	-5.44	85.67	114.56
25	AA	408	MST	C8-S7-C2	5.44	106.18	102.23
24	AB	609	CLA	C4B-C3B-CAB	5.44	138.19	127.18
31	BD	5408	LMG	O7-C8-C7	5.43	128.61	108.50
24	AC	502	CLA	C2B-C3B-CAB	-5.43	116.22	127.33
35	AD	405	PL9	C12-C13-C14	-5.43	116.06	127.81
31	AC	521	LMG	C9-O8-C28	5.43	132.49	116.99
25	BA	5409	MST	C8-S7-C2	5.43	106.17	102.23
31	AM	101	LMG	C9-O8-C28	5.42	132.46	116.99
24	AB	612	CLA	C2B-C3B-CAB	-5.41	116.25	127.33
24	BC	5513	CLA	C2B-C3B-CAB	-5.41	116.26	127.33
24	AD	404	CLA	C2B-C3B-CAB	-5.40	116.27	127.33
36	BV	5201	HEM	CBD-CAD-C3D	-5.40	102.58	114.37
36	BF	5101	HEM	CHA-C4D-ND	5.40	131.88	124.28
24	BA	5405	CLA	C2B-C3B-CAB	-5.39	116.29	127.33
24	AA	406	CLA	C2B-C3B-CAB	-5.39	116.29	127.33
27	AT	101	BCR	C38-C26-C25	5.39	130.58	124.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	605	CLA	C4B-C3B-CAB	5.39	138.09	127.18
24	AC	505	CLA	CBA-CAA-C2A	5.39	127.12	113.95
28	BA	5412	DGD	O2G-C1B-C2B	5.39	123.02	111.54
34	BD	5404	PHO	C4D-CHA-C1A	-5.39	123.15	129.57
27	BA	5411	BCR	C33-C5-C6	5.38	130.57	124.50
24	BB	5609	CLA	C4B-C3B-CAB	5.38	138.07	127.18
24	BB	5616	CLA	C2B-C3B-CAB	-5.37	116.33	127.33
27	BA	5411	BCR	C38-C26-C25	5.37	130.55	124.50
28	AA	411	DGD	O2G-C1B-C2B	5.36	122.96	111.54
36	BF	5101	HEM	C4C-NC-C1C	5.36	110.97	105.51
24	BC	5501	CLA	C4B-C3B-CAB	5.35	138.01	127.18
24	BB	5620	CLA	C4B-C3B-CAB	5.35	138.01	127.18
24	AC	513	CLA	C2B-C3B-CAB	-5.35	116.38	127.33
24	AB	606	CLA	C2B-C3B-CAB	-5.35	116.38	127.33
24	BC	5502	CLA	C2B-C3B-CAB	-5.35	116.39	127.33
24	BD	5405	CLA	C2B-C3B-CAB	-5.34	116.40	127.33
24	BC	5510	CLA	C4B-C3B-CAB	5.34	137.98	127.18
30	BA	5401	SQD	C25-C24-C23	5.34	134.22	113.51
24	BB	5608	CLA	C2B-C3B-CAB	-5.33	116.41	127.33
24	BB	5619	CLA	C4B-C3B-CAB	5.33	137.96	127.18
35	AD	405	PL9	C20-C19-C21	5.32	123.47	115.39
28	BC	5519	DGD	C6D-C5D-C4D	-5.32	99.91	111.98
32	AD	409	LMT	C1B-O1B-C4'	-5.31	104.52	118.00
30	AA	416	SQD	C25-C24-C23	5.30	134.10	113.51
24	BA	5406	CLA	C2B-C3B-CAB	-5.30	116.47	127.33
27	BC	5514	BCR	C38-C26-C25	5.30	130.48	124.50
27	BB	5621	BCR	C33-C5-C6	5.30	130.48	124.50
24	BB	5613	CLA	C4B-C3B-CAB	5.30	137.91	127.18
24	AB	604	CLA	C2B-C3B-CAB	-5.30	116.49	127.33
24	AC	503	CLA	C2B-C3B-CAB	-5.30	116.49	127.33
24	AC	505	CLA	CAA-CBA-CGA	-5.29	97.64	113.24
24	AB	616	CLA	C4B-C3B-CAB	5.29	137.90	127.18
24	AA	404	CLA	C2B-C3B-CAB	-5.29	116.50	127.33
24	AB	611	CLA	C2B-C3B-CAB	-5.28	116.51	127.33
24	BC	5505	CLA	CAA-CBA-CGA	-5.28	97.68	113.24
24	BC	5505	CLA	C4B-C3B-CAB	5.28	137.87	127.18
36	AV	201	HEM	CBD-CAD-C3D	-5.28	102.86	114.37
24	BA	5407	CLA	C2B-C3B-CAB	-5.27	116.54	127.33
24	AC	512	CLA	C2B-C3B-CAB	-5.27	116.55	127.33
24	BB	5610	CLA	C2B-C3B-CAB	-5.26	116.56	127.33
27	BJ	5101	BCR	C33-C5-C6	5.26	130.43	124.50
24	BC	5504	CLA	CBA-CAA-C2A	5.26	126.81	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	617	BCR	C33-C5-C6	5.26	130.44	124.50
28	AC	517	DGD	C6D-C5D-C4D	-5.26	100.05	111.98
28	BH	5101	DGD	C6D-O5D-C1E	-5.25	103.26	113.80
27	AJ	101	BCR	C33-C5-C6	5.25	130.42	124.50
27	AA	410	BCR	C33-C5-C6	5.25	130.42	124.50
24	AC	510	CLA	C4B-C3B-CAB	5.24	137.80	127.18
27	AA	410	BCR	C38-C26-C25	5.25	130.42	124.50
24	AC	509	CLA	C2B-C3B-CAB	-5.24	116.61	127.33
24	AC	504	CLA	CBA-CAA-C2A	5.22	126.70	113.95
28	BH	5101	DGD	O3G-C1D-C2D	-5.21	101.48	108.15
36	AF	101	HEM	CHA-C4D-ND	5.21	131.61	124.28
30	BF	5102	SQD	C44-O6-C1	5.21	124.26	113.80
24	AC	505	CLA	C4B-C3B-CAB	5.21	137.72	127.18
24	AA	405	CLA	C2B-C3B-CAB	-5.21	116.67	127.33
24	BB	5615	CLA	C2B-C3B-CAB	-5.20	116.68	127.33
28	BC	5517	DGD	C6D-C5D-C4D	-5.19	100.20	111.98
24	BC	5512	CLA	C2B-C3B-CAB	-5.15	116.80	127.33
24	AB	609	CLA	C2B-C3B-CAB	-5.14	116.81	127.33
35	BD	5406	PL9	C20-C19-C21	5.14	123.19	115.39
24	AC	507	CLA	C4B-C3B-CAB	5.13	137.56	127.18
24	BC	5510	CLA	C2B-C3B-CAB	-5.13	116.83	127.33
30	AB	622	SQD	C25-C24-C23	5.12	133.39	113.51
24	BC	5509	CLA	C2B-C3B-CAB	-5.11	116.86	127.33
30	BB	5625	SQD	C25-C24-C23	5.11	133.35	113.51
28	AH	101	DGD	O3G-C1D-C2D	-5.11	101.60	108.15
27	AB	619	BCR	C33-C5-C6	5.11	130.27	124.50
24	AB	605	CLA	C2B-C3B-CAB	-5.11	116.87	127.33
31	BL	5101	LMG	O7-C8-C7	5.10	127.36	108.50
30	BB	5625	SQD	O9-S-C6	-5.09	102.33	106.83
24	BC	5507	CLA	C4B-C3B-CAB	5.07	137.45	127.18
24	BC	5503	CLA	C2B-C3B-CAB	-5.07	116.95	127.33
24	AC	507	CLA	C2B-C3B-CAB	-5.07	116.95	127.33
31	AB	620	LMG	O7-C8-C7	5.07	127.26	108.50
27	BD	5407	BCR	C33-C5-C6	5.07	130.22	124.50
24	BC	5508	CLA	CAA-C2A-C1A	-5.07	99.09	112.51
24	BB	5613	CLA	C2B-C3B-CAB	-5.05	116.98	127.33
30	AF	102	SQD	C44-O6-C1	5.05	123.94	113.80
24	BC	5505	CLA	CAA-C2A-C1A	-5.05	99.12	112.51
28	AH	101	DGD	O5D-C6D-C5D	5.04	117.70	108.96
27	AB	619	BCR	C38-C26-C25	5.04	130.18	124.50
27	BB	5623	BCR	C38-C26-C25	5.03	130.18	124.50
24	AC	501	CLA	C2B-C3B-CAB	-5.03	117.04	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BX	5101	BCR	C33-C5-C6	5.03	130.17	124.50
28	AH	101	DGD	C6D-O5D-C1E	-5.02	103.73	113.80
24	BB	5609	CLA	C2B-C3B-CAB	-5.02	117.06	127.33
24	AB	615	CLA	C2B-C3B-CAB	-5.00	117.08	127.33
28	BC	5519	DGD	O6D-C5D-C4D	5.00	119.03	109.73
24	AB	610	CLA	C4B-C3B-CAB	5.00	137.30	127.18
27	AX	101	BCR	C33-C5-C6	4.99	130.13	124.50
24	AC	505	CLA	CAA-C2A-C1A	-4.98	99.30	112.51
24	BB	5620	CLA	C2B-C3B-CAB	-4.98	117.13	127.33
36	BV	5201	HEM	C4C-NC-C1C	4.97	110.58	105.51
24	BC	5511	CLA	CBA-CAA-C2A	4.97	126.10	113.95
36	AF	101	HEM	C4C-NC-C1C	4.96	110.56	105.51
31	AI	101	LMG	C9-O8-C28	4.96	131.14	116.99
31	AC	521	LMG	C7-O1-C1	-4.95	103.86	113.80
24	BC	5507	CLA	C2B-C3B-CAB	-4.94	117.21	127.33
24	BB	5619	CLA	C2B-C3B-CAB	-4.94	117.21	127.33
31	BD	5409	LMG	C9-C8-C7	-4.94	100.51	111.86
24	AC	510	CLA	C2B-C3B-CAB	-4.94	117.22	127.33
24	BC	5501	CLA	C2B-C3B-CAB	-4.93	117.23	127.33
31	BC	5521	LMG	C7-O1-C1	-4.93	103.90	113.80
30	AF	102	SQD	C29-C30-C31	4.93	133.58	113.73
30	BF	5102	SQD	C29-C30-C31	4.92	133.54	113.73
24	AC	511	CLA	CBA-CAA-C2A	4.92	125.98	113.95
35	BD	5406	PL9	C35-C34-C36	4.92	122.86	115.39
24	BB	5614	CLA	C4B-C3B-CAB	4.92	137.13	127.18
31	BA	5402	LMG	C9-O8-C28	4.91	131.02	116.99
31	AD	407	LMG	C9-C8-C7	-4.91	100.58	111.86
31	BI	5101	LMG	C9-O8-C28	4.91	131.01	116.99
28	AC	517	DGD	O3G-C1D-C2D	-4.90	101.87	108.15
28	BH	5101	DGD	O5D-C6D-C5D	4.90	117.47	108.96
24	AC	508	CLA	CAA-C2A-C1A	-4.90	99.52	112.51
35	AD	405	PL9	C20-C19-C18	-4.90	113.77	123.52
36	AF	101	HEM	CBD-CAD-C3D	-4.89	103.69	114.37
24	BB	5605	CLA	C4B-C3B-CAB	4.89	137.09	127.18
27	AD	406	BCR	C33-C5-C6	4.89	130.02	124.50
28	BC	5519	DGD	O2G-C2G-C1G	-4.89	90.41	108.50
30	BB	5601	SQD	O9-S-C6	-4.88	102.52	106.83
24	AB	616	CLA	C2B-C3B-CAB	-4.87	117.36	127.33
36	BF	5101	HEM	CBD-CAD-C3D	-4.87	103.74	114.37
24	BC	5511	CLA	C1C-NC-C4C	4.87	112.83	106.26
24	AC	511	CLA	C1C-NC-C4C	4.86	112.82	106.26
31	BE	5101	LMG	C7-O1-C1	-4.85	104.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AV	201	HEM	CHA-C4D-ND	4.85	131.10	124.28
31	AA	414	LMG	C7-O1-C1	-4.84	104.08	113.80
27	BB	5623	BCR	C33-C5-C6	4.84	129.96	124.50
28	AH	101	DGD	O3G-C3G-C2G	-4.83	99.50	110.99
27	AB	618	BCR	C33-C5-C6	4.82	129.94	124.50
35	BD	5406	PL9	C7-C3-C2	-4.81	119.37	123.75
31	BE	5101	LMG	C39-C38-C37	4.81	126.69	112.94
24	BB	5607	CLA	C1C-NC-C4C	4.81	112.75	106.26
35	AD	405	PL9	C35-C34-C36	4.80	122.68	115.39
31	AA	417	LMG	C9-O8-C28	4.80	130.69	116.99
24	AB	601	CLA	C4A-NA-C1A	4.80	113.14	106.38
36	BV	5201	HEM	CHA-C4D-ND	4.79	131.01	124.28
28	BH	5101	DGD	C6D-C5D-C4D	-4.78	101.12	111.98
24	AC	513	CLA	C1C-NC-C4C	4.78	112.71	106.26
24	BC	5505	CLA	C2B-C3B-CAB	-4.77	117.56	127.33
24	AB	601	CLA	C4B-C3B-CAB	4.76	136.82	127.18
24	BC	5513	CLA	C1C-NC-C4C	4.76	112.68	106.26
31	AA	414	LMG	C39-C38-C37	4.75	126.53	112.94
31	BC	5521	LMG	C13-C12-C11	-4.75	95.69	113.28
31	AC	521	LMG	C13-C12-C11	-4.74	95.72	113.28
24	BB	5609	CLA	CBA-CAA-C2A	4.74	125.53	113.95
36	AV	201	HEM	C4C-NC-C1C	4.74	110.33	105.51
28	AC	518	DGD	C6D-C5D-C4D	-4.73	101.24	111.98
28	BC	5519	DGD	C1D-O6D-C5D	-4.73	104.59	113.73
28	AH	101	DGD	C6D-C5D-C4D	-4.72	101.26	111.98
27	AJ	101	BCR	C1-C6-C5	-4.72	115.75	122.59
32	AI	103	LMT	O1B-C1B-C2B	4.71	119.38	108.11
31	BE	5101	LMG	C8-O7-C10	4.68	128.86	117.86
27	BJ	5101	BCR	C1-C6-C5	-4.68	115.81	122.59
28	BC	5517	DGD	O3G-C1D-C2D	-4.67	102.17	108.15
24	AB	605	CLA	CBA-CAA-C2A	4.66	125.35	113.95
28	AC	519	DGD	O6E-C1E-O5D	4.65	121.00	109.93
24	AC	505	CLA	C2B-C3B-CAB	-4.65	117.81	127.33
24	BB	5605	CLA	C4A-NA-C1A	4.65	112.94	106.38
30	BF	5102	SQD	O9-S-C6	-4.65	102.72	106.83
28	BC	5519	DGD	O6E-C1E-O5D	4.65	121.00	109.93
24	AC	501	CLA	CAA-C2A-C1A	-4.65	100.20	112.51
31	BD	5408	LMG	O8-C9-C8	-4.64	96.59	108.80
24	AB	603	CLA	C1C-NC-C4C	4.64	112.52	106.26
31	AA	414	LMG	C8-O7-C10	4.64	128.76	117.86
35	BD	5406	PL9	C20-C19-C18	-4.64	114.29	123.52
24	AC	508	CLA	CBA-CAA-C2A	4.63	125.28	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5501	CLA	CAA-C2A-C1A	-4.63	100.24	112.51
28	BC	5517	DGD	C4A-C3A-C2A	-4.63	96.12	113.28
27	AC	514	BCR	C33-C5-C6	4.62	129.71	124.50
28	BH	5101	DGD	O3G-C3G-C2G	-4.61	100.01	110.99
30	AF	102	SQD	O9-S-C6	-4.61	102.75	106.83
31	BD	5409	LMG	C20-C19-C18	4.60	139.00	114.56
24	AC	502	CLA	CBA-CAA-C2A	4.60	125.19	113.95
28	AC	519	DGD	O2G-C2G-C1G	-4.60	91.50	108.50
28	BC	5518	DGD	C6D-C5D-C4D	-4.59	101.56	111.98
27	AK	102	BCR	C11-C10-C9	4.58	133.91	127.29
28	BC	5518	DGD	C1D-O6D-C5D	-4.58	104.88	113.73
30	AB	622	SQD	O9-S-C6	-4.57	102.79	106.83
24	BB	5616	CLA	C1C-NC-C4C	4.57	112.43	106.26
30	AB	627	SQD	O9-S-C6	-4.57	102.79	106.83
28	AC	519	DGD	O6D-C5D-C4D	4.56	118.22	109.73
28	BC	5519	DGD	C1E-C2E-C3E	-4.56	101.15	109.99
31	AD	407	LMG	C20-C19-C18	4.55	138.73	114.56
30	BA	5414	SQD	O9-S-C6	-4.55	102.81	106.83
25	AA	408	MST	C6-N5-C4	4.54	120.34	114.05
30	AA	416	SQD	O9-S-C6	-4.54	102.81	106.83
24	AC	512	CLA	C4A-NA-C1A	4.54	112.78	106.38
28	AC	519	DGD	C1D-O6D-C5D	-4.54	104.95	113.73
24	BC	5512	CLA	C4A-NA-C1A	4.54	112.78	106.38
35	AD	405	PL9	C7-C3-C2	-4.53	119.63	123.75
30	AA	413	SQD	C44-O6-C1	4.53	122.89	113.80
24	AB	610	CLA	C2B-C3B-CAB	-4.53	118.07	127.33
31	AJ	102	LMG	O8-C9-C8	-4.52	96.92	108.80
24	BB	5614	CLA	C2B-C3B-CAB	-4.51	118.09	127.33
24	BB	5618	CLA	C1C-NC-C4C	4.51	112.34	106.26
24	BB	5619	CLA	C4A-NA-C1A	4.51	112.74	106.38
31	AJ	102	LMG	C9-O8-C28	4.51	129.86	116.99
24	AB	608	CLA	CAA-CBA-CGA	-4.51	99.96	113.24
31	BD	5410	LMG	C9-O8-C28	4.50	129.84	116.99
30	BA	5401	SQD	O9-S-C6	-4.49	102.86	106.83
27	AD	406	BCR	C38-C26-C27	-4.50	104.87	113.39
31	AD	408	LMG	C9-O8-C28	4.49	129.82	116.99
25	BA	5409	MST	C6-N5-C4	4.49	120.26	114.05
24	BC	5508	CLA	CBA-CAA-C2A	4.48	124.90	113.95
32	BC	5522	LMT	O1B-C1B-C2B	4.48	118.83	108.11
28	AC	517	DGD	C4A-C3A-C2A	-4.46	96.74	113.28
24	BC	5502	CLA	CBA-CAA-C2A	4.46	124.85	113.95
24	BC	5511	CLA	CAA-C2A-C1A	-4.46	100.70	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5501	CLA	C4A-NA-C1A	4.44	112.65	106.38
24	BB	5610	CLA	O2A-CGA-CBA	4.44	125.50	111.90
30	BA	5414	SQD	C44-O6-C1	4.44	122.71	113.80
24	AB	605	CLA	CAA-C2A-C1A	-4.44	100.74	112.51
28	AC	518	DGD	C1D-O6D-C5D	-4.43	105.16	113.73
24	BA	5406	CLA	CHD-C4C-NC	4.43	127.38	124.28
31	AA	417	LMG	C9-C8-C7	4.42	122.00	111.86
24	AB	614	CLA	C1C-NC-C4C	4.42	112.22	106.26
31	BA	5402	LMG	C9-C8-C7	4.42	122.00	111.86
24	BC	5508	CLA	C4A-NA-C1A	4.41	112.59	106.38
24	BC	5502	CLA	C4A-NA-C1A	4.40	112.59	106.38
28	AA	411	DGD	C1G-O1G-C1A	-4.40	104.42	116.99
28	BA	5412	DGD	C1G-O1G-C1A	-4.40	104.43	116.99
27	AC	516	BCR	C29-C30-C25	4.38	117.36	110.37
24	AC	511	CLA	CAA-C2A-C1A	-4.37	100.92	112.51
24	BB	5609	CLA	CAA-C2A-C1A	-4.37	100.93	112.51
27	BB	5622	BCR	C33-C5-C6	4.36	129.42	124.50
24	BC	5502	CLA	CAA-C2A-C1A	-4.35	100.97	112.51
24	AB	612	CLA	C1C-NC-C4C	4.35	112.14	106.26
31	BD	5408	LMG	C9-O8-C28	4.36	129.43	116.99
27	AJ	101	BCR	C38-C26-C27	-4.35	105.14	113.39
30	BA	5401	SQD	C44-O6-C1	4.35	122.53	113.80
24	AB	606	CLA	O2A-CGA-CBA	4.35	125.20	111.90
27	BK	5102	BCR	C11-C10-C9	4.35	133.57	127.29
24	BB	5611	CLA	O2A-CGA-CBA	4.35	125.20	111.90
34	BD	5404	PHO	C2B-C3B-CAB	-4.34	118.44	127.33
24	BB	5605	CLA	C2B-C3B-CAB	-4.34	118.44	127.33
24	AB	615	CLA	C4A-NA-C1A	4.34	112.50	106.38
31	BD	5409	LMG	C18-C17-C16	4.33	137.54	114.56
24	AB	601	CLA	C2B-C3B-CAB	-4.32	118.48	127.33
27	BC	5514	BCR	C33-C5-C6	4.32	129.37	124.50
27	AK	102	BCR	C33-C5-C4	-4.32	105.21	113.39
27	BC	5514	BCR	C24-C23-C22	4.31	132.67	126.22
24	BA	5406	CLA	O2A-CGA-CBA	4.31	125.08	111.90
28	AE	101	DGD	O2G-C1B-C2B	4.30	120.70	111.54
24	AD	404	CLA	CBA-CAA-C2A	4.30	124.45	113.95
34	AD	403	PHO	C2B-C3B-CAB	-4.30	118.54	127.33
24	AC	501	CLA	C4A-NA-C1A	4.30	112.44	106.38
24	BB	5612	CLA	CAA-CBA-CGA	-4.29	100.59	113.24
24	BD	5405	CLA	C4A-NA-C1A	4.29	112.44	106.38
28	AC	519	DGD	C1E-C2E-C3E	-4.29	101.68	109.99
25	AA	408	MST	N5-C6-N1	-4.29	119.57	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BD	5406	PL9	C15-C14-C16	4.29	121.90	115.39
24	BC	5506	CLA	CBA-CAA-C2A	4.29	124.44	113.95
28	BE	5102	DGD	O2G-C1B-C2B	4.28	120.66	111.54
27	BD	5407	BCR	C38-C26-C27	-4.28	105.28	113.39
36	AF	101	HEM	C1B-NB-C4B	4.28	109.55	105.11
36	AV	201	HEM	CAD-CBD-CGD	4.28	121.59	113.53
34	AD	402	PHO	C2B-C3B-CAB	-4.28	118.58	127.33
36	BV	5201	HEM	C1B-NB-C4B	4.27	109.53	105.11
24	AC	503	CLA	C4A-NA-C1A	4.27	112.40	106.38
24	AB	607	CLA	O2A-CGA-CBA	4.26	124.95	111.90
28	BE	5102	DGD	C6D-O5D-C1E	-4.26	105.25	113.80
25	BA	5409	MST	N5-C6-N1	-4.26	119.61	126.18
30	AA	416	SQD	C44-O6-C1	4.25	122.34	113.80
24	BB	5615	CLA	CAA-C2A-C1A	-4.25	101.23	112.51
36	BV	5201	HEM	CAD-CBD-CGD	4.25	121.54	113.53
31	AD	407	LMG	C18-C17-C16	4.25	137.13	114.56
24	AB	616	CLA	C4A-NA-C1A	4.24	112.37	106.38
24	AD	404	CLA	C4A-NA-C1A	4.24	112.36	106.38
24	AC	507	CLA	C4A-NA-C1A	4.24	112.36	106.38
31	AB	620	LMG	C8-O7-C10	4.24	127.81	117.86
32	AI	103	LMT	C1-O1'-C1'	4.24	121.39	113.91
24	BB	5620	CLA	C4A-NA-C1A	4.24	112.35	106.38
27	AK	102	BCR	C7-C8-C9	4.23	132.55	126.22
28	AE	101	DGD	O5D-C1E-C2E	4.23	113.58	108.15
24	AB	614	CLA	CAA-C2A-C1A	-4.22	101.34	112.51
27	AK	102	BCR	C2-C1-C6	4.20	117.07	110.37
24	AC	506	CLA	CBA-CAA-C2A	4.19	124.20	113.95
24	BA	5406	CLA	C4D-C3D-CAD	4.19	113.21	108.05
27	BJ	5101	BCR	C38-C26-C27	-4.19	105.45	113.39
27	AB	618	BCR	C38-C26-C27	-4.18	105.47	113.39
28	AE	101	DGD	C1G-O1G-C1A	4.18	128.93	116.99
24	BC	5507	CLA	C4A-NA-C1A	4.18	112.27	106.38
24	BB	5618	CLA	CAA-C2A-C1A	-4.18	101.44	112.51
24	AC	509	CLA	C1C-NC-C4C	4.17	111.89	106.26
24	AC	502	CLA	CAA-C2A-C1A	-4.17	101.47	112.51
31	AB	620	LMG	O1-C7-C8	4.16	120.90	110.99
31	AD	407	LMG	C15-C14-C13	-4.16	92.47	114.56
24	BC	5505	CLA	C4A-NA-C1A	4.16	112.24	106.38
24	BA	5407	CLA	O2A-CGA-CBA	4.16	124.62	111.90
35	BD	5406	PL9	C35-C34-C33	-4.15	115.25	123.52
36	AV	201	HEM	C1B-NB-C4B	4.15	109.41	105.11
24	AA	405	CLA	O2A-CGA-CBA	4.14	124.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5409	LMG	C15-C14-C13	-4.15	92.55	114.56
27	AC	514	BCR	C24-C23-C22	4.14	132.41	126.22
27	BC	5516	BCR	C29-C30-C25	4.14	116.97	110.37
28	BE	5102	DGD	C1G-O1G-C1A	4.14	128.80	116.99
24	AA	407	CLA	C4A-NA-C1A	4.14	112.21	106.38
27	BB	5622	BCR	C38-C26-C27	-4.13	105.56	113.39
35	AD	405	PL9	C15-C14-C16	4.13	121.66	115.39
31	BA	5402	LMG	O8-C9-C8	-4.12	97.96	108.80
28	AH	101	DGD	C5B-C4B-C3B	-4.12	92.68	114.56
27	AC	516	BCR	C2-C1-C6	4.12	116.94	110.37
24	AA	406	CLA	O2A-CGA-CBA	4.11	124.48	111.90
32	BC	5522	LMT	C1-O1'-C1'	4.11	121.17	113.91
27	BK	5102	BCR	C7-C8-C9	4.11	132.36	126.22
28	AE	101	DGD	C6D-O5D-C1E	-4.10	105.56	113.80
35	AD	405	PL9	C35-C34-C33	-4.11	115.35	123.52
34	BD	5403	PHO	C2B-C3B-CAB	-4.10	118.94	127.33
35	AD	405	PL9	C25-C24-C26	4.10	121.62	115.39
24	BC	5501	CLA	CBA-CAA-C2A	4.10	123.97	113.95
28	AB	628	DGD	C4B-C3B-C2B	-4.10	98.10	113.28
24	AC	505	CLA	C4A-NA-C1A	4.09	112.15	106.38
28	BH	5101	DGD	C5B-C4B-C3B	-4.09	92.85	114.56
24	BD	5405	CLA	CBA-CAA-C2A	4.09	123.94	113.95
27	BD	5407	BCR	C29-C30-C25	4.09	116.89	110.37
31	AD	408	LMG	C7-O1-C1	-4.08	105.61	113.80
24	BB	5606	CLA	C4A-NA-C1A	4.08	112.13	106.38
31	AI	101	LMG	C9-C8-C7	-4.08	102.50	111.86
27	BX	5101	BCR	C38-C26-C27	-4.08	105.66	113.39
24	BC	5510	CLA	C4A-NA-C1A	4.08	112.13	106.38
27	BK	5102	BCR	C33-C5-C4	-4.08	105.67	113.39
36	BF	5101	HEM	C1B-NB-C4B	4.07	109.33	105.11
27	BC	5516	BCR	C33-C5-C4	-4.06	105.69	113.39
24	AC	510	CLA	C4A-NA-C1A	4.06	112.11	106.38
24	BC	5509	CLA	C4A-NA-C1A	4.05	112.10	106.38
27	BB	5621	BCR	C38-C26-C27	-4.05	105.71	113.39
28	BB	5602	DGD	C4B-C3B-C2B	-4.05	98.26	113.28
24	BC	5503	CLA	C4A-NA-C1A	4.05	112.09	106.38
30	AB	622	SQD	O48-C23-C24	4.05	124.29	111.90
31	BD	5410	LMG	C7-O1-C1	-4.05	105.68	113.80
27	AT	101	BCR	C29-C30-C25	4.04	116.82	110.37
24	BC	5506	CLA	C4A-NA-C1A	4.04	112.08	106.38
29	AA	415	LHG	O7-C7-C8	4.05	120.16	111.54
31	BL	5101	LMG	C8-O7-C10	4.04	127.36	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	502	CLA	C4A-NA-C1A	4.04	112.08	106.38
29	BA	5415	LHG	O7-C7-C8	4.04	120.15	111.54
34	BD	5403	PHO	C3D-C4D-ND	4.04	111.90	106.81
24	AC	508	CLA	C4A-NA-C1A	4.03	112.07	106.38
28	AC	519	DGD	C8A-C7A-C6A	-4.02	93.20	114.56
31	BL	5101	LMG	O1-C7-C8	4.02	120.56	110.99
27	BA	5411	BCR	C7-C8-C9	4.02	132.22	126.22
27	BT	5101	BCR	C33-C5-C4	-4.01	105.79	113.39
34	AD	402	PHO	C3D-C4D-ND	4.01	111.86	106.81
27	BK	5102	BCR	C2-C1-C6	4.01	116.76	110.37
27	AX	101	BCR	C38-C26-C27	-4.01	105.80	113.39
27	AT	101	BCR	C33-C5-C4	-4.00	105.81	113.39
24	AC	509	CLA	C4A-NA-C1A	4.00	112.02	106.38
32	BB	5626	LMT	C1B-O1B-C4'	-3.99	107.85	118.00
24	BC	5509	CLA	C1C-NC-C4C	3.99	111.65	106.26
24	BD	5405	CLA	CAA-C2A-C1A	-3.99	101.94	112.51
28	BE	5102	DGD	O5D-C1E-C2E	3.99	113.27	108.15
27	BX	5101	BCR	C29-C30-C25	3.99	116.73	110.37
24	BB	5611	CLA	CBD-CHA-C1A	3.99	133.99	128.77
24	AB	611	CLA	CAA-C2A-C1A	-3.99	101.94	112.51
25	AA	408	MST	N5-C4-N3	-3.99	120.03	126.18
28	BC	5519	DGD	C8A-C7A-C6A	-3.99	93.40	114.56
24	BB	5610	CLA	C4A-NA-C1A	3.98	112.00	106.38
24	AC	506	CLA	C4A-NA-C1A	3.98	111.99	106.38
24	BB	5608	CLA	C4A-NA-C1A	3.98	111.99	106.38
24	AB	611	CLA	C4A-NA-C1A	3.98	111.99	106.38
30	AB	622	SQD	C44-O6-C1	3.97	121.78	113.80
24	AB	602	CLA	C4A-NA-C1A	3.97	111.98	106.38
30	BA	5401	SQD	O48-C23-C24	3.97	124.05	111.90
24	BB	5612	CLA	C4A-NA-C1A	3.96	111.97	106.38
24	AD	404	CLA	CAA-C2A-C1A	-3.97	102.00	112.51
30	AA	416	SQD	O48-C23-C24	3.97	124.04	111.90
28	BH	5101	DGD	O6D-C5D-C6D	3.96	114.56	106.62
28	AC	517	DGD	C1D-O6D-C5D	-3.96	106.07	113.73
24	BB	5615	CLA	C4A-NA-C1A	3.96	111.96	106.38
24	AB	608	CLA	C4A-NA-C1A	3.95	111.95	106.38
35	BD	5406	PL9	C11-C9-C8	-3.94	113.48	121.06
24	BB	5613	CLA	O2A-CGA-CBA	3.94	123.96	111.90
27	AC	514	BCR	C38-C26-C27	-3.94	105.93	113.39
32	AB	629	LMT	C1-O1'-C1'	-3.94	106.96	113.91
24	AB	606	CLA	C4A-NA-C1A	3.94	111.93	106.38
24	AB	603	CLA	C2A-C1A-CHA	3.94	131.05	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	610	CLA	C4A-NA-C1A	3.94	111.93	106.38
24	BC	5508	CLA	CHD-C4C-NC	3.93	127.03	124.28
27	AB	617	BCR	C38-C26-C27	-3.93	105.94	113.39
28	BB	5602	DGD	O1G-C1G-C2G	-3.93	98.46	108.80
28	BC	5517	DGD	C1D-O6D-C5D	-3.93	106.13	113.73
35	BD	5406	PL9	C25-C24-C26	3.93	121.36	115.39
24	AB	604	CLA	O2A-CGA-CBA	3.92	123.91	111.90
31	BD	5410	LMG	C19-C18-C17	-3.93	93.72	114.56
24	BB	5614	CLA	C4A-NA-C1A	3.92	111.91	106.38
24	AA	405	CLA	C4D-C3D-CAD	3.92	112.87	108.05
24	AD	401	CLA	C4A-NA-C1A	3.92	111.91	106.38
27	AC	515	BCR	C38-C26-C27	-3.92	105.96	113.39
27	AD	406	BCR	C24-C23-C22	3.92	132.08	126.22
27	AX	101	BCR	C29-C30-C25	3.92	116.62	110.37
24	BB	5608	CLA	O2A-CGA-CBA	3.92	123.89	111.90
27	BT	5101	BCR	C29-C30-C25	3.91	116.61	110.37
24	AC	501	CLA	CBA-CAA-C2A	3.91	123.52	113.95
24	BD	5402	CLA	C4A-NA-C1A	3.91	111.89	106.38
31	BI	5101	LMG	C9-C8-C7	-3.91	102.89	111.86
27	AC	516	BCR	C33-C5-C4	-3.91	105.99	113.39
28	AH	101	DGD	O6D-C5D-C6D	3.90	114.44	106.62
24	BA	5408	CLA	C4A-NA-C1A	3.90	111.88	106.38
27	AJ	101	BCR	C7-C8-C9	3.90	132.05	126.22
28	BC	5518	DGD	C8A-C7A-C6A	-3.90	93.86	114.56
24	BB	5607	CLA	C2A-C1A-CHA	3.89	130.97	123.87
27	BC	5515	BCR	C33-C5-C4	-3.89	106.02	113.39
24	AB	613	CLA	C4A-NA-C1A	3.89	111.86	106.38
25	BA	5409	MST	N5-C4-N3	-3.89	120.19	126.18
31	AD	408	LMG	C19-C18-C17	-3.88	93.94	114.56
31	AA	417	LMG	O8-C9-C8	-3.88	98.58	108.80
28	AC	518	DGD	C8A-C7A-C6A	-3.88	93.96	114.56
27	BB	5621	BCR	C33-C5-C4	-3.88	106.04	113.39
24	AB	609	CLA	O2A-CGA-CBA	3.88	123.77	111.90
24	BB	5617	CLA	C4A-NA-C1A	3.88	111.85	106.38
27	AC	515	BCR	C33-C5-C4	-3.87	106.05	113.39
31	AD	407	LMG	C21-C20-C19	3.87	135.14	114.56
24	BC	5505	CLA	C4D-C3D-CAD	3.87	112.81	108.05
24	AC	506	CLA	CAA-C2A-C1A	-3.87	102.26	112.51
28	AB	628	DGD	O1G-C1G-C2G	-3.87	98.63	108.80
24	AB	608	CLA	CHD-C4C-NC	3.87	126.98	124.28
24	AB	614	CLA	C2C-C1C-NC	-3.87	107.10	110.22
24	BC	5511	CLA	C2C-C1C-NC	-3.86	107.10	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BD	5406	PL9	C15-C14-C13	-3.86	115.83	123.52
28	AC	518	DGD	C3G-C2G-C1G	-3.86	103.00	111.86
30	AA	413	SQD	C45-O47-C7	3.86	126.92	117.86
28	BA	5412	DGD	O6E-C1E-O5D	3.86	119.11	109.93
27	AJ	101	BCR	C30-C25-C26	-3.86	117.00	122.59
28	AA	411	DGD	O6E-C1E-O5D	3.85	119.10	109.93
24	AB	614	CLA	C4A-NA-C1A	3.85	111.81	106.38
24	AB	607	CLA	CBD-CHA-C1A	3.85	133.81	128.77
24	BB	5615	CLA	CHD-C4C-NC	3.85	126.97	124.28
30	BA	5414	SQD	C45-O47-C7	3.85	126.89	117.86
27	BT	5101	BCR	C38-C26-C27	-3.84	106.12	113.39
28	BC	5518	DGD	C3G-C2G-C1G	-3.84	103.06	111.86
32	AB	623	LMT	C1B-O1B-C4'	-3.83	108.26	118.00
27	AC	516	BCR	C38-C26-C27	-3.83	106.13	113.39
31	AA	417	LMG	O7-C8-C7	3.83	122.67	108.50
24	BC	5506	CLA	CAA-C2A-C1A	-3.82	102.38	112.51
24	AB	603	CLA	CAA-C2A-C1A	-3.82	102.38	112.51
24	BB	5612	CLA	CHD-C4C-NC	3.82	126.95	124.28
27	AD	406	BCR	C29-C30-C25	3.82	116.46	110.37
32	BB	5603	LMT	C1-O1'-C1'	-3.82	107.17	113.91
24	BB	5615	CLA	O2A-CGA-CBA	3.82	123.58	111.90
24	AC	511	CLA	C2C-C1C-NC	-3.81	107.14	110.22
30	BB	5601	SQD	O48-C23-C24	3.81	123.57	111.90
24	BD	5402	CLA	O2A-CGA-CBA	3.81	123.56	111.90
27	BJ	5101	BCR	C33-C5-C4	-3.81	106.17	113.39
28	AH	101	DGD	C3B-C2B-C1B	-3.81	98.73	113.51
24	BA	5408	CLA	CHD-C4C-NC	3.81	126.94	124.28
24	BB	5611	CLA	C4A-NA-C1A	3.81	111.75	106.38
27	BX	5101	BCR	C2-C1-C6	3.80	116.43	110.37
24	AA	407	CLA	CAA-C2A-C1A	-3.80	102.44	112.51
30	AF	102	SQD	O48-C23-C24	3.80	123.53	111.90
24	AB	604	CLA	C4A-NA-C1A	3.80	111.73	106.38
27	AA	410	BCR	C7-C8-C9	3.79	131.89	126.22
30	BA	5401	SQD	C31-C30-C29	3.79	134.68	114.56
27	BJ	5101	BCR	C30-C25-C26	-3.79	117.11	122.59
28	BC	5519	DGD	O1G-C1G-C2G	-3.79	98.84	108.80
24	AC	508	CLA	CHD-C4C-NC	3.78	126.93	124.28
24	AB	611	CLA	O2A-CGA-CBA	3.78	123.48	111.90
27	AT	101	BCR	C38-C26-C27	-3.78	106.22	113.39
24	BC	5511	CLA	C4A-NA-C1A	3.78	111.71	106.38
28	BH	5101	DGD	C3B-C2B-C1B	-3.78	98.84	113.51
30	AB	627	SQD	O48-C23-C24	3.78	123.47	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	416	SQD	C31-C30-C29	3.78	134.63	114.56
30	BF	5102	SQD	O48-C23-C24	3.77	123.45	111.90
27	AJ	101	BCR	C23-C24-C25	3.77	138.36	127.23
31	BD	5408	LMG	O1-C7-C8	3.77	119.96	110.99
31	BC	5520	LMG	C12-C11-C10	-3.77	98.87	113.51
30	BB	5625	SQD	C44-O6-C1	3.77	121.37	113.80
31	AC	521	LMG	O7-C8-C7	3.77	122.46	108.50
35	AD	405	PL9	C11-C9-C8	-3.77	113.81	121.06
35	AD	405	PL9	C25-C24-C23	-3.77	116.01	123.52
24	BB	5613	CLA	CBA-CAA-C2A	3.77	123.17	113.95
24	AC	504	CLA	C4A-NA-C1A	3.77	111.70	106.38
27	BC	5515	BCR	C38-C26-C27	-3.77	106.25	113.39
27	AK	102	BCR	C38-C26-C27	-3.77	106.25	113.39
36	AV	201	HEM	C1A-CHA-C4D	-3.77	122.52	127.47
27	AJ	101	BCR	C33-C5-C4	-3.76	106.26	113.39
24	BB	5618	CLA	C4A-NA-C1A	3.76	111.68	106.38
24	BC	5504	CLA	C4A-NA-C1A	3.76	111.68	106.38
24	AB	607	CLA	C4A-NA-C1A	3.75	111.67	106.38
24	AB	602	CLA	O2A-CGA-CBA	3.75	123.37	111.90
24	AC	513	CLA	O2A-CGA-CBA	3.75	123.37	111.90
30	BB	5625	SQD	O48-C23-C24	3.74	123.35	111.90
24	AB	609	CLA	CBA-CAA-C2A	3.74	123.08	113.95
31	BD	5409	LMG	C21-C20-C19	3.74	134.40	114.56
28	AC	519	DGD	C6B-C5B-C4B	-3.74	94.73	114.56
31	BC	5521	LMG	O7-C8-C7	3.73	122.32	108.50
32	BD	5411	LMT	O1B-C1B-C2B	3.73	117.04	108.11
25	AA	408	MST	N3-C2-N1	-3.73	120.15	126.83
27	BD	5407	BCR	C24-C23-C22	3.73	131.79	126.22
36	BV	5201	HEM	C1A-CHA-C4D	-3.72	122.57	127.47
27	BB	5621	BCR	C29-C30-C25	3.72	116.31	110.37
24	AB	612	CLA	O2D-CGD-CBD	3.72	118.85	111.34
24	AB	609	CLA	C4A-NA-C1A	3.72	111.62	106.38
24	BB	5613	CLA	C4A-NA-C1A	3.72	111.62	106.38
24	BA	5407	CLA	C4A-NA-C1A	3.71	111.62	106.38
24	AA	405	CLA	CHD-C4C-NC	3.71	126.88	124.28
24	BB	5610	CLA	CAA-C2A-C1A	-3.71	102.67	112.51
31	AB	621	LMG	C34-C33-C32	3.71	134.27	114.56
24	BA	5406	CLA	C4A-NA-C1A	3.71	111.61	106.38
31	AC	520	LMG	C12-C11-C10	-3.71	99.12	113.51
31	BA	5402	LMG	O7-C8-C7	3.71	122.22	108.50
24	AC	505	CLA	C4D-C3D-CAD	3.71	112.61	108.05
32	AD	409	LMT	O1B-C1B-C2B	3.70	116.97	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AF	101	HEM	CAD-C3D-C2D	3.70	136.62	127.19
24	BB	5618	CLA	C2C-C1C-NC	-3.70	107.24	110.22
24	AC	511	CLA	C4A-NA-C1A	3.69	111.59	106.38
27	BC	5516	BCR	C38-C26-C27	-3.69	106.40	113.39
30	BA	5401	SQD	C11-C10-C9	3.69	134.14	114.56
24	AD	401	CLA	O2A-CGA-CBA	3.69	123.18	111.90
24	BC	5506	CLA	O2A-CGA-CBA	3.68	123.18	111.90
31	BB	5624	LMG	C34-C33-C32	3.68	134.12	114.56
31	AB	621	LMG	C14-C13-C12	-3.68	95.02	114.56
30	AA	416	SQD	C11-C10-C9	3.68	134.12	114.56
24	AA	405	CLA	O2D-CGD-CBD	3.68	118.77	111.34
35	AD	405	PL9	C15-C14-C13	-3.68	116.20	123.52
27	BK	5102	BCR	C38-C26-C27	-3.68	106.43	113.39
24	AB	603	CLA	O2A-CGA-CBA	3.67	123.14	111.90
24	AC	505	CLA	C4B-NB-C1B	3.67	110.66	107.12
24	BB	5607	CLA	CAA-C2A-C1A	-3.67	102.78	112.51
24	BB	5609	CLA	C4A-NA-C1A	3.67	111.56	106.38
24	BA	5406	CLA	O2D-CGD-CBD	3.67	118.76	111.34
27	AJ	101	BCR	C29-C30-C25	3.66	116.21	110.37
31	BB	5624	LMG	C14-C13-C12	-3.66	95.11	114.56
28	BC	5519	DGD	C6B-C5B-C4B	-3.66	95.10	114.56
31	BD	5408	LMG	C9-C8-C7	3.66	120.26	111.86
31	AJ	102	LMG	C9-C8-C7	3.66	120.25	111.86
24	AA	406	CLA	O2D-CGD-CBD	3.65	118.72	111.34
24	AB	605	CLA	C4A-NA-C1A	3.65	111.53	106.38
31	AJ	102	LMG	O1-C7-C8	3.65	119.67	110.99
24	AC	508	CLA	O2A-CGA-CBA	3.65	123.08	111.90
27	BJ	5101	BCR	C7-C8-C9	3.65	131.68	126.22
36	BF	5101	HEM	CAD-C3D-C2D	3.65	136.50	127.19
24	BB	5616	CLA	C4A-NA-C1A	3.64	111.52	106.38
24	BB	5610	CLA	C4D-C3D-CAD	3.64	112.53	108.05
31	AB	621	LMG	C37-C36-C35	-3.64	95.23	114.56
27	BJ	5101	BCR	C23-C24-C25	3.64	137.97	127.23
24	AB	603	CLA	C3A-C2A-C1A	3.64	107.61	101.70
30	AF	102	SQD	C19-C18-C17	3.64	123.33	112.94
24	BC	5503	CLA	C4D-C3D-CAD	3.63	112.52	108.05
27	BC	5515	BCR	C23-C24-C25	3.63	137.95	127.23
25	BA	5409	MST	N3-C2-N1	-3.63	120.32	126.83
31	BB	5624	LMG	C37-C36-C35	-3.63	95.28	114.56
24	AC	509	CLA	O2A-CGA-CBA	3.63	123.01	111.90
27	AB	617	BCR	C33-C5-C4	-3.62	106.52	113.39
24	BB	5606	CLA	O2A-CGA-CBA	3.62	122.99	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5408	CLA	CBA-CAA-C2A	3.62	122.81	113.95
24	AC	503	CLA	O2A-CGA-CBA	3.62	122.98	111.90
24	AA	407	CLA	CHD-C4C-NC	3.62	126.81	124.28
24	BC	5507	CLA	O2A-CGA-CBA	3.62	122.98	111.90
24	BC	5501	CLA	O2A-CGA-CBA	3.62	122.98	111.90
24	AC	509	CLA	C4D-C3D-CAD	3.62	112.50	108.05
24	AC	513	CLA	C4B-NB-C1B	3.62	110.60	107.12
24	AD	404	CLA	O2D-CGD-CBD	3.61	118.64	111.34
27	AC	515	BCR	C23-C24-C25	3.61	137.89	127.23
30	AB	622	SQD	C11-C10-C9	3.61	133.75	114.56
24	AC	507	CLA	O2A-CGA-CBA	3.61	122.95	111.90
24	BC	5505	CLA	C4B-NB-C1B	3.61	110.59	107.12
24	BB	5619	CLA	CBD-CHA-C1A	3.61	133.48	128.77
24	BC	5513	CLA	O2A-CGA-CBA	3.61	122.94	111.90
24	BA	5408	CLA	CAA-C2A-C1A	-3.61	102.96	112.51
30	AA	413	SQD	C31-C30-C29	3.60	133.70	114.56
27	BA	5411	BCR	C38-C26-C27	-3.60	106.56	113.39
36	BV	5201	HEM	C3A-C4A-NA	3.60	111.91	109.50
24	BB	5607	CLA	CBD-CHA-C1A	3.60	133.48	128.77
24	BB	5607	CLA	C3A-C2A-C1A	3.60	107.55	101.70
24	BC	5513	CLA	C4A-NA-C1A	3.60	111.46	106.38
35	BD	5406	PL9	C26-C27-C28	3.60	121.89	111.64
27	BJ	5101	BCR	C29-C30-C25	3.60	116.11	110.37
30	BB	5625	SQD	C11-C10-C9	3.59	133.64	114.56
31	BD	5409	LMG	C22-C23-C24	-3.59	99.27	113.73
24	BA	5407	CLA	C1C-NC-C4C	3.59	111.11	106.26
24	AC	506	CLA	O2A-CGA-CBA	3.59	122.88	111.90
24	AB	611	CLA	CHD-C4C-NC	3.59	126.79	124.28
27	AC	514	BCR	C33-C5-C4	-3.59	106.59	113.39
35	BD	5406	PL9	C25-C24-C23	-3.59	116.38	123.52
24	BB	5619	CLA	C2A-C1A-CHA	3.58	130.40	123.87
36	AV	201	HEM	C3A-C4A-NA	3.58	111.89	109.50
24	BD	5402	CLA	C4D-C3D-CAD	3.58	112.46	108.05
27	BB	5623	BCR	C38-C26-C27	-3.58	106.60	113.39
34	BD	5404	PHO	C3A-C2A-C1A	3.58	106.53	101.90
30	BA	5414	SQD	C31-C30-C29	3.58	133.59	114.56
27	BC	5514	BCR	C38-C26-C27	-3.58	106.61	113.39
24	AB	603	CLA	C4D-C3D-CAD	3.58	112.45	108.05
24	BC	5503	CLA	O2A-CGA-CBA	3.58	122.85	111.90
24	BB	5607	CLA	O2A-CGA-CBA	3.57	122.84	111.90
24	AC	501	CLA	CBD-CHA-C1A	3.57	133.44	128.77
27	AB	617	BCR	C29-C30-C25	3.57	116.06	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	405	CLA	C4A-NA-C1A	3.57	111.41	106.38
24	BC	5504	CLA	O2D-CGD-CBD	3.57	118.55	111.34
30	AF	102	SQD	C11-C10-C9	3.57	133.51	114.56
27	BC	5515	BCR	C29-C30-C25	3.57	116.06	110.37
28	AC	519	DGD	O1G-C1G-C2G	-3.57	99.42	108.80
27	AD	406	BCR	C30-C25-C26	-3.57	117.42	122.59
24	AB	606	CLA	CAA-C2A-C1A	-3.56	103.06	112.51
27	BD	5407	BCR	C30-C25-C26	-3.57	117.43	122.59
31	AD	408	LMG	C37-C38-C39	3.56	128.07	113.73
30	BF	5102	SQD	C11-C10-C9	3.56	133.46	114.56
27	AX	101	BCR	C2-C1-C6	3.56	116.04	110.37
24	AB	615	CLA	C4D-C3D-CAD	3.56	112.42	108.05
24	BC	5513	CLA	C4B-NB-C1B	3.56	110.54	107.12
24	BA	5407	CLA	C4D-C3D-CAD	3.55	112.42	108.05
27	AA	410	BCR	C38-C26-C27	-3.55	106.66	113.39
27	BA	5411	BCR	C33-C5-C4	-3.55	106.66	113.39
24	AB	615	CLA	C2A-C1A-CHA	3.55	130.34	123.87
24	BC	5512	CLA	C4D-C3D-CAD	3.55	112.41	108.05
30	AA	413	SQD	O9-S-C6	-3.55	103.69	106.83
24	BC	5511	CLA	C4D-C3D-CAD	3.54	112.41	108.05
30	AA	413	SQD	C11-C10-C9	3.54	133.38	114.56
31	BD	5410	LMG	C37-C38-C39	3.54	127.99	113.73
30	BA	5414	SQD	C11-C10-C9	3.54	133.37	114.56
27	AB	619	BCR	C29-C30-C25	3.54	116.02	110.37
32	BC	5522	LMT	O1'-C1-C2	-3.54	96.18	109.79
24	BB	5619	CLA	CHD-C4C-NC	3.54	126.75	124.28
24	AA	407	CLA	O2D-CGD-CBD	3.54	118.48	111.34
24	BB	5609	CLA	CHD-C4C-NC	3.53	126.75	124.28
24	BB	5616	CLA	O2D-CGD-CBD	3.53	118.48	111.34
24	AB	614	CLA	C4B-NB-C1B	3.53	110.52	107.12
24	AC	509	CLA	C2A-C1A-CHA	3.53	130.30	123.87
30	BB	5601	SQD	C11-C10-C9	3.53	133.29	114.56
24	BB	5607	CLA	C2C-C1C-NC	-3.53	107.38	110.22
24	BC	5508	CLA	O2A-CGA-CBA	3.52	122.69	111.90
24	BC	5509	CLA	C4D-C3D-CAD	3.52	112.38	108.05
24	BC	5512	CLA	C2A-C1A-CHA	3.52	130.29	123.87
30	BF	5102	SQD	C19-C18-C17	3.52	123.01	112.94
24	AA	404	CLA	C1C-NC-C4C	3.52	111.01	106.26
27	AK	102	BCR	C29-C30-C25	3.52	115.99	110.37
24	BA	5408	CLA	O2A-CGA-CBA	3.52	122.67	111.90
32	AI	103	LMT	O1'-C1-C2	-3.52	96.26	109.79
34	AD	403	PHO	O2A-CGA-CBA	3.52	122.66	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5407	CLA	O2D-CGD-CBD	3.52	118.45	111.34
31	AI	101	LMG	C7-O1-C1	-3.52	106.74	113.80
24	BB	5605	CLA	C4B-NB-C1B	3.52	110.51	107.12
24	AC	502	CLA	O2A-CGA-CBA	3.51	122.66	111.90
24	BB	5615	CLA	CBA-CAA-C2A	3.52	122.54	113.95
27	AX	101	BCR	C30-C25-C26	-3.51	117.50	122.59
27	AB	617	BCR	C23-C24-C25	3.51	137.59	127.23
24	BB	5619	CLA	C4D-C3D-CAD	3.51	112.37	108.05
24	AC	503	CLA	C4D-C3D-CAD	3.51	112.37	108.05
27	AC	515	BCR	C2-C1-C6	3.51	115.97	110.37
31	AJ	102	LMG	C12-C11-C10	3.50	127.11	113.51
24	AB	603	CLA	C4A-NA-C1A	3.50	111.32	106.38
24	AB	606	CLA	C4D-C3D-CAD	3.50	112.36	108.05
24	AC	512	CLA	O2A-CGA-CBA	3.50	122.61	111.90
24	AC	504	CLA	C1C-NC-C4C	3.50	110.98	106.26
24	AB	607	CLA	CHD-C4C-NC	3.50	126.73	124.28
24	AC	510	CLA	O2A-CGA-CBA	3.50	122.61	111.90
24	BC	5501	CLA	C4D-C3D-CAD	3.49	112.34	108.05
24	BC	5502	CLA	O2A-CGA-CBA	3.49	122.58	111.90
34	AD	403	PHO	C3D-C4D-ND	3.48	111.20	106.81
24	AC	513	CLA	C4A-NA-C1A	3.48	111.29	106.38
30	BA	5414	SQD	O48-C23-C24	3.48	122.54	111.90
28	AE	101	DGD	C2G-O2G-C1B	3.47	126.02	117.86
27	AC	516	BCR	C1-C6-C5	-3.47	117.56	122.59
24	AC	512	CLA	C2A-C1A-CHA	3.47	130.20	123.87
24	BA	5408	CLA	O2D-CGD-CBD	3.47	118.36	111.34
32	BB	5603	LMT	C1B-O1B-C4'	-3.47	109.18	118.00
27	BT	5101	BCR	C30-C25-C26	-3.47	117.56	122.59
30	AB	627	SQD	C11-C10-C9	3.47	132.99	114.56
24	AA	407	CLA	O2A-CGA-CBA	3.47	122.52	111.90
34	BD	5404	PHO	O2A-CGA-CBA	3.47	122.52	111.90
24	AC	511	CLA	O2D-CGD-CBD	3.47	118.34	111.34
27	BK	5102	BCR	C29-C30-C25	3.47	115.90	110.37
31	BI	5101	LMG	C7-O1-C1	-3.47	106.84	113.80
24	BD	5405	CLA	O2D-CGD-CBD	3.47	118.34	111.34
27	BK	5102	BCR	C8-C9-C10	-3.46	113.64	118.98
27	BC	5516	BCR	C2-C1-C6	3.46	115.89	110.37
24	AB	605	CLA	C4D-C3D-CAD	3.46	112.31	108.05
30	AA	413	SQD	O48-C23-C24	3.46	122.49	111.90
24	BB	5616	CLA	C4D-C3D-CAD	3.46	112.30	108.05
27	AK	102	BCR	C1-C6-C5	-3.46	117.58	122.59
24	BC	5510	CLA	CHD-C4C-NC	3.46	126.70	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	503	CLA	CHD-C4C-NC	3.45	126.70	124.28
27	BA	5411	BCR	C29-C30-C25	3.45	115.88	110.37
32	AB	629	LMT	C1B-O1B-C4'	-3.45	109.23	118.00
27	AT	101	BCR	C30-C25-C26	-3.45	117.59	122.59
31	AC	520	LMG	C9-O8-C28	3.45	126.84	116.99
24	AC	508	CLA	C4D-C3D-CAD	3.45	112.29	108.05
24	AB	605	CLA	O2A-CGA-CBA	3.45	122.45	111.90
27	AB	619	BCR	C38-C26-C27	-3.45	106.86	113.39
27	BC	5515	BCR	C2-C1-C6	3.45	115.86	110.37
24	AB	603	CLA	CBD-CHA-C1A	3.45	133.27	128.77
24	BB	5607	CLA	C4A-NA-C1A	3.45	111.24	106.38
35	AD	405	PL9	C26-C27-C28	3.44	121.44	111.64
27	BX	5101	BCR	C33-C5-C4	-3.44	106.86	113.39
27	BD	5407	BCR	C33-C5-C4	-3.44	106.87	113.39
24	AC	501	CLA	C3A-C2A-C1A	3.44	107.29	101.70
28	BE	5102	DGD	C2G-O2G-C1B	3.44	125.93	117.86
31	BI	5101	LMG	C8-O7-C10	3.44	125.93	117.86
24	AB	611	CLA	CBA-CAA-C2A	3.44	122.35	113.95
24	AB	601	CLA	C4D-C3D-CAD	3.44	112.28	108.05
29	AA	412	LHG	O8-C23-C24	3.44	122.42	111.90
24	BB	5618	CLA	C4B-NB-C1B	3.44	110.43	107.12
24	AB	612	CLA	C4A-NA-C1A	3.43	111.22	106.38
24	AC	504	CLA	O2A-CGA-CBA	3.43	122.41	111.90
24	BC	5509	CLA	C2A-C1A-CHA	3.43	130.13	123.87
27	AA	410	BCR	C33-C5-C4	-3.43	106.89	113.39
24	BB	5611	CLA	C4D-C3D-CAD	3.43	112.27	108.05
24	BA	5405	CLA	O2A-CGA-CBA	3.43	122.40	111.90
24	BC	5509	CLA	O2A-CGA-CBA	3.43	122.40	111.90
24	AC	504	CLA	O2D-CGD-CBD	3.43	118.27	111.34
24	AC	501	CLA	C4D-C3D-CAD	3.43	112.27	108.05
28	AB	628	DGD	O3G-C3G-C2G	3.43	119.14	110.99
24	AC	511	CLA	C4D-C3D-CAD	3.43	112.27	108.05
27	BK	5102	BCR	C1-C6-C5	-3.42	117.63	122.59
28	BC	5518	DGD	O6E-C1E-O5D	3.43	118.08	109.93
24	AA	404	CLA	O2A-CGA-CBA	3.42	122.38	111.90
24	AA	406	CLA	C4A-NA-C1A	3.42	111.21	106.38
24	BB	5618	CLA	CAA-CBA-CGA	-3.42	103.15	113.24
24	BC	5511	CLA	O2A-CGA-CBA	3.42	122.37	111.90
24	AC	511	CLA	C4B-NB-C1B	3.42	110.41	107.12
24	BC	5504	CLA	C1C-NC-C4C	3.42	110.87	106.26
24	BB	5605	CLA	C4D-C3D-CAD	3.42	112.25	108.05
24	BC	5502	CLA	CHD-C4C-NC	3.41	126.67	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	618	BCR	C29-C30-C25	3.41	115.81	110.37
31	BC	5520	LMG	C9-O8-C28	3.41	126.74	116.99
24	AD	404	CLA	C4D-C3D-CAD	3.41	112.25	108.05
27	BK	5102	BCR	C23-C24-C25	3.41	137.30	127.23
24	AB	614	CLA	C4D-C3D-CAD	3.41	112.24	108.05
24	AA	406	CLA	C1C-NC-C4C	3.41	110.86	106.26
31	BD	5408	LMG	C12-C11-C10	3.41	126.75	113.51
27	AD	406	BCR	C23-C24-C25	3.41	137.29	127.23
31	AD	407	LMG	C22-C23-C24	-3.41	100.02	113.73
27	AC	515	BCR	C29-C30-C25	3.40	115.80	110.37
27	AK	102	BCR	C23-C24-C25	3.40	137.28	127.23
24	BB	5607	CLA	C2A-C1A-NA	-3.40	106.98	111.33
24	BB	5608	CLA	C4D-C3D-CAD	3.40	112.23	108.05
24	AB	607	CLA	C1C-NC-C4C	3.40	110.85	106.26
27	BB	5623	BCR	C29-C30-C25	3.40	115.79	110.37
27	BB	5622	BCR	C2-C1-C6	3.40	115.79	110.37
24	BB	5612	CLA	C3A-C2A-C1A	3.40	107.22	101.70
24	BC	5508	CLA	C4D-C3D-CAD	3.39	112.22	108.05
24	AC	501	CLA	O2A-CGA-CBA	3.39	122.28	111.90
27	AX	101	BCR	C33-C5-C4	-3.39	106.97	113.39
24	AB	607	CLA	CAA-C2A-C3A	-3.39	104.84	113.32
27	AK	102	BCR	C30-C25-C26	-3.39	117.68	122.59
24	BB	5618	CLA	C4D-C3D-CAD	3.39	112.22	108.05
27	BX	5101	BCR	C24-C23-C22	3.39	131.28	126.22
28	BA	5412	DGD	C3A-C2A-C1A	-3.38	100.38	113.51
24	AB	615	CLA	CBD-CHA-C1A	3.38	133.19	128.77
24	AB	601	CLA	C4B-NB-C1B	3.38	110.38	107.12
24	BC	5501	CLA	CBD-CHA-C1A	3.38	133.19	128.77
24	BC	5510	CLA	C4D-C3D-CAD	3.38	112.21	108.05
24	AB	601	CLA	O2A-CGA-CBA	3.38	122.24	111.90
27	BB	5622	BCR	C29-C30-C25	3.38	115.76	110.37
24	BD	5405	CLA	C4D-C3D-CAD	3.38	112.20	108.05
27	BX	5101	BCR	C30-C25-C26	-3.38	117.70	122.59
24	AC	511	CLA	O2A-CGA-CBA	3.38	122.23	111.90
31	BB	5624	LMG	C33-C32-C31	-3.37	96.64	114.56
24	AC	513	CLA	C2C-C1C-NC	-3.37	107.50	110.22
24	AB	606	CLA	C3A-C2A-C1A	3.37	107.18	101.70
24	BA	5405	CLA	C4A-NA-C1A	3.37	111.13	106.38
24	AB	603	CLA	C2C-C1C-NC	-3.37	107.50	110.22
24	BA	5408	CLA	C4D-C3D-CAD	3.37	112.19	108.05
27	AC	514	BCR	C29-C30-C25	3.36	115.73	110.37
27	AB	618	BCR	C30-C25-C26	-3.36	117.72	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	516	BCR	C23-C24-C25	3.36	137.14	127.23
24	AB	614	CLA	CAA-CBA-CGA	-3.36	103.35	113.24
24	BC	5501	CLA	C2A-C1A-CHA	3.35	129.98	123.87
24	AC	512	CLA	C4D-C3D-CAD	3.35	112.17	108.05
27	BB	5621	BCR	C23-C24-C25	3.35	137.12	127.23
24	BC	5510	CLA	O2A-CGA-CBA	3.35	122.16	111.90
24	BB	5609	CLA	O2A-CGA-CBA	3.35	122.16	111.90
24	BC	5502	CLA	C4D-C3D-CAD	3.35	112.17	108.05
24	BC	5507	CLA	C4D-C3D-CAD	3.35	112.17	108.05
24	AA	407	CLA	CBA-CAA-C2A	3.35	122.14	113.95
24	BB	5611	CLA	C1C-NC-C4C	3.35	110.78	106.26
31	BD	5409	LMG	O1-C7-C8	-3.35	103.02	110.99
27	BD	5407	BCR	C23-C24-C25	3.35	137.11	127.23
27	AB	618	BCR	C33-C5-C4	-3.35	107.05	113.39
24	AC	501	CLA	C2A-C1A-CHA	3.35	129.97	123.87
27	AB	618	BCR	C2-C1-C6	3.34	115.70	110.37
28	AA	411	DGD	C3A-C2A-C1A	-3.34	100.54	113.51
28	AC	518	DGD	O6E-C1E-O5D	3.34	117.88	109.93
28	BA	5412	DGD	O1G-C1A-O1A	-3.34	114.75	123.48
27	BB	5623	BCR	C2-C1-C6	3.34	115.69	110.37
24	AB	604	CLA	C4D-C3D-CAD	3.33	112.15	108.05
27	BB	5622	BCR	C30-C25-C26	-3.33	117.77	122.59
24	AB	608	CLA	C3A-C2A-C1A	3.33	107.11	101.70
28	AA	411	DGD	O1G-C1A-O1A	-3.33	114.78	123.48
24	AB	603	CLA	CAA-C2A-C3A	-3.33	104.98	113.32
24	BC	5512	CLA	O2A-CGA-CBA	3.33	122.08	111.90
24	AA	404	CLA	C4A-NA-C1A	3.33	111.07	106.38
27	AT	101	BCR	C24-C23-C22	3.32	131.19	126.22
24	AC	503	CLA	CAA-C2A-C1A	-3.32	103.71	112.51
24	BB	5609	CLA	C4D-C3D-CAD	3.32	112.14	108.05
27	AD	406	BCR	C33-C5-C4	-3.32	107.09	113.39
24	AC	510	CLA	O2D-CGD-CBD	3.32	118.05	111.34
31	AI	101	LMG	C8-O7-C10	3.32	125.65	117.86
24	BB	5607	CLA	C4D-C3D-CAD	3.32	112.13	108.05
28	BC	5519	DGD	C3B-C2B-C1B	3.32	126.39	113.51
24	BB	5614	CLA	O2A-CGA-CBA	3.32	122.05	111.90
27	AK	102	BCR	C8-C9-C10	-3.32	113.87	118.98
31	AC	520	LMG	C8-O7-C10	3.31	125.64	117.86
24	BB	5610	CLA	C1C-NC-C4C	3.31	110.73	106.26
27	AA	410	BCR	C29-C30-C25	3.31	115.65	110.37
24	AC	503	CLA	O2D-CGD-CBD	3.31	118.03	111.34
27	AB	619	BCR	C33-C5-C4	-3.31	107.12	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	C3A-C2A-C1A	3.31	106.17	101.90
31	AD	408	LMG	C12-C11-C10	3.30	126.33	113.51
24	AB	612	CLA	C4D-C3D-CAD	3.30	112.11	108.05
27	AX	101	BCR	C24-C23-C22	3.30	131.15	126.22
24	BB	5610	CLA	C3A-C2A-C1A	3.30	107.06	101.70
24	BC	5503	CLA	O2D-CGD-CBD	3.30	118.01	111.34
24	AC	505	CLA	O2D-CGD-CBD	3.30	118.01	111.34
27	BC	5516	BCR	C23-C24-C25	3.30	136.96	127.23
24	AC	509	CLA	C4B-NB-C1B	3.29	110.29	107.12
28	AB	628	DGD	O6D-C5D-C6D	3.29	113.22	106.62
24	AC	501	CLA	CAA-CBA-CGA	-3.29	103.53	113.24
27	AC	516	BCR	C30-C25-C26	-3.29	117.82	122.59
24	BB	5605	CLA	O2A-CGA-CBA	3.29	121.98	111.90
31	AB	621	LMG	C33-C32-C31	-3.29	97.09	114.56
27	AC	516	BCR	C8-C7-C6	3.29	136.94	127.23
27	BT	5101	BCR	C16-C17-C18	3.29	132.04	127.29
31	BB	5624	LMG	C39-C38-C37	3.29	132.03	114.56
27	AD	406	BCR	C2-C1-C6	3.28	115.61	110.37
24	BC	5503	CLA	CAA-C2A-C1A	-3.28	103.82	112.51
31	AB	621	LMG	C12-C11-C10	-3.28	100.80	113.51
24	BB	5616	CLA	C4B-NB-C1B	3.28	110.28	107.12
28	BH	5101	DGD	C1D-O6D-C5D	-3.27	107.40	113.73
24	BC	5507	CLA	O2D-CGD-CBD	3.28	117.96	111.34
24	BC	5501	CLA	C3A-C2A-C1A	3.27	107.02	101.70
24	AD	404	CLA	CHD-C4C-NC	3.27	126.57	124.28
24	AA	406	CLA	C4D-C3D-CAD	3.27	112.07	108.05
24	BC	5506	CLA	C4D-C3D-CAD	3.27	112.07	108.05
28	BC	5517	DGD	C6B-C5B-C4B	-3.27	97.20	114.56
24	BC	5513	CLA	C2C-C1C-NC	-3.27	107.58	110.22
24	AB	610	CLA	O2A-CGA-CBA	3.27	121.89	111.90
28	AC	517	DGD	C6B-C5B-C4B	-3.27	97.22	114.56
27	BC	5516	BCR	C1-C6-C5	-3.26	117.86	122.59
34	BD	5404	PHO	C3D-C4D-ND	3.26	110.92	106.81
28	BC	5517	DGD	C3B-C2B-C1B	3.26	126.16	113.51
24	AB	605	CLA	CHD-C4C-NC	3.26	126.56	124.28
31	BD	5410	LMG	C12-C11-C10	3.26	126.15	113.51
24	BB	5611	CLA	CAA-CBA-CGA	-3.26	103.64	113.24
24	BC	5511	CLA	C4B-NB-C1B	3.25	110.25	107.12
24	AB	602	CLA	C4D-C3D-CAD	3.25	112.05	108.05
24	BB	5620	CLA	C2A-C1A-CHA	3.25	129.80	123.87
24	BA	5406	CLA	C4B-NB-C1B	3.25	110.25	107.12
31	AA	417	LMG	O1-C7-C8	3.25	118.72	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5607	CLA	CAA-C2A-C3A	-3.25	105.18	113.32
31	AB	620	LMG	C9-O8-C28	3.25	126.27	116.99
27	BK	5102	BCR	C12-C13-C14	-3.25	113.98	118.98
24	BB	5611	CLA	CAA-C2A-C3A	-3.25	105.19	113.32
24	BB	5619	CLA	C4B-NB-C1B	3.25	110.25	107.12
24	BA	5405	CLA	C4B-NB-C1B	3.25	110.24	107.12
27	BB	5622	BCR	C23-C24-C25	3.24	136.80	127.23
27	BC	5514	BCR	C2-C1-C6	3.24	115.54	110.37
24	AB	610	CLA	C4D-C3D-CAD	3.24	112.04	108.05
24	AA	407	CLA	C4D-C3D-CAD	3.24	112.04	108.05
24	AC	507	CLA	C4D-C3D-CAD	3.24	112.03	108.05
27	BC	5514	BCR	C33-C5-C4	-3.24	107.26	113.39
28	BB	5602	DGD	O6D-C5D-C6D	3.24	113.10	106.62
24	AB	616	CLA	C2A-C1A-CHA	3.23	129.76	123.87
31	AB	621	LMG	C39-C38-C37	3.23	131.74	114.56
31	BD	5408	LMG	O7-C10-C11	-3.23	104.65	111.54
34	BD	5404	PHO	O2D-CGD-CBD	3.23	117.87	111.34
24	BC	5503	CLA	CHD-C4C-NC	3.23	126.54	124.28
24	BC	5510	CLA	O2D-CGD-CBD	3.23	117.86	111.34
24	AC	504	CLA	CHD-C4C-NC	3.23	126.54	124.28
28	BB	5602	DGD	O3G-C3G-C2G	3.23	118.66	110.99
30	BB	5625	SQD	C45-O47-C7	3.22	125.43	117.86
27	AC	515	BCR	C30-C25-C26	-3.22	117.92	122.59
31	BB	5624	LMG	C12-C11-C10	-3.22	101.01	113.51
27	BT	5101	BCR	C24-C23-C22	3.22	131.03	126.22
24	BC	5510	CLA	C4B-NB-C1B	3.22	110.22	107.12
31	BL	5101	LMG	C9-O8-C28	3.22	126.17	116.99
31	AC	521	LMG	O8-C9-C8	-3.21	100.35	108.80
24	BA	5406	CLA	C3D-CAD-CBD	-3.21	103.05	107.60
31	BC	5520	LMG	C8-O7-C10	3.22	125.41	117.86
30	AA	416	SQD	C32-C31-C30	3.21	131.63	114.56
24	BB	5612	CLA	C4D-C3D-CAD	3.21	112.00	108.05
24	AC	505	CLA	C3A-C2A-C1A	3.21	106.92	101.70
24	AB	606	CLA	C1C-NC-C4C	3.21	110.59	106.26
27	AK	102	BCR	C24-C23-C22	3.21	131.02	126.22
27	BC	5515	BCR	C1-C6-C5	-3.21	117.94	122.59
24	AB	607	CLA	C4D-C3D-CAD	3.21	112.00	108.05
27	BK	5102	BCR	C24-C23-C22	3.21	131.02	126.22
24	AC	504	CLA	C4D-C3D-CAD	3.21	112.00	108.05
27	BB	5623	BCR	C33-C5-C4	-3.21	107.31	113.39
24	BC	5504	CLA	O2A-CGA-CBA	3.21	121.72	111.90
31	AI	101	LMG	C12-C11-C10	-3.21	101.06	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5501	CLA	CAA-CBA-CGA	-3.21	103.79	113.24
24	AD	404	CLA	C4B-NB-C1B	3.20	110.20	107.12
27	AT	101	BCR	C7-C8-C9	3.20	131.01	126.22
24	BC	5513	CLA	C4D-C3D-CAD	3.20	111.99	108.05
31	BI	5101	LMG	C12-C11-C10	-3.20	101.09	113.51
27	AD	406	BCR	C8-C7-C6	3.20	136.68	127.23
24	BB	5611	CLA	CHD-C4C-NC	3.20	126.52	124.28
24	AC	506	CLA	C4D-C3D-CAD	3.20	111.98	108.05
28	BH	5101	DGD	C4B-C3B-C2B	3.20	125.12	113.28
34	BD	5403	PHO	O2D-CGD-CBD	3.20	117.80	111.34
24	AB	601	CLA	O2D-CGD-CBD	3.20	117.80	111.34
34	AD	402	PHO	O2D-CGD-CBD	3.19	117.79	111.34
24	AC	512	CLA	C4B-NB-C1B	3.20	110.20	107.12
27	BC	5514	BCR	C29-C30-C25	3.20	115.47	110.37
24	BA	5405	CLA	C1C-NC-C4C	3.19	110.56	106.26
24	BB	5611	CLA	C3A-C2A-C1A	3.19	106.89	101.70
24	AD	401	CLA	C4B-NB-C1B	3.19	110.19	107.12
24	BB	5609	CLA	C3A-C2A-C1A	3.19	106.88	101.70
27	BD	5407	BCR	C8-C7-C6	3.19	136.64	127.23
24	BC	5507	CLA	C4B-NB-C1B	3.19	110.19	107.12
24	BB	5612	CLA	C4D-C3D-C2D	-3.19	103.30	107.17
24	BC	5505	CLA	C4D-C3D-C2D	-3.19	103.30	107.17
27	AB	618	BCR	C24-C23-C22	3.19	130.98	126.22
31	AD	407	LMG	O1-C7-C8	-3.19	103.41	110.99
31	AD	408	LMG	C17-C16-C15	-3.18	97.65	114.56
29	BA	5413	LHG	O8-C23-C24	3.18	121.64	111.90
27	BB	5621	BCR	C30-C25-C26	-3.18	117.98	122.59
24	BC	5504	CLA	C4D-C3D-CAD	3.18	111.96	108.05
28	AC	517	DGD	C3G-O3G-C1D	-3.18	107.41	113.80
24	BB	5612	CLA	O2A-CGA-CBA	3.18	121.63	111.90
27	BC	5516	BCR	C8-C7-C6	3.18	136.61	127.23
30	BA	5401	SQD	C32-C31-C30	3.18	131.44	114.56
24	AB	612	CLA	C4B-NB-C1B	3.18	110.18	107.12
24	AC	507	CLA	O2D-CGD-CBD	3.17	117.75	111.34
24	AB	606	CLA	C2A-C1A-CHA	3.17	129.66	123.87
24	BA	5405	CLA	C4D-C3D-CAD	3.17	111.95	108.05
24	BC	5502	CLA	C1C-NC-C4C	3.17	110.54	106.26
36	AF	101	HEM	CAD-CBD-CGD	3.17	119.50	113.53
24	BB	5610	CLA	C2A-C1A-CHA	3.17	129.65	123.87
24	AC	510	CLA	C4D-C3D-CAD	3.17	111.95	108.05
27	BX	5101	BCR	C23-C24-C25	3.17	136.58	127.23
36	AF	101	HEM	C3A-C4A-NA	3.17	111.61	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5614	CLA	O2D-CGD-CBD	3.17	117.74	111.34
24	BC	5505	CLA	C3A-C2A-C1A	3.17	106.85	101.70
24	AC	513	CLA	C4D-C3D-CAD	3.16	111.94	108.05
24	BB	5607	CLA	C4B-NB-C1B	3.16	110.17	107.12
27	AX	101	BCR	C23-C24-C25	3.16	136.56	127.23
27	BK	5102	BCR	C30-C25-C26	-3.16	118.01	122.59
24	AB	613	CLA	C4B-NB-C1B	3.16	110.16	107.12
27	AC	515	BCR	C1-C6-C5	-3.16	118.01	122.59
24	BC	5512	CLA	C4B-NB-C1B	3.16	110.16	107.12
24	BB	5620	CLA	O2D-CGD-CBD	3.16	117.72	111.34
24	AB	609	CLA	C4B-NB-C1B	3.16	110.16	107.12
24	AC	505	CLA	O2A-CGA-CBA	3.16	121.56	111.90
31	BC	5521	LMG	O8-C9-C8	-3.16	100.50	108.80
24	BB	5616	CLA	O2A-CGA-CBA	3.15	121.55	111.90
27	BD	5407	BCR	C2-C1-C6	3.15	115.40	110.37
24	AB	615	CLA	CHD-C4C-NC	3.15	126.48	124.28
24	BC	5509	CLA	C4B-NB-C1B	3.15	110.15	107.12
24	AC	505	CLA	C4D-C3D-C2D	-3.15	103.34	107.17
27	AC	514	BCR	C1-C6-C5	-3.15	118.03	122.59
24	BC	5502	CLA	C4B-NB-C1B	3.15	110.15	107.12
24	AB	608	CLA	O2A-CGA-CBA	3.15	121.53	111.90
24	BC	5501	CLA	C4B-NB-C1B	3.14	110.15	107.12
24	AA	404	CLA	C4B-NB-C1B	3.14	110.15	107.12
24	BB	5613	CLA	C4D-C3D-CAD	3.14	111.92	108.05
24	AB	603	CLA	C6-C5-C3	3.14	119.79	112.62
27	BD	5407	BCR	C7-C8-C9	3.14	130.91	126.22
28	BH	5101	DGD	C3G-C2G-C1G	-3.14	104.65	111.86
24	BC	5508	CLA	O2D-CGD-CBD	3.14	117.68	111.34
24	BD	5405	CLA	C4B-NB-C1B	3.14	110.14	107.12
36	BF	5101	HEM	O1D-CGD-CBD	-3.14	112.44	123.06
27	BX	5101	BCR	C1-C6-C5	-3.14	118.04	122.59
28	AH	101	DGD	C1D-O6D-C5D	-3.14	107.66	113.73
24	BC	5501	CLA	C2A-C1A-NA	-3.13	107.33	111.33
30	AB	627	SQD	C44-O6-C1	3.13	120.08	113.80
24	BD	5402	CLA	C4B-NB-C1B	3.13	110.13	107.12
24	AC	511	CLA	C6-C7-C8	-3.13	105.70	115.44
35	AD	405	PL9	C30-C29-C31	3.13	120.14	115.39
27	BB	5622	BCR	C33-C5-C4	-3.13	107.46	113.39
27	BB	5622	BCR	C8-C7-C6	3.13	136.47	127.23
24	AD	401	CLA	CHD-C4C-NC	3.13	126.47	124.28
31	AC	520	LMG	C14-C13-C12	-3.13	97.94	114.56
24	BC	5504	CLA	CHD-C4C-NC	3.13	126.47	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	607	CLA	C3A-C2A-C1A	3.13	106.78	101.70
24	AB	603	CLA	C4B-NB-C1B	3.13	110.13	107.12
30	BB	5601	SQD	C44-O6-C1	3.13	120.08	113.80
24	BB	5606	CLA	CHD-C4C-NC	3.12	126.47	124.28
24	AC	510	CLA	C4B-NB-C1B	3.12	110.13	107.12
31	BA	5402	LMG	O1-C7-C8	3.12	118.41	110.99
24	BB	5608	CLA	CAA-C2A-C1A	-3.12	104.24	112.51
27	BC	5516	BCR	C30-C25-C26	-3.12	118.07	122.59
34	AD	403	PHO	O2D-CGD-CBD	3.12	117.65	111.34
31	BD	5410	LMG	C17-C16-C15	-3.12	97.98	114.56
28	AH	101	DGD	C4B-C3B-C2B	3.12	124.84	113.28
24	AD	404	CLA	O2A-CGA-CBA	3.12	121.45	111.90
24	BB	5609	CLA	C1C-NC-C4C	3.12	110.47	106.26
24	BC	5512	CLA	CBD-CHA-C1A	3.12	132.84	128.77
24	BB	5610	CLA	C3D-CAD-CBD	-3.12	103.19	107.60
35	BD	5406	PL9	C50-C49-C48	-3.12	112.51	122.62
24	AA	405	CLA	CAA-CBA-CGA	-3.11	104.07	113.24
24	AB	603	CLA	C2A-C1A-NA	-3.11	107.35	111.33
24	AB	610	CLA	O2D-CGD-CBD	3.11	117.63	111.34
24	BB	5613	CLA	C4B-NB-C1B	3.11	110.11	107.12
27	AB	617	BCR	C30-C25-C26	-3.11	118.08	122.59
24	BB	5620	CLA	C4D-C3D-CAD	3.11	111.87	108.05
27	BC	5515	BCR	C30-C25-C26	-3.11	118.09	122.59
27	AD	406	BCR	C16-C17-C18	3.11	131.78	127.29
27	BB	5622	BCR	C24-C23-C22	3.11	130.87	126.22
24	AC	510	CLA	CHD-C4C-NC	3.11	126.45	124.28
27	BX	5101	BCR	C12-C13-C14	-3.11	114.20	118.98
28	BC	5517	DGD	C3G-O3G-C1D	-3.10	107.57	113.80
24	AA	407	CLA	C4B-NB-C1B	3.10	110.11	107.12
24	BB	5613	CLA	CHD-C4C-NC	3.10	126.45	124.28
24	BB	5606	CLA	C4D-C3D-CAD	3.10	111.86	108.05
24	AB	616	CLA	C4D-C3D-CAD	3.10	111.86	108.05
24	AB	613	CLA	C1C-NC-C4C	3.10	110.44	106.26
28	AC	519	DGD	C1D-C2D-C3D	-3.10	103.98	109.99
24	BB	5605	CLA	O2D-CGD-CBD	3.10	117.60	111.34
24	BB	5612	CLA	C1C-NC-C4C	3.10	110.44	106.26
24	AB	612	CLA	C3A-C2A-C1A	3.09	106.73	101.70
24	BD	5402	CLA	O2D-CGD-CBD	3.09	117.59	111.34
24	AC	502	CLA	CHD-C4C-NC	3.09	126.44	124.28
35	BD	5406	PL9	C30-C29-C31	3.09	120.09	115.39
24	AB	604	CLA	CAA-C2A-C1A	-3.09	104.31	112.51
27	AB	618	BCR	C23-C24-C25	3.09	136.35	127.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5612	CLA	O2D-CGD-CBD	3.09	117.58	111.34
24	BC	5505	CLA	O2A-CGA-CBA	3.09	121.36	111.90
24	BC	5511	CLA	O2D-CGD-CBD	3.09	117.58	111.34
28	AC	518	DGD	O2G-C2G-C3G	3.09	119.92	108.50
24	AA	407	CLA	C1C-NC-C4C	3.08	110.42	106.26
28	AC	519	DGD	C3B-C2B-C1B	3.08	125.48	113.51
32	BC	5522	LMT	O1'-C1'-C2'	-3.08	104.20	108.15
24	BB	5610	CLA	C2A-C1A-NA	-3.08	107.39	111.33
27	AC	514	BCR	C2-C1-C6	3.08	115.28	110.37
24	AC	502	CLA	C4D-C3D-CAD	3.08	111.83	108.05
24	AB	612	CLA	C2C-C1C-NC	-3.08	107.74	110.22
28	AC	517	DGD	C3B-C2B-C1B	3.07	125.45	113.51
28	BC	5518	DGD	O2G-C2G-C3G	3.08	119.88	108.50
24	BB	5611	CLA	C4B-NB-C1B	3.07	110.08	107.12
24	AB	613	CLA	C4D-C3D-CAD	3.07	111.83	108.05
31	BC	5520	LMG	C14-C13-C12	-3.07	98.27	114.56
24	BB	5606	CLA	C4B-NB-C1B	3.07	110.07	107.12
31	AC	520	LMG	C9-C8-C7	-3.07	104.82	111.86
24	BB	5608	CLA	CBA-CAA-C2A	3.06	121.44	113.95
24	AC	503	CLA	C4B-NB-C1B	3.06	110.07	107.12
27	AK	102	BCR	C12-C13-C14	-3.06	114.26	118.98
31	BC	5520	LMG	O8-C9-C8	3.06	116.85	108.80
27	AB	618	BCR	C8-C7-C6	3.06	136.26	127.23
27	BC	5515	BCR	C35-C13-C12	3.06	123.03	118.09
36	BF	5101	HEM	CAD-CBD-CGD	3.06	119.30	113.53
31	AC	521	LMG	C37-C38-C39	3.06	126.05	113.73
24	BB	5619	CLA	C1C-NC-C4C	3.06	110.38	106.26
31	BD	5408	LMG	O7-C8-C9	-3.06	97.20	108.50
27	BC	5515	BCR	C12-C13-C14	-3.05	114.28	118.98
24	AB	605	CLA	C1C-NC-C4C	3.05	110.38	106.26
31	BC	5521	LMG	C37-C38-C39	3.05	126.02	113.73
27	AX	101	BCR	C12-C13-C14	-3.05	114.28	118.98
24	BC	5511	CLA	C6-C7-C8	-3.05	105.95	115.44
24	BB	5614	CLA	C4D-C3D-CAD	3.05	111.80	108.05
24	AB	616	CLA	C4B-NB-C1B	3.05	110.06	107.12
35	AD	405	PL9	C51-C49-C50	3.05	122.30	114.62
31	BD	5408	LMG	C15-C14-C13	-3.05	98.37	114.56
24	BB	5617	CLA	C4B-NB-C1B	3.05	110.05	107.12
24	AA	406	CLA	O2A-CGA-O1A	-3.05	115.52	123.48
31	BM	5102	LMG	O7-C8-C7	3.05	119.78	108.50
35	AD	405	PL9	C50-C49-C48	-3.05	112.74	122.62
24	AD	404	CLA	C1C-NC-C4C	3.05	110.37	106.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	614	CLA	C1D-CHD-C4C	3.05	127.32	122.60
24	AB	608	CLA	C4D-C3D-CAD	3.04	111.79	108.05
31	AJ	102	LMG	C15-C14-C13	-3.04	98.41	114.56
31	AM	101	LMG	C12-C11-C10	-3.04	101.71	113.51
24	BA	5406	CLA	CAA-CBA-CGA	-3.04	104.28	113.24
24	AB	615	CLA	C4B-NB-C1B	3.04	110.05	107.12
24	BB	5615	CLA	C4D-C3D-CAD	3.04	111.79	108.05
34	BD	5404	PHO	CBD-CHA-C1A	3.04	131.94	126.67
24	BB	5608	CLA	C4B-NB-C1B	3.04	110.04	107.12
24	BC	5508	CLA	C3A-C2A-C1A	3.03	106.63	101.70
28	AA	411	DGD	O2G-C2G-C3G	3.03	119.72	108.50
24	AB	608	CLA	O2D-CGD-CBD	3.03	117.47	111.34
24	AA	405	CLA	C3D-CAD-CBD	-3.03	103.31	107.60
24	AB	606	CLA	C2A-C1A-NA	-3.03	107.46	111.33
24	AB	613	CLA	CHD-C4C-NC	3.03	126.40	124.28
32	AI	103	LMT	O1'-C1'-C2'	-3.03	104.27	108.15
28	AH	101	DGD	C3G-C2G-C1G	-3.03	104.91	111.86
24	AB	616	CLA	O2D-CGD-CBD	3.03	117.46	111.34
24	AB	607	CLA	C2A-C1A-CHA	3.03	129.39	123.87
24	AB	608	CLA	C4D-C3D-C2D	-3.03	103.49	107.17
31	AC	520	LMG	O8-C9-C8	3.03	116.76	108.80
28	BC	5519	DGD	CBA-CAA-C9A	-3.03	98.49	114.56
24	AD	401	CLA	C4D-C3D-CAD	3.02	111.77	108.05
24	AC	503	CLA	C7-C6-C5	-3.02	104.15	112.97
24	BB	5616	CLA	C3A-C2A-C1A	3.02	106.61	101.70
24	BB	5607	CLA	C6-C5-C3	3.02	119.52	112.62
27	AT	101	BCR	C16-C17-C18	3.02	131.66	127.29
24	AB	608	CLA	C11-C12-C13	3.02	124.84	115.44
27	AB	617	BCR	C2-C1-C6	3.02	115.19	110.37
31	BC	5520	LMG	C9-C8-C7	-3.02	104.93	111.86
27	AB	619	BCR	C2-C1-C6	3.02	115.18	110.37
24	AC	505	CLA	CBD-CHA-C1A	3.01	132.71	128.77
31	AJ	102	LMG	O7-C8-C9	-3.01	97.37	108.50
28	AB	628	DGD	C3B-C2B-C1B	3.01	125.19	113.51
24	BD	5405	CLA	C1C-NC-C4C	3.01	110.32	106.26
28	BA	5412	DGD	O2G-C2G-C3G	3.01	119.64	108.50
24	BB	5608	CLA	C1C-NC-C4C	3.01	110.32	106.26
24	BB	5615	CLA	C3A-C2A-C1A	3.01	106.58	101.70
24	AB	605	CLA	C3A-C2A-C1A	3.01	106.59	101.70
28	BB	5602	DGD	C3B-C2B-C1B	3.01	125.18	113.51
36	AF	101	HEM	O1D-CGD-CBD	-3.00	112.90	123.06
24	AC	501	CLA	CHD-C4C-NC	3.00	126.38	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AA	410	BCR	C30-C25-C26	-3.00	118.24	122.59
27	BB	5621	BCR	C2-C1-C6	3.00	115.15	110.37
31	AM	101	LMG	O7-C8-C7	3.00	119.61	108.50
24	AC	507	CLA	C4B-NB-C1B	3.00	110.01	107.12
24	BC	5508	CLA	C2C-C1C-NC	-3.00	107.80	110.22
24	BB	5606	CLA	O2D-CGD-CBD	3.00	117.39	111.34
24	AA	406	CLA	CHD-C4C-NC	3.00	126.38	124.28
24	AB	607	CLA	CAA-CBA-CGA	-3.00	104.41	113.24
24	AC	503	CLA	CBA-CAA-C2A	2.99	121.27	113.95
24	AB	615	CLA	O2D-CGD-CBD	2.99	117.39	111.34
31	BE	5101	LMG	O7-C10-C11	2.99	117.92	111.54
27	AC	515	BCR	C16-C17-C18	2.99	131.62	127.29
31	AD	407	LMG	C12-C11-C10	2.99	125.13	113.51
30	BA	5414	SQD	C32-C31-C30	2.99	130.46	114.56
27	BD	5407	BCR	C16-C17-C18	2.99	131.61	127.29
24	BB	5612	CLA	C11-C12-C13	2.99	124.74	115.44
27	AD	406	BCR	C12-C13-C14	-2.99	114.38	118.98
24	AB	606	CLA	C3D-CAD-CBD	-2.98	103.38	107.60
27	AC	515	BCR	C12-C13-C14	-2.99	114.38	118.98
31	AJ	102	LMG	O7-C10-C11	-2.98	105.19	111.54
24	BC	5505	CLA	CBD-CHA-C1A	2.98	132.66	128.77
24	AC	504	CLA	CAA-CBA-CGA	-2.98	104.47	113.24
24	BC	5501	CLA	CHD-C4C-NC	2.98	126.36	124.28
24	AC	501	CLA	C2A-C1A-NA	-2.97	107.53	111.33
32	BC	5522	LMT	C4-C3-C2	-2.97	98.77	114.56
24	BA	5407	CLA	O2A-CGA-O1A	-2.98	115.70	123.48
24	BA	5408	CLA	C3A-C2A-C1A	2.97	106.53	101.70
24	AC	501	CLA	C4B-NB-C1B	2.97	109.98	107.12
31	BA	5402	LMG	C12-C11-C10	2.97	125.05	113.51
27	AA	410	BCR	C2-C1-C6	2.97	115.11	110.37
27	BC	5514	BCR	C1-C6-C5	-2.97	118.29	122.59
24	AA	404	CLA	C4D-C3D-CAD	2.97	111.70	108.05
24	AB	608	CLA	C1C-NC-C4C	2.97	110.27	106.26
31	BD	5409	LMG	C12-C11-C10	2.97	125.03	113.51
24	AB	611	CLA	O2D-CGD-CBD	2.97	117.33	111.34
24	BB	5617	CLA	C4D-C3D-CAD	2.97	111.70	108.05
31	AD	407	LMG	C16-C15-C14	2.97	130.31	114.56
24	BB	5613	CLA	C1C-NC-C4C	2.97	110.26	106.26
24	BB	5619	CLA	O2A-CGA-CBA	2.96	120.97	111.90
24	BC	5503	CLA	CBA-CAA-C2A	2.96	121.20	113.95
24	BC	5504	CLA	CAA-CBA-CGA	-2.96	104.50	113.24
24	AB	609	CLA	CHD-C4C-NC	2.96	126.35	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5406	CLA	O2A-CGA-O1A	-2.97	115.73	123.48
28	AH	101	DGD	C3G-O3G-C1D	2.96	119.75	113.80
24	AB	611	CLA	C6-C5-C3	2.96	119.38	112.62
24	AC	502	CLA	C1C-NC-C4C	2.96	110.26	106.26
24	AB	604	CLA	C4B-NB-C1B	2.96	109.97	107.12
24	BC	5503	CLA	C4B-NB-C1B	2.96	109.97	107.12
35	BD	5406	PL9	C51-C49-C50	2.96	122.08	114.62
24	AC	508	CLA	O2D-CGD-CBD	2.96	117.32	111.34
24	BB	5611	CLA	C2A-C1A-CHA	2.96	129.27	123.87
24	AC	507	CLA	C2A-C1A-CHA	2.96	129.26	123.87
32	AI	103	LMT	C4-C3-C2	-2.96	98.87	114.56
24	BB	5620	CLA	C4B-NB-C1B	2.96	109.97	107.12
24	BB	5615	CLA	C1C-NC-C4C	2.96	110.25	106.26
30	AB	622	SQD	C3-C4-C5	-2.95	104.87	110.17
27	BX	5101	BCR	C8-C7-C6	2.95	135.95	127.23
24	BB	5609	CLA	CED-O2D-CGD	2.95	123.03	116.00
27	BA	5411	BCR	C30-C25-C26	-2.95	118.32	122.59
24	AB	604	CLA	C1C-NC-C4C	2.95	110.24	106.26
27	AX	101	BCR	C8-C7-C6	2.95	135.93	127.23
24	BA	5407	CLA	CHD-C4C-NC	2.95	126.34	124.28
24	BA	5408	CLA	C1C-NC-C4C	2.95	110.24	106.26
28	AC	519	DGD	O6E-C1E-C2E	2.95	116.33	110.30
31	AA	414	LMG	O7-C10-C11	2.95	117.82	111.54
24	BB	5618	CLA	C1D-CHD-C4C	2.95	127.17	122.60
28	BH	5101	DGD	C3G-O3G-C1D	2.94	119.71	113.80
28	BA	5412	DGD	C4A-C3A-C2A	2.94	124.19	113.28
24	AB	611	CLA	C1C-NC-C4C	2.94	110.23	106.26
24	AB	602	CLA	CHD-C4C-NC	2.94	126.34	124.28
24	AB	615	CLA	O2A-CGA-CBA	2.94	120.90	111.90
28	BC	5517	DGD	O6D-C1D-O3G	2.94	116.92	109.93
24	AB	609	CLA	C4D-C3D-CAD	2.94	111.66	108.05
30	BB	5625	SQD	C15-C16-C17	2.94	125.55	113.73
24	AC	508	CLA	C3A-C2A-C1A	2.93	106.47	101.70
24	BC	5513	CLA	O2D-CGD-CBD	2.93	117.27	111.34
32	BB	5603	LMT	C9-C8-C7	-2.93	98.99	114.56
24	AB	612	CLA	O2A-CGA-CBA	2.93	120.87	111.90
27	BB	5623	BCR	C30-C25-C26	-2.93	118.35	122.59
31	BD	5409	LMG	C16-C15-C14	2.93	130.13	114.56
28	AC	519	DGD	CBA-CAA-C9A	-2.93	99.00	114.56
24	BC	5503	CLA	C3D-CAD-CBD	-2.93	103.46	107.60
24	AB	610	CLA	C1C-NC-C4C	2.93	110.21	106.26
24	AB	604	CLA	CBA-CAA-C2A	2.93	121.11	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5402	CLA	CHD-C4C-NC	2.93	126.33	124.28
24	AB	601	CLA	C2A-C1A-CHA	2.93	129.20	123.87
24	AC	504	CLA	C3A-C2A-C1A	2.92	106.45	101.70
24	BC	5507	CLA	C2A-C1A-CHA	2.92	129.20	123.87
27	AD	406	BCR	C23-C22-C21	-2.92	114.48	118.98
24	BB	5610	CLA	CBD-CHA-C1A	2.92	132.59	128.77
24	BD	5405	CLA	O2A-CGA-CBA	2.92	120.84	111.90
24	AB	608	CLA	C4B-NB-C1B	2.92	109.93	107.12
32	AB	629	LMT	C9-C8-C7	-2.92	99.06	114.56
30	AA	413	SQD	C32-C31-C30	2.92	130.06	114.56
24	AC	503	CLA	C1C-NC-C4C	2.92	110.20	106.26
27	BT	5101	BCR	C7-C8-C9	2.92	130.58	126.22
31	AA	417	LMG	C12-C11-C10	2.92	124.84	113.51
36	BF	5101	HEM	C3A-C4A-NA	2.92	111.45	109.50
24	AC	508	CLA	C1C-NC-C4C	2.92	110.19	106.26
28	AA	411	DGD	C4A-C3A-C2A	2.91	124.07	113.28
24	BC	5504	CLA	C3A-C2A-C1A	2.91	106.44	101.70
27	AB	619	BCR	C30-C25-C26	-2.91	118.37	122.59
24	AB	604	CLA	CHD-C4C-NC	2.91	126.32	124.28
24	AB	612	CLA	CBD-CHA-C1A	2.91	132.58	128.77
24	BD	5402	CLA	C2A-C1A-CHA	2.91	129.18	123.87
30	AB	622	SQD	C15-C16-C17	2.91	125.45	113.73
31	BM	5102	LMG	C12-C11-C10	-2.91	102.21	113.51
27	BC	5514	BCR	C35-C13-C12	2.91	122.80	118.09
24	AB	606	CLA	CBD-CHA-C1A	2.91	132.57	128.77
24	AC	504	CLA	C4D-C3D-C2D	-2.91	103.64	107.17
24	BB	5610	CLA	CBA-CAA-C2A	2.91	121.06	113.95
27	AT	101	BCR	C2-C1-C6	2.91	115.01	110.37
27	AC	514	BCR	C30-C25-C26	-2.91	118.38	122.59
27	AD	406	BCR	C11-C10-C9	2.91	131.49	127.29
27	BD	5407	BCR	C11-C10-C9	2.91	131.49	127.29
27	BC	5514	BCR	C23-C22-C21	-2.91	114.50	118.98
28	AC	517	DGD	O6D-C1D-O3G	2.90	116.84	109.93
27	AK	102	BCR	C8-C7-C6	2.90	135.80	127.23
24	AB	610	CLA	C2A-C1A-CHA	2.90	129.16	123.87
24	AB	607	CLA	C2A-C1A-NA	-2.90	107.62	111.33
32	BB	5604	LMT	C4-C3-C2	-2.90	99.16	114.56
24	BD	5405	CLA	CHD-C4C-NC	2.90	126.31	124.28
24	BB	5615	CLA	C4B-NB-C1B	2.90	109.91	107.12
24	AA	406	CLA	C4B-NB-C1B	2.90	109.91	107.12
24	AB	614	CLA	O2A-CGA-CBA	2.90	120.76	111.90
24	AB	609	CLA	C1C-NC-C4C	2.90	110.17	106.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	O2D-CGD-CBD	2.90	117.19	111.34
34	AD	403	PHO	CBD-CHA-C1A	2.89	131.69	126.67
24	AC	502	CLA	C4B-NB-C1B	2.89	109.91	107.12
27	AT	101	BCR	C1-C6-C5	-2.89	118.40	122.59
24	BB	5613	CLA	CAA-C2A-C1A	-2.89	104.85	112.51
30	BB	5625	SQD	C3-C4-C5	-2.89	104.98	110.17
27	AJ	101	BCR	C8-C7-C6	2.89	135.76	127.23
28	BC	5519	DGD	O6E-C5E-C4E	2.89	115.11	109.73
24	BD	5402	CLA	CBA-CAA-C2A	2.89	121.02	113.95
24	BA	5405	CLA	CBD-CHA-C1A	2.89	132.55	128.77
28	BC	5519	DGD	C8B-C7B-C6B	-2.89	99.21	114.56
28	BE	5102	DGD	O5D-C6D-C5D	2.89	113.97	108.96
30	AB	622	SQD	C45-O47-C7	2.88	124.63	117.86
27	AC	515	BCR	C8-C7-C6	2.89	135.75	127.23
27	BT	5101	BCR	C2-C1-C6	2.89	114.97	110.37
28	BB	5602	DGD	O5D-C1E-C2E	2.89	111.85	108.15
24	BB	5615	CLA	C2C-C1C-NC	-2.89	107.89	110.22
24	AC	504	CLA	C4B-NB-C1B	2.88	109.89	107.12
29	AA	412	LHG	O8-C6-C5	2.88	116.38	108.80
27	BA	5411	BCR	C23-C24-C25	2.88	135.74	127.23
24	AC	506	CLA	C4B-NB-C1B	2.88	109.89	107.12
24	AA	404	CLA	CHD-C4C-NC	2.88	126.30	124.28
24	AC	501	CLA	C1C-NC-C4C	2.88	110.15	106.26
27	AX	101	BCR	C1-C6-C5	-2.88	118.42	122.59
28	AH	101	DGD	C7B-C6B-C5B	-2.88	99.28	114.56
24	AB	613	CLA	C2A-C1A-CHA	2.88	129.12	123.87
28	AE	101	DGD	O5D-C6D-C5D	2.88	113.96	108.96
32	AB	630	LMT	C4-C3-C2	-2.88	99.27	114.56
27	BX	5101	BCR	C35-C13-C12	2.88	122.74	118.09
24	BB	5614	CLA	C2A-C1A-CHA	2.88	129.11	123.87
27	BT	5101	BCR	C1-C6-C5	-2.88	118.42	122.59
24	AC	503	CLA	C3A-C2A-C1A	2.88	106.37	101.70
27	BC	5515	BCR	C8-C7-C6	2.87	135.71	127.23
27	BK	5102	BCR	C16-C17-C18	2.87	131.44	127.29
24	BC	5513	CLA	C1D-CHD-C4C	2.87	127.06	122.60
29	BA	5413	LHG	O7-C7-C8	2.87	117.66	111.54
24	AB	609	CLA	CAA-C2A-C1A	-2.87	104.90	112.51
24	BB	5607	CLA	O2D-CGD-CBD	2.87	117.14	111.34
24	BC	5508	CLA	C1C-NC-C4C	2.87	110.13	106.26
31	BB	5624	LMG	O7-C10-O9	-2.87	116.00	123.66
24	AB	605	CLA	CED-O2D-CGD	2.87	122.84	116.00
24	BB	5605	CLA	CHD-C4C-NC	2.87	126.29	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	604	CLA	CBD-CHA-C1A	2.87	132.52	128.77
24	BB	5608	CLA	CBD-CHA-C1A	2.87	132.52	128.77
24	BA	5407	CLA	C4B-NB-C1B	2.87	109.88	107.12
24	BB	5617	CLA	C1C-NC-C4C	2.87	110.13	106.26
36	AF	101	HEM	C1A-CHA-C4D	-2.87	123.70	127.47
24	BC	5503	CLA	C7-C6-C5	-2.87	104.61	112.97
28	AC	519	DGD	C8B-C7B-C6B	-2.87	99.34	114.56
24	BB	5612	CLA	C4B-NB-C1B	2.86	109.88	107.12
24	AC	513	CLA	CED-O2D-CGD	2.86	122.82	116.00
24	BB	5608	CLA	CHD-C4C-NC	2.86	126.28	124.28
29	AA	412	LHG	O7-C7-C8	2.86	117.64	111.54
24	BB	5615	CLA	C6-C5-C3	2.86	119.14	112.62
27	AD	406	BCR	C7-C8-C9	2.86	130.49	126.22
27	AA	410	BCR	C23-C24-C25	2.86	135.66	127.23
24	AB	605	CLA	O2D-CGD-CBD	2.86	117.11	111.34
24	BD	5402	CLA	CBD-CHA-C1A	2.86	132.50	128.77
24	AD	401	CLA	CBD-CHA-C1A	2.86	132.50	128.77
24	AA	407	CLA	C2A-C1A-CHA	2.86	129.08	123.87
24	BA	5406	CLA	C1C-NC-C4C	2.86	110.11	106.26
24	AC	512	CLA	CBD-CHA-C1A	2.85	132.50	128.77
24	AC	508	CLA	C2C-C1C-NC	-2.85	107.92	110.22
24	BC	5508	CLA	C3D-CAD-CBD	-2.85	103.57	107.60
24	AB	615	CLA	C1C-NC-C4C	2.85	110.11	106.26
24	AB	603	CLA	O2D-CGD-CBD	2.85	117.10	111.34
24	AB	610	CLA	C4B-NB-C1B	2.85	109.86	107.12
24	BC	5508	CLA	C4B-NB-C1B	2.85	109.86	107.12
24	BC	5508	CLA	CED-O2D-CGD	2.85	122.78	116.00
24	AC	502	CLA	O2D-CGD-CBD	2.85	117.09	111.34
24	BB	5616	CLA	C4D-C3D-C2D	-2.84	103.72	107.17
24	AC	508	CLA	CED-O2D-CGD	2.85	122.78	116.00
28	BC	5519	DGD	O6E-C1E-C2E	2.85	116.13	110.30
31	AD	407	LMG	O1-C1-C2	-2.84	104.51	108.15
24	BB	5616	CLA	C2A-C1A-CHA	2.84	129.05	123.87
24	BB	5609	CLA	C4B-NB-C1B	2.84	109.86	107.12
24	AC	513	CLA	O2D-CGD-CBD	2.84	117.08	111.34
32	BB	5603	LMT	C4-C3-C2	-2.83	99.51	114.56
24	AD	401	CLA	O2D-CGD-CBD	2.83	117.06	111.34
24	BB	5616	CLA	C1D-CHD-C4C	2.83	126.99	122.60
30	BA	5414	SQD	O8-S-O9	-2.83	105.38	111.69
28	BH	5101	DGD	C7B-C6B-C5B	-2.83	99.53	114.56
28	AA	411	DGD	O6D-C1D-C2D	-2.83	104.51	110.30
24	BC	5510	CLA	C2A-C1A-CHA	2.83	129.03	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	508	CLA	C3D-CAD-CBD	-2.83	103.60	107.60
27	AK	102	BCR	C16-C17-C18	2.83	131.38	127.29
31	BI	5101	LMG	C14-C13-C12	-2.83	99.56	114.56
27	AB	619	BCR	C23-C24-C25	2.83	135.57	127.23
31	BD	5410	LMG	C32-C31-C30	-2.82	99.56	114.56
34	BD	5404	PHO	C1C-NC-C4C	2.82	112.15	106.52
24	BC	5502	CLA	C3D-CAD-CBD	-2.82	103.61	107.60
24	AA	405	CLA	O2A-CGA-O1A	-2.82	116.11	123.48
27	AK	102	BCR	C35-C13-C12	2.82	122.65	118.09
24	AA	407	CLA	C3A-C2A-C1A	2.82	106.28	101.70
24	BC	5506	CLA	CHD-C4C-NC	2.82	126.25	124.28
24	BC	5502	CLA	CGD-CBD-CHA	-2.82	107.12	113.65
24	AC	513	CLA	C1D-CHD-C4C	2.82	126.97	122.60
24	BB	5619	CLA	O2D-CGD-CBD	2.81	117.02	111.34
30	AA	416	SQD	C3-C4-C5	-2.81	105.13	110.17
31	AB	621	LMG	O7-C10-O9	-2.81	116.17	123.66
24	AB	611	CLA	C3A-C2A-C1A	2.81	106.26	101.70
24	BC	5502	CLA	O2D-CGD-CBD	2.81	117.01	111.34
27	AC	514	BCR	C23-C22-C21	-2.81	114.66	118.98
24	AB	606	CLA	CED-O2D-CGD	2.81	122.68	116.00
36	BF	5101	HEM	C1A-CHA-C4D	-2.81	123.78	127.47
27	AB	617	BCR	C35-C13-C12	2.81	122.63	118.09
28	BB	5602	DGD	O6E-C1E-O5D	2.80	116.60	109.93
24	AD	401	CLA	CBA-CAA-C2A	2.80	120.80	113.95
24	BB	5620	CLA	O2A-CGA-CBA	2.80	120.48	111.90
24	BC	5506	CLA	C4B-NB-C1B	2.80	109.82	107.12
24	AC	505	CLA	C1C-NC-C4C	2.80	110.04	106.26
28	AC	517	DGD	C3G-C2G-C1G	2.80	118.29	111.86
24	AA	404	CLA	C4D-C3D-C2D	-2.80	103.77	107.17
27	BA	5411	BCR	C24-C23-C22	2.80	130.41	126.22
24	AB	605	CLA	C4B-NB-C1B	2.80	109.82	107.12
24	BB	5617	CLA	O2A-CGA-CBA	2.80	120.47	111.90
24	AC	511	CLA	CHD-C4C-NC	2.80	126.24	124.28
27	BJ	5101	BCR	C8-C7-C6	2.80	135.49	127.23
24	BB	5617	CLA	CHD-C4C-NC	2.80	126.24	124.28
28	BC	5517	DGD	C3G-C2G-C1G	2.80	118.28	111.86
24	AA	404	CLA	CBD-CHA-C1A	2.80	132.43	128.77
24	BC	5510	CLA	C3D-CAD-CBD	-2.80	103.64	107.60
24	BB	5605	CLA	C2A-C1A-CHA	2.80	128.97	123.87
24	BB	5611	CLA	C2A-C1A-NA	-2.80	107.76	111.33
28	AH	101	DGD	O6D-C1D-O3G	2.80	116.58	109.93
24	BA	5405	CLA	CHD-C4C-NC	2.79	126.23	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	607	CLA	C4B-NB-C1B	2.79	109.81	107.12
27	AB	617	BCR	C36-C18-C19	2.79	122.61	118.09
31	AD	408	LMG	C32-C31-C30	-2.79	99.73	114.56
31	AA	414	LMG	O8-C28-C29	2.79	120.44	111.90
31	BD	5409	LMG	O1-C1-C2	-2.79	104.58	108.15
24	BB	5618	CLA	CED-O2D-CGD	2.79	122.64	116.00
24	BC	5506	CLA	CED-O2D-CGD	2.79	122.64	116.00
28	BA	5412	DGD	O6D-C1D-C2D	-2.79	104.60	110.30
31	BE	5101	LMG	O8-C28-C29	2.79	120.43	111.90
30	BA	5401	SQD	C3-C4-C5	-2.79	105.17	110.17
27	BK	5102	BCR	C35-C13-C12	2.79	122.59	118.09
24	BC	5507	CLA	C7-C6-C5	-2.78	104.84	112.97
24	BB	5606	CLA	C1C-NC-C4C	2.78	110.02	106.26
24	BC	5512	CLA	CHD-C4C-NC	2.78	126.23	124.28
24	AA	404	CLA	CED-O2D-CGD	2.78	122.63	116.00
24	BB	5616	CLA	CBD-CHA-C1A	2.78	132.41	128.77
24	AB	602	CLA	O2D-CGD-CBD	2.78	116.96	111.34
24	BA	5405	CLA	C3D-CAD-CBD	-2.78	103.66	107.60
28	AC	519	DGD	O1G-C1A-C2A	2.78	120.42	111.90
27	BK	5102	BCR	C8-C7-C6	2.78	135.44	127.23
24	BA	5408	CLA	C4B-NB-C1B	2.78	109.80	107.12
24	AC	512	CLA	CHD-C4C-NC	2.78	126.22	124.28
24	AC	506	CLA	CED-O2D-CGD	2.78	122.61	116.00
32	BB	5603	LMT	O1B-C1B-C2B	2.77	114.75	108.11
27	BC	5515	BCR	C16-C17-C18	2.77	131.29	127.29
24	BC	5505	CLA	O2D-CGD-CBD	2.77	116.94	111.34
24	BB	5613	CLA	O2D-CGD-CBD	2.77	116.94	111.34
24	AD	401	CLA	C2A-C1A-CHA	2.77	128.92	123.87
31	BB	5624	LMG	C16-C15-C14	-2.77	99.86	114.56
34	AD	402	PHO	C3A-C4A-NA	-2.77	108.82	113.57
24	BB	5619	CLA	C3A-C2A-C1A	2.77	106.20	101.70
24	AC	509	CLA	CBD-CHA-C1A	2.77	132.39	128.77
27	AX	101	BCR	C35-C13-C12	2.77	122.56	118.09
32	AB	629	LMT	O1B-C1B-C2B	2.77	114.73	108.11
27	BT	5101	BCR	C32-C1-C6	2.77	114.91	110.33
31	BE	5101	LMG	C22-C21-C20	2.77	120.85	112.94
24	BC	5503	CLA	C3A-C2A-C1A	2.76	106.19	101.70
27	BD	5407	BCR	C23-C22-C21	-2.76	114.72	118.98
24	BC	5508	CLA	C2A-C1A-NA	-2.76	107.80	111.33
24	BC	5501	CLA	C1C-NC-C4C	2.76	109.98	106.26
24	AB	616	CLA	CHD-C4C-NC	2.76	126.21	124.28
24	BB	5618	CLA	O2A-CGA-CBA	2.76	120.35	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AD	408	LMG	O7-C8-C7	2.76	118.71	108.50
30	BB	5625	SQD	C18-C17-C16	2.76	120.82	112.94
28	BH	5101	DGD	O6D-C1D-O3G	2.75	116.48	109.93
24	BC	5508	CLA	O1D-CGD-CBD	-2.76	118.82	124.45
24	BB	5607	CLA	C4B-C3B-C2B	-2.76	104.21	107.04
24	AB	606	CLA	CBA-CAA-C2A	2.75	120.68	113.95
24	AB	611	CLA	C4B-NB-C1B	2.75	109.77	107.12
31	BL	5101	LMG	C15-C14-C13	-2.75	99.95	114.56
27	AK	102	BCR	C34-C9-C8	2.75	122.54	118.09
31	AI	101	LMG	C14-C13-C12	-2.75	99.95	114.56
24	AB	606	CLA	CHD-C4C-NC	2.75	126.20	124.28
31	AB	621	LMG	O8-C28-C29	2.75	120.30	111.90
24	BB	5616	CLA	C2C-C1C-NC	-2.75	108.00	110.22
24	BB	5617	CLA	C2A-C1A-CHA	2.74	128.87	123.87
27	AC	514	BCR	C35-C13-C12	2.74	122.52	118.09
24	BC	5504	CLA	C4B-NB-C1B	2.74	109.76	107.12
34	BD	5403	PHO	C3A-C4A-NA	-2.74	108.86	113.57
27	AB	619	BCR	C8-C7-C6	2.74	135.33	127.23
24	AC	504	CLA	C2C-C1C-NC	-2.74	108.01	110.22
24	BB	5619	CLA	C2A-C1A-NA	-2.74	107.83	111.33
35	BD	5406	PL9	C45-C44-C46	2.74	119.55	115.39
27	BB	5623	BCR	C8-C7-C6	2.74	135.32	127.23
24	AB	612	CLA	C1D-CHD-C4C	2.74	126.84	122.60
31	AB	621	LMG	C16-C15-C14	-2.74	100.03	114.56
24	BC	5509	CLA	CBD-CHA-C1A	2.74	132.35	128.77
24	AC	508	CLA	C4B-NB-C1B	2.74	109.75	107.12
27	BC	5516	BCR	C35-C13-C12	2.73	122.51	118.09
27	BB	5622	BCR	C1-C6-C5	-2.73	118.63	122.59
24	BA	5405	CLA	CAA-C2A-C3A	-2.73	106.48	113.32
27	AJ	101	BCR	C16-C15-C14	2.73	129.46	123.45
24	BB	5614	CLA	C4B-NB-C1B	2.73	109.75	107.12
27	AX	101	BCR	C11-C10-C9	2.73	131.24	127.29
24	AB	603	CLA	C7-C6-C5	-2.73	105.00	112.97
28	AB	628	DGD	O5D-C1E-C2E	2.73	111.65	108.15
34	BD	5404	PHO	C4D-CHA-CBD	-2.73	104.91	107.88
31	AA	414	LMG	C34-C33-C32	2.73	129.06	114.56
28	BC	5519	DGD	O1G-C1A-C2A	2.73	120.25	111.90
27	AJ	101	BCR	C11-C10-C9	2.72	131.23	127.29
24	AB	615	CLA	C3A-C2A-C1A	2.72	106.13	101.70
24	AB	616	CLA	O2A-CGA-CBA	2.72	120.23	111.90
27	AD	406	BCR	C1-C6-C5	-2.72	118.65	122.59
24	BA	5408	CLA	C2A-C1A-CHA	2.72	128.83	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5621	BCR	C35-C13-C12	2.72	122.49	118.09
24	BC	5506	CLA	C3A-C2A-C1A	2.72	106.12	101.70
24	AC	512	CLA	C1C-NC-C4C	2.72	109.93	106.26
36	AV	201	HEM	CAD-C3D-C2D	2.72	134.13	127.19
24	BB	5614	CLA	C1C-NC-C4C	2.72	109.93	106.26
32	AB	629	LMT	C4-C3-C2	-2.72	100.14	114.56
27	BC	5514	BCR	C1-C6-C7	2.72	123.22	115.69
34	BD	5403	PHO	CBD-CHA-C1A	2.71	131.38	126.67
31	AB	620	LMG	C15-C14-C13	-2.72	100.14	114.56
29	BA	5415	LHG	O8-C23-C24	2.71	120.21	111.90
24	AB	611	CLA	C4D-C3D-CAD	2.71	111.39	108.05
24	AC	509	CLA	C1D-CHD-C4C	2.71	126.81	122.60
24	AC	510	CLA	C2A-C1A-CHA	2.71	128.82	123.87
30	AB	622	SQD	C18-C17-C16	2.71	120.69	112.94
27	AC	515	BCR	C35-C13-C12	2.71	122.47	118.09
24	AC	506	CLA	C3A-C2A-C1A	2.71	106.10	101.70
24	AC	507	CLA	CBD-CHA-C1A	2.71	132.31	128.77
27	BC	5516	BCR	C40-C30-C29	-2.71	98.02	108.78
24	BB	5615	CLA	O2D-CGD-CBD	2.71	116.81	111.34
27	AA	410	BCR	C1-C6-C5	-2.71	118.67	122.59
24	AB	606	CLA	CAA-C2A-C3A	-2.70	106.55	113.32
24	AB	614	CLA	CED-O2D-CGD	2.71	122.44	116.00
28	AB	628	DGD	O6E-C1E-O5D	2.70	116.36	109.93
24	BC	5511	CLA	C1D-CHD-C4C	2.70	126.79	122.60
24	AB	602	CLA	C1C-NC-C4C	2.70	109.91	106.26
24	AB	602	CLA	C4D-C3D-C2D	-2.70	103.89	107.17
27	BD	5407	BCR	C1-C6-C5	-2.70	118.68	122.59
24	BC	5507	CLA	CBD-CHA-C1A	2.70	132.30	128.77
24	BC	5505	CLA	CHD-C4C-NC	2.70	126.17	124.28
31	BE	5101	LMG	C34-C33-C32	2.70	128.90	114.56
24	AB	611	CLA	C2C-C1C-NC	-2.70	108.04	110.22
27	BJ	5101	BCR	C16-C15-C14	2.70	129.39	123.45
24	BB	5607	CLA	CHD-C4C-NC	2.70	126.17	124.28
29	AA	415	LHG	O8-C23-C24	2.70	120.16	111.90
31	BD	5410	LMG	O7-C8-C7	2.70	118.49	108.50
28	BC	5518	DGD	O6D-C5D-C4D	2.70	114.75	109.73
24	BA	5406	CLA	C2A-C1A-NA	-2.70	107.88	111.33
24	AA	405	CLA	C4D-C3D-C2D	-2.70	103.89	107.17
24	BB	5607	CLA	C1D-CHD-C4C	2.70	126.78	122.60
24	AA	405	CLA	C1C-NC-C4C	2.69	109.89	106.26
24	AB	612	CLA	C2A-C1A-CHA	2.69	128.78	123.87
24	AC	506	CLA	CHD-C4C-NC	2.69	126.16	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	404	CLA	CAA-C2A-C3A	-2.69	106.58	113.32
27	BT	5101	BCR	C8-C9-C10	-2.69	114.83	118.98
24	BB	5611	CLA	C4D-C3D-C2D	-2.69	103.90	107.17
34	BD	5403	PHO	C3A-C2A-C1A	2.69	105.38	101.90
36	AF	101	HEM	CAD-C3D-C4D	-2.69	119.98	124.92
27	BB	5623	BCR	C1-C6-C5	-2.69	118.69	122.59
24	AB	603	CLA	CBA-CAA-C2A	2.69	120.53	113.95
24	AB	603	CLA	C4B-C3B-C2B	-2.69	104.27	107.04
27	BA	5411	BCR	C35-C13-C12	2.69	122.43	118.09
24	BB	5611	CLA	O2A-CGA-O1A	-2.69	116.45	123.48
24	BB	5610	CLA	O2A-CGA-O1A	-2.69	116.46	123.48
24	AA	406	CLA	C4D-C3D-C2D	-2.69	103.91	107.17
24	AC	507	CLA	C7-C6-C5	-2.68	105.14	112.97
24	BC	5503	CLA	CBD-CHA-C1A	2.68	132.27	128.77
27	AC	514	BCR	C7-C8-C9	2.68	130.23	126.22
24	BA	5405	CLA	C4D-C3D-C2D	-2.68	103.92	107.17
24	AA	406	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
24	BB	5620	CLA	CED-O2D-CGD	2.68	122.37	116.00
31	AA	414	LMG	C22-C21-C20	2.68	120.59	112.94
24	AB	604	CLA	C4D-C3D-C2D	-2.67	103.92	107.17
24	BC	5513	CLA	CED-O2D-CGD	2.67	122.37	116.00
34	AD	402	PHO	CBD-CHA-C1A	2.67	131.30	126.67
27	BX	5101	BCR	C15-C14-C13	2.67	131.15	127.29
24	AA	407	CLA	C2A-C1A-NA	-2.67	107.92	111.33
24	AB	607	CLA	C2C-C1C-NC	-2.67	108.07	110.22
24	BB	5605	CLA	CED-O2D-CGD	2.67	122.36	116.00
24	BB	5610	CLA	C4B-NB-C1B	2.67	109.69	107.12
30	AB	622	SQD	O8-S-O9	-2.66	105.76	111.69
24	AC	509	CLA	CED-O2D-CGD	2.66	122.34	116.00
30	BB	5625	SQD	O8-S-O9	-2.66	105.77	111.69
24	BB	5612	CLA	C2A-C1A-NA	-2.66	107.93	111.33
24	AA	405	CLA	CGD-CBD-CHA	-2.66	107.48	113.65
24	AB	610	CLA	CHD-C4C-NC	2.66	126.14	124.28
36	BV	5201	HEM	CAD-C3D-C2D	2.66	133.98	127.19
27	BB	5621	BCR	C16-C17-C18	2.66	131.14	127.29
27	BB	5623	BCR	C23-C24-C25	2.66	135.08	127.23
31	BD	5410	LMG	C15-C14-C13	-2.66	100.43	114.56
27	BX	5101	BCR	C11-C10-C9	2.66	131.13	127.29
24	AA	405	CLA	C3A-C2A-C1A	2.66	106.02	101.70
30	BA	5401	SQD	C45-O47-C7	2.66	124.10	117.86
24	BC	5505	CLA	C1C-NC-C4C	2.65	109.84	106.26
24	AB	613	CLA	O2A-CGA-CBA	2.65	120.02	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	607	CLA	C4D-C3D-C2D	-2.65	103.95	107.17
24	BC	5504	CLA	C4D-C3D-C2D	-2.65	103.95	107.17
27	AC	516	BCR	C40-C30-C29	-2.65	98.25	108.78
28	BC	5519	DGD	O3D-C3D-C2D	2.65	116.28	110.36
24	BC	5512	CLA	C1C-NC-C4C	2.65	109.83	106.26
24	BB	5610	CLA	CAA-C2A-C3A	-2.65	106.70	113.32
24	BB	5610	CLA	CED-O2D-CGD	2.64	122.30	116.00
30	AF	102	SQD	C45-O47-C7	2.64	124.07	117.86
32	BI	5102	LMT	C4-C3-C2	-2.64	100.52	114.56
24	BB	5606	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
27	BA	5411	BCR	C2-C1-C6	2.64	114.58	110.37
24	BB	5612	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
31	BD	5408	LMG	C22-C21-C20	2.64	120.49	112.94
24	AC	511	CLA	C1D-CHD-C4C	2.64	126.69	122.60
24	AA	407	CLA	C4D-C3D-C2D	-2.64	103.97	107.17
27	BT	5101	BCR	C19-C18-C17	-2.64	114.92	118.98
24	BC	5505	CLA	C3D-CAD-CBD	-2.64	103.87	107.60
24	AB	605	CLA	C4D-C3D-C2D	-2.64	103.97	107.17
27	AT	101	BCR	C8-C9-C10	-2.63	114.92	118.98
27	AT	101	BCR	C19-C18-C17	-2.63	114.92	118.98
27	AT	101	BCR	C23-C22-C21	-2.63	114.92	118.98
28	AC	519	DGD	O6E-C5E-C4E	2.63	114.63	109.73
24	AC	503	CLA	C3D-CAD-CBD	-2.63	103.88	107.60
32	AI	102	LMT	C4-C3-C2	-2.63	100.59	114.56
24	AC	508	CLA	C4D-C3D-C2D	-2.63	103.97	107.17
24	AB	601	CLA	CHD-C4C-NC	2.63	126.12	124.28
24	AA	406	CLA	CGD-CBD-CHA	-2.63	107.56	113.65
36	BV	5201	HEM	O1D-CGD-CBD	-2.63	114.17	123.06
28	AC	519	DGD	C3G-C2G-C1G	2.63	117.89	111.86
34	AD	403	PHO	C6-C7-C8	-2.63	107.27	115.44
27	AA	410	BCR	C16-C17-C18	2.63	131.09	127.29
24	BB	5611	CLA	C2C-C1C-NC	-2.63	108.10	110.22
24	AC	501	CLA	O2D-CGD-CBD	2.63	116.64	111.34
35	BD	5406	PL9	C2-C1-C6	2.62	123.90	118.20
24	BB	5607	CLA	CAA-CBA-CGA	-2.62	105.51	113.24
36	AV	201	HEM	O1D-CGD-CBD	-2.62	114.19	123.06
24	AA	404	CLA	C3D-CAD-CBD	-2.62	103.89	107.60
27	BB	5621	BCR	C36-C18-C19	2.62	122.32	118.09
24	AB	602	CLA	C4B-NB-C1B	2.62	109.64	107.12
24	BB	5605	CLA	CBD-CHA-C1A	2.62	132.19	128.77
24	BC	5503	CLA	O1D-CGD-CBD	-2.62	119.11	124.45
27	BC	5515	BCR	C19-C18-C17	-2.62	114.95	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5615	CLA	C4D-C3D-C2D	-2.61	104.00	107.17
24	BB	5613	CLA	C4D-C3D-C2D	-2.61	104.00	107.17
24	AA	404	CLA	C4B-C3B-C2B	-2.61	104.36	107.04
27	AC	515	BCR	C19-C18-C17	-2.61	114.96	118.98
24	BD	5402	CLA	C1C-NC-C4C	2.61	109.78	106.26
24	AB	609	CLA	O2D-CGD-CBD	2.61	116.62	111.34
24	BB	5610	CLA	CHD-C4C-NC	2.61	126.11	124.28
27	AT	101	BCR	C36-C18-C19	2.61	122.31	118.09
24	BC	5506	CLA	C1C-NC-C4C	2.61	109.78	106.26
24	BA	5407	CLA	C4D-C3D-C2D	-2.61	104.00	107.17
27	BJ	5101	BCR	C1-C6-C7	2.61	122.92	115.69
24	BB	5615	CLA	C3D-CAD-CBD	-2.61	103.91	107.60
24	AB	614	CLA	O2D-CGD-CBD	2.61	116.61	111.34
24	AB	601	CLA	CBD-CHA-C1A	2.61	132.18	128.77
27	BC	5514	BCR	C37-C22-C23	2.61	122.30	118.09
30	AA	416	SQD	C45-O47-C7	2.61	123.97	117.86
24	AB	601	CLA	CED-O2D-CGD	2.61	122.20	116.00
24	AC	506	CLA	C1C-NC-C4C	2.60	109.77	106.26
31	BB	5624	LMG	O7-C8-C7	2.60	118.13	108.50
27	AT	101	BCR	C32-C1-C6	2.60	114.64	110.33
24	BB	5607	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
27	AB	617	BCR	C8-C9-C10	-2.60	114.97	118.98
27	AX	101	BCR	C16-C17-C18	2.60	131.05	127.29
35	AD	405	PL9	C2-C1-C6	2.60	123.84	118.20
24	AA	405	CLA	C4B-NB-C1B	2.60	109.62	107.12
27	AC	514	BCR	C37-C22-C23	2.60	122.29	118.09
24	BC	5504	CLA	C3D-CAD-CBD	-2.60	103.92	107.60
24	AB	608	CLA	C3D-CAD-CBD	-2.60	103.92	107.60
27	BC	5514	BCR	C30-C25-C26	-2.60	118.83	122.59
27	AJ	101	BCR	C1-C6-C7	2.60	122.88	115.69
24	AB	606	CLA	C4B-NB-C1B	2.60	109.62	107.12
24	AB	610	CLA	CBD-CHA-C1A	2.60	132.16	128.77
24	BA	5407	CLA	C2C-C1C-NC	-2.60	108.13	110.22
27	AD	406	BCR	C35-C13-C12	2.60	122.28	118.09
24	BD	5405	CLA	C3A-C2A-C1A	2.59	105.92	101.70
24	AB	602	CLA	C3D-CAD-CBD	-2.59	103.93	107.60
27	AB	618	BCR	C1-C6-C5	-2.59	118.83	122.59
31	BB	5624	LMG	O8-C28-C29	2.59	119.84	111.90
27	AD	406	BCR	C37-C22-C23	2.59	122.28	118.09
24	BB	5607	CLA	CBA-CAA-C2A	2.59	120.29	113.95
27	AB	617	BCR	C16-C17-C18	2.59	131.04	127.29
28	AC	519	DGD	O3D-C3D-C2D	2.59	116.14	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	510	CLA	C1C-NC-C4C	2.59	109.76	106.26
24	BB	5605	CLA	C1C-NC-C4C	2.59	109.75	106.26
27	AB	619	BCR	C1-C6-C5	-2.59	118.84	122.59
27	AX	101	BCR	C15-C14-C13	2.59	131.03	127.29
34	AD	403	PHO	C1C-NC-C4C	2.59	111.68	106.52
31	AC	520	LMG	O7-C8-C7	2.59	118.07	108.50
31	BC	5521	LMG	C9-C8-C7	2.59	117.80	111.86
34	AD	402	PHO	C4B-C3B-C2B	-2.59	104.54	107.03
31	BE	5101	LMG	O8-C9-C8	2.59	115.60	108.80
27	AT	101	BCR	C20-C21-C22	2.58	131.03	127.29
27	BK	5102	BCR	C30-C25-C24	2.58	122.85	115.69
28	BC	5519	DGD	C1D-C2D-C3D	-2.58	104.98	109.99
24	AC	506	CLA	C2A-C1A-CHA	2.58	128.58	123.87
24	AC	505	CLA	CHD-C4C-NC	2.58	126.09	124.28
24	AB	604	CLA	OBD-CAD-C3D	2.58	133.38	128.15
27	AX	101	BCR	C28-C27-C26	2.58	118.06	113.81
27	BC	5516	BCR	C24-C23-C22	2.58	130.08	126.22
24	AB	603	CLA	C1D-CHD-C4C	2.58	126.61	122.60
24	BB	5611	CLA	C1D-CHD-C4C	2.58	126.61	122.60
24	BA	5406	CLA	CGD-CBD-CHA	-2.58	107.66	113.65
24	BC	5501	CLA	O2A-CGA-O1A	-2.58	116.73	123.48
24	AC	503	CLA	CBD-CHA-C1A	2.58	132.14	128.77
24	BC	5510	CLA	O1D-CGD-CBD	-2.58	119.18	124.45
27	BJ	5101	BCR	C21-C20-C19	2.58	131.90	123.23
27	AT	101	BCR	C23-C24-C25	2.58	134.84	127.23
27	BD	5407	BCR	C12-C13-C14	-2.58	115.01	118.98
24	BB	5607	CLA	C7-C6-C5	-2.58	105.45	112.97
31	BA	5402	LMG	C22-C21-C20	2.57	120.30	112.94
32	AB	623	LMT	O1B-C1B-C2B	2.57	114.28	108.11
24	AB	613	CLA	C6-C7-C8	-2.58	107.43	115.44
27	BB	5621	BCR	C1-C6-C5	-2.58	118.86	122.59
29	BA	5415	LHG	C5-O7-C7	-2.57	111.81	117.86
31	BC	5520	LMG	O7-C8-C7	2.57	118.02	108.50
27	BC	5516	BCR	C37-C22-C23	2.57	122.24	118.09
31	AJ	102	LMG	C22-C21-C20	2.57	120.29	112.94
24	BC	5510	CLA	CBD-CHA-C1A	2.57	132.13	128.77
24	AB	610	CLA	C3A-C2A-C1A	2.57	105.87	101.70
24	BB	5609	CLA	O2D-CGD-CBD	2.56	116.52	111.34
29	AA	415	LHG	C5-O7-C7	-2.57	111.83	117.86
24	BA	5406	CLA	CBD-CHA-C1A	2.57	132.12	128.77
27	AC	514	BCR	C1-C6-C7	2.56	122.80	115.69
24	BB	5615	CLA	C4-C3-C5	-2.56	111.50	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	617	BCR	C24-C23-C22	2.56	130.05	126.22
28	AC	517	DGD	C8A-C7A-C6A	-2.56	100.97	114.56
24	BB	5608	CLA	C3D-CAD-CBD	-2.56	103.98	107.60
27	BD	5407	BCR	C37-C22-C23	2.56	122.22	118.09
24	AB	612	CLA	C4D-C3D-C2D	-2.56	104.07	107.17
31	BL	5101	LMG	C12-C11-C10	2.56	123.43	113.51
24	BB	5613	CLA	C2A-C1A-CHA	2.56	128.53	123.87
24	BC	5512	CLA	CED-O2D-CGD	2.55	122.08	116.00
24	BC	5510	CLA	C1C-NC-C4C	2.55	109.71	106.26
31	AA	417	LMG	C15-C14-C13	-2.55	101.00	114.56
24	BB	5608	CLA	C3A-C2A-C1A	2.55	105.85	101.70
31	AB	621	LMG	C7-O1-C1	-2.55	108.68	113.80
31	AB	621	LMG	O7-C8-C7	2.55	117.93	108.50
24	AB	607	CLA	O2A-CGA-O1A	-2.55	116.82	123.48
24	BC	5506	CLA	C2A-C1A-CHA	2.55	128.51	123.87
28	BC	5519	DGD	C3G-C2G-C1G	2.55	117.70	111.86
34	BD	5403	PHO	C3D-CAD-CBD	-2.55	104.00	107.60
24	BB	5610	CLA	C4D-C3D-C2D	-2.55	104.08	107.17
31	AD	408	LMG	C15-C14-C13	-2.55	101.05	114.56
27	BC	5514	BCR	C12-C13-C14	-2.55	115.06	118.98
24	AA	405	CLA	CMB-C2B-C1B	-2.54	124.55	128.46
24	BC	5503	CLA	C1C-NC-C4C	2.54	109.69	106.26
24	AD	401	CLA	C1C-NC-C4C	2.54	109.69	106.26
24	AB	608	CLA	C4-C3-C5	-2.54	111.53	115.39
24	BB	5620	CLA	C1C-NC-C4C	2.54	109.69	106.26
24	BB	5608	CLA	C4B-C3B-C2B	-2.54	104.43	107.04
24	AB	616	CLA	C1C-NC-C4C	2.54	109.69	106.26
27	BK	5102	BCR	C34-C9-C8	2.54	122.19	118.09
24	AB	603	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
24	BB	5607	CLA	CED-O2D-CGD	2.54	122.05	116.00
24	AB	601	CLA	C1C-NC-C4C	2.54	109.68	106.26
27	BD	5407	BCR	C35-C13-C12	2.54	122.19	118.09
24	AB	609	CLA	CED-O2D-CGD	2.54	122.04	116.00
24	BC	5501	CLA	CED-O2D-CGD	2.53	122.03	116.00
24	AB	613	CLA	CBD-CHA-C1A	2.53	132.08	128.77
24	AA	406	CLA	CAA-CBA-CGA	-2.53	105.77	113.24
36	BF	5101	HEM	CAD-C3D-C4D	-2.53	120.27	124.92
24	AB	608	CLA	C2C-C1C-NC	-2.53	108.18	110.22
27	AK	102	BCR	C30-C25-C24	2.53	122.71	115.69
24	BA	5408	CLA	CBD-CHA-C1A	2.53	132.08	128.77
31	BA	5402	LMG	C15-C14-C13	-2.53	101.12	114.56
24	BD	5405	CLA	C4D-C3D-C2D	-2.53	104.10	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	616	CLA	C3A-C2A-C1A	2.53	105.81	101.70
24	AC	501	CLA	CED-O2D-CGD	2.53	122.03	116.00
31	AC	520	LMG	C32-C31-C30	-2.53	101.14	114.56
31	AA	414	LMG	O8-C9-C8	2.53	115.44	108.80
30	BB	5601	SQD	C3-C4-C5	-2.53	105.63	110.17
28	BC	5518	DGD	C3A-C2A-C1A	2.53	123.33	113.51
24	BB	5618	CLA	CBD-CHA-C1A	2.53	132.07	128.77
27	AC	514	BCR	C40-C30-C25	2.53	114.51	110.33
34	BD	5404	PHO	C3A-C4A-NA	-2.53	109.23	113.57
27	AC	516	BCR	C35-C13-C12	2.53	122.17	118.09
24	AB	609	CLA	C3A-C2A-C1A	2.53	105.81	101.70
30	BF	5102	SQD	O47-C7-C8	2.52	116.92	111.54
28	AC	518	DGD	C3A-C2A-C1A	2.52	123.31	113.51
24	BC	5509	CLA	C2C-C1C-NC	-2.52	108.19	110.22
35	AD	405	PL9	C45-C44-C46	2.52	119.22	115.39
24	BB	5611	CLA	OBD-CAD-C3D	2.52	133.25	128.15
34	AD	402	PHO	C3D-CAD-CBD	-2.52	104.03	107.60
24	BB	5614	CLA	C3A-C2A-C1A	2.52	105.80	101.70
28	AC	518	DGD	O6D-C5D-C4D	2.52	114.42	109.73
24	BC	5511	CLA	CHD-C4C-NC	2.52	126.04	124.28
31	AB	620	LMG	C12-C11-C10	2.52	123.29	113.51
34	AD	402	PHO	C4D-C3D-C2D	-2.52	104.00	107.01
24	AA	404	CLA	C2A-C1A-CHA	2.52	128.46	123.87
24	AB	613	CLA	C3D-CAD-CBD	-2.52	104.03	107.60
24	BB	5617	CLA	C2C-C1C-NC	-2.52	108.19	110.22
24	BC	5504	CLA	C2C-C1C-NC	-2.52	108.19	110.22
24	AC	509	CLA	C2C-C1C-NC	-2.52	108.19	110.22
24	BC	5509	CLA	C3A-C2A-C1A	2.52	105.79	101.70
24	BC	5506	CLA	C3D-CAD-CBD	-2.52	104.04	107.60
27	AA	410	BCR	C24-C23-C22	2.52	129.98	126.22
24	AD	404	CLA	C3A-C2A-C1A	2.51	105.79	101.70
24	BB	5620	CLA	CHD-C4C-NC	2.52	126.04	124.28
27	BB	5621	BCR	C12-C13-C14	-2.51	115.11	118.98
24	AC	502	CLA	CGD-CBD-CHA	-2.51	107.83	113.65
24	AB	603	CLA	CHD-C4C-NC	2.51	126.04	124.28
24	AB	608	CLA	CBD-CHA-C1A	2.51	132.05	128.77
27	AK	102	BCR	C37-C22-C23	2.51	122.15	118.09
34	BD	5403	PHO	C1C-NC-C4C	2.51	111.52	106.52
24	BC	5507	CLA	C11-C12-C13	2.51	123.25	115.44
27	BT	5101	BCR	C23-C22-C21	-2.51	115.12	118.98
28	AC	517	DGD	C3A-C2A-C1A	2.51	123.25	113.51
27	BC	5514	BCR	C7-C8-C9	2.51	129.97	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	616	CLA	CED-O2D-CGD	2.51	121.97	116.00
24	BC	5507	CLA	CHD-C4C-NC	2.50	126.03	124.28
24	BB	5606	CLA	C4D-C3D-C2D	-2.50	104.13	107.17
24	AC	502	CLA	CED-O2D-CGD	2.50	121.96	116.00
24	BA	5406	CLA	C3A-C2A-C1A	2.50	105.77	101.70
24	BC	5508	CLA	C4D-C3D-C2D	-2.50	104.13	107.17
27	AC	516	BCR	C16-C17-C18	2.50	130.91	127.29
24	AB	605	CLA	CAA-CBA-CGA	-2.50	105.86	113.24
24	BB	5620	CLA	CBD-CHA-C1A	2.50	132.04	128.77
24	BB	5612	CLA	C4-C3-C5	-2.50	111.59	115.39
29	BA	5413	LHG	O8-C6-C5	2.50	115.37	108.80
24	AB	611	CLA	C4D-C3D-C2D	-2.50	104.13	107.17
24	AC	505	CLA	C4B-C3B-C2B	-2.50	104.47	107.04
34	AD	402	PHO	C1C-NC-C4C	2.50	111.50	106.52
24	AB	608	CLA	C2A-C1A-NA	-2.50	108.14	111.33
24	AB	609	CLA	C2A-C1A-CHA	2.50	128.43	123.87
27	BK	5102	BCR	C37-C22-C23	2.50	122.13	118.09
24	BC	5512	CLA	C3D-CAD-CBD	-2.50	104.07	107.60
27	AB	619	BCR	C35-C13-C12	2.50	122.12	118.09
24	BA	5406	CLA	C4-C3-C5	-2.50	111.60	115.39
24	BB	5608	CLA	C6-C7-C8	-2.50	107.68	115.44
24	BB	5605	CLA	C4B-C3B-C2B	-2.49	104.48	107.04
27	BT	5101	BCR	C23-C24-C25	2.49	134.59	127.23
27	BJ	5101	BCR	C11-C10-C9	2.49	130.89	127.29
24	BC	5509	CLA	CHD-C4C-NC	2.49	126.02	124.28
24	BB	5608	CLA	C4D-C3D-C2D	-2.49	104.14	107.17
24	AC	512	CLA	CED-O2D-CGD	2.49	121.93	116.00
24	BC	5509	CLA	CED-O2D-CGD	2.49	121.93	116.00
24	AC	504	CLA	C3D-CAD-CBD	-2.49	104.08	107.60
24	AB	611	CLA	CED-O2D-CGD	2.49	121.93	116.00
27	AJ	101	BCR	C21-C20-C19	2.49	131.58	123.23
27	BB	5621	BCR	C19-C18-C17	-2.49	115.15	118.98
24	AC	509	CLA	CHD-C4C-NC	2.49	126.02	124.28
24	BB	5613	CLA	CED-O2D-CGD	2.48	121.91	116.00
24	AC	507	CLA	C1C-NC-C4C	2.48	109.61	106.26
30	BF	5102	SQD	O8-S-O9	-2.48	106.17	111.69
24	BB	5620	CLA	C3A-C2A-C1A	2.48	105.73	101.70
24	BB	5613	CLA	C3A-C2A-C1A	2.48	105.73	101.70
27	BD	5407	BCR	C8-C9-C10	-2.48	115.16	118.98
27	BB	5622	BCR	C1-C6-C7	2.48	122.56	115.69
24	BD	5402	CLA	C4D-C3D-C2D	-2.48	104.16	107.17
28	AC	518	DGD	O6D-C1D-O3G	2.48	115.82	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	610	CLA	C3D-CAD-CBD	-2.48	104.10	107.60
27	BA	5411	BCR	C12-C13-C14	-2.48	115.17	118.98
24	BC	5510	CLA	C3A-C2A-C1A	2.48	105.73	101.70
32	BB	5626	LMT	O1B-C1B-C2B	2.48	114.04	108.11
27	BT	5101	BCR	C36-C18-C19	2.47	122.09	118.09
24	AB	605	CLA	CAA-C2A-C3A	-2.48	107.12	113.32
31	AA	417	LMG	C32-C31-C30	-2.47	101.42	114.56
31	BC	5520	LMG	C32-C31-C30	-2.47	101.42	114.56
32	BC	5522	LMT	C1B-C2B-C3B	2.47	114.77	109.99
24	BA	5406	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
24	BC	5502	CLA	C3A-C2A-C1A	2.47	105.71	101.70
34	BD	5403	PHO	O2A-CGA-CBA	2.47	119.45	111.90
24	AD	401	CLA	C6-C7-C8	-2.47	107.76	115.44
30	BF	5102	SQD	C45-O47-C7	2.47	123.65	117.86
31	BL	5101	LMG	O1-C1-C2	2.47	111.31	108.15
28	AC	519	DGD	O6D-C1D-C2D	-2.47	105.25	110.30
24	AB	603	CLA	CAA-CBA-CGA	-2.47	105.97	113.24
27	AA	410	BCR	C35-C13-C12	2.47	122.08	118.09
24	BB	5612	CLA	CBD-CHA-C1A	2.47	131.99	128.77
24	AC	505	CLA	C2A-C1A-CHA	2.47	128.37	123.87
24	AC	508	CLA	C2A-C1A-NA	-2.47	108.18	111.33
27	BC	5514	BCR	C8-C7-C6	2.47	134.51	127.23
24	BB	5614	CLA	C3D-CAD-CBD	-2.46	104.11	107.60
30	AA	413	SQD	C32-C33-C34	2.46	123.65	113.73
27	BC	5516	BCR	C23-C22-C21	-2.46	115.18	118.98
24	BC	5508	CLA	CAA-CBA-CGA	-2.46	105.98	113.24
24	AB	612	CLA	CAA-C2A-C1A	-2.46	105.99	112.51
27	BB	5623	BCR	C24-C23-C22	2.46	129.90	126.22
24	AB	611	CLA	C7-C6-C5	-2.46	105.78	112.97
24	AB	609	CLA	CGD-CBD-CHA	-2.46	107.94	113.65
24	BB	5615	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
24	AB	605	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	AB	606	CLA	O2A-CGA-O1A	-2.46	117.05	123.48
30	BA	5414	SQD	C32-C33-C34	2.46	123.63	113.73
27	AC	514	BCR	C12-C13-C14	-2.46	115.19	118.98
24	AB	607	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	BA	5408	CLA	C4D-C3D-C2D	-2.46	104.19	107.17
24	BC	5507	CLA	C1C-NC-C4C	2.46	109.57	106.26
27	AC	516	BCR	C37-C22-C23	2.46	122.06	118.09
24	AB	604	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	BB	5617	CLA	C3D-CAD-CBD	-2.45	104.13	107.60
24	BC	5507	CLA	CED-O2D-CGD	2.45	121.84	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AA	411	DGD	C5A-C4A-C3A	-2.45	101.53	114.56
24	AC	503	CLA	C4D-C3D-C2D	-2.45	104.19	107.17
24	AC	502	CLA	C4D-C3D-C2D	-2.45	104.19	107.17
31	AM	101	LMG	O7-C10-O9	-2.45	117.11	123.66
24	BB	5609	CLA	CAA-C2A-C3A	-2.45	107.18	113.32
24	BB	5608	CLA	OBD-CAD-C3D	2.45	133.11	128.15
24	AB	614	CLA	CBD-CHA-C1A	2.45	131.97	128.77
31	BA	5402	LMG	C32-C31-C30	-2.45	101.56	114.56
24	BC	5501	CLA	O2D-CGD-CBD	2.45	116.29	111.34
24	AB	610	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
24	BB	5606	CLA	CBD-CHA-C1A	2.45	131.97	128.77
27	BD	5407	BCR	C28-C27-C26	2.45	117.84	113.81
24	AB	607	CLA	OBD-CAD-C3D	2.45	133.10	128.15
24	BB	5609	CLA	C3D-CAD-CBD	-2.45	104.14	107.60
24	AB	605	CLA	CGD-CBD-CHA	-2.45	107.97	113.65
31	AB	620	LMG	O1-C1-C2	2.45	111.29	108.15
24	BB	5614	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
24	AD	401	CLA	C4D-C3D-C2D	-2.45	104.20	107.17
27	BA	5411	BCR	C1-C6-C5	-2.44	119.05	122.59
27	AC	515	BCR	C24-C23-C22	2.44	129.87	126.22
31	AJ	102	LMG	C32-C31-C30	-2.45	101.58	114.56
24	BA	5407	CLA	CGD-CBD-CHA	-2.45	107.98	113.65
30	AA	416	SQD	C36-C35-C34	2.44	127.54	114.56
24	AB	604	CLA	C3A-C2A-C1A	2.44	105.67	101.70
27	BX	5101	BCR	C28-C27-C26	2.44	117.83	113.81
30	AF	102	SQD	O47-C7-C8	2.44	116.75	111.54
24	BB	5615	CLA	C7-C6-C5	-2.44	105.84	112.97
34	BD	5403	PHO	C4B-C3B-C2B	-2.44	104.68	107.03
28	BC	5517	DGD	C8A-C7A-C6A	-2.44	101.60	114.56
24	BB	5615	CLA	CED-O2D-CGD	2.44	121.81	116.00
27	AB	617	BCR	C12-C13-C14	-2.44	115.22	118.98
24	AB	605	CLA	C2C-C1C-NC	-2.44	108.25	110.22
24	BC	5502	CLA	C4D-C3D-C2D	-2.44	104.21	107.17
27	BB	5623	BCR	C1-C6-C7	2.44	122.45	115.69
34	AD	403	PHO	C4D-CHA-CBD	-2.44	105.22	107.88
28	BA	5412	DGD	C5A-C4A-C3A	-2.44	101.62	114.56
31	AC	521	LMG	C12-C11-C10	2.44	122.98	113.51
24	BC	5504	CLA	CBD-CHA-C1A	2.44	131.96	128.77
24	AC	502	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
24	BB	5609	CLA	CBD-CHA-C1A	2.44	131.96	128.77
24	AC	506	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
32	AI	103	LMT	C1B-C2B-C3B	2.43	114.70	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AB	627	SQD	C3-C4-C5	-2.43	105.80	110.17
24	BC	5504	CLA	OBD-CAD-C3D	2.43	133.07	128.15
24	AC	504	CLA	CBD-CHA-C1A	2.43	131.95	128.77
24	AA	407	CLA	C2C-C1C-NC	-2.43	108.26	110.22
24	BB	5610	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
24	AB	615	CLA	C2A-C1A-NA	-2.43	108.22	111.33
27	AC	514	BCR	C8-C7-C6	2.43	134.41	127.23
24	BC	5509	CLA	O2D-CGD-CBD	2.43	116.26	111.34
24	BD	5402	CLA	C6-C7-C8	-2.43	107.88	115.44
24	BD	5405	CLA	CBD-CHA-C1A	2.43	131.95	128.77
27	AC	515	BCR	C36-C18-C19	2.43	122.02	118.09
28	BC	5517	DGD	C3A-C2A-C1A	2.43	122.94	113.51
24	AA	406	CLA	OBD-CAD-C3D	2.43	133.06	128.15
24	AB	616	CLA	CBD-CHA-C1A	2.43	131.94	128.77
24	AB	616	CLA	C2A-C1A-NA	-2.43	108.23	111.33
24	BC	5506	CLA	O2D-CGD-CBD	2.43	116.25	111.34
24	AB	611	CLA	C4B-C3B-C2B	-2.43	104.55	107.04
24	BB	5616	CLA	O1D-CGD-CBD	-2.43	119.49	124.45
31	AA	417	LMG	C22-C21-C20	2.43	119.88	112.94
24	BB	5609	CLA	CAA-CBA-CGA	-2.43	106.09	113.24
24	BB	5615	CLA	C5-C3-C2	2.43	125.73	121.06
24	AC	510	CLA	CED-O2D-CGD	2.43	121.78	116.00
24	AC	507	CLA	C11-C12-C13	2.42	122.98	115.44
24	BB	5617	CLA	CBD-CHA-C1A	2.42	131.94	128.77
34	AD	402	PHO	C3A-C2A-C1A	2.42	105.03	101.90
24	AA	405	CLA	CAA-C2A-C3A	-2.42	107.25	113.32
24	AC	505	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
27	BC	5514	BCR	C40-C30-C25	2.43	114.34	110.33
28	AB	628	DGD	C4A-C3A-C2A	-2.42	104.30	113.28
24	BA	5406	CLA	C4D-C3D-C2D	-2.42	104.23	107.17
24	BC	5502	CLA	CED-O2D-CGD	2.42	121.77	116.00
24	BB	5608	CLA	O2A-CGA-O1A	-2.42	117.15	123.48
24	BC	5513	CLA	C3D-CAD-CBD	-2.42	104.17	107.60
34	AD	402	PHO	O2A-CGA-CBA	2.42	119.30	111.90
31	BB	5624	LMG	C7-O1-C1	-2.42	108.95	113.80
24	AC	507	CLA	CHD-C4C-NC	2.42	125.97	124.28
24	BB	5616	CLA	C3D-CAD-CBD	-2.42	104.18	107.60
34	AD	402	PHO	C3A-C4A-CHB	2.41	126.46	121.69
31	AC	520	LMG	C13-C12-C11	2.41	122.22	113.28
24	AD	401	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
24	AB	610	CLA	C4D-C3D-C2D	-2.41	104.24	107.17
24	BB	5617	CLA	CED-O2D-CGD	2.41	121.74	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5606	CLA	C4B-C3B-C2B	-2.41	104.56	107.04
24	AC	508	CLA	CBD-CHA-C1A	2.41	131.92	128.77
24	AB	601	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
27	BX	5101	BCR	C16-C17-C18	2.41	130.78	127.29
24	BB	5611	CLA	C11-C12-C13	2.41	122.94	115.44
30	BB	5625	SQD	C15-C14-C13	2.41	127.36	114.56
24	BC	5511	CLA	CGD-CBD-CHA	-2.41	108.07	113.65
24	BB	5614	CLA	C4D-C3D-C2D	-2.41	104.24	107.17
24	BC	5508	CLA	CBD-CHA-C1A	2.41	131.92	128.77
24	BC	5510	CLA	CED-O2D-CGD	2.41	121.74	116.00
24	AB	607	CLA	C11-C12-C13	2.41	122.94	115.44
27	AB	617	BCR	C11-C10-C9	2.41	130.77	127.29
27	AC	516	BCR	C24-C23-C22	2.41	129.82	126.22
24	AC	510	CLA	C4D-C3D-C2D	-2.41	104.24	107.17
24	BB	5605	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
31	BD	5408	LMG	C36-C35-C34	-2.41	101.78	114.56
34	BD	5403	PHO	CED-O2D-CGD	2.41	121.73	116.00
30	BA	5401	SQD	O47-C7-C8	2.41	116.67	111.54
27	BC	5516	BCR	C30-C25-C24	2.41	122.36	115.69
24	AB	602	CLA	CBD-CHA-C1A	2.41	131.91	128.77
24	AC	512	CLA	C3D-CAD-CBD	-2.41	104.19	107.60
24	AC	513	CLA	C3D-CAD-CBD	-2.40	104.20	107.60
28	AC	517	DGD	O2G-C2G-C1G	-2.40	99.61	108.50
24	BA	5405	CLA	CED-O2D-CGD	2.40	121.72	116.00
31	BM	5102	LMG	O7-C10-O9	-2.40	117.25	123.66
24	BB	5609	CLA	C2A-C1A-CHA	2.40	128.25	123.87
24	AB	603	CLA	C2B-C1B-CHB	-2.40	121.44	126.00
24	AD	401	CLA	O2A-CGA-O1A	-2.40	117.20	123.48
28	AC	518	DGD	C5A-C4A-C3A	2.40	127.32	114.56
27	AB	617	BCR	C1-C6-C5	-2.40	119.11	122.59
24	BC	5506	CLA	C4D-C3D-C2D	-2.40	104.25	107.17
24	AC	507	CLA	CED-O2D-CGD	2.40	121.72	116.00
24	AB	611	CLA	CAA-CBA-CGA	-2.40	106.17	113.24
24	BB	5616	CLA	CAA-C2A-C1A	-2.40	106.15	112.51
24	AC	508	CLA	CAA-CBA-CGA	-2.40	106.17	113.24
27	AB	617	BCR	C37-C22-C23	2.40	121.97	118.09
28	BC	5518	DGD	C5A-C4A-C3A	2.40	127.31	114.56
24	AA	404	CLA	OBD-CAD-C3D	2.40	133.00	128.15
24	BC	5505	CLA	C4B-C3B-C2B	-2.40	104.58	107.04
24	AB	608	CLA	C2D-C3D-CAD	2.40	144.71	134.94
24	AB	611	CLA	OBD-CAD-C3D	2.39	132.99	128.15
24	BB	5612	CLA	C2D-C3D-CAD	2.39	144.70	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5402	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
34	AD	403	PHO	C3A-C4A-NA	-2.39	109.47	113.57
30	AB	622	SQD	C15-C14-C13	2.39	127.27	114.56
36	BF	5101	HEM	C2D-C1D-ND	-2.39	110.10	112.93
24	BA	5408	CLA	C2C-C1C-NC	-2.39	108.29	110.22
31	AC	521	LMG	C9-C8-C7	2.39	117.35	111.86
27	BC	5514	BCR	C32-C1-C6	2.39	114.29	110.33
24	AC	509	CLA	O2D-CGD-CBD	2.39	116.17	111.34
24	AB	607	CLA	C2B-C1B-NB	2.39	111.09	109.50
24	AB	604	CLA	C6-C7-C8	-2.39	108.00	115.44
27	AC	514	BCR	C32-C1-C6	2.39	114.28	110.33
24	AC	502	CLA	C2C-C1C-NC	-2.39	108.29	110.22
24	BB	5612	CLA	C2A-C1A-CHA	2.38	128.22	123.87
24	BD	5405	CLA	C2A-C1A-CHA	2.38	128.21	123.87
27	BC	5515	BCR	C36-C18-C19	2.38	121.94	118.09
27	AC	516	BCR	C30-C25-C24	2.38	122.30	115.69
27	BD	5407	BCR	C34-C9-C8	2.38	121.94	118.09
24	AB	612	CLA	C3D-CAD-CBD	-2.38	104.23	107.60
31	BD	5408	LMG	C32-C31-C30	-2.38	101.92	114.56
31	BB	5624	LMG	C13-C12-C11	2.38	122.10	113.28
24	BC	5509	CLA	C1D-CHD-C4C	2.38	126.29	122.60
24	BC	5505	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
31	AD	408	LMG	O7-C8-C9	-2.38	99.70	108.50
24	AB	610	CLA	CED-O2D-CGD	2.38	121.66	116.00
24	AB	613	CLA	C1D-CHD-C4C	2.38	126.29	122.60
24	AC	508	CLA	O2A-CGA-O1A	-2.38	117.26	123.48
24	BB	5609	CLA	C2A-C1A-NA	-2.38	108.29	111.33
27	AD	406	BCR	C36-C18-C19	2.38	121.93	118.09
27	BB	5622	BCR	C32-C1-C6	2.38	114.27	110.33
30	AA	413	SQD	O8-S-O9	-2.38	106.40	111.69
24	AD	404	CLA	C4D-C3D-C2D	-2.38	104.28	107.17
24	AA	404	CLA	C3A-C2A-C1A	2.38	105.56	101.70
24	AA	405	CLA	C4B-C3B-C2B	-2.37	104.60	107.04
31	AC	521	LMG	C15-C14-C13	-2.38	101.95	114.56
24	BA	5407	CLA	C3A-C2A-C1A	2.38	105.56	101.70
27	AB	617	BCR	C19-C18-C17	-2.38	115.32	118.98
30	BA	5401	SQD	C36-C35-C34	2.37	127.17	114.56
24	BB	5616	CLA	CAA-CBA-CGA	-2.37	106.25	113.24
24	AB	605	CLA	C2A-C1A-CHA	2.37	128.19	123.87
24	BC	5512	CLA	C2A-C1A-NA	-2.37	108.30	111.33
30	AF	102	SQD	O8-S-O9	-2.37	106.41	111.69
27	AB	619	BCR	C1-C6-C7	2.37	122.26	115.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BB	5627	LMT	C4-C3-C2	-2.37	101.98	114.56
24	BB	5611	CLA	C2B-C1B-NB	2.37	111.08	109.50
24	AB	616	CLA	C4D-C3D-C2D	-2.37	104.30	107.17
27	BB	5621	BCR	C8-C9-C10	-2.37	115.33	118.98
24	AA	407	CLA	OBD-CAD-C3D	2.37	132.94	128.15
24	BC	5506	CLA	C2A-C1A-NA	-2.37	108.31	111.33
24	AA	406	CLA	C3D-CAD-CBD	-2.37	104.25	107.60
28	BC	5519	DGD	C1E-O6E-C5E	2.37	118.31	113.73
24	AA	406	CLA	C2C-C1C-NC	-2.36	108.31	110.22
31	BC	5521	LMG	C12-C11-C10	2.36	122.69	113.51
30	BF	5102	SQD	C3-C4-C5	-2.36	105.93	110.17
28	BE	5102	DGD	C3G-C2G-C1G	2.36	117.28	111.86
24	BB	5620	CLA	C2A-C1A-NA	-2.36	108.31	111.33
24	BB	5609	CLA	C4D-C3D-C2D	-2.36	104.30	107.17
24	AC	504	CLA	OBD-CAD-C3D	2.36	132.92	128.15
24	AB	612	CLA	CAA-CBA-CGA	-2.36	106.29	113.24
24	AD	404	CLA	CBD-CHA-C1A	2.36	131.85	128.77
28	AC	518	DGD	CBA-CAA-C9A	-2.36	102.03	114.56
24	BA	5407	CLA	CAA-CBA-CGA	-2.36	106.29	113.24
34	BD	5403	PHO	C4D-C3D-C2D	-2.36	104.19	107.01
24	BA	5407	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
28	BC	5518	DGD	CBA-CAA-C9A	-2.36	102.05	114.56
31	BC	5521	LMG	C15-C14-C13	-2.36	102.05	114.56
34	AD	402	PHO	OBD-CAD-C3D	2.36	132.91	128.15
28	AB	628	DGD	O2G-C2G-C3G	2.35	117.21	108.50
24	AC	503	CLA	C6-C5-C3	2.35	117.99	112.62
31	AB	621	LMG	C13-C12-C11	2.35	122.00	113.28
24	BC	5511	CLA	C3D-CAD-CBD	-2.35	104.27	107.60
24	AB	612	CLA	O1D-CGD-CBD	-2.35	119.65	124.45
24	AD	404	CLA	C2A-C1A-CHA	2.35	128.16	123.87
24	AA	404	CLA	C2D-C3D-CAD	2.35	144.53	134.94
27	BT	5101	BCR	C37-C22-C23	2.35	121.89	118.09
24	AB	607	CLA	O2D-CGD-CBD	2.35	116.09	111.34
31	AB	620	LMG	O7-C8-C9	-2.35	99.81	108.50
24	AA	405	CLA	C2B-C1B-NB	2.35	111.07	109.50
31	BC	5520	LMG	O1-C7-C8	-2.35	105.40	110.99
24	AC	511	CLA	C3D-CAD-CBD	-2.35	104.28	107.60
24	AB	615	CLA	CED-O2D-CGD	2.35	121.59	116.00
31	BB	5624	LMG	C40-C39-C38	-2.35	102.10	114.56
24	AC	511	CLA	CGD-CBD-CHA	-2.35	108.21	113.65
24	AC	503	CLA	C2A-C1A-CHA	2.35	128.15	123.87
28	BB	5602	DGD	C4A-C3A-C2A	-2.35	104.59	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BD	5404	PHO	C6-C7-C8	-2.35	108.14	115.44
24	BA	5407	CLA	OBD-CAD-C3D	2.35	132.89	128.15
24	AC	506	CLA	CGD-CBD-CHA	-2.34	108.22	113.65
24	AD	401	CLA	C4B-C3B-C2B	-2.34	104.63	107.04
24	AB	610	CLA	C4B-C3B-C2B	-2.34	104.63	107.04
24	BC	5509	CLA	C3D-CAD-CBD	-2.34	104.28	107.60
30	AA	416	SQD	O47-C7-C8	2.34	116.53	111.54
24	AB	611	CLA	C2D-C3D-CAD	2.34	144.48	134.94
24	AA	407	CLA	CBD-CHA-C1A	2.34	131.83	128.77
24	AC	501	CLA	O2A-CGA-O1A	-2.34	117.36	123.48
27	BK	5102	BCR	C15-C14-C13	2.34	130.67	127.29
24	AC	507	CLA	C4D-C3D-C2D	-2.34	104.33	107.17
31	BD	5409	LMG	O8-C28-C29	2.34	119.05	111.90
24	BA	5405	CLA	OBD-CAD-C3D	2.34	132.88	128.15
24	BC	5505	CLA	C2A-C1A-CHA	2.34	128.13	123.87
34	BD	5404	PHO	C4-C3-C5	-2.34	111.84	115.39
24	BB	5607	CLA	C2B-C1B-CHB	-2.34	121.57	126.00
32	AB	624	LMT	C4-C3-C2	-2.34	102.15	114.56
24	BB	5615	CLA	OBD-CAD-C3D	2.33	132.87	128.15
27	BA	5411	BCR	C30-C25-C24	2.33	122.15	115.69
24	AB	608	CLA	C2A-C1A-CHA	2.33	128.12	123.87
28	BC	5519	DGD	O1G-C1A-O1A	-2.33	117.38	123.48
27	BA	5411	BCR	C16-C17-C18	2.33	130.66	127.29
31	AB	621	LMG	C40-C39-C38	-2.33	102.18	114.56
27	AA	410	BCR	C30-C25-C24	2.33	122.14	115.69
24	BB	5611	CLA	C3D-CAD-CBD	-2.33	104.30	107.60
28	AC	519	DGD	O3G-C3G-C2G	2.33	116.53	110.99
24	BB	5613	CLA	CGD-CBD-CHA	-2.33	108.25	113.65
27	AJ	101	BCR	C3-C4-C5	2.33	117.64	113.81
24	AB	612	CLA	C2A-C1A-NA	-2.33	108.36	111.33
28	BC	5517	DGD	CBA-CAA-C9A	-2.33	102.21	114.56
31	AD	408	LMG	O8-C9-C8	-2.33	102.68	108.80
24	BB	5611	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
28	BH	5101	DGD	C1G-O1G-C1A	2.32	123.63	116.99
27	AB	618	BCR	C32-C1-C6	2.32	114.17	110.33
24	BC	5508	CLA	O2A-CGA-O1A	-2.32	117.41	123.48
27	BA	5411	BCR	C36-C18-C19	2.32	121.84	118.09
31	AD	407	LMG	C39-C38-C37	2.32	126.90	114.56
24	BC	5506	CLA	CGD-CBD-CHA	-2.32	108.27	113.65
24	AC	513	CLA	CHD-C4C-NC	2.32	125.91	124.28
24	AC	510	CLA	CBD-CHA-C1A	2.32	131.81	128.77
34	BD	5404	PHO	O1D-CGD-CBD	-2.32	119.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5613	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
31	BL	5101	LMG	O7-C8-C9	-2.32	99.92	108.50
24	BC	5503	CLA	C4B-C3B-C2B	-2.32	104.66	107.04
24	AB	614	CLA	C4D-C3D-C2D	-2.32	104.35	107.17
24	AC	509	CLA	CBA-CAA-C2A	2.32	119.62	113.95
24	AC	510	CLA	O2A-CGA-O1A	-2.32	117.42	123.48
24	BC	5513	CLA	CHD-C4C-NC	2.32	125.90	124.28
24	BB	5611	CLA	O2D-CGD-CBD	2.32	116.03	111.34
24	AC	503	CLA	O1D-CGD-CBD	-2.32	119.72	124.45
24	BB	5620	CLA	C4D-C3D-C2D	-2.32	104.36	107.17
24	BB	5616	CLA	C2A-C1A-NA	-2.32	108.37	111.33
24	AB	604	CLA	O2D-CGD-CBD	2.32	116.02	111.34
30	BA	5414	SQD	C15-C14-C13	2.32	126.86	114.56
24	BA	5408	CLA	C2A-C1A-NA	-2.32	108.37	111.33
27	BJ	5101	BCR	C16-C17-C18	2.31	130.63	127.29
31	BD	5410	LMG	O8-C9-C8	-2.31	102.71	108.80
27	AJ	101	BCR	C28-C27-C26	2.31	117.61	113.81
24	BB	5614	CLA	CBD-CHA-C1A	2.31	131.79	128.77
24	AA	405	CLA	C4-C3-C5	-2.31	111.88	115.39
27	BC	5516	BCR	C19-C18-C17	-2.31	115.42	118.98
34	AD	403	PHO	O1D-CGD-CBD	-2.31	119.73	124.45
24	AB	602	CLA	C3A-C2A-C1A	2.31	105.46	101.70
24	BC	5503	CLA	C6-C5-C3	2.31	117.90	112.62
28	AC	517	DGD	CBA-CAA-C9A	-2.31	102.29	114.56
24	AC	504	CLA	C2D-C3D-CAD	2.31	144.36	134.94
34	BD	5404	PHO	C3D-CAD-CBD	-2.31	104.33	107.60
31	BC	5520	LMG	C13-C12-C11	2.31	121.84	113.28
27	AA	410	BCR	C8-C9-C10	-2.31	115.42	118.98
27	BA	5411	BCR	C37-C22-C23	2.31	121.82	118.09
24	AA	407	CLA	C3D-CAD-CBD	-2.31	104.33	107.60
24	AC	513	CLA	C4D-C3D-C2D	-2.31	104.37	107.17
31	AM	101	LMG	C22-C21-C20	2.31	119.54	112.94
24	BB	5613	CLA	O2A-CGA-O1A	-2.31	117.45	123.48
27	AT	101	BCR	C37-C22-C23	2.30	121.81	118.09
31	BM	5102	LMG	C14-C13-C12	-2.30	102.33	114.56
24	BB	5615	CLA	CBD-CHA-C1A	2.30	131.78	128.77
24	BC	5512	CLA	C3A-C2A-C1A	2.30	105.44	101.70
24	AA	405	CLA	C2A-C1A-NA	-2.30	108.39	111.33
27	AX	101	BCR	C1-C6-C7	2.30	122.07	115.69
31	BD	5410	LMG	O7-C8-C9	-2.30	99.99	108.50
24	BB	5606	CLA	C2A-C1A-CHA	2.30	128.06	123.87
24	AB	606	CLA	C4D-C3D-C2D	-2.30	104.38	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	C4-C3-C5	-2.30	111.90	115.39
31	BC	5521	LMG	C34-C33-C32	2.30	126.78	114.56
31	BD	5409	LMG	C39-C38-C37	2.30	126.77	114.56
24	BC	5509	CLA	CBA-CAA-C2A	2.30	119.57	113.95
24	BB	5614	CLA	CHD-C4C-NC	2.30	125.89	124.28
24	AA	405	CLA	C2C-C1C-NC	-2.30	108.37	110.22
24	AB	611	CLA	O1D-CGD-CBD	-2.30	119.76	124.45
24	AD	401	CLA	CED-O2D-CGD	2.29	121.46	116.00
24	AA	404	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
24	BA	5408	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
24	AC	506	CLA	O2D-CGD-CBD	2.29	115.97	111.34
36	AF	101	HEM	C2D-C1D-ND	-2.29	110.22	112.93
27	AX	101	BCR	C36-C18-C19	2.29	121.80	118.09
24	AB	602	CLA	C2A-C1A-CHA	2.29	128.05	123.87
27	BC	5515	BCR	C34-C9-C8	2.29	121.80	118.09
24	AA	406	CLA	O1D-CGD-CBD	-2.29	119.77	124.45
24	AC	508	CLA	O1D-CGD-CBD	-2.29	119.77	124.45
27	AC	516	BCR	C23-C22-C21	-2.29	115.45	118.98
30	AA	413	SQD	C15-C14-C13	2.29	126.72	114.56
24	AB	608	CLA	C4B-C3B-C2B	-2.29	104.69	107.04
24	BD	5402	CLA	C4B-C3B-C2B	-2.29	104.69	107.04
27	BA	5411	BCR	C8-C9-C10	-2.28	115.46	118.98
24	AC	509	CLA	C3A-C2A-C1A	2.28	105.41	101.70
28	BB	5602	DGD	O2G-C2G-C3G	2.29	116.96	108.50
36	BF	5101	HEM	C4D-ND-C1D	2.28	107.48	105.11
28	AB	628	DGD	C6B-C5B-C4B	-2.28	102.44	114.56
24	BC	5503	CLA	C4D-C3D-C2D	-2.28	104.40	107.17
24	AB	614	CLA	C3A-C2A-C1A	2.28	105.41	101.70
24	BC	5504	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
24	AB	601	CLA	C4B-C3B-C2B	-2.28	104.69	107.04
31	AM	101	LMG	C14-C13-C12	-2.28	102.44	114.56
24	AB	604	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
24	AC	506	CLA	C4D-C3D-C2D	-2.28	104.40	107.17
27	AB	618	BCR	C23-C22-C21	-2.28	115.47	118.98
24	AC	511	CLA	C4D-C3D-C2D	-2.28	104.40	107.17
24	BA	5405	CLA	C3A-C2A-C1A	2.28	105.41	101.70
24	AC	510	CLA	O1D-CGD-CBD	-2.28	119.79	124.45
24	BC	5511	CLA	CAA-CBA-CGA	-2.28	106.53	113.24
27	BB	5623	BCR	C35-C13-C12	2.28	121.77	118.09
31	BM	5102	LMG	C22-C21-C20	2.28	119.45	112.94
31	AJ	102	LMG	C36-C35-C34	-2.28	102.47	114.56
24	BA	5405	CLA	C2A-C1A-CHA	2.28	128.02	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5508	CLA	C2A-C1A-CHA	2.28	128.02	123.87
24	BB	5609	CLA	CGD-CBD-CHA	-2.28	108.37	113.65
24	AC	511	CLA	CED-O2D-CGD	2.27	121.42	116.00
24	AC	503	CLA	CED-O2D-CGD	2.27	121.42	116.00
31	AC	521	LMG	C19-C18-C17	-2.27	102.48	114.56
31	AD	407	LMG	O8-C28-C29	2.27	118.86	111.90
24	BB	5615	CLA	C2D-C3D-CAD	2.27	144.22	134.94
27	AB	619	BCR	C12-C13-C14	-2.27	115.48	118.98
24	AC	506	CLA	C2A-C1A-NA	-2.27	108.43	111.33
28	BC	5517	DGD	O2G-C2G-C1G	-2.27	100.10	108.50
27	BC	5515	BCR	C37-C22-C23	2.27	121.76	118.09
24	BA	5407	CLA	C4B-C3B-C2B	-2.27	104.70	107.04
27	AC	515	BCR	C34-C9-C8	2.27	121.76	118.09
31	AC	521	LMG	C34-C33-C32	2.27	126.62	114.56
27	AA	410	BCR	C37-C22-C23	2.27	121.76	118.09
28	BE	5102	DGD	C5B-C4B-C3B	-2.27	102.52	114.56
27	AC	515	BCR	C15-C14-C13	2.27	130.57	127.29
28	BC	5518	DGD	O6D-C1D-O3G	2.27	115.33	109.93
24	AC	511	CLA	CAA-CBA-CGA	-2.27	106.56	113.24
24	AB	613	CLA	C3A-C2A-C1A	2.27	105.39	101.70
24	AC	501	CLA	C4B-C3B-C2B	-2.27	104.71	107.04
24	BB	5617	CLA	C6-C7-C8	-2.26	108.40	115.44
34	BD	5403	PHO	C3A-C4A-CHB	2.27	126.17	121.69
27	BC	5516	BCR	C36-C18-C19	2.26	121.75	118.09
27	AD	406	BCR	C8-C9-C10	-2.26	115.49	118.98
27	AK	102	BCR	C32-C1-C2	-2.26	99.78	108.78
27	AA	410	BCR	C1-C6-C7	2.26	121.97	115.69
30	AB	627	SQD	O47-C7-C8	2.26	116.36	111.54
24	AD	404	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
27	AA	410	BCR	C36-C18-C19	2.26	121.75	118.09
24	AB	615	CLA	C4D-C3D-C2D	-2.26	104.42	107.17
24	AB	611	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
24	AC	501	CLA	C4D-C3D-C2D	-2.26	104.42	107.17
24	AB	615	CLA	C4B-C3B-C2B	-2.26	104.72	107.04
24	BA	5407	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
24	BA	5408	CLA	O1D-CGD-CBD	-2.26	119.83	124.45
24	AC	508	CLA	C2A-C1A-CHA	2.26	127.99	123.87
27	AB	618	BCR	C1-C6-C7	2.26	121.95	115.69
27	AB	619	BCR	C37-C22-C23	2.26	121.74	118.09
34	AD	403	PHO	C3D-CAD-CBD	-2.26	104.41	107.60
27	BD	5407	BCR	C36-C18-C19	2.26	121.74	118.09
24	AA	405	CLA	CBD-CHA-C1A	2.26	131.72	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	609	CLA	C6-C7-C8	-2.25	108.43	115.44
24	AC	501	CLA	CAA-C2A-C3A	-2.25	107.68	113.32
24	BB	5613	CLA	OBD-CAD-C3D	2.25	132.71	128.15
27	AK	102	BCR	C15-C14-C13	2.25	130.55	127.29
27	BT	5101	BCR	C8-C7-C6	2.25	133.88	127.23
24	BA	5405	CLA	C2D-C3D-CAD	2.25	144.13	134.94
24	BB	5609	CLA	C2C-C1C-NC	-2.25	108.40	110.22
24	BB	5616	CLA	OBD-CAD-C3D	2.25	132.70	128.15
27	AB	619	BCR	C24-C23-C22	2.25	129.58	126.22
30	AF	102	SQD	C3-C4-C5	-2.25	106.13	110.17
27	AD	406	BCR	C19-C18-C17	-2.25	115.51	118.98
24	AC	501	CLA	C1D-CHD-C4C	2.25	126.09	122.60
27	BJ	5101	BCR	C28-C27-C26	2.25	117.51	113.81
27	AA	410	BCR	C12-C13-C14	-2.25	115.52	118.98
24	BD	5405	CLA	CAA-CBA-CGA	-2.25	106.62	113.24
31	BL	5101	LMG	C22-C23-C24	-2.25	104.69	113.73
24	AA	404	CLA	C6-C7-C8	-2.25	108.45	115.44
27	BT	5101	BCR	C40-C30-C25	2.25	114.05	110.33
24	BB	5608	CLA	O2D-CGD-CBD	2.25	115.88	111.34
31	AC	520	LMG	O1-C7-C8	-2.25	105.64	110.99
28	BH	5101	DGD	O2G-C1B-O1B	-2.24	117.67	123.66
24	AA	404	CLA	C2B-C1B-NB	2.25	111.00	109.50
28	BB	5602	DGD	C6B-C5B-C4B	-2.24	102.64	114.56
27	BJ	5101	BCR	C3-C4-C5	2.24	117.50	113.81
34	AD	402	PHO	C2D-C3D-CAD	2.24	144.08	134.94
24	BB	5610	CLA	OBD-CAD-C3D	2.24	132.68	128.15
24	AC	506	CLA	OBD-CAD-C3D	2.24	132.68	128.15
27	AJ	101	BCR	C40-C30-C25	2.24	114.04	110.33
24	BC	5504	CLA	C2D-C3D-CAD	2.24	144.08	134.94
31	AC	520	LMG	O9-C10-C11	-2.24	114.69	123.78
24	BB	5613	CLA	C2D-C3D-CAD	2.24	144.08	134.94
24	AB	611	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
24	AB	604	CLA	O2A-CGA-O1A	-2.24	117.62	123.48
24	BB	5610	CLA	C1D-CHD-C4C	2.24	126.07	122.60
24	AC	509	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
31	BC	5520	LMG	O9-C10-C11	-2.24	114.70	123.78
27	BT	5101	BCR	C20-C21-C22	2.24	130.53	127.29
27	AC	514	BCR	C15-C14-C13	2.24	130.53	127.29
24	AC	505	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
24	BA	5406	CLA	C4B-C3B-C2B	-2.24	104.74	107.04
24	AA	407	CLA	O2A-CGA-O1A	-2.24	117.63	123.48
24	BC	5509	CLA	C2A-C1A-NA	-2.24	108.47	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	416	SQD	C15-C14-C13	2.24	126.44	114.56
24	AB	605	CLA	CBD-CHA-C1A	2.24	131.69	128.77
30	BB	5601	SQD	O47-C7-C8	2.24	116.31	111.54
24	AB	602	CLA	C2D-C3D-CAD	2.24	144.06	134.94
34	BD	5404	PHO	C2A-C1A-NA	-2.24	108.48	111.93
24	BC	5511	CLA	CED-O2D-CGD	2.23	121.32	116.00
24	BB	5619	CLA	CED-O2D-CGD	2.23	121.32	116.00
24	AB	608	CLA	CED-O2D-CGD	2.24	121.32	116.00
24	AB	615	CLA	C1D-CHD-C4C	2.23	126.06	122.60
31	BD	5409	LMG	C32-C31-C30	-2.23	102.70	114.56
24	AA	406	CLA	C4B-C3B-C2B	-2.23	104.74	107.04
31	AC	520	LMG	O7-C10-O9	-2.23	117.70	123.66
24	AB	607	CLA	C2D-C3D-CAD	2.23	144.05	134.94
24	AC	505	CLA	C2D-C3D-CAD	2.23	144.05	134.94
24	BB	5612	CLA	C2C-C1C-NC	-2.23	108.42	110.22
27	AT	101	BCR	C8-C7-C6	2.23	133.82	127.23
35	BD	5406	PL9	C42-C41-C39	-2.23	105.38	112.75
28	AE	101	DGD	C5B-C4B-C3B	-2.23	102.71	114.56
24	BD	5405	CLA	C4B-C3B-C2B	-2.23	104.75	107.04
24	AD	401	CLA	C2D-C3D-CAD	2.23	144.03	134.94
24	AB	616	CLA	C4B-C3B-C2B	-2.23	104.75	107.04
24	AC	509	CLA	C2A-C1A-NA	-2.23	108.48	111.33
28	AC	517	DGD	C6B-C7B-C8B	-2.23	104.76	113.73
24	BB	5619	CLA	C1D-CHD-C4C	2.23	126.05	122.60
24	AB	611	CLA	C3D-CAD-CBD	-2.23	104.45	107.60
24	AB	609	CLA	CAA-C2A-C3A	-2.23	107.75	113.32
24	AA	406	CLA	C2D-C3D-CAD	2.22	144.01	134.94
24	AC	513	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
24	AC	512	CLA	C4D-C3D-C2D	-2.23	104.47	107.17
24	BB	5618	CLA	C4D-C3D-C2D	-2.23	104.47	107.17
27	AB	617	BCR	C8-C7-C6	2.23	133.80	127.23
27	AJ	101	BCR	C31-C1-C2	2.22	117.62	108.78
24	BC	5507	CLA	C4D-C3D-C2D	-2.22	104.47	107.17
24	BB	5606	CLA	C2D-C3D-CAD	2.22	144.01	134.94
27	BX	5101	BCR	C1-C6-C7	2.22	121.85	115.69
34	AD	403	PHO	C4D-C3D-CAD	2.22	112.02	107.67
24	BC	5503	CLA	CED-O2D-CGD	2.22	121.29	116.00
24	AA	407	CLA	C2D-C3D-CAD	2.22	144.00	134.94
24	BC	5501	CLA	C4B-C3B-C2B	-2.22	104.76	107.04
27	BJ	5101	BCR	C31-C1-C2	2.22	117.60	108.78
24	AB	607	CLA	C1D-CHD-C4C	2.22	126.04	122.60
30	BB	5601	SQD	O8-S-O9	-2.22	106.75	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	413	SQD	O8-S-O7	2.22	116.62	111.69
24	BB	5616	CLA	C2D-C3D-CAD	2.22	143.98	134.94
24	AC	502	CLA	C2D-C3D-CAD	2.22	143.98	134.94
27	BD	5407	BCR	C19-C18-C17	-2.22	115.56	118.98
31	BD	5409	LMG	C1-O6-C5	-2.21	109.45	113.73
24	AC	512	CLA	O2D-CGD-CBD	2.21	115.81	111.34
34	BD	5403	PHO	C4D-C3D-CAD	2.21	112.01	107.67
24	AB	609	CLA	C4D-C3D-C2D	-2.21	104.48	107.17
24	AB	603	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
27	AD	406	BCR	C15-C14-C13	2.21	130.49	127.29
31	AB	620	LMG	C22-C23-C24	-2.21	104.83	113.73
28	BC	5519	DGD	O2E-C2E-C3E	2.21	115.30	110.36
24	BA	5408	CLA	CED-O2D-CGD	2.21	121.27	116.00
24	BB	5612	CLA	OBD-CAD-C3D	2.21	132.62	128.15
24	BB	5614	CLA	C2D-C3D-CAD	2.21	143.96	134.94
24	BC	5506	CLA	OBD-CAD-C3D	2.21	132.62	128.15
24	AB	603	CLA	CED-O2D-CGD	2.21	121.26	116.00
24	BB	5613	CLA	C6-C7-C8	-2.21	108.56	115.44
24	BC	5507	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
31	BL	5101	LMG	C19-C18-C17	-2.21	102.83	114.56
27	BX	5101	BCR	C7-C8-C9	2.21	129.52	126.22
34	BD	5404	PHO	C4A-NA-C1A	2.21	111.33	108.42
34	BD	5404	PHO	C4D-C3D-CAD	2.21	112.00	107.67
24	AB	610	CLA	O1D-CGD-CBD	-2.21	119.94	124.45
24	BB	5618	CLA	C3A-C2A-C1A	2.21	105.29	101.70
24	BB	5606	CLA	C3A-C2A-C1A	2.21	105.28	101.70
24	AB	609	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
24	BB	5611	CLA	CMC-C2C-C1C	2.21	128.09	124.95
27	AC	515	BCR	C37-C22-C23	2.20	121.65	118.09
27	BT	5101	BCR	C40-C30-C29	-2.21	100.02	108.78
34	BD	5403	PHO	OBD-CAD-C3D	2.20	132.61	128.15
31	AC	520	LMG	C39-C38-C37	2.20	126.26	114.56
24	AB	604	CLA	C2D-C3D-CAD	2.20	143.93	134.94
24	AB	611	CLA	C4-C3-C5	-2.20	112.04	115.39
24	AB	613	CLA	C4D-C3D-C2D	-2.20	104.50	107.17
24	AC	512	CLA	C4B-C3B-C2B	-2.20	104.78	107.04
34	BD	5403	PHO	O1D-CGD-CBD	-2.20	119.95	124.45
24	BB	5614	CLA	C4B-C3B-C2B	-2.20	104.78	107.04
24	AA	407	CLA	C1D-CHD-C4C	2.20	126.01	122.60
24	BB	5607	CLA	O1D-CGD-CBD	-2.20	119.96	124.45
24	BA	5408	CLA	O2A-CGA-O1A	-2.20	117.73	123.48
24	AA	405	CLA	OBD-CAD-C3D	2.20	132.59	128.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	606	CLA	C4B-C3B-C2B	-2.20	104.78	107.04
24	BB	5616	CLA	C4B-C3B-C2B	-2.20	104.78	107.04
24	BA	5405	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
31	AD	407	LMG	C32-C31-C30	-2.20	102.89	114.56
27	BK	5102	BCR	C32-C1-C2	-2.20	100.04	108.78
24	BA	5406	CLA	C12-C11-C10	-2.20	102.16	113.00
27	BB	5621	BCR	C8-C7-C6	2.20	133.71	127.23
24	BC	5505	CLA	C2D-C3D-CAD	2.19	143.89	134.94
27	AB	618	BCR	C16-C17-C18	2.19	130.46	127.29
24	BC	5503	CLA	CAA-CBA-CGA	-2.19	106.78	113.24
27	BC	5516	BCR	C16-C17-C18	2.19	130.46	127.29
24	AB	602	CLA	CED-O2D-CGD	2.19	121.22	116.00
27	BK	5102	BCR	C23-C22-C21	-2.19	115.60	118.98
24	BC	5502	CLA	O1D-CGD-CBD	-2.19	119.98	124.45
24	BD	5405	CLA	C2A-C1A-NA	-2.19	108.53	111.33
28	AC	519	DGD	C5B-C4B-C3B	2.19	126.19	114.56
24	BC	5502	CLA	OBD-CAD-C3D	2.19	132.57	128.15
24	BD	5402	CLA	O2A-CGA-O1A	-2.19	117.76	123.48
31	BD	5409	LMG	C6-C5-C4	-2.19	107.70	113.04
24	BD	5402	CLA	CED-O2D-CGD	2.19	121.21	116.00
24	BB	5616	CLA	CAA-C2A-C3A	-2.19	107.84	113.32
24	BB	5615	CLA	O1D-CGD-CBD	-2.19	119.98	124.45
24	BB	5605	CLA	C4D-C3D-C2D	-2.19	104.51	107.17
24	AB	609	CLA	C2D-C3D-CAD	2.19	143.85	134.94
27	BB	5622	BCR	C16-C17-C18	2.19	130.45	127.29
24	BB	5617	CLA	C4D-C3D-C2D	-2.18	104.52	107.17
24	BD	5402	CLA	C4-C3-C5	-2.18	112.07	115.39
24	AC	513	CLA	OBD-CAD-C3D	2.18	132.57	128.15
27	BX	5101	BCR	C36-C18-C19	2.18	121.62	118.09
24	BA	5406	CLA	C2C-C1C-NC	-2.18	108.46	110.22
24	AB	616	CLA	C2D-C3D-CAD	2.18	143.84	134.94
24	BB	5618	CLA	C3D-CAD-CBD	-2.18	104.51	107.60
28	AE	101	DGD	C3G-C2G-C1G	2.18	116.86	111.86
24	BB	5615	CLA	CAA-CBA-CGA	-2.18	106.81	113.24
24	BB	5613	CLA	C2A-C1A-NA	-2.18	108.55	111.33
24	AB	612	CLA	C2D-C3D-CAD	2.18	143.82	134.94
28	AC	518	DGD	C1G-O1G-C1A	2.18	123.21	116.99
24	BC	5504	CLA	O1D-CGD-CBD	-2.18	120.00	124.45
24	AC	502	CLA	CAA-CBA-CGA	-2.18	106.82	113.24
36	BF	5101	HEM	O2D-CGD-CBD	2.18	121.72	114.19
27	AB	619	BCR	C23-C22-C21	-2.18	115.62	118.98
28	BC	5518	DGD	C1G-O1G-C1A	2.18	123.21	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5611	CLA	C2D-C3D-CAD	2.18	143.82	134.94
24	AB	614	CLA	C3D-CAD-CBD	-2.18	104.52	107.60
24	BB	5617	CLA	OBD-CAD-C3D	2.17	132.55	128.15
34	BD	5403	PHO	C2D-C3D-CAD	2.17	143.80	134.94
27	AX	101	BCR	C7-C8-C9	2.17	129.47	126.22
28	AC	518	DGD	CDB-CCB-CBB	-2.18	103.01	114.56
24	BC	5504	CLA	C2A-C1A-NA	-2.18	108.55	111.33
24	AD	401	CLA	O1D-CGD-CBD	-2.17	120.01	124.45
24	AC	511	CLA	OBD-CAD-C3D	2.17	132.55	128.15
24	AC	503	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
24	AC	510	CLA	C2D-C3D-CAD	2.17	143.81	134.94
24	BC	5512	CLA	C4D-C3D-C2D	-2.17	104.53	107.17
34	AD	402	PHO	C4D-C3D-CAD	2.17	111.92	107.67
30	BF	5102	SQD	C6-C5-C4	-2.17	107.28	111.86
24	AB	615	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
24	AB	611	CLA	C5-C3-C2	2.17	125.24	121.06
24	BC	5510	CLA	O2A-CGA-O1A	-2.17	117.80	123.48
27	BA	5411	BCR	C1-C6-C7	2.17	121.70	115.69
24	BB	5617	CLA	C2D-C3D-CAD	2.17	143.78	134.94
36	AF	101	HEM	C4D-ND-C1D	2.17	107.36	105.11
24	AA	407	CLA	CED-O2D-CGD	2.17	121.17	116.00
24	BC	5506	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
27	BB	5622	BCR	C37-C22-C23	2.17	121.60	118.09
28	AH	101	DGD	O2G-C1B-O1B	-2.17	117.87	123.66
34	AD	403	PHO	C4B-C3B-C2B	-2.17	104.95	107.03
24	BB	5615	CLA	C4B-C3B-C2B	-2.17	104.81	107.04
31	AB	620	LMG	C34-C33-C32	2.17	126.07	114.56
24	AA	405	CLA	O1D-CGD-CBD	-2.17	120.02	124.45
30	AB	627	SQD	O8-S-O9	-2.17	106.86	111.69
34	AD	403	PHO	CED-O2D-CGD	2.17	121.16	116.00
24	AB	602	CLA	OBD-CAD-C3D	2.17	132.53	128.15
28	BC	5518	DGD	O2G-C2G-C1G	2.17	116.53	108.50
24	BB	5620	CLA	C2D-C3D-CAD	2.17	143.77	134.94
24	AC	502	CLA	C3A-C2A-C1A	2.17	105.22	101.70
24	BC	5506	CLA	CBD-CHA-C1A	2.16	131.60	128.77
27	BB	5622	BCR	C23-C22-C21	-2.17	115.64	118.98
24	BB	5617	CLA	CBA-CAA-C2A	2.16	119.24	113.95
31	AB	620	LMG	C19-C18-C17	-2.16	103.08	114.56
30	AA	413	SQD	C35-C34-C33	2.16	119.12	112.94
27	AC	516	BCR	C36-C18-C19	2.16	121.58	118.09
31	BC	5521	LMG	C19-C18-C17	-2.16	103.07	114.56
24	AD	404	CLA	CMB-C2B-C1B	-2.16	125.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5613	CLA	C3D-CAD-CBD	-2.16	104.54	107.60
27	BC	5514	BCR	C30-C25-C24	2.16	121.68	115.69
24	BA	5408	CLA	CAA-C2A-C3A	-2.16	107.91	113.32
24	AB	603	CLA	C4D-C3D-C2D	-2.16	104.55	107.17
27	AA	410	BCR	C34-C9-C8	2.16	121.58	118.09
28	BC	5518	DGD	CDB-CCB-CBB	-2.16	103.09	114.56
24	BA	5406	CLA	CAA-C2A-C3A	-2.16	107.91	113.32
24	BB	5610	CLA	C4B-C3B-C2B	-2.16	104.82	107.04
24	AA	406	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
24	AB	608	CLA	OBD-CAD-C3D	2.16	132.52	128.15
30	BA	5401	SQD	C15-C14-C13	2.16	126.02	114.56
28	AC	518	DGD	C8B-C7B-C6B	-2.16	103.11	114.56
30	AF	102	SQD	C15-C14-C13	2.16	126.01	114.56
35	AD	405	PL9	C42-C41-C39	-2.16	105.62	112.75
24	BB	5619	CLA	C4B-C3B-C2B	-2.15	104.83	107.04
24	AB	610	CLA	C2D-C3D-CAD	2.15	143.73	134.94
24	AC	508	CLA	C2D-C3D-CAD	2.16	143.73	134.94
24	AC	510	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
24	BB	5617	CLA	C1D-CHD-C4C	2.15	125.94	122.60
30	BA	5401	SQD	O8-S-O9	-2.15	106.90	111.69
24	BD	5405	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
24	AB	605	CLA	C2D-C3D-CAD	2.15	143.72	134.94
24	BB	5612	CLA	CED-O2D-CGD	2.15	121.12	116.00
28	AA	411	DGD	C3G-C2G-C1G	2.15	116.79	111.86
27	AT	101	BCR	C28-C27-C26	2.15	117.35	113.81
31	AB	620	LMG	C17-C16-C15	-2.15	103.15	114.56
30	BF	5102	SQD	C15-C14-C13	2.15	125.97	114.56
27	AC	514	BCR	C28-C27-C26	2.15	117.34	113.81
35	BD	5406	PL9	C31-C29-C28	-2.15	116.93	121.06
24	BB	5609	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
34	BD	5404	PHO	CED-O2D-CGD	2.15	121.12	116.00
24	AB	612	CLA	C4B-C3B-C2B	-2.15	104.83	107.04
24	BD	5402	CLA	C3D-CAD-CBD	-2.15	104.56	107.60
24	BD	5405	CLA	C2D-C3D-CAD	2.15	143.70	134.94
24	AC	513	CLA	C2D-C3D-CAD	2.15	143.69	134.94
34	BD	5403	PHO	C4-C3-C5	-2.14	112.13	115.39
24	AB	610	CLA	C2A-C1A-NA	-2.14	108.59	111.33
24	BB	5606	CLA	CED-O2D-CGD	2.14	121.11	116.00
24	AC	502	CLA	OBD-CAD-C3D	2.14	132.49	128.15
24	AC	508	CLA	OBD-CAD-C3D	2.14	132.49	128.15
24	BA	5407	CLA	OBD-CAD-CBD	-2.14	122.70	125.94
28	BC	5518	DGD	C8B-C7B-C6B	-2.15	103.17	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	413	SQD	O47-C7-C8	2.14	116.11	111.54
24	AB	613	CLA	C2D-C3D-CAD	2.14	143.68	134.94
35	AD	405	PL9	C31-C29-C28	-2.14	116.94	121.06
24	AC	503	CLA	CAA-CBA-CGA	-2.14	106.93	113.24
24	BC	5506	CLA	C2D-C3D-CAD	2.14	143.67	134.94
28	BC	5519	DGD	C5B-C4B-C3B	2.14	125.94	114.56
27	BC	5515	BCR	C24-C23-C22	2.14	129.42	126.22
32	AM	102	LMT	O1B-C1B-C2B	2.14	113.23	108.11
27	AC	516	BCR	C19-C18-C17	-2.14	115.69	118.98
24	BC	5508	CLA	C2D-C3D-CAD	2.13	143.64	134.94
27	BA	5411	BCR	C34-C9-C8	2.13	121.54	118.09
24	BC	5506	CLA	C4B-C3B-C2B	-2.14	104.84	107.04
27	BJ	5101	BCR	C40-C30-C25	2.13	113.86	110.33
30	AA	416	SQD	C34-C33-C32	2.13	125.90	114.56
24	AC	512	CLA	C2A-C1A-NA	-2.13	108.60	111.33
24	AC	507	CLA	C2D-C3D-CAD	2.13	143.64	134.94
24	BD	5402	CLA	O1D-CGD-CBD	-2.13	120.09	124.45
28	BC	5518	DGD	C7A-C6A-C5A	2.13	125.89	114.56
24	AC	507	CLA	C3D-CAD-CBD	-2.13	104.58	107.60
24	AB	602	CLA	C4B-C3B-C2B	-2.13	104.85	107.04
24	AB	614	CLA	C2A-C1A-CHA	2.13	127.75	123.87
27	BB	5621	BCR	C11-C10-C9	2.13	130.37	127.29
24	BB	5608	CLA	C2D-C3D-CAD	2.13	143.62	134.94
24	BC	5502	CLA	C2D-C3D-CAD	2.13	143.62	134.94
24	BB	5612	CLA	C4B-C3B-C2B	-2.13	104.85	107.04
31	BL	5101	LMG	C17-C16-C15	-2.13	103.25	114.56
27	AC	514	BCR	C36-C18-C19	2.13	121.53	118.09
24	BA	5408	CLA	C2D-C3D-CAD	2.13	143.62	134.94
24	BC	5508	CLA	C3D-C4D-CHA	2.13	111.57	108.16
30	AA	416	SQD	O8-S-O9	-2.13	106.95	111.69
27	BC	5514	BCR	C8-C9-C10	-2.13	115.70	118.98
27	AB	619	BCR	C30-C25-C24	2.13	121.59	115.69
24	BC	5512	CLA	C4B-C3B-C2B	-2.13	104.85	107.04
24	AC	506	CLA	C2D-C3D-CAD	2.13	143.61	134.94
31	BA	5402	LMG	O1-C1-C2	2.13	110.88	108.15
24	AA	407	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
32	AI	103	LMT	C3'-C4'-C5'	-2.13	106.11	110.86
24	AB	606	CLA	OBD-CAD-C3D	2.12	132.45	128.15
24	BB	5619	CLA	C2C-C1C-NC	-2.12	108.51	110.22
24	AB	606	CLA	O2D-CGD-CBD	2.12	115.63	111.34
24	BB	5620	CLA	C4B-C3B-C2B	-2.12	104.86	107.04
31	AD	407	LMG	C14-C13-C12	2.12	125.84	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BC	5520	LMG	C39-C38-C37	2.12	125.84	114.56
24	AC	506	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
24	BB	5619	CLA	O1D-CGD-CBD	-2.12	120.12	124.45
27	BC	5515	BCR	C8-C9-C10	-2.12	115.71	118.98
24	AB	611	CLA	CBD-CHA-C1A	2.12	131.54	128.77
24	AB	614	CLA	OBD-CAD-C3D	2.12	132.44	128.15
24	AA	407	CLA	O1D-CGD-CBD	-2.12	120.12	124.45
24	AB	605	CLA	O1D-CGD-CBD	-2.12	120.12	124.45
24	BB	5618	CLA	CHD-C4C-NC	2.12	125.76	124.28
24	AB	602	CLA	O2A-CGA-O1A	-2.12	117.94	123.48
24	AC	503	CLA	OBD-CAD-C3D	2.12	132.43	128.15
24	BB	5606	CLA	CAA-CBA-CGA	-2.12	107.00	113.24
28	BB	5602	DGD	O5D-C6D-C5D	2.12	112.64	108.96
24	BA	5407	CLA	C2D-C3D-CAD	2.12	143.57	134.94
31	BC	5521	LMG	C17-C16-C15	-2.12	103.31	114.56
24	BC	5501	CLA	C4D-C3D-C2D	-2.12	104.60	107.17
24	AA	406	CLA	C3A-C2A-C1A	2.12	105.14	101.70
24	AC	508	CLA	C4B-C3B-C2B	-2.12	104.86	107.04
28	AC	517	DGD	O2G-C2G-C3G	2.12	116.34	108.50
30	AA	413	SQD	C6-C5-C4	-2.11	107.40	111.86
24	AB	612	CLA	CHD-C4C-NC	2.11	125.76	124.28
24	AB	610	CLA	OBD-CAD-C3D	2.11	132.43	128.15
27	BC	5515	BCR	C7-C8-C9	2.11	129.38	126.22
24	AB	613	CLA	C4B-C3B-C2B	-2.11	104.87	107.04
27	BT	5101	BCR	C28-C27-C26	2.11	117.29	113.81
27	BB	5623	BCR	C37-C22-C23	2.11	121.50	118.09
28	AH	101	DGD	O2G-C2G-C3G	2.11	116.33	108.50
24	AB	606	CLA	C1D-CHD-C4C	2.11	125.88	122.60
27	BB	5621	BCR	C24-C23-C22	2.11	129.38	126.22
24	BB	5609	CLA	C4B-C3B-C2B	-2.11	104.87	107.04
24	BB	5609	CLA	C2D-C3D-CAD	2.11	143.56	134.94
28	BC	5519	DGD	O3G-C3G-C2G	2.11	116.02	110.99
24	BB	5609	CLA	O1D-CGD-CBD	-2.11	120.13	124.45
24	AC	504	CLA	C2A-C1A-NA	-2.11	108.63	111.33
24	BC	5501	CLA	C1D-CHD-C4C	2.11	125.87	122.60
32	AB	624	LMT	C1'-O5'-C5'	-2.11	109.65	113.73
28	BH	5101	DGD	O2G-C2G-C3G	2.11	116.31	108.50
24	AA	405	CLA	C2A-C1A-CHA	2.11	127.72	123.87
24	BB	5613	CLA	OBD-CAD-CBD	-2.11	122.75	125.94
24	BC	5511	CLA	C3A-C2A-C1A	2.11	105.13	101.70
24	BA	5405	CLA	C2C-C1C-NC	-2.11	108.52	110.22
31	BL	5101	LMG	C34-C33-C32	2.11	125.75	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AC	520	LMG	O7-C8-C9	2.11	116.30	108.50
27	AT	101	BCR	C40-C30-C29	-2.11	100.41	108.78
30	BA	5401	SQD	C34-C33-C32	2.10	125.74	114.56
28	BA	5412	DGD	O1A-C1A-C2A	-2.10	115.25	123.78
24	AB	608	CLA	C5-C3-C2	2.10	125.11	121.06
27	BB	5621	BCR	C34-C9-C8	2.10	121.49	118.09
27	AC	516	BCR	C12-C13-C14	-2.10	115.74	118.98
24	BC	5501	CLA	CAA-C2A-C3A	-2.10	108.06	113.32
34	AD	403	PHO	C4A-NA-C1A	2.10	111.19	108.42
24	BC	5503	CLA	OBD-CAD-C3D	2.10	132.40	128.15
27	BT	5101	BCR	C34-C9-C8	2.10	121.49	118.09
24	BA	5405	CLA	C4B-C3B-C2B	-2.10	104.88	107.04
24	BC	5503	CLA	C2A-C1A-CHA	2.10	127.70	123.87
31	AC	520	LMG	O1-C1-C2	-2.10	105.46	108.15
24	AB	607	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
27	AA	410	BCR	C19-C18-C17	-2.10	115.74	118.98
24	BB	5618	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
34	AD	402	PHO	CED-O2D-CGD	2.10	121.00	116.00
24	AC	506	CLA	CBD-CHA-C1A	2.10	131.51	128.77
24	AB	612	CLA	OBD-CAD-C3D	2.10	132.39	128.15
28	AH	101	DGD	C1G-O1G-C1A	2.10	122.98	116.99
24	AB	613	CLA	O2D-CGD-CBD	2.10	115.58	111.34
27	BB	5623	BCR	C23-C22-C21	-2.10	115.75	118.98
32	BM	5101	LMT	O1B-C1B-C2B	2.10	113.13	108.11
24	AC	512	CLA	C1D-CHD-C4C	2.10	125.85	122.60
27	BX	5101	BCR	C37-C22-C23	2.10	121.48	118.09
24	BD	5405	CLA	O1D-CGD-CBD	-2.09	120.17	124.45
24	BC	5509	CLA	C4B-C3B-C2B	-2.09	104.89	107.04
27	BX	5101	BCR	C34-C9-C8	2.09	121.47	118.09
27	AJ	101	BCR	C30-C25-C24	2.09	121.49	115.69
24	AB	606	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
24	BD	5405	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
24	AA	406	CLA	CBD-CHA-C1A	2.09	131.51	128.77
24	BC	5507	CLA	O1D-CGD-CBD	-2.09	120.18	124.45
24	AD	401	CLA	C3A-C2A-C1A	2.09	105.10	101.70
24	AD	404	CLA	C2D-C3D-CAD	2.09	143.47	134.94
31	BM	5102	LMG	C6-C5-C4	-2.09	107.93	113.04
24	BC	5512	CLA	O2D-CGD-CBD	2.09	115.56	111.34
24	AB	613	CLA	CBA-CAA-C2A	2.09	119.06	113.95
34	BD	5404	PHO	C4B-C3B-C2B	-2.09	105.02	107.03
31	AM	101	LMG	C6-C5-C4	-2.09	107.94	113.04
24	BB	5607	CLA	C4D-C3D-C2D	-2.09	104.63	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5402	CLA	C3A-C2A-C1A	2.09	105.09	101.70
24	BB	5620	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
31	BD	5409	LMG	C14-C13-C12	2.09	125.65	114.56
31	AC	520	LMG	O8-C28-C29	2.09	118.29	111.90
28	BC	5518	DGD	O6E-C1E-C2E	2.09	114.58	110.30
24	AB	601	CLA	C3A-C2A-C1A	2.09	105.09	101.70
27	BC	5514	BCR	C36-C18-C19	2.09	121.46	118.09
31	BC	5520	LMG	O1-C1-C2	-2.09	105.48	108.15
31	BC	5520	LMG	O7-C8-C9	2.09	116.23	108.50
28	AC	518	DGD	C7A-C6A-C5A	2.09	125.64	114.56
24	AB	616	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
24	AC	507	CLA	C3A-C2A-C1A	2.09	105.09	101.70
24	AC	503	CLA	C2D-C3D-CAD	2.09	143.44	134.94
24	AC	503	CLA	C4-C3-C5	-2.09	112.22	115.39
30	BA	5414	SQD	C35-C34-C33	2.09	118.91	112.94
27	AK	102	BCR	C19-C18-C17	-2.09	115.77	118.98
27	AB	618	BCR	C37-C22-C23	2.09	121.46	118.09
24	AC	504	CLA	C4B-C3B-C2B	-2.08	104.90	107.04
24	BC	5508	CLA	C4B-C3B-C2B	-2.08	104.90	107.04
31	AC	521	LMG	O1-C7-C8	2.08	115.94	110.99
24	AC	502	CLA	O1D-CGD-CBD	-2.08	120.19	124.45
30	BA	5401	SQD	C17-C16-C15	2.08	125.61	114.56
24	BB	5614	CLA	C2A-C1A-NA	-2.08	108.68	111.33
27	BB	5623	BCR	C30-C25-C24	2.08	121.45	115.69
24	BC	5503	CLA	C4-C3-C5	-2.08	112.23	115.39
36	BF	5101	HEM	C2A-C1A-NA	2.08	112.62	109.73
27	AC	514	BCR	C30-C25-C24	2.08	121.45	115.69
24	AB	605	CLA	C2A-C1A-NA	-2.08	108.68	111.33
24	BC	5513	CLA	C3A-C2A-C1A	2.08	105.08	101.70
24	BB	5608	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
24	BC	5510	CLA	C4D-C3D-C2D	-2.08	104.65	107.17
27	AT	101	BCR	C34-C9-C8	2.08	121.45	118.09
27	AJ	101	BCR	C16-C17-C18	2.08	130.29	127.29
24	AB	614	CLA	C2D-C3D-CAD	2.08	143.40	134.94
24	AC	507	CLA	C2A-C1A-NA	-2.07	108.68	111.33
24	BB	5610	CLA	C2D-C3D-CAD	2.07	143.39	134.94
24	AB	613	CLA	OBD-CAD-C3D	2.07	132.34	128.15
24	BC	5502	CLA	C2C-C1C-NC	-2.07	108.55	110.22
24	BB	5606	CLA	OBD-CAD-C3D	2.07	132.34	128.15
24	AB	609	CLA	C3D-CAD-CBD	-2.07	104.67	107.60
24	AC	505	CLA	C1D-CHD-C4C	2.07	125.81	122.60
31	BC	5520	LMG	C6-C5-C4	-2.07	107.98	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	OBD-CAD-C3D	2.07	132.34	128.15
24	AA	405	CLA	C12-C11-C10	-2.07	102.80	113.00
24	BB	5608	CLA	C2C-C1C-NC	-2.07	108.55	110.22
24	BD	5402	CLA	C2D-C3D-CAD	2.07	143.38	134.94
24	AB	609	CLA	O2A-CGA-O1A	-2.07	118.07	123.48
32	BC	5522	LMT	C6B-C5B-C4B	2.07	118.11	113.04
36	AF	101	HEM	O2D-CGD-CBD	2.07	121.34	114.19
24	BB	5614	CLA	CED-O2D-CGD	2.07	120.93	116.00
28	AC	518	DGD	O2G-C2G-C1G	2.07	116.16	108.50
27	AT	101	BCR	C40-C30-C25	2.07	113.75	110.33
31	BC	5520	LMG	O7-C10-O9	-2.07	118.14	123.66
30	AA	413	SQD	O6-C44-C45	-2.06	106.08	110.99
28	AB	628	DGD	C6D-O5D-C1E	-2.06	109.66	113.80
24	BC	5507	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
24	BC	5507	CLA	C2D-C3D-CAD	2.07	143.36	134.94
24	AC	503	CLA	C2A-C1A-NA	-2.06	108.69	111.33
27	BK	5102	BCR	C19-C18-C17	-2.06	115.80	118.98
24	AC	512	CLA	C2D-C3D-CAD	2.06	143.36	134.94
24	BC	5508	CLA	OBD-CAD-C3D	2.06	132.32	128.15
24	AB	614	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	AB	611	CLA	O2A-CGA-O1A	-2.06	118.09	123.48
34	BD	5404	PHO	C2D-C3D-CAD	2.06	143.35	134.94
24	AB	612	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	BB	5612	CLA	C2B-C1B-NB	2.06	110.87	109.50
30	BF	5102	SQD	O3-C3-C2	-2.06	105.75	110.36
28	AA	411	DGD	O1A-C1A-C2A	-2.06	115.43	123.78
28	AC	518	DGD	O6E-C5E-C4E	2.06	113.56	109.73
28	BC	5517	DGD	C6B-C7B-C8B	-2.06	105.45	113.73
24	AB	602	CLA	C2B-C1B-NB	2.06	110.87	109.50
24	AC	508	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
34	BD	5403	PHO	C6-C7-C8	-2.06	109.04	115.44
24	BC	5506	CLA	O2A-CGA-O1A	-2.06	118.10	123.48
24	AB	601	CLA	C3D-C4D-CHA	2.06	111.46	108.16
27	AB	617	BCR	C34-C9-C8	2.06	121.42	118.09
24	BC	5513	CLA	O2A-CGA-O1A	-2.06	118.10	123.48
24	AC	511	CLA	C3A-C2A-C1A	2.06	105.04	101.70
24	AC	511	CLA	C2D-C3D-CAD	2.06	143.33	134.94
31	AC	521	LMG	O7-C8-C9	-2.06	100.89	108.50
24	AC	513	CLA	C3A-C2A-C1A	2.06	105.05	101.70
27	BC	5514	BCR	C34-C9-C8	2.06	121.41	118.09
24	BC	5513	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
34	AD	402	PHO	O1D-CGD-CBD	-2.05	120.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5619	CLA	C4D-CHA-CBD	-2.05	104.63	109.45
24	AC	509	CLA	C4B-C3B-C2B	-2.05	104.93	107.04
24	AC	501	CLA	C2D-C3D-CAD	2.05	143.31	134.94
27	BJ	5101	BCR	C30-C25-C24	2.05	121.38	115.69
30	AF	102	SQD	C6-C5-C4	-2.05	107.53	111.86
27	BC	5514	BCR	C32-C1-C2	-2.05	100.62	108.78
24	BB	5618	CLA	C2D-C3D-CAD	2.05	143.32	134.94
24	BC	5508	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
32	BM	5101	LMT	C6B-C5B-C4B	2.05	118.06	113.04
24	BC	5504	CLA	C6-C7-C8	-2.05	109.06	115.44
24	AB	608	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
30	BA	5414	SQD	C6-C5-C4	-2.05	107.53	111.86
27	AK	102	BCR	C11-C12-C13	2.05	132.25	126.37
24	AD	401	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
27	BA	5411	BCR	C19-C18-C17	-2.05	115.82	118.98
27	AD	406	BCR	C34-C9-C8	2.05	121.40	118.09
24	BB	5615	CLA	O2A-CGA-O1A	-2.05	118.12	123.48
24	AC	512	CLA	C3A-C2A-C1A	2.05	105.03	101.70
30	BA	5414	SQD	C17-C16-C15	2.05	125.44	114.56
24	AB	605	CLA	OBD-CAD-C3D	2.05	132.29	128.15
24	BC	5513	CLA	C2D-C3D-CAD	2.05	143.29	134.94
24	AD	404	CLA	CAA-CBA-CGA	-2.05	107.21	113.24
24	BC	5510	CLA	C3B-CAB-CBB	-2.05	121.72	125.95
28	AE	101	DGD	C3G-O3G-C1D	-2.05	109.69	113.80
24	AC	513	CLA	O2A-CGA-O1A	-2.05	118.13	123.48
31	AC	521	LMG	C17-C16-C15	-2.05	103.69	114.56
24	AB	603	CLA	OBD-CAD-C3D	2.05	132.29	128.15
24	BC	5512	CLA	C4D-CHA-CBD	-2.04	104.65	109.45
32	BB	5627	LMT	C1'-O5'-C5'	-2.04	109.78	113.73
24	AC	511	CLA	O1D-CGD-CBD	-2.04	120.27	124.45
24	AC	509	CLA	C4D-C3D-C2D	-2.05	104.69	107.17
24	AC	510	CLA	C2A-C3A-C4A	2.05	105.20	101.89
27	BC	5514	BCR	C23-C24-C25	2.05	133.27	127.23
24	BC	5503	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
27	AC	514	BCR	C23-C24-C25	2.04	133.26	127.23
30	AA	416	SQD	O8-S-O7	2.04	116.23	111.69
24	AC	510	CLA	C3A-C2A-C1A	2.04	105.02	101.70
32	BD	5411	LMT	C5-C6-C7	2.04	121.96	113.73
24	AB	606	CLA	C2D-C3D-CAD	2.04	143.26	134.94
36	AF	101	HEM	C2A-C1A-NA	2.04	112.57	109.73
34	AD	403	PHO	OBD-CAD-C3D	2.04	132.28	128.15
31	BD	5409	LMG	C9-O8-C28	2.04	122.82	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	607	CLA	C2B-C1B-CHB	-2.04	122.13	126.00
24	BB	5619	CLA	C4D-C3D-C2D	-2.04	104.69	107.17
27	AX	101	BCR	C34-C9-C8	2.04	121.39	118.09
24	AD	404	CLA	C4B-C3B-C2B	-2.04	104.94	107.04
24	BA	5405	CLA	C7-C6-C5	-2.04	107.02	112.97
31	BD	5408	LMG	C17-C16-C15	-2.04	103.73	114.56
24	BB	5615	CLA	C2A-C1A-NA	-2.04	108.73	111.33
28	BA	5412	DGD	O1B-C1B-C2B	-2.04	115.52	123.78
24	AC	511	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
28	AA	411	DGD	O3D-C3D-C2D	2.04	114.91	110.36
34	AD	403	PHO	C2D-C3D-CAD	2.04	143.25	134.94
31	AD	407	LMG	C1-O6-C5	-2.04	109.79	113.73
30	BA	5414	SQD	O47-C7-C8	2.04	115.88	111.54
30	BA	5414	SQD	O8-S-O7	2.04	116.22	111.69
24	AB	612	CLA	CAA-C2A-C3A	-2.03	108.22	113.32
28	BE	5102	DGD	C6E-C5E-C4E	-2.04	108.07	113.04
27	AK	102	BCR	C28-C27-C26	2.04	117.16	113.81
24	BB	5607	CLA	C2D-C3D-CAD	2.03	143.24	134.94
24	AB	605	CLA	CMB-C2B-C1B	-2.04	125.34	128.46
24	AA	405	CLA	C2D-C3D-CAD	2.03	143.23	134.94
27	BC	5515	BCR	C1-C6-C7	2.03	121.33	115.69
24	BB	5605	CLA	C2D-C3D-CAD	2.03	143.24	134.94
24	BB	5606	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
28	AE	101	DGD	C4A-C3A-C2A	-2.03	105.75	113.28
24	AC	513	CLA	C2A-C1A-CHA	2.03	127.58	123.87
24	AB	608	CLA	C2B-C1B-NB	2.03	110.86	109.50
27	AC	516	BCR	C7-C8-C9	2.03	129.25	126.22
30	BA	5414	SQD	C3-C4-C5	-2.03	106.52	110.17
27	BD	5407	BCR	C15-C14-C13	2.03	130.23	127.29
24	AD	404	CLA	OBD-CAD-C3D	2.03	132.25	128.15
28	BA	5412	DGD	O3D-C3D-C2D	2.03	114.89	110.36
24	AB	613	CLA	CED-O2D-CGD	2.03	120.84	116.00
24	BB	5615	CLA	CHC-C1C-NC	2.03	127.45	123.42
24	BC	5502	CLA	CAA-CBA-CGA	-2.03	107.26	113.24
24	BC	5512	CLA	C1D-CHD-C4C	2.03	125.75	122.60
24	BB	5608	CLA	CAA-CBA-CGA	-2.03	107.26	113.24
28	AC	518	DGD	O6E-C1E-C2E	2.03	114.45	110.30
24	AB	602	CLA	CAA-CBA-CGA	-2.03	107.26	113.24
24	BA	5405	CLA	C6-C7-C8	-2.03	109.13	115.44
27	AD	406	BCR	C1-C6-C7	2.03	121.31	115.69
24	BA	5406	CLA	O1D-CGD-CBD	-2.03	120.31	124.45
24	AB	601	CLA	C4D-CHA-CBD	-2.03	104.69	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5512	CLA	OBD-CAD-C3D	2.03	132.25	128.15
24	AC	504	CLA	C6-C7-C8	-2.03	109.14	115.44
32	AB	629	LMT	C6'-C5'-C4'	-2.03	107.47	113.27
24	BB	5619	CLA	C3D-CAD-CBD	-2.02	104.73	107.60
28	AC	519	DGD	C4D-C3D-C2D	2.02	114.53	110.80
24	BA	5408	CLA	OBD-CAD-C3D	2.02	132.24	128.15
28	BH	5101	DGD	O1G-C1A-C2A	2.02	118.09	111.90
24	BB	5608	CLA	C2A-C1A-CHA	2.02	127.56	123.87
24	BB	5610	CLA	O2D-CGD-CBD	2.02	115.42	111.34
24	AC	504	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
24	AC	506	CLA	O2A-CGA-O1A	-2.02	118.20	123.48
24	AA	406	CLA	CED-O2D-CGD	2.02	120.81	116.00
30	BA	5414	SQD	O3-C3-C2	-2.02	105.84	110.36
24	BC	5501	CLA	C3A-C4A-NA	-2.02	108.36	110.81
27	BB	5623	BCR	C36-C18-C19	2.02	121.35	118.09
24	AB	610	CLA	CAA-C2A-C3A	-2.02	108.27	113.32
27	AC	515	BCR	C30-C25-C24	2.02	121.29	115.69
31	AJ	102	LMG	C35-C34-C33	2.02	125.29	114.56
24	BC	5513	CLA	C4D-C3D-C2D	-2.02	104.72	107.17
28	AB	628	DGD	O5D-C6D-C5D	2.02	112.46	108.96
24	BC	5507	CLA	C3A-C2A-C1A	2.02	104.98	101.70
27	BC	5516	BCR	C12-C13-C14	-2.02	115.87	118.98
31	BD	5408	LMG	C35-C34-C33	2.02	125.28	114.56
34	BD	5404	PHO	O2A-CGA-O1A	-2.02	118.20	123.48
24	BB	5619	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
28	AA	411	DGD	O1B-C1B-C2B	-2.01	115.62	123.78
24	AB	615	CLA	C2D-C3D-CAD	2.01	143.15	134.94
27	BC	5515	BCR	C30-C25-C24	2.01	121.27	115.69
24	BC	5510	CLA	C2D-C3D-CAD	2.01	143.15	134.94
24	AC	505	CLA	C2A-C1A-NA	-2.01	108.76	111.33
31	AD	407	LMG	C6-C5-C4	-2.01	108.13	113.04
28	AE	101	DGD	C6D-C5D-C4D	-2.01	107.41	111.98
24	AC	512	CLA	OBD-CAD-C3D	2.01	132.22	128.15
27	BB	5622	BCR	C30-C25-C24	2.01	121.26	115.69
31	BC	5521	LMG	O7-C8-C9	-2.01	101.06	108.50
24	BB	5608	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
30	BA	5401	SQD	O3-C3-C2	-2.01	105.87	110.36
34	AD	403	PHO	C2A-C1A-NA	-2.01	108.83	111.93
24	AD	401	CLA	C4-C3-C5	-2.01	112.34	115.39
24	AB	616	CLA	C3D-CAD-CBD	-2.01	104.75	107.60
24	AC	509	CLA	O1D-CGD-CBD	-2.01	120.34	124.45
24	BA	5405	CLA	C2B-C1B-NB	2.01	110.84	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5613	CLA	CAA-C2A-C3A	-2.01	108.29	113.32
24	AB	604	CLA	C4B-C3B-C2B	-2.01	104.97	107.04
27	AK	102	BCR	C36-C18-C19	2.01	121.33	118.09
27	AB	617	BCR	C7-C8-C9	2.01	129.22	126.22
24	BC	5513	CLA	C2A-C1A-CHA	2.01	127.53	123.87
30	BB	5601	SQD	C15-C14-C13	2.01	125.23	114.56
24	BC	5511	CLA	O1D-CGD-CBD	-2.01	120.35	124.45
30	BB	5601	SQD	O48-C23-O10	-2.01	118.23	123.48
24	AB	611	CLA	C2A-C1A-NA	-2.01	108.77	111.33
30	AA	416	SQD	O3-C3-C2	-2.01	105.87	110.36
24	AC	510	CLA	C4B-C3B-C2B	-2.01	104.98	107.04
27	AB	619	BCR	C40-C30-C25	2.00	113.65	110.33
24	BB	5611	CLA	CED-O2D-CGD	2.01	120.78	116.00
31	AB	620	LMG	O7-C10-C11	-2.00	107.27	111.54
30	AA	413	SQD	C17-C16-C15	2.00	125.21	114.56
24	BB	5620	CLA	C3D-CAD-CBD	-2.00	104.76	107.60
24	AB	613	CLA	C2C-C1C-NC	-2.00	108.60	110.22
32	AM	102	LMT	C6B-C5B-C4B	2.00	117.94	113.04
32	BI	5102	LMT	C9-C8-C7	-2.00	103.92	114.56
24	BC	5503	CLA	C5-C3-C2	2.00	124.91	121.06
27	AC	515	BCR	C1-C6-C7	2.00	121.23	115.69
24	AC	512	CLA	CHA-C1A-NA	-2.00	121.19	126.00
24	BC	5513	CLA	OBD-CAD-C3D	2.00	132.20	128.15
31	AC	520	LMG	C36-C35-C34	-2.00	103.94	114.56
24	AB	604	CLA	C2C-C1C-NC	-2.00	108.61	110.22

All (82) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	C8
24	BC	5511	CLA	C8
24	AC	507	CLA	C8
24	BB	5617	CLA	C8
34	BD	5403	PHO	C2A
34	BD	5403	PHO	C13
24	BB	5612	CLA	C8
24	AC	504	CLA	C8
24	BC	5512	CLA	C8
34	AD	402	PHO	C2A
34	AD	402	PHO	C13
24	AC	506	CLA	C8
24	BB	5619	CLA	C8

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Mol	Chain	Res	Type	Atom
24	BB	5614	CLA	C8
24	AA	405	CLA	C8
24	BC	5507	CLA	C8
24	AB	612	CLA	C8
24	BC	5508	CLA	C8
24	BB	5608	CLA	C8
24	BC	5501	CLA	C8
24	BD	5402	CLA	C8
24	BB	5610	CLA	C8
24	AB	606	CLA	C8
24	BD	5405	CLA	C8
24	AD	401	CLA	C8
24	AD	404	CLA	C8
34	AD	403	PHO	C2A
34	AD	403	PHO	C13
28	AC	518	DGD	C1E
24	AB	602	CLA	C8
24	AC	511	CLA	C8
24	AC	503	CLA	C8
24	AA	404	CLA	C8
24	BC	5503	CLA	C8
24	AB	615	CLA	C8
24	BB	5620	CLA	C8
24	AB	610	CLA	C8
24	BB	5606	CLA	C8
24	AB	616	CLA	C8
24	AB	614	CLA	C8
24	AB	611	CLA	C8
24	AB	613	CLA	C8
24	AC	509	CLA	C8
24	AA	407	CLA	C8
24	BC	5510	CLA	C8
24	AC	501	CLA	C8
24	BB	5616	CLA	C8
24	BA	5405	CLA	C8
24	AA	406	CLA	C8
24	BC	5504	CLA	C8
24	AB	609	CLA	C8
24	AC	502	CLA	C8
24	BC	5509	CLA	C8
24	AB	607	CLA	C8
28	AC	519	DGD	C1E

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Mol	Chain	Res	Type	Atom
24	BC	5506	CLA	C8
24	AC	505	CLA	C8
24	AC	508	CLA	C8
24	AC	513	CLA	C8
24	BB	5609	CLA	C8
24	BC	5505	CLA	C8
34	BD	5404	PHO	C2A
34	BD	5404	PHO	C13
24	AB	603	CLA	C8
24	BB	5615	CLA	C8
24	BA	5407	CLA	C8
24	AB	601	CLA	C8
24	AC	512	CLA	C8
24	BB	5613	CLA	C8
24	BB	5607	CLA	C8
24	AB	608	CLA	C8
24	AC	510	CLA	C8
28	BC	5519	DGD	C1E
24	BB	5605	CLA	C8
24	AB	605	CLA	C8
24	AB	604	CLA	C8
24	BA	5408	CLA	C8
24	BC	5513	CLA	C8
28	BC	5518	DGD	C1E
24	BA	5406	CLA	C8
24	BB	5611	CLA	C8
24	BB	5618	CLA	C8

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	AD	405	PL9	C49-C48-C47-C46
35	BD	5406	PL9	C49-C48-C47-C46
35	AD	405	PL9	C29-C28-C27-C26

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%)	-0.09	1 (0%) 91 58	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.06	2 (0%) 86 41	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.11	1 (0%) 93 66	81, 103, 136, 152	0
2	BB	490/510 (96%)	-0.02	5 (1%) 79 29	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.10	2 (0%) 90 51	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.09	6 (1%) 74 24	91, 124, 149, 159	0
4	AD	341/352 (96%)	-0.09	1 (0%) 91 58	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.09	3 (0%) 81 32	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.13	1 (1%) 75 26	104, 126, 151, 155	0
5	BE	82/84 (97%)	0.59	4 (4%) 28 6	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.06	2 (5%) 23 5	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.04	0 100 100	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.19	0 100 100	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.16	2 (3%) 47 10	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.13	1 (2%) 49 10	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.16	3 (8%) 11 3	108, 116, 142, 147	0
9	AJ	38/40 (95%)	-0.08	0 100 100	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.08	1 (2%) 53 11	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.16	1 (2%) 52 11	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.18	1 (2%) 52 11	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.07	1 (2%) 52 11	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.18	2 (5%) 25 5	90, 104, 158, 160	0
12	AM	34/36 (94%)	-0.04	0 100 100	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.20	1 (2%) 49 10	90, 99, 140, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.08	2 (0%) 83 35	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.09	3 (1%) 75 26	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.23	2 (6%) 19 4	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.10	2 (6%) 19 4	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.08	0 100 100	93, 105, 116, 125	0
15	BU	97/104 (93%)	-0.03	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	-0.01	1 (0%) 84 38	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.21	0 100 100	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.18	1 (3%) 41 8	141, 154, 160, 160	0
17	By	28/46 (60%)	0.44	1 (3%) 41 8	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.12	2 (5%) 25 5	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.13	0 100 100	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.23	5 (8%) 12 3	134, 148, 160, 160	0
20	BZ	62/62 (100%)	0.85	6 (9%) 8 2	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.04	66 (1%) 74 24	81, 113, 149, 160	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	6.0
20	BZ	5001	MET	5.0
20	BZ	5061	VAL	4.7
17	By	5046	LEU	4.5
11	BL	5001	MET	3.6
5	BE	5008	ARG	3.3
7	BH	5066	GLY	3.3
12	BM	5034	LYS	3.2
14	AT	32	LYS	3.1
13	BO	5084	ASN	3.0
6	AF	11	VAL	3.0
2	BB	5491	VAL	2.9
3	BC	5135	ARG	2.9
7	BH	5065	LEU	2.8
18	AX	47	GLN	2.7
8	BI	5034	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
3	AC	137	PRO	2.7
5	BE	5007	GLU	2.7
18	AX	45	LYS	2.7
20	BZ	5060	PHE	2.7
20	BZ	5033	TRP	2.7
4	BD	5233	ARG	2.6
11	BL	5002	GLU	2.6
8	BI	5032	PRO	2.6
1	BA	5011	ALA	2.6
1	AA	242	GLU	2.6
9	BJ	5004	GLU	2.6
2	BB	5490	GLN	2.6
13	AO	84	ASN	2.4
4	AD	241	GLU	2.4
8	BI	5033	LYS	2.4
16	AV	116	GLU	2.4
4	BD	5012	ARG	2.4
14	AT	31	LYS	2.3
13	BO	5112	LYS	2.3
4	BD	5239	GLN	2.3
3	BC	5204	LEU	2.3
14	BT	5032	LYS	2.3
13	AO	88	GLU	2.3
1	BA	5233	ALA	2.3
14	BT	5028	ARG	2.2
2	BB	5002	GLY	2.2
20	AZ	60	PHE	2.2
13	BO	5030	THR	2.2
6	AF	13	TYR	2.2
11	AL	1	MET	2.2
2	AB	379	ALA	2.1
3	BC	5137	PRO	2.1
10	AK	46	ARG	2.1
8	AI	35	LYS	2.1
20	AZ	34	ASP	2.1
3	AC	141	GLU	2.1
3	BC	5138	GLU	2.1
5	BE	5059	GLU	2.1
5	AE	83	LEU	2.1
2	BB	5124	ARG	2.0
5	BE	5006	GLY	2.0
20	AZ	57	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	BC	5207	ARG	2.0
20	AZ	62	VAL	2.0
3	BC	5057	ALA	2.0
20	BZ	5002	THR	2.0
17	Ay	42	ARG	2.0
10	BK	5014	ALA	2.0
2	BB	5123	PHE	2.0
20	AZ	33	TRP	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
27	BCR	AJ	101	40/40	0.74	17.34	158,160,160,160	0
28	DGD	AE	101	63/66	0.70	12.39	146,160,160,160	0
32	LMT	BB	5626	35/35	0.54	12.12	131,160,160,160	0
28	DGD	BB	5602	52/66	0.45	7.76	152,160,160,160	0
31	LMG	BA	5402	42/55	0.48	7.11	144,157,160,160	0
27	BCR	BJ	5101	40/40	0.58	6.70	160,160,160,160	0
28	DGD	AC	518	62/66	0.44	5.55	146,155,160,160	0
28	DGD	AB	628	52/66	0.57	5.53	154,160,160,160	0
33	DMS	BB	5628	4/4	0.46	5.45	156,157,157,157	0
31	LMG	AA	417	42/55	0.40	5.22	145,157,160,160	0
33	DMS	AV	202	4/4	0.50	5.01	148,148,148,149	0
28	DGD	BC	5518	62/66	0.45	4.88	147,156,160,160	0
32	LMT	AB	624	35/35	0.54	4.81	156,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	LMG	BD	5410	48/55	0.48	4.69	126,131,141,141	0
32	LMT	AB	629	35/35	0.45	4.49	133,160,160,160	0
31	LMG	AJ	102	46/55	0.39	4.39	139,144,160,160	0
32	LMT	BB	5603	35/35	0.40	4.15	132,160,160,160	0
33	DMS	AB	625	4/4	0.54	4.14	156,157,157,157	0
28	DGD	AC	519	66/66	0.38	4.12	110,120,157,158	0
27	BCR	BB	5621	40/40	0.35	4.10	112,120,124,125	0
28	DGD	BE	5102	63/66	0.68	4.10	145,160,160,160	0
31	LMG	AB	621	49/55	0.44	4.09	145,150,157,160	0
30	SQD	BA	5401	54/54	0.53	3.95	136,160,160,160	0
32	LMT	BI	5102	35/35	0.73	3.92	151,160,160,160	0
31	LMG	BB	5624	49/55	0.37	3.73	145,150,157,160	0
33	DMS	BV	5203	4/4	0.38	3.40	160,160,160,160	0
31	LMG	AD	408	48/55	0.43	3.37	121,130,139,139	0
31	LMG	AD	407	49/55	0.37	3.33	126,133,143,145	0
28	DGD	BC	5519	66/66	0.37	3.32	112,121,158,159	0
31	LMG	AA	414	44/55	0.44	3.31	140,160,160,160	0
31	LMG	AI	101	43/55	0.81	3.27	159,160,160,160	0
31	LMG	AC	520	48/55	0.49	3.22	136,157,160,160	0
31	LMG	AB	620	51/55	0.45	3.20	125,139,150,151	0
32	LMT	AM	102	35/35	0.44	3.13	126,149,154,154	0
32	LMT	BB	5604	35/35	0.47	3.10	131,160,160,160	0
29	LHG	BA	5415	37/49	0.61	3.03	151,160,160,160	0
24	CLA	BA	5408	65/65	0.34	3.03	95,103,150,150	0
24	CLA	AD	404	65/65	0.36	3.03	126,130,148,149	0
27	BCR	AK	102	40/40	0.38	3.00	133,139,151,152	0
27	BCR	AB	617	40/40	0.32	2.98	112,121,125,125	0
31	LMG	BI	5101	43/55	0.67	2.95	160,160,160,160	0
30	SQD	AB	622	43/54	0.40	2.95	133,149,160,160	0
37	CA	BO	5301	1/1	0.43	2.91	160,160,160,160	0
32	LMT	BB	5627	35/35	0.42	2.90	156,160,160,160	0
27	BCR	AT	101	40/40	0.36	2.89	126,140,146,147	0
31	LMG	BD	5408	46/55	0.39	2.82	139,145,160,160	0
33	DMS	AB	626	4/4	0.28	2.81	129,130,130,130	0
24	CLA	AB	601	65/65	0.50	2.79	146,159,160,160	0
27	BCR	BT	5101	40/40	0.32	2.78	124,143,147,147	0
30	SQD	BB	5625	43/54	0.39	2.75	132,148,160,160	0
24	CLA	AA	407	65/65	0.35	2.74	93,101,150,151	0
28	DGD	AC	517	53/66	0.35	2.73	121,128,135,140	0
27	BCR	AX	101	40/40	0.58	2.71	135,143,158,159	0
32	LMT	BC	5522	35/35	0.63	2.67	157,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	PL9	AD	405	55/55	0.34	2.66	99,109,113,113	0
24	CLA	BB	5605	65/65	0.60	2.64	146,159,160,160	0
27	BCR	BD	5407	40/40	0.28	2.64	112,127,132,132	0
24	CLA	AA	406	65/65	0.32	2.63	105,112,138,139	0
24	CLA	BB	5609	65/65	0.33	2.56	103,110,124,124	0
28	DGD	BA	5412	56/66	0.46	2.55	150,160,160,160	0
31	LMG	BC	5520	48/55	0.46	2.51	138,159,160,160	0
30	SQD	AF	102	45/54	0.51	2.45	154,160,160,160	0
28	DGD	AA	411	56/66	0.51	2.44	148,158,160,160	0
27	BCR	AD	406	40/40	0.32	2.44	110,126,131,131	0
24	CLA	BC	5504	65/65	0.31	2.43	132,135,160,160	0
27	BCR	BB	5623	40/40	0.39	2.42	111,116,131,131	0
32	LMT	AD	409	31/35	0.39	2.40	139,154,160,160	0
32	LMT	BM	5101	35/35	0.42	2.40	126,149,154,155	0
27	BCR	AC	516	40/40	0.45	2.35	135,138,143,143	0
31	LMG	BE	5101	44/55	0.44	2.35	140,160,160,160	0
32	LMT	AI	102	35/35	0.66	2.34	149,158,160,160	0
24	CLA	AC	504	65/65	0.34	2.29	129,134,160,160	0
32	LMT	AI	103	35/35	0.43	2.24	156,158,160,160	0
24	CLA	AB	605	65/65	0.26	2.22	105,113,122,124	0
27	BCR	BX	5101	40/40	0.55	2.18	136,143,157,158	0
31	LMG	BL	5101	51/55	0.41	2.17	122,138,151,152	0
32	LMT	AB	623	35/35	0.56	2.16	135,160,160,160	0
24	CLA	AB	616	65/65	0.43	2.15	143,147,160,160	0
24	CLA	BB	5612	65/65	0.37	2.12	122,127,136,139	0
24	CLA	AB	615	65/65	0.39	2.11	134,139,155,157	0
24	CLA	BD	5405	65/65	0.37	2.10	125,131,148,149	0
24	CLA	AB	608	65/65	0.35	2.09	123,127,135,140	0
27	BCR	AC	515	40/40	0.42	2.02	149,152,155,155	0
24	CLA	BB	5617	65/65	0.30	1.99	98,102,138,141	0
32	LMT	AB	630	35/35	0.50	1.95	132,160,160,160	0
27	BCR	BC	5515	40/40	0.53	1.92	150,152,155,156	0
24	CLA	AC	505	65/65	0.38	1.86	121,146,150,151	0
31	LMG	AC	521	45/55	0.59	1.85	154,160,160,160	0
34	PHO	BD	5403	64/64	0.32	1.79	102,109,118,118	0
28	DGD	BH	5101	58/66	0.30	1.77	107,118,156,160	0
24	CLA	AC	503	65/65	0.44	1.76	137,144,147,152	0
24	CLA	AB	610	65/65	0.34	1.66	117,121,123,127	0
24	CLA	BA	5407	65/65	0.28	1.66	110,114,138,139	0
30	SQD	AA	416	54/54	0.32	1.63	136,160,160,160	0
24	CLA	AB	603	65/65	0.33	1.61	107,109,119,121	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	CLA	BB	5614	65/65	0.32	1.59	117,123,124,128	0
24	CLA	AC	507	65/65	0.38	1.59	137,149,152,153	0
35	PL9	BD	5406	55/55	0.32	1.55	103,110,115,116	0
27	BCR	AB	619	40/40	0.30	1.53	111,117,131,131	0
24	CLA	AB	609	65/65	0.35	1.51	126,136,141,143	0
24	CLA	BC	5502	65/65	0.30	1.50	108,111,143,144	0
31	LMG	BD	5409	49/55	0.36	1.50	128,133,144,146	0
27	BCR	BK	5102	40/40	0.36	1.50	136,140,152,152	0
27	BCR	BA	5411	40/40	0.30	1.47	94,122,132,132	0
24	CLA	BC	5513	65/65	0.57	1.45	158,160,160,160	0
27	BCR	BC	5514	40/40	0.44	1.44	123,126,129,129	0
24	CLA	AC	508	65/65	0.36	1.42	140,144,157,158	0
30	SQD	AA	413	51/54	0.37	1.42	143,150,160,160	0
29	LHG	AA	415	37/49	0.40	1.40	149,160,160,160	0
32	LMT	BD	5411	31/35	0.49	1.40	140,152,160,160	0
24	CLA	BC	5505	65/65	0.35	1.38	123,148,152,153	0
34	PHO	AD	402	64/64	0.29	1.36	99,109,116,117	0
24	CLA	BA	5406	65/65	0.25	1.36	89,94,108,112	0
24	CLA	AC	502	65/65	0.35	1.31	103,109,142,143	0
27	BCR	AA	410	40/40	0.29	1.30	91,122,130,130	0
24	CLA	BB	5611	65/65	0.25	1.25	95,102,132,136	0
34	PHO	AD	403	64/64	0.26	1.22	119,123,128,129	0
30	SQD	BF	5102	45/54	0.47	1.21	154,160,160,160	0
24	CLA	BB	5607	65/65	0.28	1.16	108,111,120,123	0
24	CLA	AB	606	65/65	0.32	1.15	120,133,140,141	0
24	CLA	BB	5613	65/65	0.30	1.12	127,135,140,142	0
28	DGD	AH	101	58/66	0.27	1.11	108,120,155,157	0
24	CLA	AC	501	65/65	0.34	1.10	133,136,139,143	0
27	BCR	AB	618	40/40	0.24	1.08	109,117,122,122	0
33	DMS	BB	5629	4/4	0.22	1.08	125,126,127,127	0
24	CLA	BB	5616	65/65	0.31	1.07	108,110,120,122	0
24	CLA	AC	506	65/65	0.32	1.05	136,143,160,160	0
24	CLA	BC	5507	65/65	0.36	1.04	136,150,153,154	0
24	CLA	AB	614	65/65	0.34	1.03	129,133,160,160	0
24	CLA	BB	5608	65/65	0.31	1.01	96,103,124,125	0
31	LMG	AM	101	42/55	0.42	1.01	136,158,160,160	0
24	CLA	AB	612	65/65	0.29	0.99	107,111,120,121	0
34	PHO	BD	5404	64/64	0.29	0.99	123,125,129,130	0
24	CLA	AB	602	65/65	0.28	0.98	124,127,129,132	0
24	CLA	AB	604	65/65	0.29	0.86	96,104,125,127	0
24	CLA	AD	401	65/65	0.25	0.84	93,100,115,119	0
29	LHG	AA	412	39/49	0.28	0.83	110,118,128,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	CLA	AB	607	65/65	0.24	0.83	94,100,132,135	0
24	CLA	AC	509	65/65	0.38	0.83	115,128,135,137	0
24	CLA	BD	5402	65/65	0.25	0.82	97,101,117,119	0
36	HEM	AF	101	43/43	0.33	0.81	148,152,159,160	0
27	BCR	BB	5622	40/40	0.26	0.81	110,117,120,121	0
28	DGD	BC	5517	53/66	0.27	0.80	124,130,136,139	0
30	SQD	BB	5601	47/54	0.35	0.80	137,156,160,160	0
24	CLA	BA	5405	65/65	0.27	0.78	90,101,105,109	0
30	SQD	AB	627	47/54	0.33	0.77	138,157,160,160	0
37	CA	AO	301	1/1	0.31	0.75	152,152,152,152	0
24	CLA	AB	611	65/65	0.29	0.74	99,113,116,122	0
24	CLA	BC	5511	65/65	0.44	0.73	154,158,159,160	0
27	BCR	AC	514	40/40	0.31	0.72	120,123,127,128	0
24	CLA	BC	5510	65/65	0.35	0.71	113,116,130,131	0
24	CLA	AC	513	65/65	0.47	0.71	158,160,160,160	0
24	CLA	BC	5503	65/65	0.32	0.69	137,147,148,152	0
24	CLA	AA	404	65/65	0.24	0.68	89,99,106,108	0
24	CLA	BC	5506	65/65	0.35	0.68	136,143,160,160	0
24	CLA	BB	5618	65/65	0.30	0.68	128,133,160,160	0
37	CA	BK	5101	1/1	0.21	0.67	145,145,145,145	0
27	BCR	BC	5516	40/40	0.39	0.65	136,140,145,145	0
31	LMG	BM	5102	42/55	0.40	0.63	136,160,160,160	0
23	CL	BA	5404[A]	1/1	0.22	0.60	29,29,29,29	1
24	CLA	AC	510	65/65	0.34	0.58	110,113,129,130	0
24	CLA	AC	512	65/65	0.38	0.56	154,158,160,160	0
24	CLA	BB	5606	65/65	0.28	0.54	124,127,130,131	0
24	CLA	BC	5501	65/65	0.29	0.51	134,137,141,144	0
24	CLA	BC	5508	65/65	0.29	0.51	142,146,157,159	0
24	CLA	BB	5610	65/65	0.30	0.50	121,132,140,141	0
23	CL	AA	403[B]	1/1	0.27	0.50	108,108,108,108	1
23	CL	AA	403[A]	1/1	0.27	0.49	33,33,33,33	1
30	SQD	BA	5414	51/54	0.36	0.47	145,150,160,160	0
24	CLA	BC	5509	65/65	0.30	0.42	116,128,138,138	0
24	CLA	BC	5512	65/65	0.35	0.40	157,160,160,160	0
36	HEM	BV	5201	43/43	0.25	0.39	97,102,106,109	0
24	CLA	BB	5619	65/65	0.31	0.37	135,137,155,157	0
26	OEC	AA	409	5/9	0.28	0.36	82,83,90,110	0
36	HEM	AV	201	43/43	0.26	0.35	94,100,102,103	0
29	LHG	BA	5413	39/49	0.27	0.35	113,122,128,129	0
31	LMG	BC	5521	45/55	0.49	0.35	154,160,160,160	0
25	MST	AA	408	16/16	0.25	0.33	123,126,129,130	0
24	CLA	AA	405	65/65	0.24	0.32	88,93,108,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	DMS	AU	201	4/4	0.28	0.29	160,160,160,160	0
24	CLA	AC	511	65/65	0.31	0.27	152,155,157,158	0
24	CLA	AB	613	65/65	0.23	0.26	99,102,136,140	0
36	HEM	BF	5101	43/43	0.42	0.25	148,152,160,160	0
24	CLA	BB	5615	65/65	0.24	0.22	101,113,117,120	0
24	CLA	BB	5620	65/65	0.30	0.11	143,147,160,160	0
23	CL	BA	5404[B]	1/1	0.22	-0.14	115,115,115,115	1
37	CA	AK	101	1/1	0.12	-0.23	146,146,146,146	0
25	MST	BA	5409	16/16	0.20	-0.25	124,129,131,132	0
26	OEC	BA	5410	5/9	0.22	-0.41	23,88,99,134	0
33	DMS	BV	5202	4/4	0.19	-0.59	148,149,149,150	0
22	BCT	AA	402	4/4	0.19	-0.93	135,136,137,137	0
21	FE2	AA	401	1/1	0.15	-1.32	115,115,115,115	0
22	BCT	BA	5403	4/4	0.14	-1.32	135,136,136,137	0
21	FE2	BD	5401	1/1	0.08	-2.97	119,119,119,119	0
37	CA	AF	103	1/1	0.20	-5.12	150,150,150,150	0
37	CA	BF	5103	1/1	0.17	-9.15	146,146,146,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.