



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:09 pm GMT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk28620

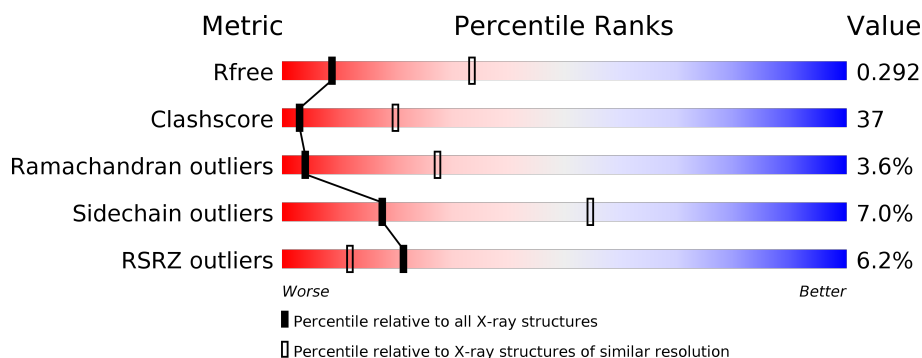
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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

Mol	Chain	Length	Quality of chain
1	AA	344	<div> <div>2%</div> <div>40%</div> <div>53%</div> <div>5%</div> </div>
1	BA	344	<div> <div>4%</div> <div>39%</div> <div>53%</div> <div>5%</div> </div>
2	AB	510	<div> <div>2%</div> <div>46%</div> <div>45%</div> <div>5%</div> </div>
2	BB	510	<div> <div>4%</div> <div>46%</div> <div>45%</div> <div>5%</div> </div>
3	AC	461	<div> <div>5%</div> <div>40%</div> <div>51%</div> <div>5%</div> </div>
3	BC	461	<div> <div>6%</div> <div>39%</div> <div>52%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
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	

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CL	BA	5404[A]	-	-	-	X
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	X
24	CLA	AA	407	X	-	-	X
24	CLA	AB	601	X	-	-	X
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	X
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	X
24	CLA	AB	609	X	-	-	-
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-
24	CLA	AB	616	X	-	-	-
24	CLA	AC	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AC	502	X	-	-	-
24	CLA	AC	503	X	-	-	X
24	CLA	AC	504	X	-	-	X
24	CLA	AC	505	X	-	-	X
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	X
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	X	-
24	CLA	AC	512	X	-	-	X
24	CLA	AC	513	X	-	-	X
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	X
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	X	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	X
24	CLA	BB	5605	X	-	-	X
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	X
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	X
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	X
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	X
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	-
24	CLA	BC	5507	X	-	-	-
24	CLA	BC	5508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	X	X
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	X
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
27	BCR	AB	617	-	-	-	X
27	BCR	AC	515	-	-	-	X
27	BCR	AC	516	-	-	-	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	5622	-	-	-	X
27	BCR	BC	5514	-	-	-	X
27	BCR	BC	5515	-	-	-	X
27	BCR	BC	5516	-	-	-	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	-	-	X
28	DGD	AC	519	X	-	X	X
28	DGD	AE	101	-	-	-	X
28	DGD	BA	5412	-	-	-	X
28	DGD	BB	5602	-	-	-	X
28	DGD	BC	5518	X	-	-	X
28	DGD	BC	5519	X	-	X	X
28	DGD	BE	5102	-	-	-	X
28	DGD	BH	5101	-	-	-	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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	BF	5102	-	-	-	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
31	LMG	AD	407	-	-	-	X
31	LMG	AD	408	-	-	-	X
31	LMG	AJ	102	-	-	-	X
31	LMG	AM	101	-	-	-	X
31	LMG	BA	5402	-	-	-	X
31	LMG	BB	5624	-	-	-	X
31	LMG	BC	5520	-	-	-	X
31	LMG	BC	5521	-	-	-	X
31	LMG	BD	5408	-	-	-	X
31	LMG	BD	5409	-	-	-	X
31	LMG	BD	5410	-	-	-	X
31	LMG	BE	5101	-	-	-	X
31	LMG	BL	5101	-	-	-	X
31	LMG	BM	5102	-	-	-	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	5627	-	-	-	X
32	LMT	BC	5522	-	-	-	X
32	LMT	BD	5411	-	-	-	X
32	LMT	BI	5102	-	-	-	X
32	LMT	BM	5101	-	-	-	X
33	DMS	AB	625	-	-	-	X
33	DMS	AV	202	-	-	-	X
33	DMS	BB	5628	-	-	-	X
33	DMS	BB	5629	-	-	-	X
33	DMS	BV	5203	-	-	-	X
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-
35	PL9	AD	405	-	-	-	X
36	HEM	BF	5101	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	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				

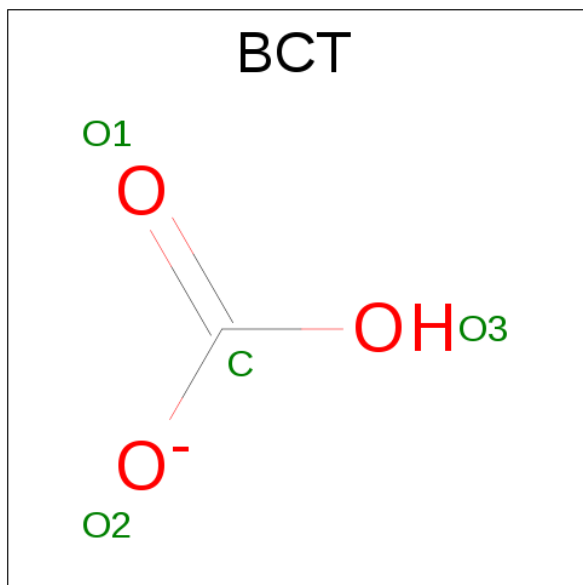
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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).

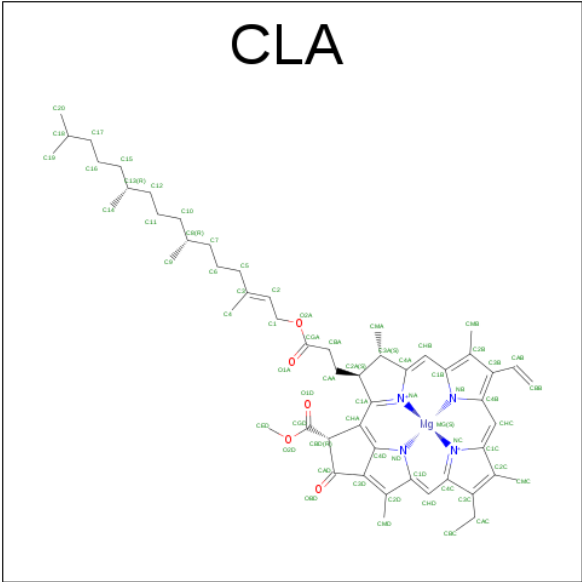


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- 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 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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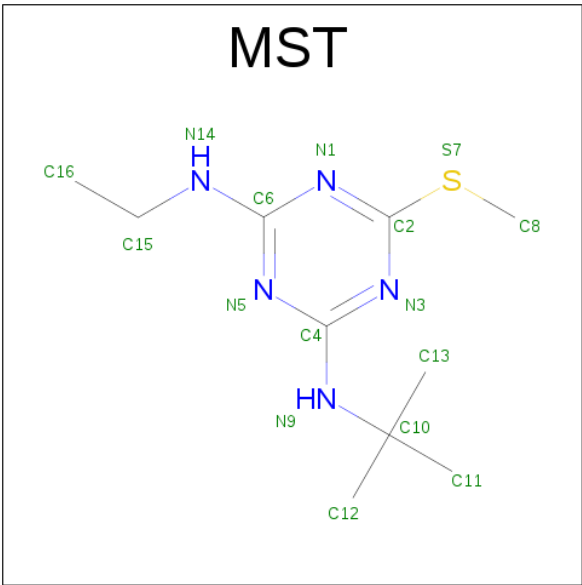
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55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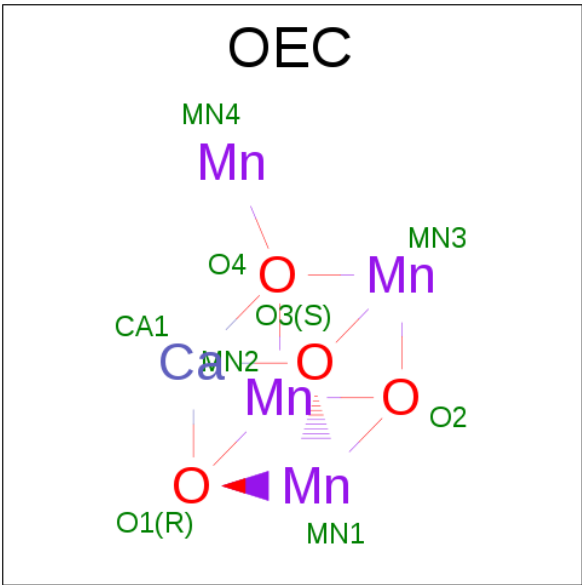
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55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

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



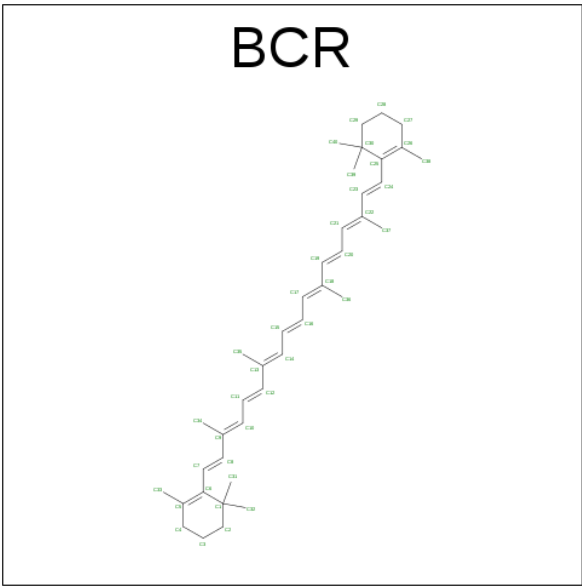
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- 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: C₄₀H₅₆).



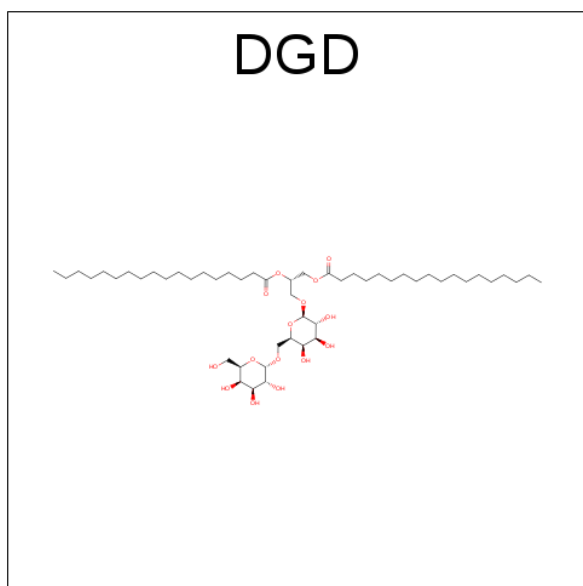
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
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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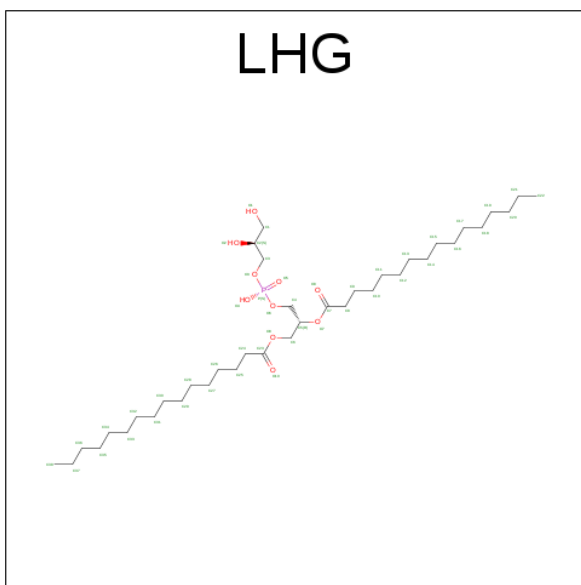
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

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



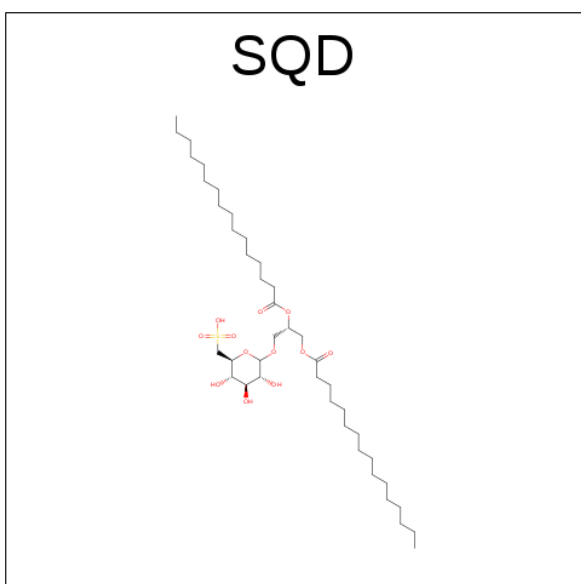
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA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



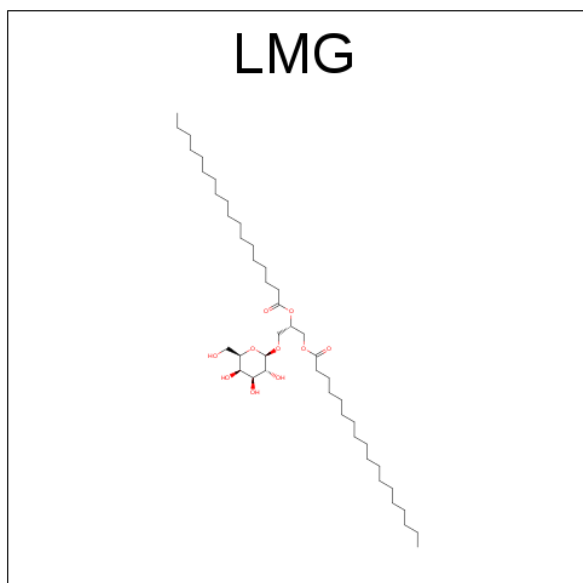
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



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: $C_{45}H_{86}O_{10}$).



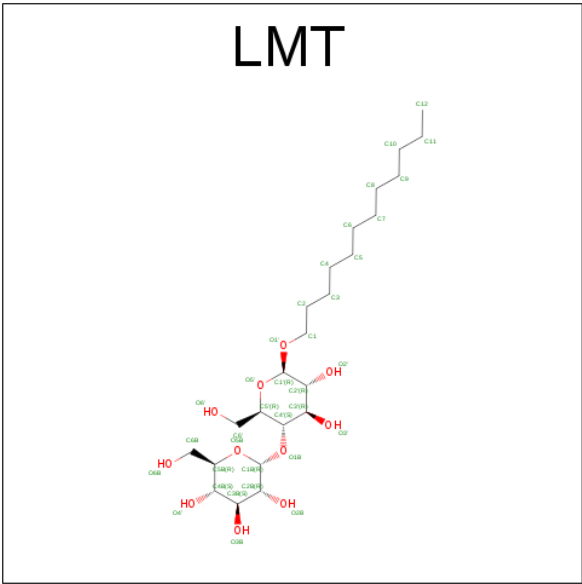
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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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: $C_{24}H_{46}O_{11}$).



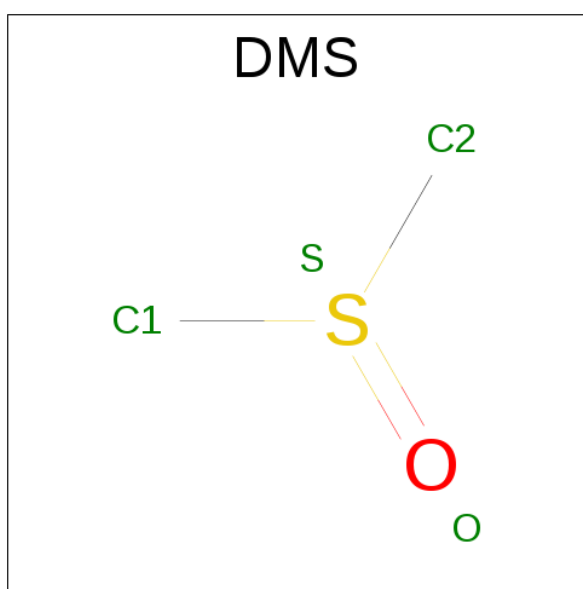
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM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



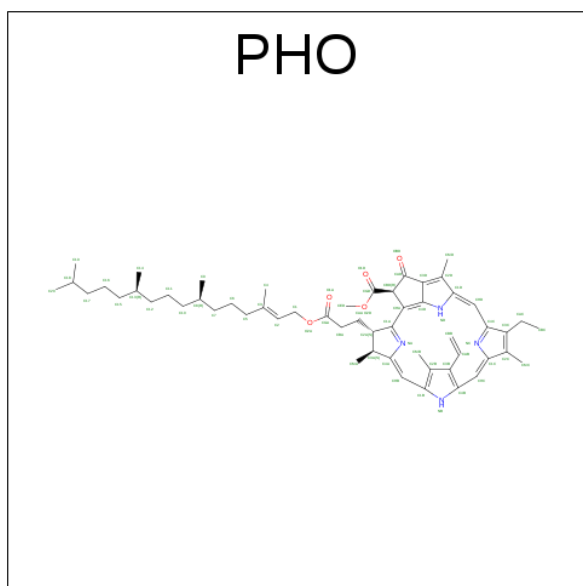
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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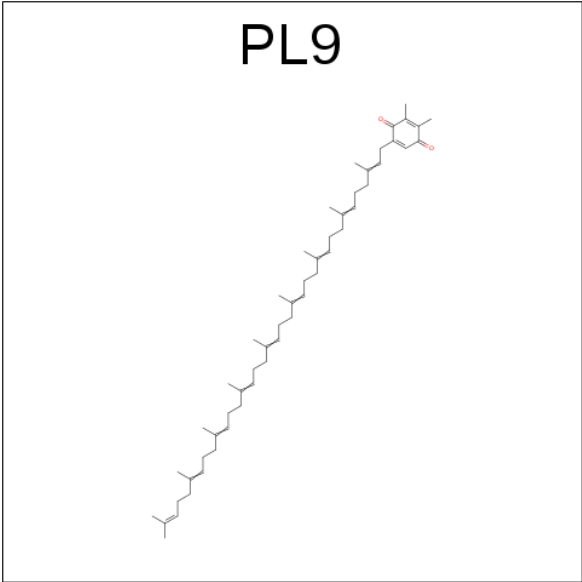
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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



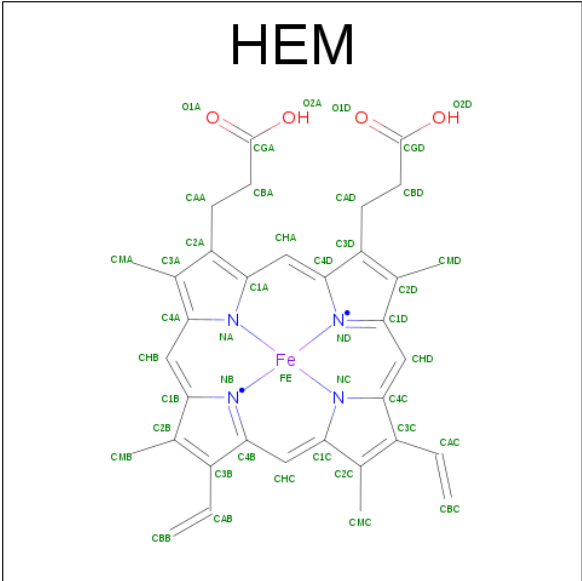
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- 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

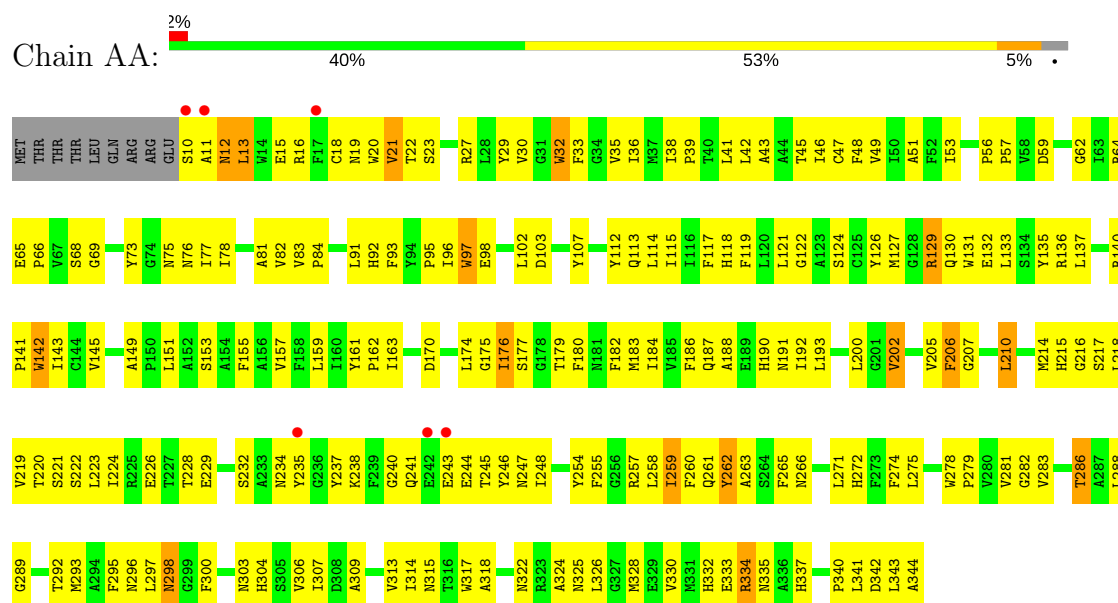
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

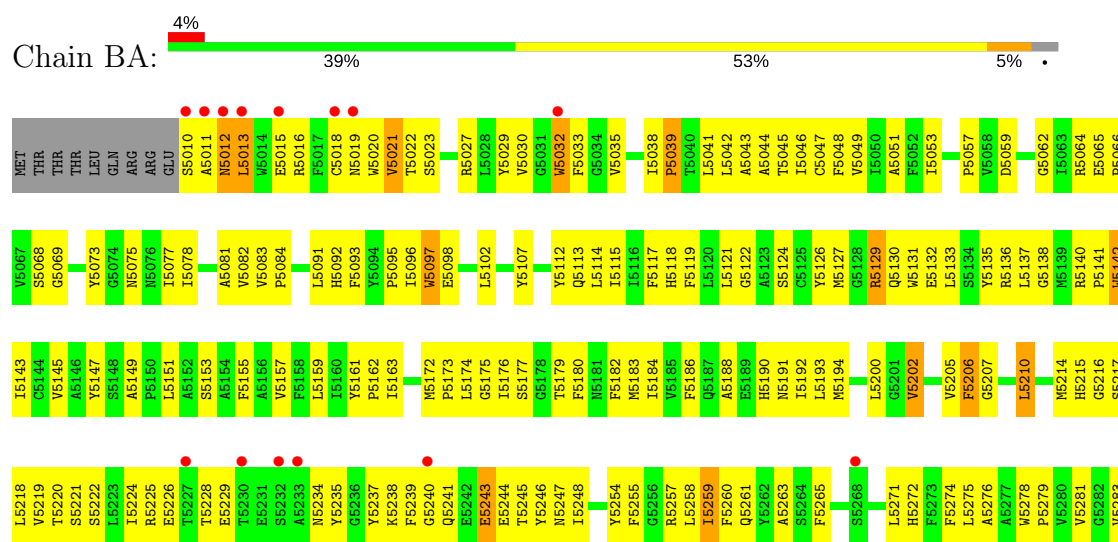
3 Residue-property plots

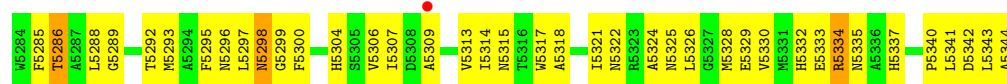
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Photosystem Q(B) protein 1

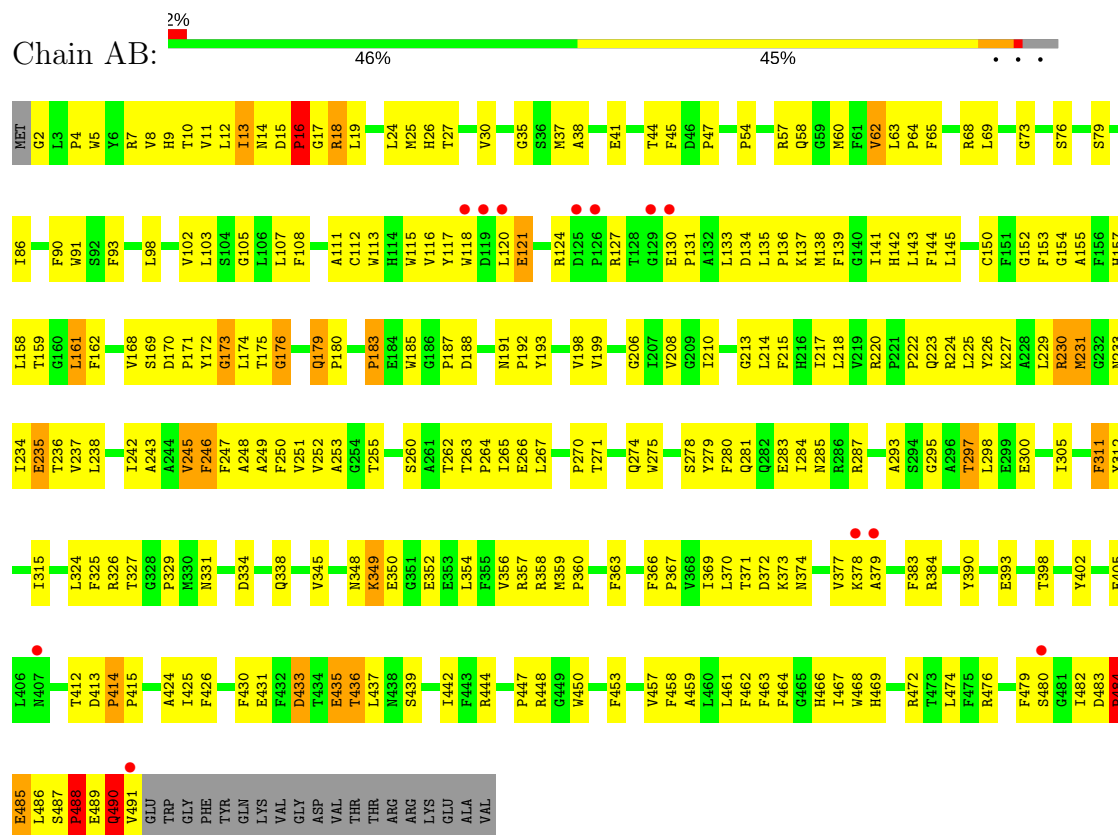


• Molecule 1: Photosystem Q(B) protein 1

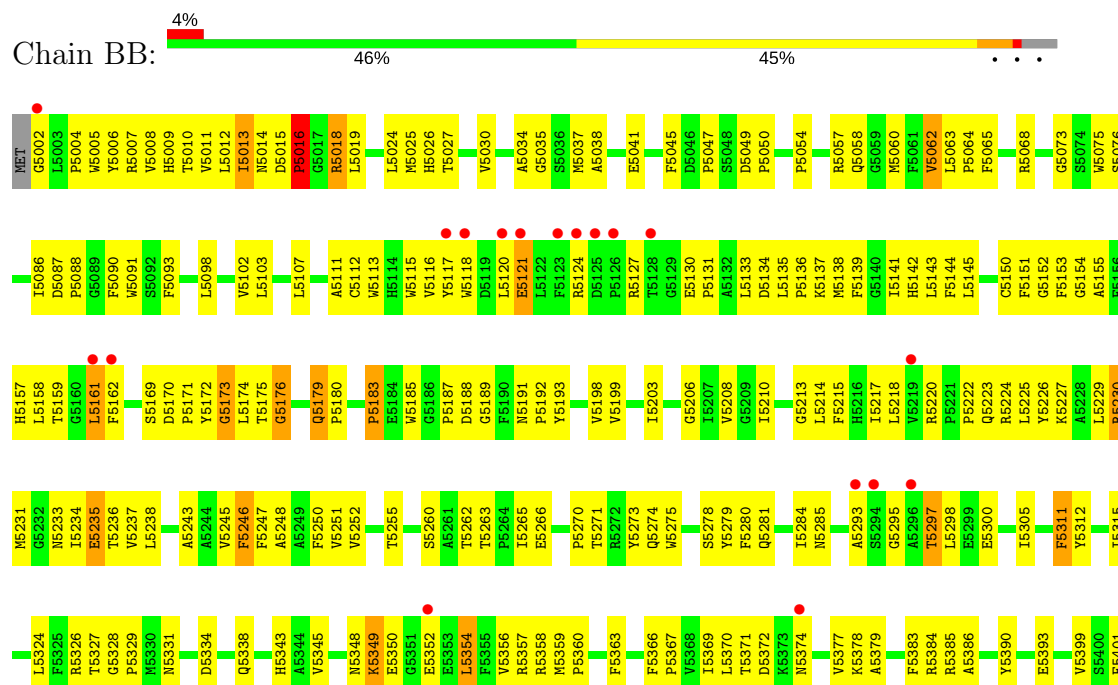


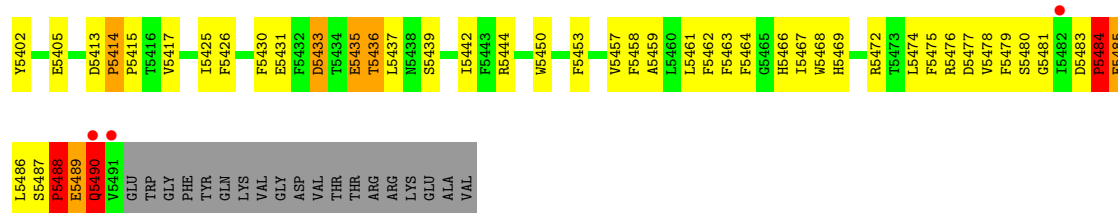


- Molecule 2: Photosystem II core light harvesting protein

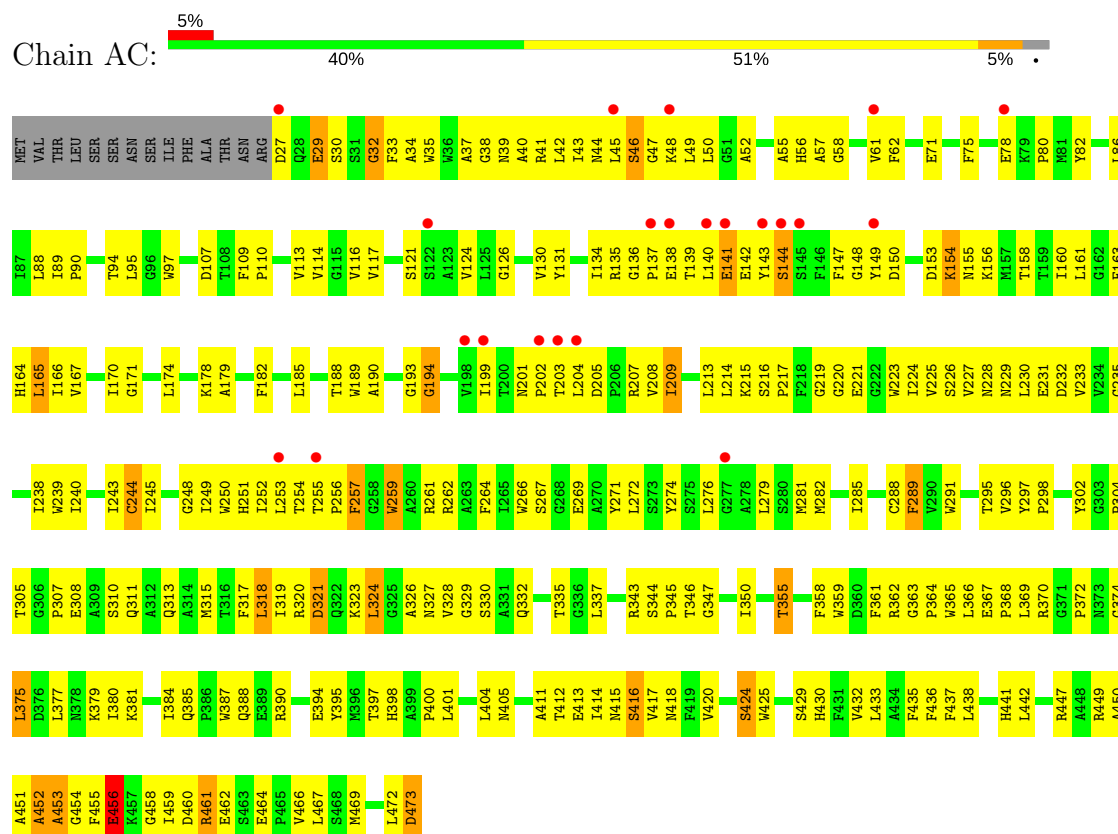


- Molecule 2: Photosystem II core light harvesting protein

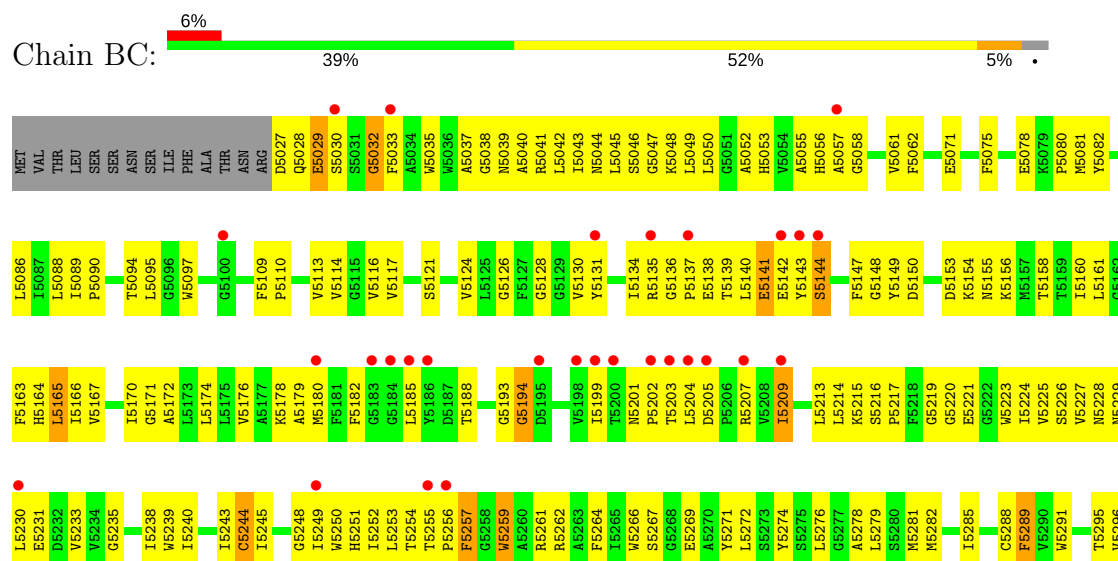


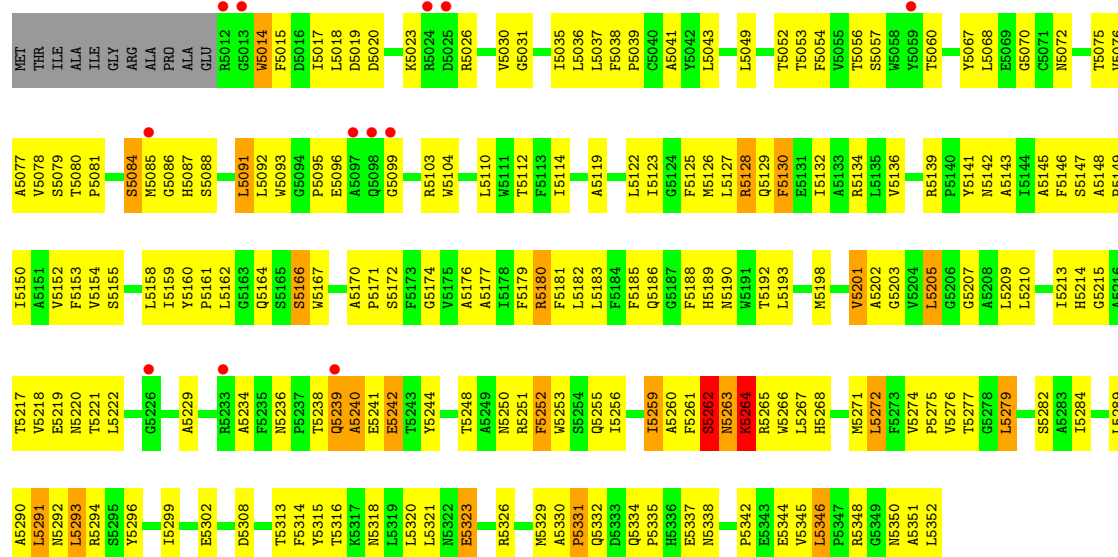


• Molecule 3: Photosystem II CP43 protein

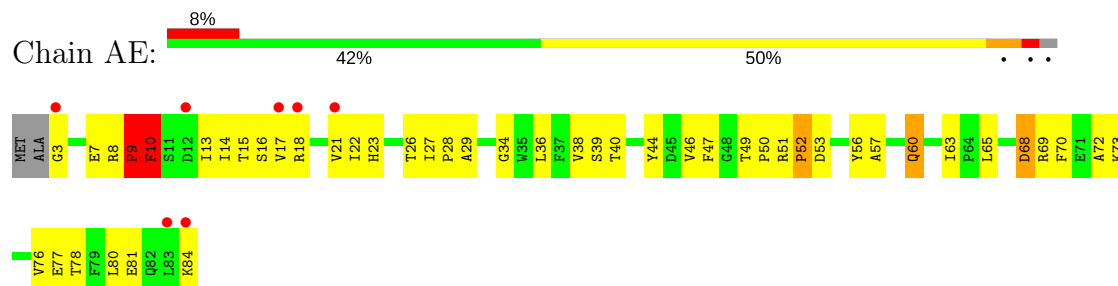


• Molecule 3: Photosystem II CP43 protein

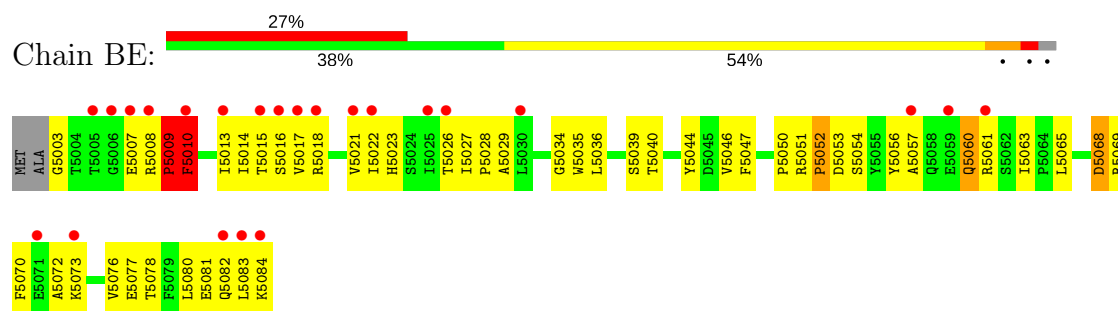




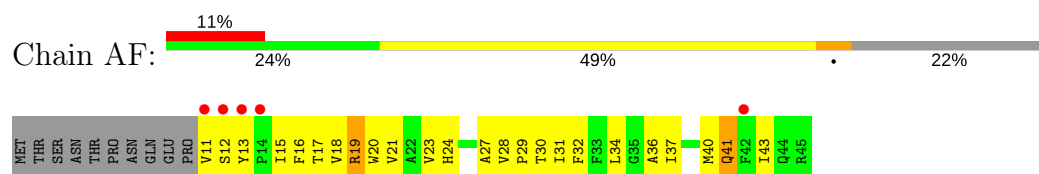
- Molecule 5: Cytochrome b559 subunit alpha



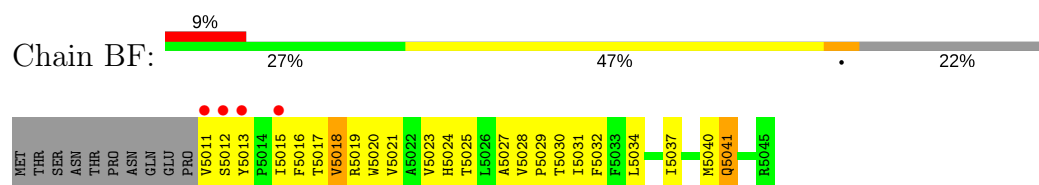
- Molecule 5: Cytochrome b559 subunit alpha



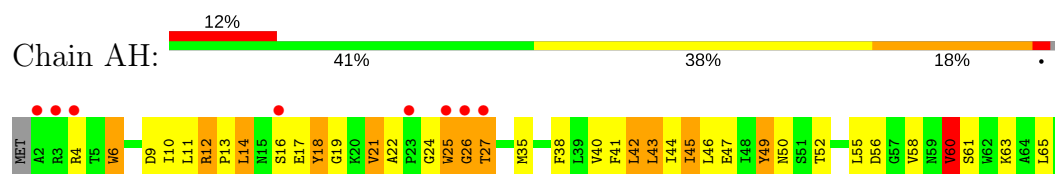
- Molecule 6: Cytochrome b559 subunit beta



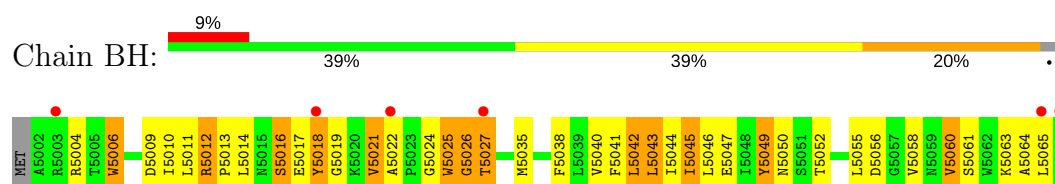
- Molecule 6: Cytochrome b559 subunit beta



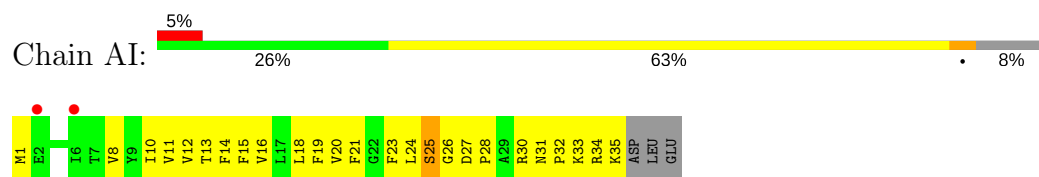
- Molecule 7: Photosystem II reaction center protein H



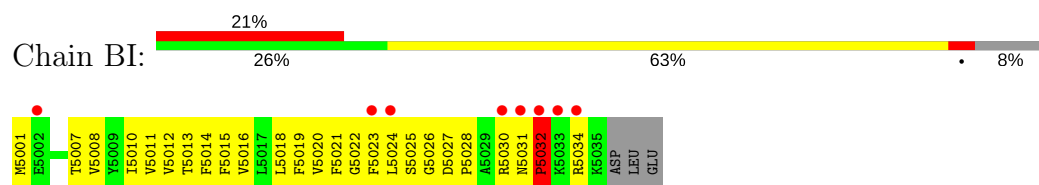
- Molecule 7: Photosystem II reaction center protein H



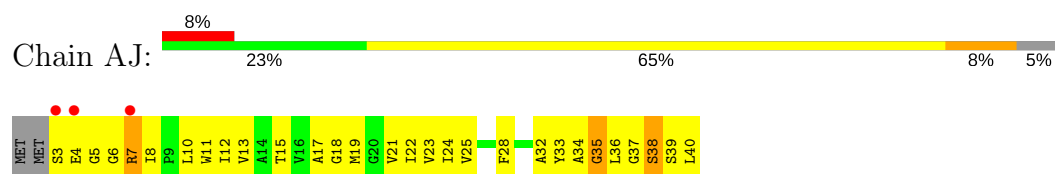
- Molecule 8: Photosystem II reaction center protein I



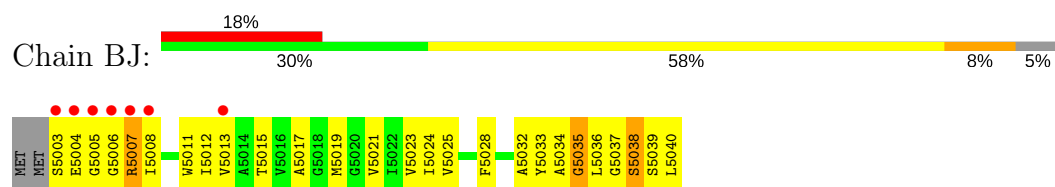
- Molecule 8: Photosystem II reaction center protein I



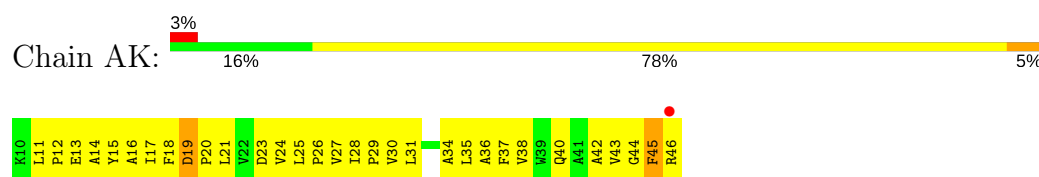
- Molecule 9: Photosystem II reaction center protein J



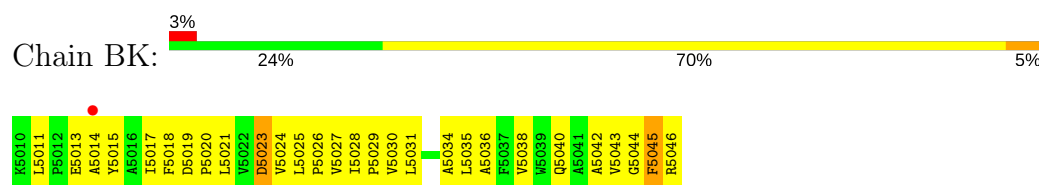
- Molecule 9: Photosystem II reaction center protein J



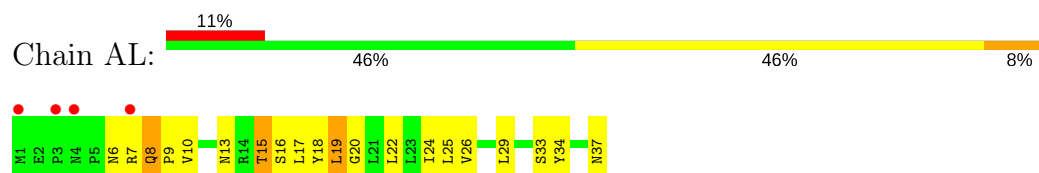
- Molecule 10: Photosystem II reaction center protein K



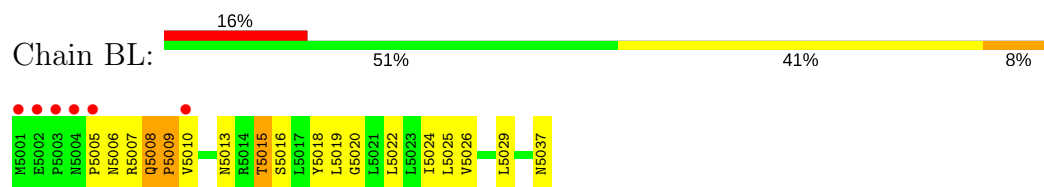
- Molecule 10: Photosystem II reaction center protein K



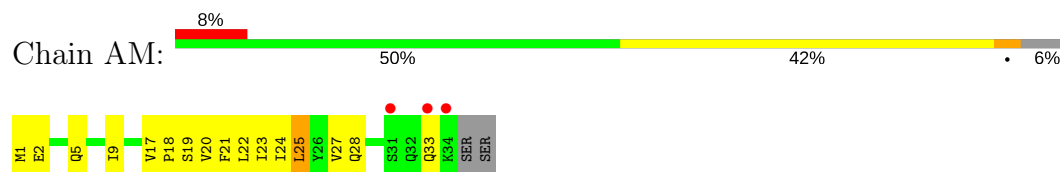
- Molecule 11: Photosystem II reaction center protein L



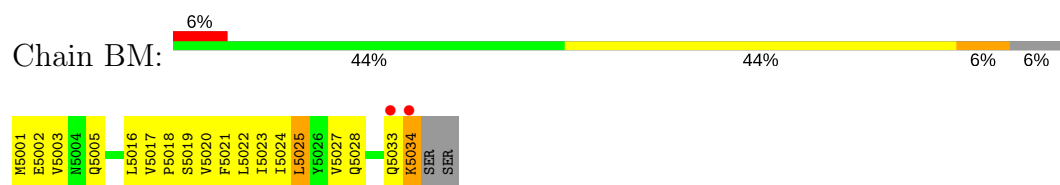
- Molecule 11: Photosystem II reaction center protein L



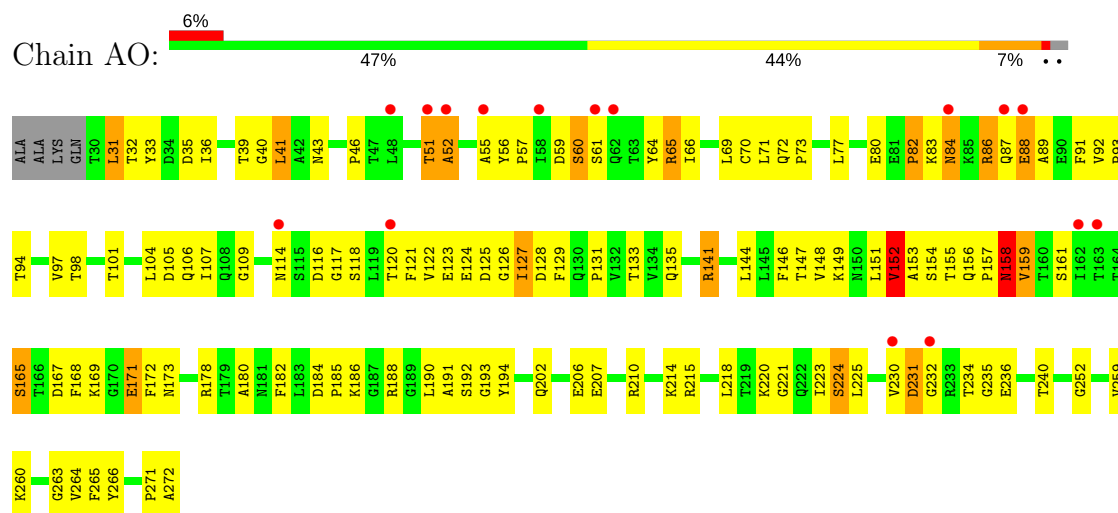
- Molecule 12: Photosystem II reaction center protein M



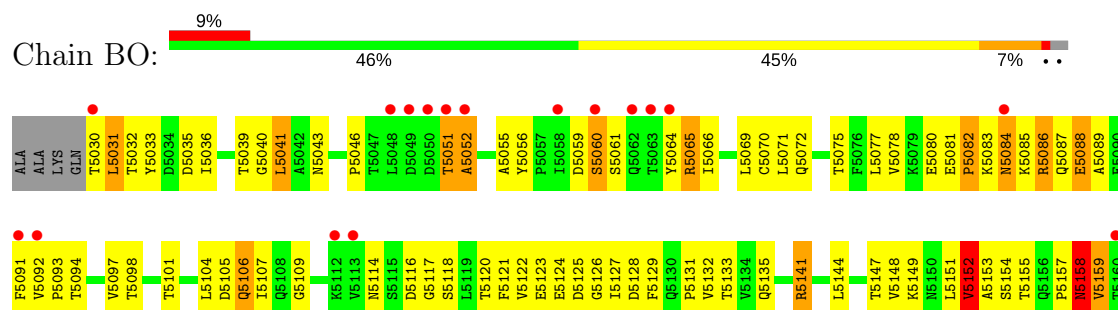
- Molecule 12: Photosystem II reaction center protein M

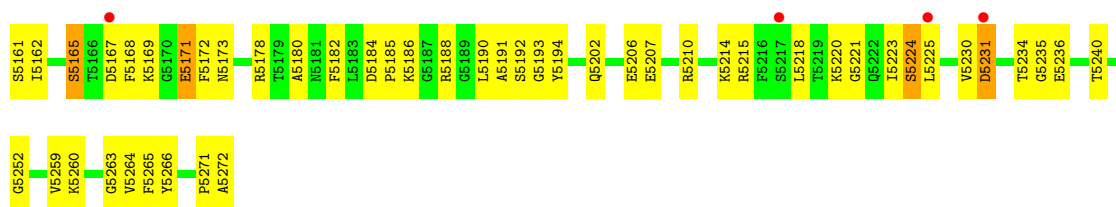


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

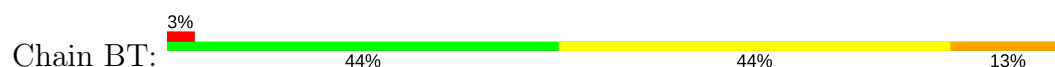




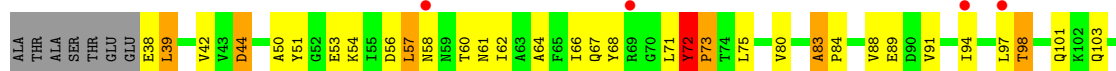
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

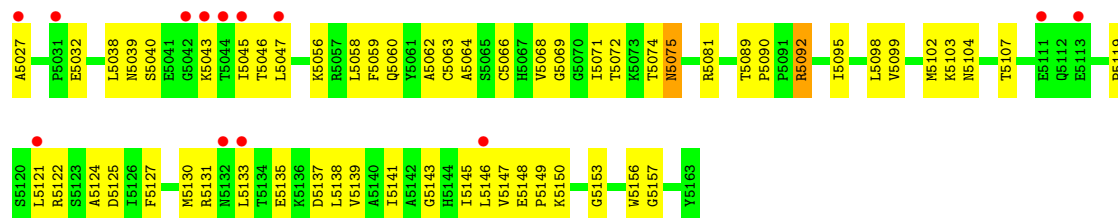


- Molecule 16: Cytochrome c-550

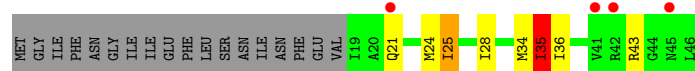
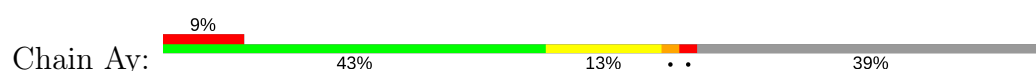




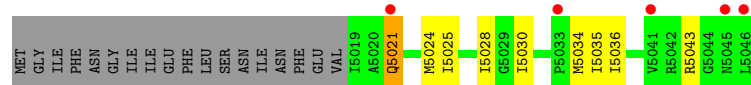
• Molecule 16: Cytochrome c-550



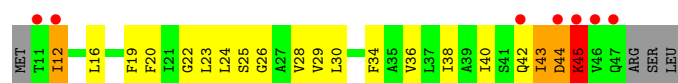
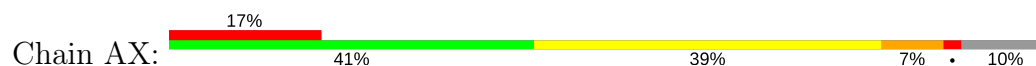
• Molecule 17: Photosystem II reaction center protein ycf12



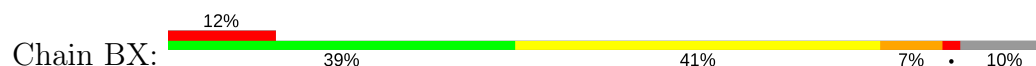
• Molecule 17: Photosystem II reaction center protein ycf12



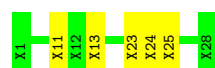
• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: PHOTOSYSTEM II PSBX PROTEIN



- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:  68% 32%



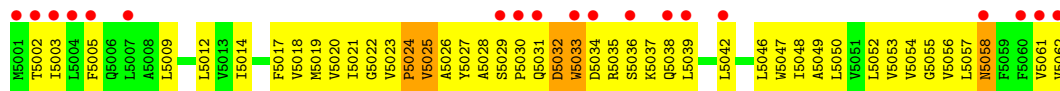
- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:  18% 32% 60% 8%



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:  31% 29% 63% 8%



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 0.272 , 0.292	Depositor DCC
R_{free} test set	2905 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 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
11	BL	304	0	313	35	0
12	AM	267	0	289	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
27	AK	40	0	56	5	0
27	AT	40	0	56	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (3700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.35	1.04
28:BA:5412:DGD:O2D	3:BC:5216:SER:HB2	1.57	1.04
9:BJ:5015:THR:HG21	10:BK:5038:VAL:HG13	1.35	1.04
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.22	1.04
13:BO:5082:PRO:HG3	13:BO:5089:ALA:HB2	1.34	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
2:AB:476:ARG:HH11	2:AB:476:ARG:HB3	1.32	0.94
13:BO:5069:LEU:HB3	13:BO:5107:ILE:HB	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:248:ALA:HA	24:AB:603:CLA:H42	1.49	0.93
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
3:BC:5461:ARG:HG3	3:BC:5461:ARG:HH11	1.33	0.93
4:BD:5274:VAL:HA	35:BD:5406:PL9:H253	1.51	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
1:BA:5102:LEU:HB2	31:BA:5402:LMG:H351	1.51	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
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:HBB1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:5061:SER:HA	28:BH:5101:DGD:HE4	1.54	0.87
3:AC:451:ALA:HA	3:AC:456:GLU:OE2	1.74	0.87
13:BO:5230:VAL:HG12	13:BO:5231:ASP:H	1.39	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
2:AB:179:GLN:HE21	2:AB:179:GLN:HA	1.43	0.84
7:AH:61:SER:HA	28:AH:101:DGD:HE4	1.59	0.84
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.58	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
1:AA:177:SER:HA	1:AA:180:PHE:HD2	1.42	0.84
2:BB:5383:PHE:O	13:BO:5192:SER:HA	1.78	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: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
24:AA:405:CLA:H93	34:AD:402:PHO:HMA1	1.60	0.83
1:BA:5289:GLY:O	1:BA:5292:THR:HG22	1.77	0.83
13:AO:32:THR:O	13:AO:36:ILE:HD12	1.79	0.83
2:BB:5464:PHE:HD2	24:BB:5615:CLA:HAC2	1.43	0.83
13:BO:5032:THR:O	13:BO:5036:ILE:HD12	1.77	0.83
5:AE:15:THR:HG22	9:AJ:7:ARG:N	1.93	0.83
3:BC:5130:VAL:HG13	24:BC:5511:CLA:H92	1.60	0.83
4:BD:5148:ALA:HB2	4:BD:5276:VAL:HG13	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5031:LEU:H	13:BO:5031:LEU:HD12	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
24:BC:5504:CLA:C15	28:BC:5519:DGD:HA91	2.08	0.82
7:AH:55:LEU:HD21	18:AX:16:LEU:HD23	1.59	0.82
1:BA:5278:TRP:CH2	28:BC:5519:DGD:HBG1	2.13	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
2:AB:155:ALA:O	2:AB:161:LEU:HD22	1.79	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
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
4:AD:17:ILE:HG21	18:AX:42:GLN:HG2	1.63	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
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.80	0.81
2:BB:5354:LEU:CD2	2:BB:5378:LYS:HB2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5464:GLU:HB3	3:BC:5467:LEU:HD12	1.64	0.80
31:AA:414:LMG:O3	5:AE:9:PRO:HB3	1.81	0.80
2:AB:297:THR:HG23	2:AB:300:GLU:H	1.47	0.80
2:AB:357:ARG:HG3	2:AB:357:ARG:HH11	1.46	0.80
4:AD:122:LEU:HD21	24:AD:401:CLA:H92	1.64	0.80
4:BD:5221:THR:HG23	4:BD:5244:TYR:HB2	1.63	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
2:AB:383:PHE:O	13:AO:192:SER:HA	1.82	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
3:AC:116:VAL:HG21	27:AC:515:BCR:H323	1.63	0.79
31:AI:101:LMG:H152	32:AI:102:LMT:H52	1.64	0.79
1:BA:5143:ILE:HD11	4:BD:5217:THR:HA	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
5:BE:5009:PRO:HB3	31:BE:5101:LMG:O3	1.81	0.79
3:AC:372:PRO:O	13:AO:36:ILE:HD13	1.82	0.79
1:BA:5177:SER:HA	1:BA:5180:PHE:HD2	1.47	0.79
1:AA:84:PRO:HA	1:AA:112:TYR:CD2	2.16	0.79
24:AA:407:CLA:H43	24:AC:505:CLA:H201	1.64	0.79
1:AA:278:TRP:CH2	28:AC:519:DGD:HBG1	2.18	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
1:AA:258:LEU:HB3	1:AA:259:ILE:HD13	1.63	0.78
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
2:AB:354:LEU:HD23	2:AB:378:LYS:HB2	1.63	0.78
20:AZ:19:MET:O	20:AZ:23:VAL:HG23	1.83	0.78
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HD1	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:461:ARG:CG	3:AC:461:ARG:HH11	1.96	0.78
24:BA:5408:CLA:H43	24:BC:5505:CLA:H201	1.66	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
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
3:AC:48:LYS:HE2	3:AC:138:GLU:HG3	1.67	0.77
1:AA:127:MET:HE3	3:AC:442:LEU:HD21	1.67	0.77
10:AK:27:VAL:O	10:AK:30:VAL:HG12	1.82	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:AC:464:GLU:HB3	3:AC:467:LEU:HD12	1.65	0.77
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	2.00	0.77
3:BC:5219:GLY:HA2	28:BC:5517:DGD:O3D	1.85	0.77
3:AC:117:VAL:HG11	31:AC:521:LMG:H192	1.67	0.77
24:AC:511:CLA:H202	20:AZ:20:VAL:HA	1.66	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
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.67	0.76
2:BB:5297:THR:HG23	2:BB:5300:GLU:H	1.50	0.76
24:AC:504:CLA:C15	28:AC:519:DGD:HA91	2.14	0.76
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.67	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
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.66	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
1:AA:262:TYR:CE1	31:AA:414:LMG:HC5	2.21	0.76
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.49	0.76
1:BA:5259:ILE:N	1:BA:5259:ILE:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:BB:5121:GLU:HG3	7:BH:5004:ARG:HA	1.67	0.75
3:BC:5372:PRO:O	13:BO:5036:ILE:HD13	1.86	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
3:BC:5385:GLN:H	3:BC:5388:GLN:NE2	1.85	0.74
4:BD:5103:ARG:NH1	5:BE:5077:GLU:HG3	2.02	0.74
10:BK:5027:VAL:O	10:BK:5030:VAL:HG12	1.86	0.74
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.69	0.74
1:BA:5315:ASN:HD21	4:BD:5332:GLN:HE22	1.35	0.74
31:AA:417:LMG:H201	2:BB:5098:LEU:HD13	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
1:AA:13:LEU:HA	1:AA:16:ARG:HD3	1.69	0.74
13:AO:230:VAL:HG12	13:AO:231:ASP:N	2.03	0.74
10:AK:18:PHE:HE1	20:AZ:9:LEU:HG	1.51	0.74
13:AO:31:LEU:HD12	13:AO:31:LEU:H	1.51	0.74
13:BO:5178:ARG:HH11	13:BO:5178:ARG:HG3	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	13:BO:5031:LEU:HD12	2.03	0.73
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.21	0.73
2:AB:16:PRO:CG	2:AB:133:LEU:HD11	2.17	0.73
13:AO:171:GLU:HG2	13:AO:172:PHE:N	2.02	0.73
2:BB:5483:ASP:CB	2:BB:5484:PRO:HD2	2.16	0.73
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
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.69	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
10:BK:5018:PHE:HE1	20:BZ:5009:LEU:HG	1.53	0.73
24:AC:513:CLA:HMC2	27:AC:515:BCR:H372	1.70	0.73
3:AC:397:THR:HG21	16:AV:66:CYS:SG	2.27	0.73
2:BB:5474:LEU:HD13	30:BB:5625:SQD:H81	1.68	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
3:AC:248:GLY:O	3:AC:252:ILE:HG12	1.89	0.73
3:AC:55:ALA:HB1	27:AC:514:BCR:H373	1.69	0.73
24:BB:5612:CLA:H52	24:BB:5613:CLA:H8	1.71	0.73
1:AA:18:CYS:O	1:AA:22:THR:HG22	1.89	0.73
1:AA:300:PHE:HE2	28:AC:519:DGD:O1A	1.71	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
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
24:BC:5509:CLA:H121	24:BC:5509:CLA:HBD	1.71	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:5086:ILE:HD12	2:BB:5086:ILE:O	1.89	0.72
2:BB:5371:THR:HG22	2:BB:5377:VAL:HA	1.71	0.72
2:BB:5214:LEU:O	2:BB:5218:LEU:HG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5018:LEU:HD22	18:BX:5038:ILE:HD13	1.71	0.72
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.90	0.72
7:BH:5021:VAL:HG23	7:BH:5022:ALA:O	1.88	0.72
8:BI:5016:VAL:O	8:BI:5020:VAL:HG23	1.90	0.72
2:AB:86:ILE:HD12	2:AB:86:ILE:O	1.90	0.72
1:BA:5013:LEU:HA	1:BA:5016:ARG:HD3	1.69	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
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
4:AD:91:LEU:HD22	7:AH:52:THR:HG21	1.70	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
2:AB:137:LYS:O	2:AB:141:ILE:HG13	1.90	0.71
35:AD:405:PL9:H303	35:AD:405:PL9:H23	1.70	0.71
2:BB:5425:ILE:HG22	2:BB:5426:PHE:CD2	2.25	0.71
4:BD:5053:THR:HG22	4:BD:5067:TYR:CE2	2.25	0.71
1:AA:133:LEU:HD23	4:AD:252:PHE:CD1	2.26	0.71
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.72	0.71
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.55	0.71
3:BC:5397:THR:HG21	16:BV:5066:CYS:SG	2.30	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
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
4:AD:134:ARG:HA	4:AD:134:ARG:HE	1.56	0.71
12:AM:20:VAL:HG21	12:BM:5020:VAL:HG21	1.72	0.71
20:BZ:5019:MET:O	20:BZ:5023:VAL:HG23	1.90	0.71
2:AB:425:ILE:HG22	2:AB:426:PHE:CD2	2.26	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
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
20:AZ:52:LEU:O	20:AZ:56:VAL:HG23	1.91	0.71
11:BL:5013:ASN:HD21	11:BL:5015:THR:HG22	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:235:GLU:HG2	2:AB:235:GLU:O	1.91	0.70
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.91	0.70
5:AE:18:ARG:O	5:AE:22:ILE:HG13	1.90	0.70
2:BB:5004:PRO:HD2	2:BB:5007:ARG:HB2	1.71	0.70
5:BE:5034:GLY:HA2	6:BF:5032:PHE:CE1	2.26	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
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
10:BK:5028:ILE:HA	10:BK:5031:LEU:CD1	2.18	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
2:AB:98:LEU:HD13	31:BA:5402:LMG:H201	1.73	0.70
24:BB:5618:CLA:OBD	11:BL:5010:VAL:HG21	1.90	0.70
1:AA:49:VAL:O	1:AA:53:ILE:HG13	1.92	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
2:AB:183:PRO:HG3	2:AB:199:VAL:CG1	2.21	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
1:AA:288:LEU:HD13	3:AC:432:VAL:HG23	1.74	0.70
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	1.92	0.70
1:BA:5260:PHE:CE1	1:BA:5263:ALA:HB2	2.27	0.70
2:BB:5068:ARG:HH12	24:BB:5608:CLA:HED1	1.56	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
2:BB:5137:LYS:O	2:BB:5141:ILE:HG13	1.92	0.69
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
1:BA:5032:TRP:HA	1:BA:5032:TRP:CE3	2.27	0.69
2:BB:5297:THR:HG22	2:BB:5300:GLU:OE1	1.92	0.69
7:BH:5058:VAL:O	7:BH:5058:VAL:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AA:334:ARG:HD3	4:AD:320:LEU:CD1	2.23	0.69
2:AB:298:LEU:HD23	2:AB:402:TYR:CZ	2.28	0.69
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.75	0.69
4:BD:5018:LEU:HD22	18:BX:5038:ILE:CD1	2.22	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
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
3:BC:5154:LYS:HE2	3:BC:5261:ARG:HD2	1.74	0.69
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.27	0.69
6:AF:27:ALA:HB1	36:AF:101:HEM:HBC2	1.74	0.69
7:AH:55:LEU:O	7:AH:58:VAL:HG12	1.92	0.69
3:BC:5158:THR:O	3:BC:5251:HIS:HB3	1.92	0.69
4:BD:5274:VAL:HB	4:BD:5275:PRO:HD3	1.74	0.69
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.22	0.69
1:BA:5271:LEU:HD12	25:BA:5409:MST:H162	1.73	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
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.23	0.69
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.93	0.69
1:AA:177:SER:HA	1:AA:180:PHE:CD2	2.28	0.69
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.75	0.69
1:AA:278:TRP:CD2	28:AC:519:DGD:HAG2	2.25	0.69
24:BC:5502:CLA:HBB2	24:BC:5510:CLA:H152	1.74	0.69
1:BA:5300:PHE:HE2	28:BC:5519:DGD:O1A	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
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
3:BC:5415:ASN:O	3:BC:5416:SER:HB3	1.93	0.68
6:BF:5027:ALA:HB1	36:BF:5101:HEM:HBC2	1.73	0.68
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.74	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
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
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AC:515:BCR:H312	20:AZ:55:GLY:HA2	1.74	0.68
1:BA:5038:ILE:HG23	30:BA:5401:SQD:H131	1.76	0.68
1:BA:5234:ASN:HD21	4:BD:5266:TRP:HB2	1.57	0.68
1:BA:5278:TRP:CZ3	28:BC:5519:DGD:HAG2	2.27	0.68
4:BD:5250:ASN:HD22	4:BD:5262:SER:HB3	1.57	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
5:AE:23:HIS:HA	5:AE:26:THR:OG1	1.93	0.68
8:AI:11:VAL:HG22	32:AI:102:LMT:H101	1.76	0.68
1:BA:5288:LEU:HD13	3:BC:5432:VAL:HG23	1.76	0.68
24:BC:5513:CLA:HMC2	27:BC:5515:BCR:H372	1.76	0.68
4:BD:5129:GLN:NE2	4:BD:5143:ALA:HA	2.08	0.68
1:BA:5234:ASN:ND2	4:BD:5266:TRP:HB2	2.09	0.68
4:BD:5192:THR:HG23	24:BD:5402:CLA:HBC2	1.75	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
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
18:AX:12:ILE:HG13	18:AX:12:ILE:O	1.94	0.68
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.93	0.68
2:BB:5005:TRP:O	2:BB:5008:VAL:HG13	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
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.59	0.68
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.08	0.68
16:AV:66:CYS:SG	36:AV:201:HEM:CAC	2.81	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
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	1.94	0.67
3:AC:62:PHE:HE2	10:AK:28:ILE:HB	1.59	0.67
3:AC:262:ARG:HH21	32:AI:103:LMT:H5'	1.59	0.67
12:AM:33:GLN:HB3	12:BM:5033:GLN:CB	2.23	0.67
3:BC:5150:ASP:HB3	3:BC:5153:ASP:HB2	1.75	0.67
2:AB:121:GLU:HG2	7:AH:4:ARG:HD2	1.74	0.67
2:BB:5065:PHE:O	24:BB:5609:CLA:HBA1	1.94	0.67
10:BK:5040:GLN:HA	10:BK:5043:VAL:HG12	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:5025:LEU:O	12:BM:5028:GLN:HG3	1.95	0.67
1:BA:5239:PHE:O	14:BT:5029:ILE:HA	1.95	0.67
2:AB:297:THR:HG22	2:AB:300:GLU:OE1	1.94	0.67
27:AC:515:BCR:C31	20:AZ:55:GLY:HA2	2.24	0.67
13:AO:114:ASN:HD21	13:AO:120:THR:HG23	1.59	0.67
2:BB:5068:ARG:HH12	24:BB:5608:CLA:CED	2.07	0.67
13:BO:5092:VAL:CG1	13:BO:5093:PRO:HD2	2.24	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:HD23	1.76	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:BB:5250:PHE:CD2	2:BB:5459:ALA:HB1	2.30	0.67
1:AA:214:MET:HE3	1:AA:214:MET:HA	1.74	0.67
2:AB:103:LEU:HD21	24:AB:605:CLA:HMC3	1.76	0.67
2:AB:130:GLU:HB2	2:AB:131:PRO:HD2	1.76	0.67
24:AC:502:CLA:HBB2	24:AC:510:CLA:H152	1.76	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:CD2	2.24	0.67
7:AH:9:ASP:O	7:AH:12:ARG:HB2	1.95	0.67
2:BB:5379:ALA:HA	2:BB:5390:TYR:HB3	1.76	0.67
14:BT:5029:ILE:HD12	14:BT:5029:ILE:H	1.58	0.67
2:AB:8:VAL:HB	24:AB:614:CLA:O1D	1.95	0.67
1:BA:5190:HIS:HB3	1:BA:5293:MET:HE2	1.76	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
2:AB:234:ILE:HD12	2:AB:237:VAL:HG21	1.77	0.67
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.77	0.67
31:AA:414:LMG:HO2	5:AE:10:PHE:HD2	1.43	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
3:BC:5347:GLY:HA3	13:BO:5043:ASN:HB2	1.75	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
3:BC:5199:ILE:H	3:BC:5199:ILE:HD12	1.60	0.67
3:BC:5308:GLU:HB2	3:BC:5361:PHE:CE1	2.29	0.67
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CZ	2.29	0.67
16:BV:5063:CYS:SG	36:BV:5201:HEM:CAB	2.81	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
3:AC:199:ILE:HD12	3:AC:199:ILE:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5297:LEU:HD11	3:BC:5404:LEU:HD12	1.77	0.66
13:BO:5169:LYS:HG2	13:BO:5224:SER:HB3	1.77	0.66
3:AC:134:ILE:HD11	24:AC:511:CLA:H93	1.77	0.66
15:AU:66:ILE:O	15:AU:66:ILE:HG22	1.95	0.66
2:BB:5224:ARG:HG3	7:BH:5025:TRP:CD1	2.30	0.66
3:BC:5040:ALA:O	3:BC:5043:ILE:HG13	1.95	0.66
2:BB:5222:PRO:HG3	7:BH:5027:THR:H	1.58	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
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	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:5248:GLY:O	3:BC:5252:ILE:HG12	1.94	0.66
3:BC:5254:THR:CG2	3:BC:5255:THR:H	2.06	0.66
16:BV:5133:LEU:H	16:BV:5133:LEU:HD12	1.59	0.66
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.76	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
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.59	0.66
10:AK:28:ILE:HA	10:AK:31:LEU:CD1	2.17	0.66
18:AX:36:VAL:O	18:AX:40:ILE:HG22	1.96	0.66
4:BD:5261:PHE:HA	31:BD:5410:LMG:O2	1.96	0.66
5:BE:5027:ILE:HB	5:BE:5028:PRO:HD3	1.78	0.66
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.77	0.66
2:AB:357:ARG:HG3	2:AB:357:ARG:NH1	2.06	0.66
2:AB:5:TRP:O	2:AB:8:VAL:HG13	1.95	0.66
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.76	0.66
20:AZ:32:ASP:HA	20:AZ:34:ASP:OD2	1.95	0.66
1:BA:5033:PHE:CE1	24:BC:5505:CLA:H92	2.27	0.66
2:AB:120:LEU:HD13	24:AB:616:CLA:HMD2	1.78	0.66
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.77	0.66
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.29	0.66
13:AO:31:LEU:N	13:AO:31:LEU:HD12	2.11	0.66
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	1.96	0.66
1:BA:5330:VAL:HG11	4:BD:5348:ARG:HG2	1.77	0.66
24:BC:5504:CLA:H172	28:BC:5519:DGD:HAE1	1.76	0.66
10:BK:5019:ASP:N	10:BK:5020:PRO:HD2	2.10	0.66
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:BC:5305:THR:HG23	3:BC:5308:GLU:H	1.59	0.66
1:BA:5221:SER:HB2	4:BD:5139:ARG:O	1.96	0.66
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.17	0.66
13:AO:87:GLN:O	13:AO:88:GLU:CG	2.41	0.66
2:BB:5008:VAL:HB	24:BB:5618:CLA:O1D	1.95	0.66
1:AA:39:PRO:HB2	24:AA:407:CLA:CBB	2.25	0.66
30:AB:627:SQD:H242	30:AB:627:SQD:H81	1.76	0.66
3:AC:254:THR:CG2	3:AC:255:THR:H	2.07	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
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
4:BD:5103:ARG:HG3	5:BE:5073:LYS:CG	2.26	0.66
13:BO:5114:ASN:HD21	13:BO:5120:THR:HG23	1.60	0.66
3:AC:405:ASN:HB2	28:AC:519:DGD:HG32	1.77	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
1:BA:5278:TRP:CD2	28:BC:5519:DGD:HAG2	2.29	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
2:AB:489:GLU:HB2	5:AE:3:GLY:N	2.11	0.65
2:AB:65:PHE:O	24:AB:605:CLA:HBA1	1.96	0.65
24:AB:614:CLA:OBD	11:AL:10:VAL:HG21	1.95	0.65
31:AI:101:LMG:O9	31:AI:101:LMG:O8	2.14	0.65
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.79	0.65
3:BC:5262:ARG:HH21	32:BC:5522:LMT:H5'	1.61	0.65
3:BC:5282:MET:HG2	24:BC:5501:CLA:H71	1.78	0.65
15:BU:5066:ILE:O	15:BU:5066:ILE:HG22	1.95	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
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.60	0.65
2:AB:468:TRP:HD1	2:AB:469:HIS:ND1	1.94	0.65
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.10	0.65
8:AI:19:PHE:CE1	8:AI:23:PHE:HE2	2.14	0.65
20:AZ:2:THR:HG23	20:AZ:3:ILE:H	1.60	0.65
1:BA:5039:PRO:HB2	24:BA:5408:CLA:CBB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5183:PRO:HG3	2:BB:5199:VAL:CG1	2.27	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
13:BO:5087:GLN:O	13:BO:5088:GLU:CG	2.41	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: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
3:BC:5416:SER:C	28:BC:5519:DGD:O3E	2.35	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
16:AV:71:ILE:HD12	16:AV:72:THR:N	2.11	0.65
3:BC:5405:ASN:HB2	28:BC:5519:DGD:HG32	1.77	0.65
5:BE:5023:HIS:HA	5:BE:5026:THR:OG1	1.96	0.65
5:BE:5010:PHE:HD2	31:BE:5101:LMG:HO2	1.45	0.65
31:BI:5101:LMG:O8	31:BI:5101:LMG:O9	2.15	0.65
1:AA:271:LEU:HD12	25:AA:408:MST:H162	1.78	0.65
2:AB:213:GLY:O	2:AB:217:ILE:HG13	1.97	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
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:BA:5097:TRP:HA	8:BI:5001:MET:SD	2.36	0.65
2:BB:5062:VAL:HG13	24:BB:5609:CLA:HED3	1.78	0.65
3:BC:5062:PHE:CE2	10:BK:5028:ILE:HB	2.32	0.65
31:BD:5410:LMG:O6	11:BL:5015:THR:HG21	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
3:BC:5320:ARG:O	3:BC:5324:LEU:HD23	1.96	0.65
16:BV:5071:ILE:HD12	16:BV:5072:THR:N	2.12	0.65
3:AC:179:ALA:HB1	3:AC:199:ILE:HD13	1.79	0.65
3:AC:282:MET:HG2	24:AC:501:CLA:H71	1.79	0.65
5:AE:51:ARG:HG3	5:AE:51:ARG:HH11	1.62	0.65
2:BB:5009:HIS:HB2	24:BB:5615:CLA:HBA2	1.79	0.65
2:BB:5222:PRO:HG3	7:BH:5026:GLY:HA3	1.78	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:AB:224:ARG:HG2	7:AH:24:GLY:O	1.97	0.65
4:AD:153:PHE:HB2	24:AD:401:CLA:H41	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:78:THR:HA	5:AE:81:GLU:HG2	1.78	0.65
1:AA:257:ARG:HG3	1:AA:257:ARG:HH11	1.62	0.64
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.32	0.64
3:AC:362:ARG:HE	3:AC:370:ARG:HH11	1.45	0.64
2:BB:5150:CYS:HB2	24:BB:5607:CLA:HMC3	1.78	0.64
2:BB:5393:GLU:HG2	15:BU:5044:ASP:O	1.97	0.64
15:BU:5058:ASN:ND2	15:BU:5114:VAL:HG13	2.11	0.64
1:AA:288:LEU:HD22	3:AC:432:VAL:HG23	1.80	0.64
1:AA:300:PHE:CE2	28:AC:519:DGD:O1A	2.50	0.64
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.79	0.64
3:BC:5416:SER:C	28:BC:5519:DGD:HO3E	2.01	0.64
3:AC:320:ARG:O	3:AC:324:LEU:HD23	1.97	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
16:AV:135:GLU:O	16:AV:139:VAL:HG23	1.97	0.64
3:BC:5052:ALA:HA	24:BC:5511:CLA:CMB	2.24	0.64
1:BA:5048:PHE:HB2	1:BA:5115:ILE:HD13	1.79	0.64
3:BC:5149:TYR:HA	3:BC:5156:LYS:HD3	1.77	0.64
2:AB:384:ARG:HD3	15:AU:132:LEU:CD1	2.28	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: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
1:BA:5228:THR:HG22	1:BA:5229:GLU:H	1.61	0.64
3:BC:5179:ALA:HB1	3:BC:5199:ILE:HD13	1.77	0.64
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.12	0.64
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.31	0.64
1:BA:5010:SER:HB3	1:BA:5016:ARG:NH1	2.13	0.64
2:BB:5246:PHE:CD1	2:BB:5246:PHE:C	2.71	0.64
2:AB:278:SER:HB3	2:AB:281:GLN:HE21	1.63	0.64
2:AB:9:HIS:HB2	24:AB:611:CLA:HBA2	1.79	0.64
3:BC:5418:ASN:CA	28:BC:5519:DGD:HE2	2.27	0.64
3:BC:5030:SER:HB3	10:BK:5046:ARG:O	1.98	0.64
1:AA:281:VAL:CG1	28:AC:519:DGD:HAG3	2.27	0.64
2:AB:214:LEU:O	2:AB:218:LEU:HG	1.97	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
3:AC:42:LEU:HD23	24:AC:511:CLA:HED3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:38:PHE:HB2	27:AX:101:BCR:H10C	1.78	0.64
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	1.98	0.64
2:BB:5103:LEU:HD21	24:BB:5609:CLA:HMC3	1.80	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
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.81	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
31:AB:620:LMG:H202	11:AL:26:VAL:HG21	1.79	0.63
3:BC:5449:ARG:HG2	24:BC:5505:CLA:HED1	1.80	0.63
8:BI:5014:PHE:CZ	8:BI:5018:LEU:HD11	2.33	0.63
2:BB:5191:ASN:HB2	7:BH:5058:VAL:HG23	1.79	0.63
2:BB:5187:PRO:HB3	24:BB:5605:CLA:HMB2	1.79	0.63
28:BC:5518:DGD:HG11	31:BC:5520:LMG:H301	1.81	0.63
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:C40	2.26	0.63
4:BD:5236:ASN:ND2	4:BD:5239:GLN:O	2.29	0.63
8:BI:5011:VAL:HG22	32:BI:5102:LMT:H101	1.80	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
3:AC:304:PRO:HB3	3:AC:395:TYR:CD1	2.33	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
4:BD:5041:ALA:HB1	34:BD:5404:PHO:H42	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:AC:518:DGD:HG11	31:AC:520:LMG:H301	1.81	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
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
1:AA:274:PHE:CE2	25:AA:408:MST:H133	2.33	0.63
2:AB:124:ARG:HH11	2:AB:124:ARG:HG3	1.63	0.63
3:AC:461:ARG:CG	3:AC:461:ARG:NH1	2.60	0.63
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.63
2:AB:191:ASN:HB2	7:AH:58:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	1.99	0.63
3:BC:5437:PHE:CZ	24:BC:5502:CLA:HMC1	2.34	0.63
5:BE:5076:VAL:O	5:BE:5080:LEU:HD22	1.98	0.63
1:AA:221:SER:HB2	4:AD:139:ARG:O	1.99	0.63
1:BA:5343:LEU:O	1:BA:5344:ALA:HB2	1.99	0.63
11:BL:5016:SER:HA	11:BL:5019:LEU:HG	1.80	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
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.29	0.62
4:BD:5053:THR:HG22	4:BD:5067:TYR:CD2	2.34	0.62
7:BH:5038:PHE:HB2	27:BX:5101:BCR:H10C	1.81	0.62
2:AB:150:CYS:HB2	24:AB:603:CLA:HMC3	1.82	0.62
3:BC:5413:GLU:HG3	3:BC:5414:ILE:H	1.64	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:265:PHE:CD1	1:AA:271:LEU:HA	2.34	0.62
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.14	0.62
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.62
4:AD:207:GLY:HA3	4:AD:275:PRO:HG3	1.80	0.62
35:AD:405:PL9:H303	35:AD:405:PL9:C23	2.30	0.62
1:BA:5228:THR:HG22	1:BA:5229:GLU:N	2.15	0.62
2:BB:5008:VAL:HG23	2:BB:5009:HIS:CD2	2.34	0.62
4:BD:5241:GLU:H	4:BD:5241:GLU:CD	2.01	0.62
11:BL:5018:TYR:CE2	14:BT:5020:ALA:HA	2.35	0.62
16:BV:5047:LEU:HD11	16:BV:5143:GLY:HA3	1.81	0.62
4:AD:103:ARG:HG3	5:AE:73:LYS:CG	2.28	0.62
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.34	0.62
4:AD:80:THR:HB	4:AD:81:PRO:HD2	1.80	0.62
5:BE:5008:ARG:HH22	5:BE:5016:SER:HB3	1.64	0.62
3:AC:432:VAL:CG1	3:AC:433:LEU:N	2.63	0.62
4:AD:261:PHE:CD2	4:AD:267:LEU:HD12	2.35	0.62
5:AE:34:GLY:CA	6:AF:32:PHE:CE1	2.83	0.62
1:BA:5193:LEU:HD13	4:BD:5179:PHE:HB3	1.81	0.62
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BV:5092:ARG:HG3	16:BV:5092:ARG:HH11	1.65	0.62
1:AA:48:PHE:HB2	1:AA:115:ILE:HD13	1.81	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:5062:PHE:HD2	10:BK:5029:PRO:HG3	1.65	0.62
3:BC:5039:ASN:HB3	24:BC:5509:CLA:CBB	2.30	0.62
2:AB:179:GLN:HE21	2:AB:180:PRO:HD2	1.64	0.62
4:AD:14:TRP:CD1	4:AD:15:PHE:N	2.68	0.62
15:AU:58:ASN:HD22	15:AU:114:VAL:HG13	1.64	0.62
1:BA:5296:ASN:HB2	3:BC:5400:PRO:O	2.00	0.62
1:BA:5306:VAL:HG13	1:BA:5314:ILE:O	2.00	0.62
2:BB:5284:ILE:HG23	2:BB:5305:ILE:HD12	1.82	0.62
18:BX:5036:VAL:O	18:BX:5040:ILE:HG22	1.99	0.62
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.00	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
3:AC:40:ALA:O	3:AC:43:ILE:HG13	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
3:AC:62:PHE:HD2	10:AK:29:PRO:HG3	1.65	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
4:BD:5080:THR:HB	4:BD:5081:PRO:HD2	1.81	0.62
6:BF:5017:THR:HG23	6:BF:5020:TRP:H	1.65	0.62
24:AB:608:CLA:H143	24:AD:404:CLA:HMB2	1.82	0.61
5:AE:26:THR:HB	36:AF:101:HEM:HAB	1.81	0.61
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.34	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
3:BC:5041:ARG:NH1	24:BC:5511:CLA:OBD	2.33	0.61
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.65	0.61
16:AV:99:VAL:O	16:AV:103:LYS:HG3	2.00	0.61
1:BA:5012:ASN:HD22	1:BA:5015:GLU:HB2	1.66	0.61
2:BB:5284:ILE:HG23	2:BB:5305:ILE:CD1	2.30	0.61
4:BD:5239:GLN:O	4:BD:5240:ALA:HB3	2.00	0.61
31:AB:621:LMG:H411	4:AD:284:ILE:HG12	1.82	0.61
2:AB:453:PHE:HB2	4:AD:291:LEU:HD23	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
11:BL:5007:ARG:O	11:BL:5007:ARG:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:142:HIS:HA	2:AB:145:LEU:HD12	1.83	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
5:BE:5051:ARG:HG3	5:BE:5051:ARG:HH11	1.65	0.61
13:BO:5151:LEU:HD12	13:BO:5152:VAL:H	1.65	0.61
2:BB:5247:PHE:HB2	24:BB:5612:CLA:HBC1	1.81	0.61
29:AA:412:LHG:HC11	3:AC:447:ARG:NH2	2.16	0.61
24:AB:611:CLA:H201	24:AB:613:CLA:H92	1.82	0.61
1:BA:5200:LEU:HD13	28:BC:5519:DGD:HAW2	1.78	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:5324:LEU:N	3:BC:5324:LEU:HD22	2.15	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:5033:PHE:CE1	4:BD:5229:ALA:CB	2.84	0.61
1:AA:10:SER:HB3	1:AA:16:ARG:NH1	2.14	0.61
2:AB:179:GLN:NE2	2:AB:180:PRO:HD2	2.15	0.61
3:AC:324:LEU:HD22	3:AC:324:LEU:N	2.16	0.61
1:BA:5131:TRP:CE3	1:BA:5132:GLU:N	2.69	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
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
27:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.81	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
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
2:BB:5278:SER:HB3	2:BB:5281:GLN:HE21	1.65	0.61
7:BH:5009:ASP:O	7:BH:5012:ARG:HB2	2.01	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.01	0.61
2:AB:246:PHE:C	2:AB:246:PHE:CD1	2.72	0.61
3:AC:30:SER:HB3	10:AK:46:ARG:O	2.00	0.61
13:AO:151:LEU:HD12	13:AO:152:VAL:H	1.64	0.61
13:AO:169:LYS:HG2	13:AO:224:SER:HB3	1.82	0.61
2:BB:5173:GLY:CA	2:BB:5265:ILE:HD11	2.31	0.61
1:AA:262:TYR:CZ	31:AA:414:LMG:HC5	2.36	0.60
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG11	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:222:PRO:HD2	2:AB:225:LEU:HD12	1.83	0.60
3:AC:113:VAL:HG11	31:AC:521:LMG:H132	1.83	0.60
2:BB:5133:LEU:HB3	2:BB:5138:MET:CE	2.30	0.60
1:AA:262:TYR:OH	31:AA:414:LMG:HC5	2.00	0.60
2:AB:153:PHE:N	24:AB:606:CLA:HMC3	2.16	0.60
16:AV:92:ARG:HH11	16:AV:92:ARG:HG3	1.66	0.60
1:BA:5300:PHE:CE2	28:BC:5519:DGD:O1A	2.54	0.60
7:BH:5006:TRP:CE2	7:BH:5010:ILE:HD11	2.36	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
4:BD:5253:TRP:HA	4:BD:5256:ILE:HG22	1.84	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
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.02	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
1:AA:324:ALA:HB2	4:AD:329:MET:SD	2.42	0.60
9:AJ:17:ALA:O	9:AJ:21:VAL:HG23	2.01	0.60
12:AM:19:SER:O	12:AM:23:ILE:HD13	2.01	0.60
24:BC:5504:CLA:H152	28:BC:5519:DGD:HA91	1.84	0.60
10:BK:5018:PHE:CE1	20:BZ:5009:LEU:HG	2.36	0.60
15:BU:5113:THR:O	15:BU:5114:VAL:HG23	2.01	0.60
4:AD:80:THR:HG23	4:AD:172:SER:OG	2.01	0.60
2:BB:5068:ARG:NH2	24:BB:5608:CLA:HED1	2.17	0.60
29:AA:415:LHG:HC41	29:AA:415:LHG:O9	2.02	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
1:AA:297:LEU:HD11	3:AC:404:LEU:HD12	1.84	0.60
3:AC:437:PHE:CZ	24:AC:502:CLA:HMC1	2.36	0.60
16:AV:104:ASN:HA	16:AV:122:ARG:HD3	1.83	0.60
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.36	0.60
2:BB:5384:ARG:HD3	15:BU:5132:LEU:CD1	2.32	0.60
3:BC:5044:ASN:C	3:BC:5045:LEU:HD12	2.21	0.60
24:BC:5503:CLA:H171	24:BC:5510:CLA:HBB2	1.83	0.60
12:BM:5001:MET:CG	12:BM:5002:GLU:H	2.13	0.60
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.84	0.60
2:AB:113:TRP:CE2	2:AB:117:TYR:HD1	2.20	0.60
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.83	0.60
3:AC:41:ARG:NH1	24:AC:511:CLA:OBD	2.34	0.60
24:AB:603:CLA:H161	7:AH:38:PHE:HE2	1.65	0.60
1:BA:5289:GLY:O	1:BA:5292:THR:CG2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5124:ARG:HH11	2:BB:5124:ARG:HG3	1.67	0.60
24:BB:5608:CLA:HMD2	24:BB:5616:CLA:H193	1.83	0.60
4:BD:5145:ALA:HB2	4:BD:5272:LEU:HD21	1.83	0.60
13:BO:5118:SER:HB3	13:BO:5157:PRO:HA	1.84	0.60
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.84	0.60
30:AB:622:SQD:H442	4:AD:23:LYS:HE2	1.82	0.60
13:AO:64:TYR:HD1	13:AO:271:PRO:HA	1.67	0.60
2:BB:5142:HIS:HA	2:BB:5145:LEU:HD12	1.83	0.60
3:BC:5156:LYS:O	3:BC:5160:ILE:HG13	2.02	0.60
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.37	0.60
3:BC:5143:TYR:O	3:BC:5144:SER:HB2	2.02	0.60
3:BC:5216:SER:HB3	3:BC:5221:GLU:HB2	1.84	0.60
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NH2	2.17	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
3:AC:167:VAL:HG11	24:AC:512:CLA:H3A	1.84	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:5413:GLU:HG3	3:BC:5414:ILE:N	2.17	0.59
3:BC:5042:LEU:HD23	24:BC:5511:CLA:HED3	1.82	0.59
9:BJ:5017:ALA:O	9:BJ:5021:VAL:HG23	2.01	0.59
24:AA:405:CLA:HBA2	31:AB:620:LMG:C25	2.32	0.59
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.25	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
2:AB:359:MET:HB2	2:AB:425:ILE:HG23	1.84	0.59
5:AE:8:ARG:HH22	5:AE:16:SER:HB3	1.67	0.59
16:AV:47:LEU:HD11	16:AV:143:GLY:HA3	1.83	0.59
1:BA:5265:PHE:CD1	1:BA:5271:LEU:HA	2.36	0.59
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HG23	1.82	0.59
2:BB:5265:ILE:HG13	2:BB:5266:GLU:N	2.17	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
10:BK:5024:VAL:O	10:BK:5027:VAL:HG12	2.02	0.59
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.38	0.59
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.13	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
3:AC:324:LEU:CD2	3:AC:324:LEU:N	2.66	0.59
6:AF:19:ARG:HH11	6:AF:19:ARG:HG3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:206:GLU:CD	13:AO:206:GLU:H	2.05	0.59
1:BA:5257:ARG:HH11	1:BA:5257:ARG:HG3	1.66	0.59
4:BD:5014:TRP:CD1	4:BD:5015:PHE:N	2.70	0.59
3:BC:5415:ASN:HB3	9:BJ:5039:SER:OG	2.03	0.59
10:BK:5017:ILE:N	10:BK:5017:ILE:HD12	2.17	0.59
24:AB:604:CLA:H121	24:AB:615:CLA:HBA1	1.83	0.59
3:AC:362:ARG:HE	3:AC:370:ARG:NH1	1.99	0.59
1:BA:5220:THR:HG23	4:BD:5141:TYR:HD1	1.68	0.59
2:BB:5487:SER:N	2:BB:5488:PRO:HD2	2.17	0.59
3:AC:305:THR:HG22	3:AC:308:GLU:HB3	1.81	0.59
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.84	0.59
1:BA:5083:VAL:HG22	4:BD:5314:PHE:CE2	2.36	0.59
35:BD:5406:PL9:C30	35:BD:5406:PL9:H262	2.32	0.59
11:BL:5013:ASN:ND2	11:BL:5015:THR:HG22	2.18	0.59
16:BV:5099:VAL:O	16:BV:5103:LYS:HG3	2.02	0.59
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.02	0.59
1:AA:97:TRP:HA	8:AI:1:MET:SD	2.43	0.59
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.84	0.59
4:AD:299:ILE:HG13	11:AL:37:ASN:HD21	1.67	0.59
5:AE:51:ARG:NH1	5:AE:51:ARG:HG3	2.15	0.59
8:AI:14:PHE:CZ	8:AI:18:LEU:HD11	2.38	0.59
24:AC:511:CLA:H151	20:AZ:24:PRO:HG3	1.84	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:BC:5504:CLA:H151	28:BC:5519:DGD:C9A	2.31	0.59
5:BE:5026:THR:HB	36:BF:5101:HEM:HAB	1.85	0.59
6:BF:5037:ILE:HA	6:BF:5040:MET:SD	2.43	0.59
2:AB:483:ASP:HB3	2:AB:484:PRO:HD2	1.85	0.59
1:BA:5032:TRP:HA	1:BA:5032:TRP:HE3	1.67	0.59
3:BC:5170:ILE:HG22	3:BC:5174:LEU:CD2	2.33	0.59
3:BC:5033:PHE:CE1	4:BD:5229:ALA:HB3	2.38	0.59
2:AB:384:ARG:HD3	15:AU:132:LEU:HD11	1.85	0.59
35:AD:405:PL9:H262	35:AD:405:PL9:C30	2.33	0.59
15:AU:68:TYR:HB2	15:AU:71:LEU:HD12	1.84	0.59
1:BA:5188:ALA:HB2	1:BA:5328:MET:HB2	1.85	0.59
3:BC:5405:ASN:HB2	28:BC:5519:DGD:C3G	2.32	0.59
7:BH:5055:LEU:O	7:BH:5058:VAL:HG12	2.02	0.59
10:BK:5031:LEU:O	10:BK:5034:ALA:HB3	2.03	0.59
24:AA:405:CLA:H92	34:AD:402:PHO:HMB3	1.85	0.59
1:AA:64:ARG:N	1:AA:64:ARG:HD3	2.17	0.59
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:AD:150:ILE:O	4:AD:154:VAL:HG23	2.03	0.59
6:AF:15:ILE:HG22	6:AF:16:PHE:HD1	1.68	0.59
15:AU:98:THR:HG23	15:AU:101:GLN:OE1	2.03	0.59
24:BB:5612:CLA:H202	7:BH:5043:LEU:HD11	1.83	0.59
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.85	0.58
1:AA:180:PHE:CD1	4:AD:192:THR:HB	2.38	0.58
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.03	0.58
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.03	0.58
1:BA:5013:LEU:CA	1:BA:5016:ARG:HD3	2.33	0.58
2:BB:5458:PHE:HB3	24:BB:5608:CLA:HBC2	1.84	0.58
3:BC:5324:LEU:CD2	3:BC:5324:LEU:N	2.65	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
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.02	0.58
6:BF:5015:ILE:HG22	6:BF:5016:PHE:HD1	1.68	0.58
7:BH:5012:ARG:N	7:BH:5013:PRO:HD2	2.18	0.58
10:BK:5026:PRO:O	10:BK:5029:PRO:HD2	2.02	0.58
4:BD:5299:ILE:HG13	11:BL:5037:ASN:HD21	1.68	0.58
1:BA:5020:TRP:CD1	1:BA:5020:TRP:C	2.75	0.58
28:BC:5519:DGD:HG2	9:BJ:5033:TYR:OH	2.03	0.58
9:BJ:5011:TRP:CE3	10:BK:5042:ALA:HB2	2.39	0.58
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.68	0.58
2:AB:144:PHE:CE1	2:AB:210:ILE:HG23	2.39	0.58
2:AB:490:GLN:OE1	2:AB:490:GLN:O	2.21	0.58
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.03	0.58
15:AU:54:LYS:HD2	15:AU:113:THR:HG23	1.86	0.58
1:BA:5163:ILE:HG12	28:BC:5517:DGD:HB31	1.85	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
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
1:AA:271:LEU:C	1:AA:271:LEU:HD23	2.24	0.58
2:BB:5246:PHE:HD1	2:BB:5246:PHE:C	2.07	0.58
2:BB:5359:MET:HB2	2:BB:5425:ILE:HG23	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5349:LYS:HG3	2:BB:5350:GLU:OE1	2.03	0.58
3:BC:5432:VAL:CG1	3:BC:5433:LEU:N	2.65	0.58
6:BF:5011:VAL:HG12	6:BF:5012:SER:H	1.69	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
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.04	0.58
3:AC:257:PHE:O	3:AC:261:ARG:HG3	2.03	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
2:BB:5170:ASP:HB2	2:BB:5171:PRO:CD	2.32	0.58
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.38	0.58
3:AC:39:ASN:HB2	24:AC:508:CLA:HBA2	1.84	0.58
4:AD:244:TYR:OH	4:AD:264:LYS:HD2	2.03	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.03	0.58
1:BA:5272:HIS:HD2	4:BD:5218:VAL:HG21	1.68	0.58
2:BB:5479:PHE:O	2:BB:5480:SER:HB2	2.03	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
6:BF:5018:VAL:HG12	6:BF:5019:ARG:N	2.19	0.58
16:BV:5133:LEU:H	16:BV:5133:LEU:CD1	2.16	0.58
1:AA:219:VAL:HG11	4:AD:268:HIS:CD2	2.38	0.58
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.03	0.58
4:AD:171:PRO:HG3	4:AD:181:PHE:CZ	2.39	0.58
2:BB:5179:GLN:NE2	2:BB:5180:PRO:HD2	2.18	0.58
24:BB:5618:CLA:H202	31:BL:5101:LMG:H422	1.86	0.58
3:BC:5367:GLU:HB2	3:BC:5368:PRO:HD3	1.86	0.58
4:BD:5244:TYR:OH	4:BD:5264:LYS:HD2	2.04	0.58
8:BI:5027:ASP:N	8:BI:5028:PRO:CD	2.66	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: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:BB:5113:TRP:CE2	2:BB:5117:TYR:HD1	2.22	0.58
1:BA:5219:VAL:HG11	4:BD:5268:HIS:CD2	2.38	0.58
1:AA:330:VAL:CG1	4:AD:348:ARG:HG2	2.34	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AX:16:LEU:O	18:AX:16:LEU:HD13	2.04	0.57
1:BA:5341:LEU:HB2	3:BC:5313:GLN:NE2	2.10	0.57
3:BC:5226:SER:O	28:BC:5517:DGD:HE62	2.04	0.57
3:BC:5377:LEU:O	3:BC:5381:LYS:HB2	2.04	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
14:BT:5022:PHE:C	14:BT:5023:PHE:HD2	2.06	0.57
1:AA:260:PHE:CZ	1:AA:263:ALA:HB2	2.39	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
3:AC:449:ARG:HG2	24:AC:505:CLA:HED1	1.86	0.57
6:AF:37:ILE:HA	6:AF:40:MET:SD	2.44	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
3:BC:5297:TYR:HA	3:BC:5302:TYR:HE2	1.69	0.57
24:BB:5606:CLA:H11	7:BH:5049:TYR:HD2	1.69	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
13:AO:32:THR:O	13:AO:36:ILE:CD1	2.52	0.57
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.05	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
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.69	0.57
2:AB:458:PHE:HB3	24:AB:604:CLA:HBC2	1.86	0.57
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
2:BB:5262:THR:HG23	2:BB:5263:THR:HG23	1.86	0.57
32:BB:5627:LMT:H112	7:BH:5035:MET:HE2	1.87	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
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.24	0.57
1:BA:5317:TRP:CD1	4:BD:5177:ALA:HB2	2.38	0.57
3:BC:5220:GLY:N	28:BC:5517:DGD:O3D	2.35	0.57
3:AC:199:ILE:HD12	3:AC:199:ILE:N	2.18	0.57
4:AD:335:PRO:HB2	5:AE:65:LEU:HD21	1.86	0.57
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.87	0.57
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:BC:5039:ASN:HB2	24:BC:5508:CLA:HBA2	1.85	0.57
4:BD:5056:THR:HG21	5:BE:5050:PRO:HD3	1.87	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
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.87	0.57
2:AB:246:PHE:C	2:AB:246:PHE:HD1	2.08	0.57
24:AC:504:CLA:H2	28:AC:518:DGD:HA21	1.87	0.57
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.38	0.57
24:BB:5614:CLA:O1D	24:BB:5614:CLA:H121	2.04	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
13:BO:5114:ASN:ND2	13:BO:5120:THR:HG23	2.20	0.57
2:AB:327:THR:O	2:AB:444:ARG:NE	2.36	0.57
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.05	0.57
24:AC:504:CLA:H172	28:AC:519:DGD:HAE1	1.85	0.57
1:BA:5191:ASN:HB2	3:BC:5411:ALA:HB1	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
18:BX:5045:LYS:N	18:BX:5045:LYS:HD3	2.19	0.57
24:BB:5613:CLA:HMC2	27:BX:5101:BCR:H343	1.85	0.57
25:AA:408:MST:H122	25:AA:408:MST:N3	2.20	0.56
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.35	0.56
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.05	0.56
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.87	0.56
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.04	0.56
32:AB:624:LMT:H92	7:AH:35:MET:CE	2.35	0.56
1:BA:5278:TRP:O	1:BA:5281:VAL:HG12	2.05	0.56
24:BB:5606:CLA:HBD	24:BB:5606:CLA:H43	1.86	0.56
32:BB:5627:LMT:H92	7:BH:5035:MET:CE	2.35	0.56
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
5:BE:5077:GLU:HA	5:BE:5080:LEU:HD23	1.87	0.56
3:BC:5062:PHE:HZ	10:BK:5028:ILE:HD12	1.69	0.56
13:BO:5098:THR:HG23	13:BO:5133:THR:HB	1.87	0.56
28:AA:411:DGD:O1B	28:AA:411:DGD:C1G	2.53	0.56
13:AO:114:ASN:ND2	13:AO:120:THR:HG23	2.19	0.56
1:BA:5180:PHE:CE1	4:BD:5192:THR:HB	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:5058:VAL:O	7:BH:5058:VAL:CG1	2.53	0.56
1:AA:15:GLU:O	1:AA:19:ASN:OD1	2.23	0.56
1:AA:262:TYR:CE1	31:AA:414:LMG:C5	2.89	0.56
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.20	0.56
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.56
27:AC:516:BCR:HC41	8:AI:20:VAL:HG13	1.86	0.56
5:AE:56:TYR:HE1	5:AE:63:ILE:HD12	1.69	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
2:BB:5271:THR:OG1	2:BB:5274:GLN:HG3	2.05	0.56
3:BC:5199:ILE:N	3:BC:5199:ILE:HD12	2.20	0.56
3:BC:5304:PRO:HB3	3:BC:5395:TYR:CD1	2.40	0.56
4:BD:5221:THR:CG2	4:BD:5244:TYR:HB2	2.35	0.56
2:BB:5453:PHE:HB2	4:BD:5291:LEU:HD23	1.87	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
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.68	0.56
2:BB:5462:PHE:HA	24:BB:5615:CLA:CMC	2.35	0.56
3:BC:5362:ARG:HE	3:BC:5370:ARG:HH11	1.52	0.56
3:BC:5375:LEU:HB3	3:BC:5380:ILE:HD11	1.87	0.56
4:BD:5158:LEU:O	4:BD:5162:LEU:HG	2.06	0.56
4:BD:5086:GLY:C	4:BD:5166:SER:HB2	2.25	0.56
20:BZ:5014:ILE:O	20:BZ:5018:VAL:HG23	2.05	0.56
1:AA:126:TYR:O	1:AA:130:GLN:HG3	2.06	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
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.05	0.56
2:BB:5027:THR:HG22	2:BB:5107:LEU:CD1	2.24	0.56
3:BC:5297:TYR:HA	3:BC:5302:TYR:CE2	2.40	0.56
1:BA:5326:LEU:HD21	3:BC:5412:THR:HB	1.87	0.56
5:BE:5051:ARG:HG3	5:BE:5051:ARG:NH1	2.19	0.56
8:BI:5013:THR:HA	8:BI:5016:VAL:HG12	1.85	0.56
5:BE:5014:ILE:CG2	9:BJ:5013:VAL:HG11	2.35	0.56
13:BO:5154:SER:O	13:BO:5168:PHE:HA	2.05	0.56
2:AB:262:THR:HG23	2:AB:263:THR:HG23	1.88	0.56
2:AB:271:THR:OG1	2:AB:274:GLN:HG3	2.05	0.56
24:AB:611:CLA:C5	24:AB:614:CLA:HBC2	2.36	0.56
16:AV:133:LEU:CD1	16:AV:133:LEU:H	2.18	0.56
3:BC:5149:TYR:HA	3:BC:5156:LYS:CD	2.35	0.56
13:BO:5173:ASN:ND2	13:BO:5220:LYS:HD3	2.20	0.56
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AC:505:CLA:O1A	8:AI:23:PHE:CE1	2.59	0.56
3:AC:114:VAL:HG22	31:AC:521:LMG:H141	1.87	0.56
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	2.05	0.56
4:AD:145:ALA:HB2	4:AD:272:LEU:HD21	1.86	0.56
8:AI:13:THR:O	8:AI:16:VAL:HG12	2.06	0.56
13:AO:148:VAL:HA	13:AO:172:PHE:CD2	2.40	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
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
1:BA:5221:SER:HB3	4:BD:5141:TYR:HB2	1.86	0.56
13:BO:5215:ARG:NH1	13:BO:5252:GLY:O	2.38	0.56
15:BU:5083:ALA:CB	15:BU:5084:PRO:CD	2.82	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
3:AC:170:ILE:HG22	3:AC:174:LEU:CD2	2.36	0.56
3:AC:44:ASN:O	3:AC:45:LEU:HD12	2.05	0.56
3:AC:42:LEU:CD2	24:AC:511:CLA:HED3	2.36	0.56
4:AD:241:GLU:H	4:AD:241:GLU:CD	2.08	0.56
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.88	0.56
5:AE:57:ALA:H	5:AE:60:GLN:NE2	2.04	0.56
1:BA:5092:HIS:HD2	3:BC:5219:GLY:HA3	1.71	0.56
1:BA:5124:SER:O	1:BA:5127:MET:HB3	2.06	0.56
1:BA:5133:LEU:O	1:BA:5137:LEU:HG	2.06	0.56
2:BB:5179:GLN:HE21	2:BB:5180:PRO:HD2	1.71	0.56
2:BB:5329:PRO:HD3	24:BB:5611:CLA:HED1	1.86	0.56
4:BD:5129:GLN:HE22	4:BD:5143:ALA:HA	1.70	0.56
5:BE:5056:TYR:HE1	5:BE:5063:ILE:HD12	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
1:AA:180:PHE:CE1	4:AD:192:THR:HB	2.41	0.56
1:AA:157:VAL:HG21	24:AA:405:CLA:CMC	2.36	0.56
3:AC:57:ALA:HB1	24:AC:512:CLA:HED2	1.88	0.56
5:AE:15:THR:HB	9:AJ:6:GLY:HA2	1.87	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
2:BB:5462:PHE:CZ	24:BB:5617:CLA:HMB3	2.41	0.56
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB3	1.83	0.56
5:BE:5069:ARG:HG3	5:BE:5070:PHE:N	2.20	0.56
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CD2	2.41	0.56
3:BC:5343:ARG:NH1	3:BC:5347:GLY:O	2.39	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
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.87	0.56
24:BA:5406:CLA:H93	34:BD:5403:PHO:HHB	1.88	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
15:BU:5058:ASN:HD22	15:BU:5114:VAL:HG13	1.69	0.56
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
24:AC:513:CLA:H42	24:AC:513:CLA:HAA1	1.88	0.55
3:AC:405:ASN:HA	28:AC:519:DGD:HG11	1.88	0.55
35:AD:405:PL9:H301	35:AD:405:PL9:C33	2.34	0.55
14:AT:29:ILE:N	14:AT:29:ILE:HD12	2.06	0.55
18:AX:12:ILE:HA	27:AX:101:BCR:H401	1.88	0.55
1:BA:5048:PHE:HA	1:BA:5115:ILE:HD11	1.88	0.55
3:BC:5124:VAL:HB	27:BC:5515:BCR:H362	1.88	0.55
28:BC:5518:DGD:HB22	28:BC:5519:DGD:HA21	1.88	0.55
16:AV:81:ARG:HH11	16:AV:81:ARG:HG2	1.70	0.55
24:BA:5406:CLA:H92	34:BD:5403:PHO:HMB3	1.87	0.55
2:BB:5144:PHE:CE1	2:BB:5210:ILE:HG23	2.41	0.55
2:BB:5483:ASP:CG	2:BB:5484:PRO:HD2	2.26	0.55
24:BB:5605:CLA:HMB1	27:BX:5101:BCR:H393	1.88	0.55
3:BC:5033:PHE:HE1	4:BD:5229:ALA:CB	2.19	0.55
3:BC:5416:SER:N	28:BC:5519:DGD:O3E	2.37	0.55
5:BE:5076:VAL:O	5:BE:5080:LEU:CD2	2.54	0.55
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.89	0.55
1:AA:304:HIS:CE1	3:AC:414:ILE:HD12	2.41	0.55
24:AB:601:CLA:HMB1	27:AX:101:BCR:H393	1.88	0.55
25:BA:5409:MST:N3	25:BA:5409:MST:H131	2.20	0.55
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CIA	2.36	0.55
8:BI:5013:THR:O	8:BI:5016:VAL:HG12	2.06	0.55
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.55
24:AA:405:CLA:H201	14:AT:14:ILE:HD11	1.86	0.55
4:AD:86:GLY:C	4:AD:166:SER:HB2	2.26	0.55
2:BB:5154:GLY:O	2:BB:5159:THR:HG23	2.06	0.55
3:BC:5170:ILE:HG22	3:BC:5174:LEU:HD23	1.88	0.55
3:BC:5225:VAL:HG22	3:BC:5289:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5239:GLN:O	4:BD:5240:ALA:CB	2.54	0.55
4:BD:5014:TRP:NE1	7:BH:5025:TRP:HH2	1.95	0.55
9:BJ:5011:TRP:CG	10:BK:5042:ALA:HA	2.41	0.55
12:BM:5005:GLN:HE22	32:BM:5101:LMT:H3'	1.71	0.55
13:BO:5092:VAL:HG13	13:BO:5093:PRO:HD2	1.87	0.55
15:BU:5098:THR:HG23	15:BU:5101:GLN:OE1	2.07	0.55
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD11	1.89	0.55
2:AB:231:MET:HG2	24:AB:610:CLA:HMC1	1.89	0.55
4:AD:253:TRP:HA	4:AD:256:ILE:HG22	1.89	0.55
3:BC:5155:ASN:O	3:BC:5158:THR:HG22	2.07	0.55
4:BD:5266:TRP:CD1	31:BD:5410:LMG:HC1	2.42	0.55
15:BU:5066:ILE:HG12	15:BU:5072:TYR:CG	2.42	0.55
20:BZ:5033:TRP:CD1	20:BZ:5033:TRP:O	2.60	0.55
1:AA:124:SER:O	1:AA:127:MET:HB3	2.07	0.55
1:AA:191:ASN:HB2	3:AC:411:ALA:HB1	1.89	0.55
1:AA:340:PRO:HG2	3:AC:317:PHE:CZ	2.42	0.55
1:AA:205:VAL:HG21	24:AA:404:CLA:CMA	2.37	0.55
2:AB:121:GLU:HG3	7:AH:4:ARG:CA	2.36	0.55
24:AB:602:CLA:H11	7:AH:49:TYR:HD2	1.71	0.55
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.07	0.55
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.36	0.55
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.06	0.55
1:BA:5176:ILE:HG22	1:BA:5180:PHE:HE2	1.71	0.55
1:BA:5271:LEU:HD21	25:BA:5409:MST:H83	1.89	0.55
2:BB:5176:GLY:HA3	2:BB:5266:GLU:OE1	2.06	0.55
2:BB:5275:TRP:CH2	2:BB:5358:ARG:HD3	2.41	0.55
3:BC:5461:ARG:CG	3:BC:5461:ARG:NH1	2.61	0.55
27:BC:5515:BCR:H312	20:BZ:5055:GLY:HA2	1.88	0.55
4:BD:5049:LEU:O	4:BD:5053:THR:HG23	2.06	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
32:AB:630:LMT:H41	8:BI:5001:MET:CE	2.36	0.55
12:AM:20:VAL:HG22	12:BM:5020:VAL:HG11	1.89	0.55
29:BA:5415:LHG:HC41	29:BA:5415:LHG:O9	2.05	0.55
2:BB:5348:ASN:OD1	2:BB:5352:GLU:HB2	2.06	0.55
3:BC:5257:PHE:O	3:BC:5261:ARG:HG3	2.06	0.55
7:BH:5055:LEU:HB2	7:BH:5058:VAL:HG12	1.89	0.55
1:AA:341:LEU:HB2	3:AC:313:GLN:NE2	2.17	0.55
2:AB:90:PHE:CE2	2:AB:91:TRP:CZ3	2.94	0.55
3:AC:35:TRP:O	24:AC:511:CLA:HMD3	2.07	0.55
4:AD:259:ILE:HG12	31:AD:408:LMG:H301	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AM:23:ILE:HG12	31:AM:101:LMG:H212	1.89	0.55
13:AO:64:TYR:CD1	13:AO:271:PRO:HA	2.41	0.55
1:BA:5217:SER:HA	1:BA:5220:THR:HG22	1.89	0.55
1:BA:5289:GLY:C	1:BA:5292:THR:HG22	2.27	0.55
1:BA:5157:VAL:HG21	24:BA:5406:CLA:CMC	2.36	0.55
2:BB:5354:LEU:HD21	2:BB:5378:LYS:HB2	1.89	0.55
3:BC:5281:MET:O	3:BC:5285:ILE:HG13	2.06	0.55
24:BC:5513:CLA:H42	24:BC:5513:CLA:HAA1	1.88	0.55
4:BD:5313:THR:OG1	4:BD:5315:TYR:HB3	2.07	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:HE1	1.89	0.55
13:BO:5064:TYR:HD1	13:BO:5271:PRO:HA	1.72	0.55
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:N	2.57	0.55
25:AA:408:MST:H131	25:AA:408:MST:N3	2.21	0.55
3:AC:62:PHE:HZ	10:AK:28:ILE:HD12	1.71	0.55
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.22	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
7:BH:5011:LEU:C	7:BH:5013:PRO:HD2	2.28	0.55
3:BC:5453:ALA:C	8:BI:5034:ARG:HB2	2.27	0.55
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.22	0.55
1:AA:288:LEU:HD13	3:AC:432:VAL:CG2	2.37	0.55
24:AC:512:CLA:H203	31:AC:521:LMG:H381	1.88	0.55
24:AB:613:CLA:H203	31:AD:407:LMG:H401	1.89	0.55
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.88	0.55
1:BA:5064:ARG:HD3	1:BA:5064:ARG:H	1.72	0.55
1:BA:5281:VAL:CG1	28:BC:5519:DGD:CIA	2.84	0.55
1:BA:5330:VAL:HG12	4:BD:5348:ARG:HA	1.87	0.55
2:AB:76:SER:HB3	31:BA:5402:LMG:H301	1.88	0.55
28:BA:5412:DGD:C1G	28:BA:5412:DGD:O1B	2.55	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
3:BC:5326:ALA:HB2	15:BU:5128:TYR:CG	2.42	0.55
27:BC:5515:BCR:C31	20:BZ:5055:GLY:HA2	2.37	0.55
1:AA:38:ILE:HB	1:AA:39:PRO:HD3	1.89	0.54
30:AA:416:SQD:H302	24:BB:5620:CLA:H51	1.88	0.54
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	1.87	0.54
28:AC:519:DGD:HE62	9:AJ:40:LEU:HD11	1.89	0.54
13:AO:116:ASP:C	13:AO:116:ASP:OD2	2.46	0.54
15:AU:57:LEU:HD11	15:AU:112:PHE:HB3	1.89	0.54
1:BA:5234:ASN:HB2	31:BL:5101:LMG:O3	2.05	0.54
3:BC:5259:TRP:HD1	3:BC:5259:TRP:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:5222:PRO:HD2	2:BB:5225:LEU:HD12	1.88	0.54
2:BB:5068:ARG:NH1	24:BB:5608:CLA:HED1	2.22	0.54
3:BC:5035:TRP:O	24:BC:5511:CLA:HMD3	2.07	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
24:BB:5617:CLA:H203	31:BD:5409:LMG:H401	1.88	0.54
7:BH:5017:GLU:CD	7:BH:5017:GLU:H	2.10	0.54
8:BI:5010:ILE:HG21	32:BI:5102:LMT:H82	1.88	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
3:AC:466:VAL:HA	3:AC:469:MET:HE1	1.89	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
4:BD:5330:ALA:HB3	4:BD:5331:PRO:HD3	1.89	0.54
15:BU:5064:ALA:O	15:BU:5067:GLN:HG2	2.06	0.54
20:BZ:5023:VAL:O	20:BZ:5026:ALA:HB3	2.08	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
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
13:AO:117:GLY:O	13:AO:159:VAL:HG12	2.07	0.54
1:BA:5069:GLY:HA2	1:BA:5075:ASN:ND2	2.22	0.54
2:BB:5183:PRO:HB2	2:BB:5185:TRP:CH2	2.42	0.54
5:BE:5034:GLY:CA	6:BF:5032:PHE:CE1	2.90	0.54
1:AA:214:MET:HE2	1:AA:214:MET:HA	1.90	0.54
1:AA:261:GLN:NE2	2:AB:489:GLU:HG3	2.22	0.54
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.28	0.54
24:AB:603:CLA:H161	7:AH:38:PHE:CE2	2.43	0.54
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.07	0.54
3:AC:281:MET:O	3:AC:285:ILE:HG13	2.07	0.54
4:AD:128:ARG:HG2	4:AD:129:GLN:N	2.22	0.54
4:AD:152:VAL:HG11	24:AD:401:CLA:H11	1.88	0.54
16:AV:71:ILE:C	16:AV:71:ILE:HD12	2.28	0.54
2:BB:5018:ARG:HD3	2:BB:5118:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BD:5407:BCR:H343	27:BD:5407:BCR:H321	1.89	0.54
31:BD:5410:LMG:H192	31:BL:5101:LMG:H201	1.89	0.54
13:BO:5180:ALA:HB1	13:BO:5191:ALA:HB2	1.90	0.54
20:BZ:5032:ASP:C	20:BZ:5034:ASP:N	2.60	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
20:AZ:33:TRP:O	20:AZ:33:TRP:HD1	1.90	0.54
2:BB:5058:GLN:O	24:BB:5611:CLA:HED3	2.07	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
1:BA:5064:ARG:HG3	1:BA:5064:ARG:HH11	1.71	0.54
1:BA:5315:ASN:ND2	4:BD:5332:GLN:NE2	2.56	0.54
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE2	1.89	0.54
3:BC:5042:LEU:CD2	24:BC:5511:CLA:HED3	2.37	0.54
35:BD:5406:PL9:H401	11:BL:5029:LEU:HD23	1.90	0.54
1:BA:5240:GLY:HA3	14:BT:5029:ILE:HG22	1.88	0.54
2:AB:237:VAL:HG22	24:AB:610:CLA:HBC2	1.88	0.54
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.90	0.54
24:AA:405:CLA:H93	34:AD:402:PHO:HHB	1.89	0.54
35:AD:405:PL9:H401	11:AL:29:LEU:HD23	1.90	0.54
11:AL:18:TYR:CE2	14:AT:20:ALA:HA	2.43	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
24:BA:5406:CLA:C9	34:BD:5403:PHO:HHB	2.37	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
4:BD:5259:ILE:HG12	31:BD:5410:LMG:H301	1.89	0.54
4:BD:5335:PRO:HB2	5:BE:5065:LEU:HD21	1.89	0.54
24:BA:5405:CLA:H202	34:BD:5403:PHO:HMA2	1.89	0.54
6:BF:5011:VAL:HG12	6:BF:5012:SER:N	2.23	0.54
2:BB:5011:VAL:HG23	11:BL:5006:ASN:O	2.07	0.54
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.73	0.54
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.08	0.54
5:AE:76:VAL:O	5:AE:80:LEU:CD2	2.56	0.54
1:BA:5012:ASN:ND2	1:BA:5015:GLU:HB2	2.22	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
2:BB:5246:PHE:CE2	2:BB:5463:PHE:HA	2.43	0.54
3:BC:5223:TRP:CE3	3:BC:5224:ILE:HG13	2.43	0.54
1:AA:64:ARG:HH11	1:AA:64:ARG:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.21	0.54
3:AC:259:TRP:HD1	3:AC:259:TRP:H	1.56	0.54
10:AK:43:VAL:HG21	10:AK:46:ARG:HE	1.72	0.54
1:BA:5260:PHE:CZ	1:BA:5263:ALA:HB2	2.43	0.54
1:BA:5340:PRO:HG2	3:BC:5317:PHE:CZ	2.43	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
3:BC:5250:TRP:C	3:BC:5250:TRP:CD1	2.81	0.54
4:BD:5238:THR:O	4:BD:5239:GLN:O	2.26	0.54
3:BC:5472:LEU:HG	4:BD:5251:ARG:HH12	1.72	0.54
12:BM:5023:ILE:HG12	31:BM:5102:LMG:H212	1.90	0.54
16:BV:5104:ASN:HA	16:BV:5122:ARG:HD3	1.90	0.54
18:BX:5022:GLY:HA2	18:BX:5025:SER:OG	2.08	0.54
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.91	0.53
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
16:AV:38:LEU:HD12	16:AV:95:ILE:HB	1.89	0.53
1:BA:5126:TYR:O	1:BA:5130:GLN:HG3	2.07	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:262:TYR:HE1	31:AA:414:LMG:HC5	1.72	0.53
2:AB:157:HIS:HD2	2:AB:158:LEU:HD23	1.73	0.53
3:AC:163:PHE:O	3:AC:167:VAL:HG23	2.09	0.53
3:AC:170:ILE:HG22	3:AC:174:LEU:HD23	1.91	0.53
24:AA:404:CLA:H202	34:AD:402:PHO:HMA2	1.89	0.53
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.70	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
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
1:AA:315:ASN:HD21	4:AD:332:GLN:NE2	2.05	0.53
2:AB:215:PHE:C	2:AB:215:PHE:CD2	2.82	0.53
3:AC:432:VAL:HG13	3:AC:433:LEU:N	2.23	0.53
9:AJ:19:MET:O	9:AJ:23:VAL:HG23	2.07	0.53
3:BC:5044:ASN:O	3:BC:5045:LEU:HD12	2.08	0.53
3:BC:5155:ASN:HA	3:BC:5158:THR:CG2	2.34	0.53
4:BD:5068:LEU:HD11	5:BE:5044:TYR:CE1	2.43	0.53
1:BA:5332:HIS:HB3	4:BD:5321:LEU:HD21	1.90	0.53
9:BJ:5011:TRP:CE2	9:BJ:5012:ILE:HG13	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.72	0.53
3:AC:311:GLN:OE1	3:AC:355:THR:HG22	2.08	0.53
3:AC:415:ASN:O	3:AC:416:SER:CB	2.55	0.53
4:AD:86:GLY:CA	4:AD:166:SER:HB2	2.38	0.53
4:AD:26:ARG:HH11	4:AD:26:ARG:HG3	1.72	0.53
24:BA:5406:CLA:H201	14:BT:5014:ILE:HD11	1.90	0.53
20:BZ:5049:ALA:O	20:BZ:5053:VAL:HG23	2.07	0.53
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.08	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
3:AC:124:VAL:HB	27:AC:515:BCR:H362	1.89	0.53
13:AO:98:THR:HG23	13:AO:133:THR:HB	1.89	0.53
31:AD:408:LMG:H392	27:AT:101:BCR:HC32	1.91	0.53
15:AU:64:ALA:O	15:AU:67:GLN:HG2	2.08	0.53
18:AX:12:ILE:HG23	18:AX:12:ILE:O	2.09	0.53
1:BA:5190:HIS:O	1:BA:5298:ASN:HB3	2.09	0.53
2:BB:5327:THR:O	2:BB:5444:ARG:NE	2.39	0.53
24:BC:5504:CLA:H2	28:BC:5518:DGD:HA21	1.89	0.53
4:BD:5088:SER:CB	5:BE:5069:ARG:NH2	2.69	0.53
1:BA:5324:ALA:HB2	4:BD:5329:MET:SD	2.49	0.53
5:BE:5010:PHE:HD2	31:BE:5101:LMG:O2	1.92	0.53
3:AC:437:PHE:CZ	24:AC:510:CLA:HMB3	2.44	0.53
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.43	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:279:LEU:HD22	24:AC:503:CLA:H143	1.90	0.53
3:AC:405:ASN:HB2	28:AC:519:DGD:C3G	2.38	0.53
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.39	0.53
27:AD:406:BCR:H321	27:AD:406:BCR:H343	1.91	0.53
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.90	0.53
1:BA:5155:PHE:CE1	28:BA:5412:DGD:HBE1	2.44	0.53
2:BB:5087:ASP:OD1	28:BB:5602:DGD:HD62	2.08	0.53
2:BB:5363:PHE:HD1	4:BD:5326:ARG:HD2	1.74	0.53
8:AI:1:MET:CE	32:BB:5604:LMT:H41	2.39	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
3:BC:5368:PRO:O	3:BC:5379:LYS:HE2	2.08	0.53
4:BD:5037:LEU:HD13	4:BD:5125:PHE:N	2.24	0.53
1:BA:5254:TYR:CD1	4:BD:5132:ILE:HG22	2.43	0.53
16:BV:5074:THR:O	16:BV:5075:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:307:ILE:HG22	1:AA:313:VAL:HA	1.89	0.53
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.08	0.53
2:AB:183:PRO:HG3	2:AB:199:VAL:HG12	1.90	0.53
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.44	0.53
2:AB:462:PHE:HA	24:AB:611:CLA:CMC	2.37	0.53
1:AA:332:HIS:HB3	4:AD:321:LEU:HD21	1.91	0.53
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.91	0.53
13:AO:218:LEU:CD2	15:AU:119:THR:HG21	2.39	0.53
20:AZ:12:LEU:O	20:AZ:12:LEU:HD12	2.08	0.53
1:BA:5333:GLU:HB2	1:BA:5337:HIS:HE1	1.74	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
1:AA:234:ASN:HB2	31:AB:620:LMG:O3	2.09	0.53
1:AA:289:GLY:O	1:AA:292:THR:CG2	2.53	0.53
2:AB:68:ARG:HH22	24:AB:604:CLA:CED	2.21	0.53
24:AC:504:CLA:H151	28:AC:519:DGD:C9A	2.36	0.53
1:AA:220:THR:HG23	4:AD:141:TYR:HD1	1.73	0.53
4:AD:313:THR:OG1	4:AD:315:TYR:HB3	2.09	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
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
12:AM:20:VAL:O	12:AM:24:ILE:HG13	2.07	0.53
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.09	0.53
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.09	0.53
24:BA:5406:CLA:H152	24:BA:5406:CLA:H102	1.91	0.53
3:BC:5166:ILE:HG23	3:BC:5245:ILE:HG23	1.91	0.53
3:BC:5233:VAL:HA	27:BC:5516:BCR:C28	2.38	0.53
4:BD:5134:ARG:HE	4:BD:5134:ARG:CA	2.21	0.53
1:BA:5142:TRP:HB2	4:BD:5220:ASN:OD1	2.09	0.53
5:BE:5008:ARG:HD3	5:BE:5013:ILE:HG12	1.91	0.53
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:CD1	2.38	0.53
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.56	0.52
24:AA:405:CLA:C9	34:AD:402:PHO:HHB	2.39	0.52
24:BB:5614:CLA:HHC	24:BB:5614:CLA:HBB1	1.89	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
2:BB:5005:TRP:CH2	31:BL:5101:LMG:H291	2.44	0.52
20:BZ:5030:PRO:C	20:BZ:5032:ASP:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BZ:5035:ARG:O	20:BZ:5038:GLN:HB3	2.09	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
2:AB:246:PHE:CE2	2:AB:463:PHE:HA	2.44	0.52
30:AB:622:SQD:H152	32:AB:624:LMT:H81	1.90	0.52
4:AD:238:THR:O	4:AD:239:GLN:O	2.28	0.52
4:AD:267:LEU:C	4:AD:267:LEU:HD23	2.30	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
1:BA:5202:VAL:HG11	24:BA:5407:CLA:OBD	2.10	0.52
3:BC:5113:VAL:CG1	31:BC:5521:LMG:H132	2.40	0.52
3:BC:5126:GLY:O	3:BC:5130:VAL:HG23	2.09	0.52
3:BC:5279:LEU:HD23	3:BC:5282:MET:CE	2.39	0.52
3:BC:5337:LEU:HD12	13:BO:5131:PRO:CG	2.39	0.52
3:BC:5042:LEU:HD13	24:BC:5511:CLA:HMA3	1.90	0.52
1:BA:5254:TYR:OH	4:BD:5129:GLN:HB3	2.09	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
24:AB:611:CLA:H51	24:AB:614:CLA:HBC2	1.92	0.52
3:AC:149:TYR:HA	3:AC:156:LYS:CD	2.40	0.52
3:AC:259:TRP:N	3:AC:259:TRP:CD1	2.78	0.52
3:AC:38:GLY:HA3	24:AC:511:CLA:HMD3	1.92	0.52
24:AC:504:CLA:H61	28:AC:518:DGD:HA61	1.89	0.52
24:AC:504:CLA:H152	28:AC:519:DGD:HA91	1.90	0.52
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.21	0.52
16:AV:56:LYS:O	16:AV:60:GLN:HG3	2.09	0.52
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.10	0.52
1:BA:5035:VAL:HA	27:BA:5411:BCR:H333	1.90	0.52
2:BB:5143:LEU:HD12	2:BB:5143:LEU:O	2.10	0.52
2:BB:5030:VAL:HG22	24:BB:5617:CLA:C3C	2.39	0.52
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD21	1.91	0.52
4:BD:5302:GLU:OE2	4:BD:5302:GLU:HA	2.10	0.52
24:BB:5613:CLA:OBD	7:BH:5027:THR:HB	2.10	0.52
13:BO:5144:LEU:HD13	13:BO:5259:VAL:HG11	1.90	0.52
14:BT:5022:PHE:C	14:BT:5023:PHE:CD2	2.83	0.52
2:AB:62:VAL:CG1	24:AB:605:CLA:HED3	2.39	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.25	0.52
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
2:BB:5238:LEU:HB2	24:BB:5616:CLA:HMD3	1.91	0.52
13:BO:5210:ARG:HA	15:BU:5039:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:5054:LYS:HD2	15:BU:5113:THR:HG23	1.90	0.52
16:BV:5081:ARG:HH11	16:BV:5081:ARG:HG2	1.73	0.52
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.45	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:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
3:AC:220:GLY:N	28:AC:517:DGD:O3D	2.42	0.52
4:AD:308:ASP:OD1	4:AD:308:ASP:C	2.47	0.52
10:AK:17:ILE:N	10:AK:17:ILE:HD12	2.23	0.52
12:AM:27:VAL:HG12	12:BM:5028:GLN:HB3	1.90	0.52
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.44	0.52
1:BA:5157:VAL:HG11	24:BA:5406:CLA:HMC3	1.92	0.52
1:BA:5220:THR:CG2	4:BD:5141:TYR:HD1	2.23	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
2:AB:10:THR:C	2:AB:12:LEU:H	2.11	0.52
2:AB:260:SER:HG	2:AB:262:THR:HG22	1.70	0.52
2:AB:331:ASN:HB3	2:AB:437:LEU:HD22	1.92	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
13:AO:215:ARG:NH1	13:AO:252:GLY:O	2.43	0.52
2:BB:5139:PHE:CZ	24:BB:5613:CLA:HMB3	2.45	0.52
3:BC:5140:LEU:HB2	3:BC:5148:GLY:HA2	1.91	0.52
3:BC:5141:GLU:CD	3:BC:5141:GLU:H	2.13	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:H	2.22	0.52
2:AB:238:LEU:N	24:AB:612:CLA:HMD3	2.25	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
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
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.10	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.52
1:BA:5289:GLY:CA	1:BA:5292:THR:HG22	2.38	0.52
2:BB:5010:THR:C	2:BB:5012:LEU:H	2.11	0.52
3:BC:5418:ASN:HA	28:BC:5519:DGD:HE2	1.91	0.52
4:BD:5128:ARG:HG2	4:BD:5129:GLN:N	2.24	0.52
31:BL:5101:LMG:H302	12:BM:5022:LEU:HD21	1.91	0.52
1:AA:193:LEU:HD13	4:AD:179:PHE:HB3	1.91	0.52
2:AB:30:VAL:HG22	24:AB:613:CLA:C3C	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.40	0.52
2:AB:354:LEU:HD21	2:AB:378:LYS:HB2	1.90	0.52
24:AB:601:CLA:HBB1	24:AB:601:CLA:HHC	1.91	0.52
3:AC:366:LEU:HD23	3:AC:366:LEU:C	2.29	0.52
4:AD:236:ASN:ND2	4:AD:239:GLN:O	2.37	0.52
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.92	0.52
13:AO:91:PHE:CE1	13:AO:260:LYS:HB2	2.45	0.52
13:AO:46:PRO:HD2	13:AO:266:TYR:HD2	1.74	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
3:BC:5366:LEU:C	3:BC:5366:LEU:HD23	2.30	0.52
4:BD:5154:VAL:O	4:BD:5158:LEU:HB2	2.10	0.52
20:BZ:5042:LEU:O	20:BZ:5046:LEU:HB2	2.10	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
3:AC:149:TYR:CB	3:AC:156:LYS:HD3	2.40	0.52
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.52
3:AC:252:ILE:HG22	3:AC:253:LEU:HD23	1.91	0.52
4:AD:158:LEU:O	4:AD:162:LEU:HG	2.09	0.52
5:AE:26:THR:HB	36:AF:101:HEM:CAB	2.40	0.52
4:AD:88:SER:CB	5:AE:69:ARG:NH2	2.69	0.52
5:AE:8:ARG:HD3	5:AE:13:ILE:HG12	1.92	0.52
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.25	0.52
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.92	0.52
1:BA:5064:ARG:HG3	1:BA:5064:ARG:NH1	2.25	0.52
25:BA:5409:MST:H122	25:BA:5409:MST:N3	2.24	0.52
3:BC:5037:ALA:O	24:BC:5508:CLA:HBA1	2.10	0.52
3:BC:5362:ARG:HE	3:BC:5370:ARG:NH1	2.07	0.52
3:BC:5052:ALA:CA	24:BC:5511:CLA:HMB3	2.28	0.52
4:BD:5072:ASN:HA	31:BD:5408:LMG:HC72	1.92	0.52
1:BA:5315:ASN:ND2	4:BD:5332:GLN:HE22	2.06	0.52
13:BO:5059:ASP:C	13:BO:5061:SER:H	2.13	0.52
2:AB:369:ILE:O	2:AB:370:LEU:HD23	2.09	0.52
27:AT:101:BCR:H19C	27:BB:5622:BCR:H363	1.91	0.52
1:BA:5027:ARG:NH1	1:BA:5027:ARG:O	2.43	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
3:BC:5214:LEU:N	3:BC:5214:LEU:HD22	2.24	0.52
4:BD:5026:ARG:HG3	4:BD:5026:ARG:HH11	1.75	0.52
4:BD:5201:VAL:O	4:BD:5205:LEU:HB2	2.09	0.52
13:BO:5230:VAL:CG1	13:BO:5231:ASP:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:315:ASN:ND2	4:AD:332:GLN:NE2	2.57	0.51
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.20	0.51
10:AK:18:PHE:C	10:AK:20:PRO:HD2	2.29	0.51
13:AO:84:ASN:ND2	2:BB:5431:GLU:OE2	2.43	0.51
1:BA:5159:LEU:HD11	28:BC:5517:DGD:HB51	1.92	0.51
1:BA:5082:VAL:HB	1:BA:5174:LEU:HB2	1.91	0.51
2:BB:5121:GLU:HG3	7:BH:5004:ARG:CA	2.39	0.51
3:BC:5038:GLY:HA3	24:BC:5511:CLA:HMD3	1.92	0.51
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:HD11	1.93	0.51
4:BD:5274:VAL:HA	35:BD:5406:PL9:C25	2.34	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
20:BZ:5031:GLN:O	20:BZ:5032:ASP:HB3	2.11	0.51
1:AA:283:VAL:HG21	34:AD:402:PHO:HBC3	1.91	0.51
4:AD:92:LEU:HA	4:AD:104:TRP:CD1	2.45	0.51
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.51
4:AD:35:ILE:O	24:AD:404:CLA:HBB2	2.11	0.51
20:AZ:42:LEU:O	20:AZ:46:LEU:HB2	2.09	0.51
1:BA:5011:ALA:O	1:BA:5012:ASN:CB	2.58	0.51
1:BA:5288:LEU:HD13	3:BC:5432:VAL:CG2	2.37	0.51
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE2	2.46	0.51
4:BD:5188:PHE:CZ	4:BD:5326:ARG:HG2	2.46	0.51
10:BK:5020:PRO:O	10:BK:5023:ASP:HB2	2.11	0.51
27:BK:5102:BCR:H331	27:BK:5102:BCR:HC8	1.92	0.51
11:BL:5008:GLN:HB3	11:BL:5009:PRO:HD2	1.93	0.51
12:BM:5020:VAL:O	12:BM:5024:ILE:HG13	2.11	0.51
13:BO:5046:PRO:HD2	13:BO:5266:TYR:HD2	1.75	0.51
13:BO:5180:ALA:HB2	15:BU:5120:ALA:O	2.09	0.51
1:AA:289:GLY:C	1:AA:292:THR:HG22	2.31	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
3:AC:297:TYR:HA	3:AC:302:TYR:CE2	2.46	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5163:PHE:O	3:BC:5167:VAL:HG23	2.09	0.51
3:BC:5259:TRP:N	3:BC:5259:TRP:CD1	2.77	0.51
4:BD:5259:ILE:HD13	14:BT:5021:ILE:HG12	1.93	0.51
9:BJ:5019:MET:O	9:BJ:5023:VAL:HG23	2.10	0.51
24:BD:5405:CLA:H42	18:BX:5023:LEU:HA	1.92	0.51
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.51
3:AC:377:LEU:O	3:AC:381:LYS:HB2	2.10	0.51
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	1.93	0.51
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	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
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
24:BC:5504:CLA:H61	28:BC:5518:DGD:HA61	1.92	0.51
4:BD:5334:GLN:N	4:BD:5335:PRO:HD3	2.24	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
16:BV:5058:LEU:HD13	16:BV:5137:ASP:HB3	1.92	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
2:AB:461:LEU:HD21	31:AB:621:LMG:C43	2.41	0.51
3:AC:453:ALA:HA	8:AI:34:ARG:O	2.10	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	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
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
3:BC:5458:GLY:HA2	4:BD:5222:LEU:O	2.11	0.51
1:BA:5129:ARG:NH2	4:BD:5256:ILE:HA	2.26	0.51
4:BD:5266:TRP:HE1	31:BD:5410:LMG:HC72	1.74	0.51
18:BX:5022:GLY:HA2	18:BX:5025:SER:HG	1.75	0.51
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.92	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
4:AD:302:GLU:OE2	4:AD:302:GLU:HA	2.11	0.51
5:BE:5072:ALA:O	5:BE:5076:VAL:HG23	2.10	0.51
2:AB:173:GLY:CA	2:AB:265:ILE:HD11	2.41	0.51
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	1.93	0.51
24:AB:611:CLA:H142	31:AB:620:LMG:H371	1.92	0.51
3:AC:321:ASP:OD2	15:AU:129:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5280:PHE:O	2:BB:5284:ILE:HG13	2.10	0.51
2:BB:5315:ILE:HG22	2:BB:5426:PHE:HB3	1.92	0.51
2:BB:5187:PRO:HB3	24:BB:5605:CLA:CMB	2.41	0.51
3:BC:5297:TYR:HD1	3:BC:5302:TYR:CE2	2.29	0.51
13:BO:5071:LEU:HD23	13:BO:5265:PHE:HB3	1.91	0.51
15:BU:5080:VAL:HG22	15:BU:5127:ARG:HH21	1.76	0.51
18:BX:5024:LEU:O	18:BX:5028:VAL:HG23	2.10	0.51
2:AB:356:VAL:HA	2:AB:370:LEU:HD22	1.93	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CE2	2.29	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
3:AC:42:LEU:HD13	24:AC:511:CLA:HMA3	1.93	0.51
3:AC:37:ALA:O	24:AC:508:CLA:HBA1	2.11	0.51
1:AA:244:GLU:OE2	4:AD:264:LYS:NZ	2.43	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB2	1.93	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.93	0.51
32:AB:624:LMT:H92	7:AH:35:MET:HE2	1.92	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.41	0.51
11:AL:8:GLN:HE21	11:AL:8:GLN:N	2.08	0.51
20:AZ:2:THR:CG2	20:AZ:3:ILE:H	2.23	0.51
24:BB:5615:CLA:H142	31:BL:5101:LMG:H371	1.92	0.51
3:AC:264:PHE:HE1	27:AC:516:BCR:C32	2.24	0.51
31:AC:520:LMG:H292	27:AJ:101:BCR:H363	1.93	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:AB:383:PHE:HE1	13:AO:194:TYR:CD2	2.29	0.51
2:BB:5015:ASP:N	2:BB:5016:PRO:HD3	2.26	0.51
2:BB:5063:LEU:N	2:BB:5064:PRO:HD2	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
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:5094:THR:HG22	3:BC:5298:PRO:HD2	1.93	0.51
3:BC:5315:MET:HE1	3:BC:5369:LEU:HD12	1.92	0.51
3:BC:5028:GLN:HB2	24:BC:5511:CLA:CED	2.41	0.51
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CE2	2.45	0.51
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CE2	2.29	0.51
14:BT:5018:PHE:HB2	27:BT:5101:BCR:H10C	1.93	0.51
20:BZ:5034:ASP:OD1	20:BZ:5035:ARG:N	2.44	0.51
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.46	0.51
2:AB:30:VAL:HG12	24:AB:605:CLA:HHD	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.51
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.46	0.51
2:AB:238:LEU:HB2	24:AB:612:CLA:HMD3	1.93	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:HE2	1.75	0.51
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.10	0.51
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.25	0.51
15:AU:66:ILE:CG1	15:AU:72:TYR:CD1	2.94	0.51
3:BC:5288:CYS:HB3	28:BC:5517:DGD:HG2	1.92	0.51
13:BO:5092:VAL:HG12	13:BO:5093:PRO:HD2	1.91	0.51
1:AA:262:TYR:HE1	31:AA:414:LMG:C5	2.24	0.50
2:AB:176:GLY:HA3	2:AB:266:GLU:OE1	2.12	0.50
2:AB:2:GLY:HA3	11:AL:9:PRO:HG2	1.93	0.50
31:AB:620:LMG:HC91	11:AL:19:LEU:CD1	2.41	0.50
3:AC:458:GLY:HA2	4:AD:222:LEU:O	2.10	0.50
4:AD:87:HIS:HB2	28:AH:101:DGD:O2D	2.11	0.50
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.10	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:BX:5044:ASP:O	18:BX:5045:LYS:HB3	2.11	0.50
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.41	0.50
31:AM:101:LMG:O2	11:BL:5009:PRO:HB3	2.11	0.50
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.92	0.50
2:BB:5354:LEU:N	2:BB:5354:LEU:HD12	2.26	0.50
29:BA:5413:LHG:HC11	3:BC:5447:ARG:CZ	2.41	0.50
4:BD:5253:TRP:HB2	4:BD:5260:ALA:HB2	1.93	0.50
2:BB:5172:TYR:OH	7:BH:5063:LYS:HE2	2.11	0.50
27:AB:618:BCR:H363	27:BT:5101:BCR:H19C	1.92	0.50
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	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
20:AZ:23:VAL:HG12	20:AZ:27:TYR:CE2	2.46	0.50
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CE2	2.47	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:H83	1.93	0.50
24:BC:5505:CLA:HAA1	24:BC:5505:CLA:H2	1.94	0.50
3:BC:5033:PHE:CD1	4:BD:5229:ALA:HB3	2.45	0.50
16:BV:5133:LEU:N	16:BV:5133:LEU:HD12	2.24	0.50
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.60	0.50
1:AA:200:LEU:HD11	28:AC:519:DGD:CCA	2.29	0.50
1:AA:48:PHE:HA	1:AA:115:ILE:HD11	1.92	0.50
24:AB:612:CLA:H171	24:AB:613:CLA:HBB2	1.92	0.50
3:AC:262:ARG:HH21	32:AI:103:LMT:C5'	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:PHE:HE1	32:AI:103:LMT:H41	1.75	0.50
8:AI:19:PHE:CZ	8:AI:23:PHE:HE2	2.29	0.50
10:AK:14:ALA:O	10:AK:17:ILE:HD13	2.10	0.50
13:AO:46:PRO:HD2	13:AO:266:TYR:CD2	2.45	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
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
24:BA:5406:CLA:H92	34:BD:5403:PHO:CMB	2.41	0.50
3:BC:5415:ASN:CB	9:BJ:5039:SER:OG	2.60	0.50
11:BL:5019:LEU:CD1	31:BL:5101:LMG:HC91	2.42	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
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.12	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
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
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.11	0.50
24:BB:5616:CLA:H171	24:BB:5617:CLA:HBB2	1.93	0.50
3:BC:5193:GLY:O	3:BC:5194:GLY:C	2.48	0.50
3:BC:5321:ASP:OD1	3:BC:5321:ASP:N	2.44	0.50
3:BC:5377:LEU:CD2	13:BO:5126:GLY:HA2	2.41	0.50
13:BO:5032:THR:O	13:BO:5036:ILE:CD1	2.54	0.50
18:BX:5012:ILE:O	18:BX:5012:ILE:HG13	2.11	0.50
20:BZ:5033:TRP:O	20:BZ:5037:LYS:HB2	2.12	0.50
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.39	0.50
13:AO:155:THR:HG23	13:AO:168:PHE:CE2	2.47	0.50
1:BA:5182:PHE:O	1:BA:5186:PHE:HB2	2.12	0.50
2:BB:5377:VAL:HG11	4:BD:5342:PRO:HG2	1.93	0.50
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CB	2.23	0.50
13:BO:5091:PHE:CE1	13:BO:5260:LYS:HB2	2.47	0.50
14:BT:5022:PHE:O	14:BT:5023:PHE:CD2	2.64	0.50
1:AA:190:HIS:HB3	1:AA:293:MET:CE	2.41	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:368:PRO:O	3:AC:379:LYS:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:225:VAL:CG2	28:AC:517:DGD:HG11	2.41	0.50
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.47	0.50
7:AH:11:LEU:HA	7:AH:14:LEU:HD12	1.93	0.50
27:AK:102:BCR:HC8	27:AK:102:BCR:H331	1.93	0.50
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.24	0.50
13:AO:234:THR:HG1	13:AO:236:GLU:HG2	1.76	0.50
3:BC:5335:THR:HA	13:BO:5178:ARG:HD3	1.94	0.50
4:BD:5279:LEU:HD22	24:BD:5402:CLA:HMA2	1.93	0.50
10:BK:5017:ILE:H	10:BK:5017:ILE:CD1	2.25	0.50
2:AB:25:MET:HE2	27:AB:617:BCR:H393	1.93	0.50
3:AC:418:ASN:CA	28:AC:519:DGD:HE2	2.42	0.50
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.12	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
24:BA:5406:CLA:HMD2	24:BD:5402:CLA:CBB	2.42	0.50
3:BC:5055:ALA:CB	27:BC:5514:BCR:H373	2.38	0.50
27:BC:5516:BCR:HC41	8:BI:5020:VAL:CG1	2.41	0.50
5:BE:5014:ILE:O	5:BE:5014:ILE:HG22	2.12	0.50
12:BM:5025:LEU:N	12:BM:5025:LEU:HD23	2.27	0.50
13:BO:5225:LEU:N	13:BO:5225:LEU:HD12	2.27	0.50
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.50
3:AC:109:PHE:O	3:AC:113:VAL:HG23	2.11	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.23	0.50
31:AB:620:LMG:H302	12:AM:22:LEU:HD21	1.93	0.50
13:AO:86:ARG:NE	13:AO:86:ARG:O	2.45	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:C8	2.42	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
6:BF:5018:VAL:CG1	6:BF:5019:ARG:N	2.74	0.50
11:BL:5022:LEU:HD13	14:BT:5016:LEU:HD23	1.94	0.50
13:BO:5064:TYR:CD1	13:BO:5271:PRO:HA	2.47	0.50
1:AA:258:LEU:HB3	1:AA:259:ILE:CD1	2.39	0.49
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
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:271:LEU:HD21	25:AA:408:MST:C8	2.41	0.49
1:AA:289:GLY:CA	1:AA:292:THR:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:69:GLY:HA2	1:AA:75:ASN:ND2	2.27	0.49
2:AB:311:PHE:HA	2:AB:430:PHE:CZ	2.47	0.49
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.12	0.49
4:AD:193:LEU:O	4:AD:193:LEU:HG	2.11	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
4:AD:141:TYR:OH	31:AD:407:LMG:HC2	2.11	0.49
9:AJ:18:GLY:HA3	27:AK:102:BCR:H371	1.94	0.49
28:AC:519:DGD:HG2	9:AJ:33:TYR:OH	2.12	0.49
1:BA:5043:ALA:HB3	1:BA:5118:HIS:HD2	1.77	0.49
1:BA:5257:ARG:NH1	1:BA:5257:ARG:HG3	2.26	0.49
2:BB:5311:PHE:HA	2:BB:5430:PHE:CZ	2.47	0.49
2:BB:5235:GLU:OE1	2:BB:5472:ARG:NH1	2.44	0.49
3:BC:5225:VAL:CG2	28:BC:5517:DGD:HG11	2.42	0.49
4:BD:5053:THR:HA	4:BD:5067:TYR:CD2	2.47	0.49
4:BD:5141:TYR:OH	31:BD:5409:LMG:HC2	2.13	0.49
13:BO:5186:LYS:HA	13:BO:5186:LYS:HE2	1.92	0.49
15:BU:5080:VAL:HG22	15:BU:5127:ARG:NH2	2.27	0.49
2:AB:371:THR:HG22	2:AB:377:VAL:CA	2.41	0.49
2:AB:91:TRP:CZ3	24:AB:606:CLA:O1A	2.65	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	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
5:AE:7:GLU:O	5:AE:9:PRO:HD3	2.12	0.49
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.49
3:BC:5109:PHE:O	3:BC:5113:VAL:HG23	2.12	0.49
24:BB:5605:CLA:HBC3	7:BH:5041:PHE:CE1	2.47	0.49
20:BZ:5029:SER:C	20:BZ:5031:GLN:H	2.16	0.49
2:AB:243:ALA:HB2	2:AB:466:HIS:ND1	2.27	0.49
2:AB:384:ARG:HD3	15:AU:132:LEU:HD13	1.94	0.49
3:AC:55:ALA:CB	27:AC:514:BCR:H373	2.40	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
13:AO:225:LEU:N	13:AO:225:LEU:HD12	2.28	0.49
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.80	0.49
20:AZ:2:THR:CG2	20:AZ:3:ILE:N	2.73	0.49
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HA	1.94	0.49
2:BB:5372:ASP:OD1	2:BB:5374:ASN:N	2.44	0.49
2:BB:5450:TRP:HB3	24:BB:5611:CLA:HMB2	1.95	0.49
3:BC:5332:GLN:HG3	13:BO:5129:PHE:CE2	2.47	0.49
31:BC:5520:LMG:H292	27:BJ:5101:BCR:H363	1.93	0.49
3:BC:5114:VAL:CG2	31:BC:5521:LMG:H141	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:5017:VAL:HG12	12:BM:5018:PRO:N	2.26	0.49
14:BT:5025:GLU:O	14:BT:5026:PRO:C	2.50	0.49
1:AA:163:ILE:HG12	28:AC:517:DGD:HB31	1.93	0.49
1:AA:257:ARG:NH1	1:AA:257:ARG:HG3	2.24	0.49
1:AA:57:PRO:HD3	1:AA:73:TYR:CE2	2.48	0.49
4:AD:279:LEU:HD22	24:AD:401:CLA:HMA2	1.94	0.49
6:AF:19:ARG:HG3	6:AF:19:ARG:NH1	2.28	0.49
28:AC:519:DGD:O3D	9:AJ:37:GLY:O	2.25	0.49
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.46	0.49
13:AO:186:LYS:HE2	13:AO:186:LYS:HA	1.95	0.49
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE1	1.93	0.49
3:BC:5252:ILE:HG22	3:BC:5253:LEU:HD23	1.95	0.49
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC1	1.93	0.49
3:BC:5452:ALA:O	3:BC:5454:GLY:N	2.44	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
16:BV:5090:PRO:O	16:BV:5092:ARG:HD3	2.13	0.49
2:AB:41:GLU:HB3	2:AB:60:MET:SD	2.52	0.49
2:AB:44:THR:HB	32:AB:629:LMT:O6'	2.13	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	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
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.48	0.49
18:AX:24:LEU:O	18:AX:28:VAL:HG23	2.12	0.49
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.95	0.49
2:BB:5252:VAL:HG12	24:BB:5607:CLA:O1A	2.13	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
1:BA:5077:ILE:HG12	14:BT:5006:TYR:CD1	2.47	0.49
1:AA:207:GLY:O	1:AA:210:LEU:HB3	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
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.49
1:BA:5038:ILE:HB	1:BA:5039:PRO:HD3	1.93	0.49
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NE	2.27	0.49
4:BD:5308:ASP:C	4:BD:5308:ASP:OD1	2.49	0.49
9:BJ:5024:ILE:HG23	9:BJ:5025:VAL:N	2.27	0.49
3:BC:5337:LEU:CD1	13:BO:5131:PRO:HG3	2.41	0.49
13:BO:5148:VAL:HA	13:BO:5172:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:5072:TYR:CB	15:BU:5073:PRO:HD3	2.40	0.49
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.94	0.49
3:AC:297:TYR:HA	3:AC:302:TYR:HE2	1.77	0.49
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.48	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
2:BB:5008:VAL:HG23	2:BB:5009:HIS:HD2	1.76	0.49
13:AO:83:LYS:HE2	2:BB:5338:GLN:HA	1.94	0.49
24:BB:5612:CLA:HMA1	4:BD:5130:PHE:CE1	2.48	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
3:BC:5089:ILE:N	3:BC:5090:PRO:CD	2.74	0.49
4:BD:5186:GLN:HB2	24:BD:5402:CLA:HBC1	1.95	0.49
9:BJ:5034:ALA:O	9:BJ:5035:GLY:O	2.31	0.49
16:BV:5071:ILE:C	16:BV:5071:ILE:HD12	2.33	0.49
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.12	0.49
28:AC:518:DGD:HB22	28:AC:519:DGD:HA21	1.95	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
4:AD:57:SER:CA	4:AD:60:THR:HG22	2.43	0.49
1:AA:22:THR:HG21	8:AI:30:ARG:HE	1.78	0.49
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.48	0.49
13:AO:71:LEU:HD23	13:AO:265:PHE:HB3	1.94	0.49
4:BD:5052:THR:HG22	4:BD:5067:TYR:CE2	2.48	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
13:BO:5155:THR:HG23	13:BO:5168:PHE:CE2	2.48	0.49
13:BO:5240:THR:HA	13:BO:5264:VAL:HA	1.95	0.49
1:AA:59:ASP:OD1	1:AA:64:ARG:N	2.46	0.49
2:AB:187:PRO:HB3	24:AB:601:CLA:CMB	2.42	0.49
2:AB:27:THR:HG23	24:AB:605:CLA:HMC1	1.94	0.49
2:AB:8:VAL:HG23	2:AB:9:HIS:HD2	1.77	0.49
3:AC:149:TYR:CA	3:AC:156:LYS:HD3	2.42	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
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.61	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.27	0.49
3:BC:5346:THR:O	13:BO:5040:GLY:HA2	2.13	0.49
3:BC:5271:TYR:CE1	24:BC:5507:CLA:HAC2	2.48	0.49
18:BX:5043:ILE:HG22	18:BX:5043:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:64:ARG:NH1	1:AA:64:ARG:HG3	2.27	0.48
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
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.78	0.48
20:AZ:48:ILE:O	20:AZ:52:LEU:HG	2.13	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
2:BB:5270:PRO:HG3	2:BB:5312:TYR:CD2	2.48	0.48
2:BB:5293:ALA:C	2:BB:5295:GLY:H	2.15	0.48
24:BB:5606:CLA:H191	4:BD:5158:LEU:HB3	1.96	0.48
3:BC:5296:VAL:HG23	3:BC:5297:TYR:CD2	2.48	0.48
3:BC:5380:ILE:CA	3:BC:5384:ILE:HD11	2.37	0.48
5:BE:5026:THR:HB	36:BF:5101:HEM:CAB	2.43	0.48
13:BO:5116:ASP:C	13:BO:5116:ASP:OD2	2.50	0.48
2:BB:5384:ARG:HH11	15:BU:5132:LEU:HD13	1.77	0.48
20:BZ:5023:VAL:HB	20:BZ:5024:PRO:HD3	1.95	0.48
20:BZ:5032:ASP:OD1	20:BZ:5036:SER:HB2	2.13	0.48
20:BZ:5048:ILE:O	20:BZ:5052:LEU:HG	2.13	0.48
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.48
2:AB:384:ARG:NH1	15:AU:132:LEU:HD13	2.28	0.48
24:AB:604:CLA:HMC2	24:AB:611:CLA:H191	1.95	0.48
3:AC:49:LEU:HD23	3:AC:149:TYR:OH	2.13	0.48
4:AD:266:TRP:CD1	31:AD:408:LMG:HC1	2.47	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
1:BA:5057:PRO:HG3	1:BA:5068:SER:CB	2.43	0.48
2:BB:5238:LEU:N	24:BB:5616:CLA:HMD3	2.28	0.48
2:BB:5324:LEU:CA	4:BD:5293:LEU:HD23	2.38	0.48
3:BC:5235:GLY:O	3:BC:5238:ILE:HB	2.13	0.48
3:BC:5249:ILE:O	3:BC:5253:LEU:HG	2.13	0.48
4:BD:5266:TRP:NE1	31:BD:5410:LMG:HC72	2.28	0.48
13:BO:5066:ILE:HD12	13:BO:5121:PHE:CD1	2.48	0.48
15:BU:5057:LEU:HD11	15:BU:5112:PHE:CB	2.42	0.48
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	2.97	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.48
13:AO:159:VAL:HG13	13:AO:159:VAL:O	2.13	0.48
15:AU:73:PRO:HG2	16:AV:107:THR:HB	1.95	0.48
1:BA:5092:HIS:CD2	3:BC:5219:GLY:HA3	2.48	0.48
29:BA:5413:LHG:C1	3:BC:5447:ARG:HE	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BB:5605:CLA:HHC	24:BB:5605:CLA:HBB1	1.94	0.48
29:BA:5413:LHG:HC11	3:BC:5447:ARG:HH21	1.78	0.48
13:BO:5065:ARG:NH1	13:BO:5065:ARG:HB2	2.28	0.48
13:BO:5147:THR:OG1	13:BO:5148:VAL:N	2.47	0.48
1:AA:27:ARG:NH1	1:AA:27:ARG:O	2.47	0.48
2:AB:354:LEU:N	2:AB:354:LEU:HD12	2.28	0.48
24:AB:611:CLA:H92	31:AD:407:LMG:H232	1.95	0.48
1:AA:254:TYR:CD1	4:AD:132:ILE:HG22	2.48	0.48
1:AA:318:ALA:HB2	4:AD:75:THR:HG22	1.95	0.48
7:AH:35:MET:SD	27:AX:101:BCR:H322	2.53	0.48
1:BA:5330:VAL:CG1	4:BD:5348:ARG:HG2	2.42	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
20:BZ:5032:ASP:OD1	20:BZ:5033:TRP:N	2.41	0.48
1:AA:45:THR:CG2	1:AA:46:ILE:N	2.76	0.48
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.48
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.44	0.48
3:AC:337:LEU:HD12	13:AO:131:PRO:CG	2.44	0.48
24:AC:506:CLA:HMC2	24:AC:507:CLA:H8	1.95	0.48
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.34	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
5:BE:5061:ARG:NH2	16:BV:5153:GLY:HA3	2.28	0.48
7:BH:5011:LEU:HA	7:BH:5014:LEU:HD12	1.94	0.48
13:BO:5135:GLN:HG2	13:BO:5141:ARG:HG3	1.96	0.48
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.14	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
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
2:BB:5012:LEU:HD12	2:BB:5019:LEU:HD12	1.96	0.48
24:BC:5511:CLA:H143	20:BZ:5024:PRO:HG2	1.96	0.48
1:BA:5220:THR:HG23	4:BD:5141:TYR:CD1	2.49	0.48
5:BE:5078:THR:O	5:BE:5081:GLU:HB2	2.14	0.48
6:BF:5015:ILE:HG22	6:BF:5016:PHE:CD1	2.47	0.48
13:BO:5120:THR:HA	13:BO:5153:ALA:O	2.14	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
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
1:AA:248:ILE:CG1	1:AA:248:ILE:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.48
2:AB:245:VAL:HG22	24:AB:612:CLA:H192	1.95	0.48
3:AC:214:LEU:HD22	3:AC:214:LEU:N	2.28	0.48
3:AC:271:TYR:CE1	24:AC:507:CLA:HAC2	2.49	0.48
4:AD:188:PHE:CZ	4:AD:326:ARG:HG2	2.49	0.48
3:AC:461:ARG:NH2	4:AD:242:GLU:O	2.46	0.48
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.96	0.48
16:AV:143:GLY:O	16:AV:147:VAL:HG23	2.14	0.48
18:AX:22:GLY:HA2	18:AX:25:SER:HG	1.79	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
1:BA:5281:VAL:HG13	28:BC:5519:DGD:HAG3	1.93	0.48
3:BC:5418:ASN:HB2	28:BC:5519:DGD:HE2	1.92	0.48
7:BH:5013:PRO:HG2	7:BH:5014:LEU:H	1.78	0.48
1:AA:315:ASN:ND2	4:AD:332:GLN:HE22	2.07	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
1:BA:5047:CYS:SG	1:BA:5114:LEU:HD22	2.53	0.48
1:BA:5131:TRP:CE3	1:BA:5132:GLU:CA	2.97	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
4:BD:5209:LEU:HD23	4:BD:5209:LEU:C	2.34	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
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
2:AB:326:ARG:HD3	2:AB:442:ILE:HG22	1.95	0.48
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.16	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
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.48
2:BB:5329:PRO:HD2	31:BB:5624:LMG:O4	2.14	0.48
24:BB:5610:CLA:H52	27:BB:5623:BCR:H321	1.96	0.48
4:BD:5152:VAL:HG11	24:BD:5402:CLA:H11	1.94	0.48
16:BV:5121:LEU:CD2	16:BV:5138:LEU:HD11	2.44	0.48
1:AA:183:MET:HA	24:AA:404:CLA:HMD2	1.96	0.47
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:AO:236:GLU:O	13:AO:236:GLU:HG3	2.14	0.47
15:AU:38:GLU:O	15:AU:39:LEU:O	2.32	0.47
16:AV:81:ARG:NH1	16:AV:81:ARG:HG2	2.29	0.47
1:BA:5048:PHE:CA	1:BA:5115:ILE:HD11	2.44	0.47
1:BA:5322:ASN:OD1	3:BC:5412:THR:HA	2.14	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
4:BD:5096:GLU:H	4:BD:5096:GLU:CD	2.17	0.47
5:BE:5051:ARG:O	5:BE:5053:ASP:N	2.47	0.47
13:BO:5071:LEU:HD12	13:BO:5104:LEU:HD12	1.96	0.47
13:BO:5157:PRO:O	13:BO:5158:ASN:O	2.32	0.47
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.47
1:AA:275:LEU:HD13	25:AA:408:MST:C8	2.44	0.47
1:AA:295:PHE:O	3:AC:424:SER:OG	2.32	0.47
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.49	0.47
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.29	0.47
24:AC:507:CLA:HBB1	24:AC:507:CLA:HHC	1.96	0.47
4:AD:221:THR:HG23	4:AD:221:THR:O	2.13	0.47
4:AD:261:PHE:HE1	4:AD:266:TRP:CD1	2.33	0.47
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.13	0.47
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.96	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
2:BB:5012:LEU:HD22	2:BB:5018:ARG:HB2	1.95	0.47
3:BC:5441:HIS:HD2	3:BC:5442:LEU:HD12	1.78	0.47
24:BC:5504:CLA:H192	28:BC:5518:DGD:HBN2	1.96	0.47
1:BA:5281:VAL:HG11	28:BC:5519:DGD:HAV1	1.96	0.47
4:BD:5160:TYR:HB3	4:BD:5161:PRO:CD	2.44	0.47
11:BL:5026:VAL:HG11	31:BL:5101:LMG:H202	1.96	0.47
20:BZ:5036:SER:HA	20:BZ:5039:LEU:CG	2.40	0.47
20:BZ:5047:TRP:O	20:BZ:5050:LEU:HB2	2.14	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5084:SER:HB3	5:BE:5068:ASP:HA	1.95	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
1:AA:153:SER:CB	24:AA:404:CLA:H11	2.45	0.47
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.14	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
24:AC:504:CLA:H192	28:AC:518:DGD:HBN2	1.96	0.47
13:AO:155:THR:HG23	13:AO:168:PHE:CD2	2.50	0.47
1:BA:5091:LEU:HD11	1:BA:5163:ILE:HA	1.94	0.47
1:BA:5119:PHE:HD1	34:BD:5403:PHO:H92	1.78	0.47
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HA	1.95	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
7:BH:5050:ASN:HD22	28:BH:5101:DGD:HA21	1.79	0.47
8:BI:5014:PHE:CE2	8:BI:5018:LEU:HD11	2.49	0.47
13:BO:5039:THR:HB	13:BO:5041:LEU:HD22	1.95	0.47
2:AB:54:PRO:HD2	2:AB:57:ARG:HG3	1.95	0.47
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.79	0.47
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.67	0.47
1:AA:326:LEU:CD2	3:AC:412:THR:HB	2.44	0.47
29:AA:412:LHG:HC11	3:AC:447:ARG:HH21	1.78	0.47
1:AA:272:HIS:HD2	4:AD:218:VAL:HG21	1.76	0.47
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	1.96	0.47
4:AD:274:VAL:HA	35:AD:405:PL9:C25	2.37	0.47
4:AD:299:ILE:HG13	11:AL:37:ASN:ND2	2.29	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
28:AC:519:DGD:HE62	9:AJ:40:LEU:CD1	2.45	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
1:BA:5029:TYR:CD2	1:BA:5133:LEU:HD13	2.49	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
3:BC:5131:TYR:HE1	3:BC:5135:ARG:HD2	1.80	0.47
24:BC:5506:CLA:HMC2	24:BC:5507:CLA:H8	1.96	0.47
5:BE:5027:ILE:CB	5:BE:5028:PRO:HD3	2.43	0.47
11:BL:5024:ILE:HG21	12:BM:5019:SER:OG	2.14	0.47
3:BC:5327:ASN:HB3	13:BO:5125:ASP:OD1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:43:ALA:HB3	1:AA:118:HIS:HD2	1.80	0.47
1:AA:13:LEU:N	1:AA:16:ARG:HH11	2.13	0.47
1:AA:223:LEU:O	2:AB:482:ILE:HG12	2.13	0.47
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.14	0.47
2:AB:405:GLU:OE1	2:AB:405:GLU:HA	2.14	0.47
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.47
5:AE:27:ILE:CB	5:AE:28:PRO:HD3	2.44	0.47
31:AB:620:LMG:H202	11:AL:26:VAL:HG11	1.95	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
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.47
4:BD:5087:HIS:HD2	4:BD:5166:SER:HA	1.72	0.47
4:BD:5180:ARG:HG3	4:BD:5181:PHE:N	2.29	0.47
7:BH:5025:TRP:O	7:BH:5026:GLY:C	2.53	0.47
3:BC:5330:SER:HB2	13:BO:5149:LYS:NZ	2.29	0.47
15:BU:5099:GLU:HA	15:BU:5102:LYS:HE3	1.97	0.47
1:AA:119:PHE:HD1	34:AD:402:PHO:H92	1.79	0.47
1:AA:288:LEU:HD22	3:AC:432:VAL:HA	1.96	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:AC:437:PHE:HZ	24:AC:510:CLA:HMB3	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
2:AB:325:PHE:CD1	11:AL:34:TYR:HB3	2.49	0.47
13:AO:65:ARG:NH1	13:AO:65:ARG:HB2	2.29	0.47
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.29	0.47
1:BA:5015:GLU:O	1:BA:5019:ASN:OD1	2.32	0.47
1:BA:5183:MET:HG3	24:BA:5406:CLA:HBC1	1.96	0.47
24:BB:5615:CLA:H92	31:BD:5409:LMG:H232	1.95	0.47
3:BC:5075:PHE:CD1	3:BC:5086:LEU:HD21	2.50	0.47
3:BC:5394:GLU:OE2	3:BC:5398:HIS:CD2	2.68	0.47
24:BC:5510:CLA:H122	24:BC:5510:CLA:H161	1.81	0.47
5:BE:5015:THR:O	9:BJ:5008:ILE:CD1	2.63	0.47
2:BB:5250:PHE:O	28:BH:5101:DGD:HB82	2.15	0.47
13:BO:5236:GLU:HG3	13:BO:5236:GLU:O	2.14	0.47
1:AA:47:CYS:SG	1:AA:114:LEU:HD22	2.54	0.47
2:AB:143:LEU:HD12	2:AB:143:LEU:O	2.14	0.47
2:AB:324:LEU:CA	4:AD:293:LEU:HD23	2.43	0.47
2:AB:9:HIS:HB2	24:AB:611:CLA:CBA	2.44	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.95	0.47
3:AC:472:LEU:O	3:AC:473:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:416:SER:CA	28:AC:519:DGD:O3E	2.62	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
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
1:BA:5059:ASP:OD2	1:BA:5062:GLY:HA2	2.15	0.47
1:BA:5153:SER:HB2	24:BA:5405:CLA:H11	1.97	0.47
1:BA:5248:ILE:O	1:BA:5248:ILE:CG1	2.62	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:5262:ARG:HH21	32:BC:5522:LMT:C5'	2.26	0.47
3:BC:5271:TYR:HA	3:BC:5274:TYR:CD2	2.49	0.47
3:BC:5318:LEU:HD21	3:BC:5380:ILE:HG23	1.97	0.47
4:BD:5263:ASN:O	4:BD:5266:TRP:N	2.47	0.47
1:AA:214:MET:HE1	4:AD:142:ASN:OD1	2.14	0.47
1:AA:39:PRO:CB	24:AA:407:CLA:HBB1	2.44	0.47
2:AB:250:PHE:O	28:AH:101:DGD:HB82	2.15	0.47
2:AB:329:PRO:HD2	31:AB:621:LMG:O4	2.15	0.47
2:AB:356:VAL:HA	2:AB:370:LEU:CD2	2.45	0.47
2:AB:384:ARG:HH11	15:AU:132:LEU:HD13	1.79	0.47
3:AC:319:ILE:O	3:AC:323:LYS:HG3	2.15	0.47
3:AC:387:TRP:CE2	3:AC:388:GLN:HG3	2.49	0.47
4:AD:68:LEU:HD11	5:AE:44:TYR:CE1	2.49	0.47
11:AL:17:LEU:HD11	12:AM:23:ILE:HD12	1.97	0.47
11:AL:8:GLN:N	11:AL:8:GLN:NE2	2.62	0.47
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.79	0.47
15:AU:58:ASN:OD1	15:AU:84:PRO:CA	2.61	0.47
29:BA:5415:LHG:H102	31:BE:5101:LMG:H142	1.97	0.47
2:BB:5250:PHE:HD1	28:BH:5101:DGD:HB92	1.80	0.47
1:BA:5135:TYR:HE1	3:BC:5449:ARG:O	1.97	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
16:BV:5143:GLY:O	16:BV:5147:VAL:HG23	2.14	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
2:AB:425:ILE:HG22	2:AB:426:PHE:HD2	1.75	0.47
2:AB:485:GLU:HG2	2:AB:486:LEU:N	2.29	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
3:AC:436:PHE:O	24:AC:508:CLA:HAC1	2.15	0.47
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5329:GLU:O	1:BA:5332:HIS:ND1	2.45	0.47
2:BB:5369:ILE:C	2:BB:5370:LEU:HD23	2.35	0.47
24:BB:5614:CLA:H111	24:BB:5619:CLA:CAA	2.44	0.47
2:BB:5025:MET:HE2	27:BB:5621:BCR:H393	1.97	0.47
5:BE:5014:ILE:HG22	9:BJ:5013:VAL:HG11	1.96	0.47
10:BK:5015:TYR:OH	20:BZ:5058:ASN:ND2	2.48	0.47
13:BO:5031:LEU:N	13:BO:5031:LEU:CD1	2.72	0.47
13:BO:5070:CYS:SG	13:BO:5105:ASP:OD1	2.72	0.47
13:BO:5171:GLU:HA	13:BO:5221:GLY:O	2.15	0.47
1:AA:13:LEU:HD12	1:AA:16:ARG:NH1	2.29	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
2:AB:115:TRP:CZ2	24:AB:614:CLA:HBA2	2.50	0.47
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.97	0.47
3:AC:375:LEU:HB3	3:AC:380:ILE:HD11	1.96	0.47
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.68	0.47
24:AB:601:CLA:HBC3	7:AH:41:PHE:CE1	2.50	0.47
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.30	0.47
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CBA	2.45	0.47
2:BB:5175:THR:O	2:BB:5176:GLY:O	2.33	0.47
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG12	1.95	0.47
3:BC:5042:LEU:HD21	24:BC:5511:CLA:H2A	1.97	0.47
3:BC:5143:TYR:O	3:BC:5144:SER:CB	2.62	0.47
3:BC:5473:ASP:HB2	14:BT:5026:PRO:HB3	1.96	0.47
5:BE:5078:THR:HA	5:BE:5081:GLU:CG	2.43	0.47
28:BC:5518:DGD:O3D	27:BJ:5101:BCR:H382	2.14	0.47
13:BO:5077:LEU:HB3	13:BO:5091:PHE:HB3	1.97	0.47
16:BV:5081:ARG:CZ	16:BV:5157:GLY:HA3	2.45	0.47
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.15	0.46
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	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
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
1:BA:5222:SER:O	1:BA:5246:TYR:HB2	2.14	0.46
2:BB:5112:CYS:HB3	27:BB:5623:BCR:H393	1.96	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
3:BC:5420:VAL:HB	3:BC:5425:TRP:HE1	1.80	0.46
3:BC:5432:VAL:HG13	3:BC:5433:LEU:N	2.29	0.46
24:BC:5510:CLA:HBB1	24:BC:5510:CLA:HHC	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BD:5405:CLA:C4	18:BX:5023:LEU:HA	2.45	0.46
5:BE:5036:LEU:HA	5:BE:5039:SER:OG	2.15	0.46
11:BL:5016:SER:O	11:BL:5019:LEU:HD12	2.14	0.46
15:BU:5072:TYR:O	15:BU:5073:PRO:C	2.51	0.46
20:BZ:5023:VAL:HG12	20:BZ:5027:TYR:CE2	2.49	0.46
1:AA:12:ASN:ND2	1:AA:15:GLU:HB2	2.29	0.46
1:AA:210:LEU:HD23	1:AA:210:LEU:C	2.36	0.46
2:AB:489:GLU:C	2:AB:490:GLN:HG3	2.36	0.46
24:AB:602:CLA:H191	4:AD:158:LEU:HB3	1.97	0.46
5:AE:78:THR:O	5:AE:81:GLU:HB2	2.15	0.46
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	1.97	0.46
8:AI:33:LYS:O	8:AI:35:LYS:HG2	2.14	0.46
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.98	0.46
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
2:BB:5153:PHE:CZ	2:BB:5158:LEU:HD21	2.50	0.46
2:BB:5007:ARG:HA	24:BB:5615:CLA:HBA1	1.97	0.46
4:BD:5093:TRP:HA	4:BD:5099:GLY:H	1.81	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
16:BV:5098:LEU:O	16:BV:5102:MET:HG3	2.14	0.46
18:BX:5012:ILE:CD1	18:BX:5016:LEU:HD12	2.44	0.46
18:BX:5024:LEU:HA	18:BX:5024:LEU:HD12	1.74	0.46
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.15	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
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.30	0.46
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.16	0.46
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.29	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
1:BA:5138:GLY:HA3	8:BI:5032:PRO:HG2	1.98	0.46
2:BB:5005:TRP:CZ2	31:BL:5101:LMG:H291	2.50	0.46
2:BB:5384:ARG:NH1	15:BU:5132:LEU:HD13	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
1:BA:5326:LEU:CD2	3:BC:5412:THR:HB	2.46	0.46
4:BD:5036:LEU:O	4:BD:5039:PRO:HD2	2.15	0.46
4:BD:5299:ILE:HG13	11:BL:5037:ASN:ND2	2.30	0.46
5:BE:5017:VAL:HA	9:BJ:5008:ILE:HD11	1.96	0.46
6:BF:5023:VAL:O	6:BF:5027:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5086:ARG:O	13:BO:5086:ARG:CG	2.63	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
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
2:AB:242:ILE:HG22	2:AB:466:HIS:HB2	1.96	0.46
2:AB:298:LEU:HD23	2:AB:402:TYR:CE1	2.51	0.46
2:AB:112:CYS:HB3	27:AB:619:BCR:H393	1.98	0.46
3:AC:420:VAL:HB	3:AC:425:TRP:HE1	1.79	0.46
4:AD:251:ARG:HG2	4:AD:255:GLN:OE1	2.16	0.46
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.15	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.46
1:BA:5244:GLU:HG3	1:BA:5246:TYR:H	1.80	0.46
31:AA:417:LMG:H301	2:BB:5076:SER:HB3	1.96	0.46
3:BC:5057:ALA:O	3:BC:5061:VAL:HG23	2.15	0.46
3:BC:5094:THR:CG2	3:BC:5298:PRO:HD2	2.44	0.46
24:BC:5511:CLA:H141	20:BZ:5020:VAL:O	2.16	0.46
4:BD:5136:VAL:O	4:BD:5136:VAL:HG12	2.15	0.46
1:BA:5064:ARG:NH1	13:BO:5098:THR:HG21	2.31	0.46
16:BV:5148:GLU:HA	16:BV:5148:GLU:OE1	2.15	0.46
1:AA:131:TRP:CE3	1:AA:132:GLU:HA	2.50	0.46
29:AA:412:LHG:HC11	3:AC:447:ARG:NE	2.31	0.46
2:AB:179:GLN:HE21	2:AB:179:GLN:CA	2.18	0.46
2:AB:237:VAL:HB	24:AB:612:CLA:CMD	2.46	0.46
1:AA:220:THR:CG2	4:AD:141:TYR:HD1	2.29	0.46
4:AD:209:LEU:HD23	4:AD:209:LEU:C	2.35	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
3:BC:5029:GLU:HA	10:BK:5046:ARG:HH12	1.80	0.46
3:BC:5380:ILE:HA	3:BC:5384:ILE:CD1	2.37	0.46
4:BD:5250:ASN:ND2	4:BD:5262:SER:HB3	2.28	0.46
6:BF:5021:VAL:HG21	30:BF:5102:SQD:H101	1.97	0.46
13:BO:5072:GLN:O	13:BO:5263:GLY:HA3	2.14	0.46
20:BZ:5021:ILE:O	20:BZ:5025:VAL:HG22	2.16	0.46
1:AA:214:MET:HE1	34:AD:403:PHO:OBD	2.14	0.46
24:AA:407:CLA:HMA2	28:AA:411:DGD:HB42	1.98	0.46
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.50	0.46
2:AB:334:ASP:HB3	13:AO:202:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:155:SER:HA	4:AD:159:ILE:HG13	1.98	0.46
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.97	0.46
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.46
4:AD:72:ASN:HA	31:AJ:102:LMG:HC72	1.97	0.46
4:AD:88:SER:HA	7:AH:50:ASN:OD1	2.15	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
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:BA:5140:ARG:HD3	4:BD:5219:GLU:O	2.15	0.46
4:BD:5253:TRP:HA	4:BD:5256:ILE:CG2	2.45	0.46
13:BO:5071:LEU:HD23	13:BO:5265:PHE:CB	2.45	0.46
20:BZ:5032:ASP:C	20:BZ:5034:ASP:H	2.17	0.46
1:AA:153:SER:HB2	24:AA:404:CLA:H11	1.98	0.46
1:AA:210:LEU:C	1:AA:210:LEU:CD2	2.84	0.46
24:AA:405:CLA:H72	31:AB:620:LMG:C25	2.46	0.46
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.46
2:AB:135:LEU:HD21	2:AB:234:ILE:HD13	1.98	0.46
3:AC:418:ASN:HB2	28:AC:519:DGD:HE2	1.98	0.46
3:AC:57:ALA:O	3:AC:61:VAL:HG23	2.16	0.46
4:AD:119:ALA:O	4:AD:123:ILE:HG13	2.16	0.46
5:AE:26:THR:HB	36:AF:101:HEM:C3B	2.51	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:5371:THR:HG22	2:BB:5377:VAL:CA	2.42	0.46
2:BB:5490:GLN:OE1	2:BB:5490:GLN:O	2.33	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
3:BC:5319:ILE:O	3:BC:5323:LYS:HG3	2.15	0.46
4:BD:5057:SER:HA	4:BD:5060:THR:HG22	1.97	0.46
4:BD:5210:LEU:HD13	4:BD:5271:MET:HG2	1.98	0.46
6:BF:5031:ILE:HG12	36:BF:5101:HEM:HMC2	1.97	0.46
16:BV:5059:PHE:HA	16:BV:5063:CYS:SG	2.56	0.46
2:AB:107:LEU:HD21	24:AB:615:CLA:H42	1.97	0.46
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.96	0.46
2:AB:363:PHE:HD1	4:AD:326:ARG:HD2	1.80	0.46
3:AC:164:HIS:HA	3:AC:167:VAL:HG23	1.97	0.46
1:AA:135:TYR:HE1	3:AC:449:ARG:O	1.99	0.46
3:AC:62:PHE:HZ	10:AK:28:ILE:CD1	2.29	0.46
4:AD:162:LEU:HD21	4:AD:167:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:180:ARG:HG3	4:AD:181:PHE:N	2.31	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
1:BA:5179:THR:HG22	1:BA:5183:MET:CE	2.46	0.46
24:BA:5406:CLA:H61	34:BD:5403:PHO:HMB3	1.97	0.46
2:BB:5179:GLN:CA	2:BB:5179:GLN:HE21	2.17	0.46
2:BB:5356:VAL:HG22	2:BB:5370:LEU:HD21	1.97	0.46
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD13	1.98	0.46
24:BB:5612:CLA:CAB	4:BD:5123:ILE:HG23	2.46	0.46
3:BC:5272:LEU:HA	24:BC:5509:CLA:HMD3	1.97	0.46
4:BD:5217:THR:O	4:BD:5221:THR:HB	2.15	0.46
2:AB:187:PRO:HG2	2:AB:188:ASP:H	1.80	0.46
2:AB:152:GLY:C	24:AB:606:CLA:HMC3	2.36	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
2:AB:121:GLU:HG2	7:AH:4:ARG:CD	2.43	0.46
9:AJ:11:TRP:CE3	10:AK:42:ALA:HB2	2.51	0.46
11:AL:22:LEU:HD13	14:AT:16:LEU:HD23	1.98	0.46
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.84	0.46
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.67	0.46
1:BA:5114:LEU:HD23	1:BA:5114:LEU:C	2.37	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
2:BB:5121:GLU:HG2	7:BH:5004:ARG:CD	2.42	0.46
2:BB:5425:ILE:HG22	2:BB:5426:PHE:HD2	1.78	0.46
30:BB:5601:SQD:H92	24:BB:5618:CLA:H42	1.98	0.46
3:BC:5335:THR:HA	13:BO:5178:ARG:CD	2.46	0.46
3:BC:5465:PRO:O	3:BC:5469:MET:HE3	2.16	0.46
4:BD:5193:LEU:O	4:BD:5193:LEU:HG	2.16	0.46
9:BJ:5003:SER:CA	9:BJ:5007:ARG:HH22	2.29	0.46
13:BO:5086:ARG:CD	13:BO:5086:ARG:O	2.64	0.46
13:BO:5159:VAL:O	13:BO:5159:VAL:HG13	2.16	0.46
4:BD:5323:GLU:HG2	13:BO:5194:TYR:OH	2.16	0.46
2:AB:226:TYR:HA	2:AB:231:MET:HE2	1.97	0.46
2:AB:485:GLU:CG	2:AB:486:LEU:N	2.78	0.46
2:AB:9:HIS:HB2	24:AB:611:CLA:CGA	2.46	0.46
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	2.16	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
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.81	0.46
1:BA:5021:VAL:HG11	1:BA:5032:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5285:ASN:HD22	2:BB:5285:ASN:N	2.14	0.46
2:BB:5354:LEU:HD21	2:BB:5378:LYS:CB	2.46	0.46
2:BB:5485:GLU:CG	2:BB:5486:LEU:N	2.79	0.46
3:BC:5185:LEU:HD12	3:BC:5230:LEU:HD12	1.97	0.46
3:BC:5460:ASP:O	3:BC:5461:ARG:C	2.54	0.46
1:BA:5318:ALA:HB2	4:BD:5075:THR:HG22	1.97	0.46
4:BD:5084:SER:HB3	5:BE:5068:ASP:CA	2.46	0.46
35:BD:5406:PL9:H303	35:BD:5406:PL9:H262	1.97	0.46
7:BH:5006:TRP:O	7:BH:5010:ILE:HG13	2.16	0.46
12:BM:5019:SER:O	12:BM:5023:ILE:HD13	2.16	0.46
13:BO:5036:ILE:HG23	13:BO:5041:LEU:CB	2.46	0.46
13:BO:5271:PRO:HG2	13:BO:5272:ALA:H	1.81	0.46
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.45
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.80	0.45
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	1.99	0.45
2:AB:398:THR:HG22	2:AB:412:THR:HG22	1.96	0.45
24:AB:604:CLA:H111	24:AB:615:CLA:H2	1.97	0.45
31:AC:520:LMG:H202	9:AJ:22:ILE:HG21	1.97	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
1:BA:5084:PRO:HA	1:BA:5112:TYR:CG	2.49	0.45
2:BB:5356:VAL:HA	2:BB:5370:LEU:CD2	2.45	0.45
3:BC:5229:ASN:ND2	3:BC:5231:GLU:HB2	2.31	0.45
13:BO:5215:ARG:HD2	15:BU:5039:LEU:HD22	1.98	0.45
14:BT:5014:ILE:HD13	14:BT:5017:PHE:CD2	2.52	0.45
1:AA:29:TYR:HD2	1:AA:133:LEU:HB2	1.80	0.45
2:AB:144:PHE:CE1	2:AB:210:ILE:CG2	2.99	0.45
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.52	0.45
3:AC:55:ALA:HB1	27:AC:514:BCR:C37	2.43	0.45
3:AC:75:PHE:CD1	3:AC:86:LEU:HD21	2.51	0.45
4:AD:126:MET:HE1	4:AD:147:SER:HA	1.99	0.45
1:BA:5042:LEU:HD21	30:BA:5401:SQD:H152	1.97	0.45
1:BA:5214:MET:HE1	34:BD:5404:PHO:OBD	2.16	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:5414:ILE:HG22	3:BC:5415:ASN:N	2.32	0.45
3:BC:5435:PHE:O	3:BC:5438:LEU:N	2.47	0.45
3:BC:5450:ALA:HA	3:BC:5455:PHE:CE2	2.51	0.45
4:BD:5119:ALA:O	4:BD:5123:ILE:HG13	2.16	0.45
6:BF:5016:PHE:N	6:BF:5016:PHE:HD1	2.14	0.45
16:BV:5141:ILE:O	16:BV:5145:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:179:GLN:NE2	2:AB:179:GLN:HA	2.22	0.45
3:AC:318:LEU:HD21	3:AC:380:ILE:HG23	1.97	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:5055:ALA:HB1	27:BC:5514:BCR:C37	2.41	0.45
3:BC:5202:PRO:HB2	3:BC:5235:GLY:HA2	1.98	0.45
3:BC:5438:LEU:HD23	28:BC:5517:DGD:HAW2	1.97	0.45
4:BD:5079:SER:HA	4:BD:5172:SER:HB3	1.97	0.45
7:BH:5044:ILE:HG12	18:BX:5019:PHE:CE2	2.51	0.45
11:BL:5022:LEU:HG	31:BL:5101:LMG:C19	2.46	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
20:BZ:5036:SER:C	20:BZ:5038:GLN:N	2.70	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
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.16	0.45
1:AA:342:ASP:HB2	4:AD:352:LEU:HD21	1.98	0.45
35:AD:405:PL9:H262	35:AD:405:PL9:H303	1.98	0.45
6:AF:24:HIS:NE2	36:AF:101:HEM:NB	2.65	0.45
13:AO:135:GLN:HB3	13:AO:135:GLN:HE21	1.48	0.45
16:AV:118:HIS:ND1	16:AV:119:PRO:HD2	2.31	0.45
1:BA:5041:LEU:HD21	1:BA:5122:GLY:HA3	1.99	0.45
1:BA:5292:THR:HB	28:BC:5518:DGD:HAH2	1.99	0.45
24:BA:5408:CLA:HMA2	28:BA:5412:DGD:HB42	1.98	0.45
2:BB:5041:GLU:HB3	2:BB:5060:MET:SD	2.55	0.45
24:BB:5612:CLA:HAA1	24:BB:5612:CLA:C1	2.45	0.45
4:BD:5057:SER:CA	4:BD:5060:THR:HG22	2.46	0.45
4:BD:5088:SER:HA	7:BH:5050:ASN:OD1	2.16	0.45
8:BI:5024:LEU:O	8:BI:5026:GLY:N	2.41	0.45
1:AA:234:ASN:HD21	4:AD:266:TRP:CA	2.30	0.45
1:AA:65:GLU:N	1:AA:66:PRO:HD3	2.32	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
3:AC:213:LEU:HD21	27:AC:516:BCR:C19	2.47	0.45
24:AC:507:CLA:O1D	24:AC:509:CLA:H101	2.17	0.45
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.45
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.16	0.45
5:AE:17:VAL:HG22	9:AJ:8:ILE:CD1	2.47	0.45
13:AO:215:ARG:HD2	15:AU:39:LEU:HD22	1.97	0.45
18:AX:43:ILE:CG2	18:AX:43:ILE:O	2.64	0.45
1:BA:5045:THR:CG2	1:BA:5046:ILE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5172:TYR:O	2:BB:5173:GLY:C	2.52	0.45
24:BB:5608:CLA:H111	24:BB:5619:CLA:H2	1.99	0.45
2:BB:5007:ARG:HG2	24:BB:5615:CLA:HED1	1.97	0.45
10:BK:5021:LEU:HD11	27:BK:5102:BCR:HC42	1.99	0.45
1:AA:29:TYR:CD2	1:AA:133:LEU:HB2	2.51	0.45
2:AB:226:TYR:HA	2:AB:231:MET:CE	2.47	0.45
3:AC:365:TRP:HA	3:AC:387:TRP:CH2	2.51	0.45
5:AE:14:ILE:HG22	9:AJ:13:VAL:HG11	1.99	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
20:AZ:30:PRO:HA	20:AZ:33:TRP:CE3	2.51	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
2:BB:5278:SER:HB3	2:BB:5281:GLN:NE2	2.31	0.45
2:BB:5390:TYR:HD2	4:BD:5344:GLU:OE1	2.00	0.45
32:BB:5627:LMT:H92	7:BH:5035:MET:HE2	1.98	0.45
3:BC:5193:GLY:O	3:BC:5194:GLY:O	2.34	0.45
4:BD:5038:PHE:CE2	4:BD:5128:ARG:NH2	2.85	0.45
4:BD:5176:ALA:HA	4:BD:5179:PHE:CD2	2.52	0.45
4:BD:5251:ARG:HG2	4:BD:5255:GLN:OE1	2.17	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
2:BB:5279:TYR:HE1	7:BH:5063:LYS:HE3	1.80	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
13:BO:5184:ASP:HB2	13:BO:5185:PRO:HD2	1.99	0.45
12:BM:5003:VAL:HG11	14:BT:5002:GLU:HG2	1.99	0.45
13:BO:5210:ARG:HA	15:BU:5039:LEU:HD13	1.97	0.45
15:BU:5056:ASP:OD2	15:BU:5115:THR:OG1	2.34	0.45
16:BV:5081:ARG:HG2	16:BV:5081:ARG:NH1	2.31	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
3:AC:38:GLY:HA3	24:AC:511:CLA:C2D	2.46	0.45
8:AI:10:ILE:HG21	32:AI:102:LMT:H82	1.98	0.45
8:AI:14:PHE:CE2	8:AI:18:LEU:HD11	2.52	0.45
28:AC:518:DGD:O3D	27:AJ:101:BCR:H382	2.16	0.45
27:AB:617:BCR:HC41	12:AM:9:ILE:HG23	1.98	0.45
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.17	0.45
20:AZ:9:LEU:HD13	20:AZ:54:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5013:LEU:CA	1:BA:5016:ARG:HH11	2.30	0.45
1:BA:5180:PHE:O	1:BA:5184:ILE:HG13	2.17	0.45
1:BA:5295:PHE:O	3:BC:5424:SER:OG	2.31	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:HA	3:BC:5276:LEU:HD23	1.75	0.45
4:BD:5035:ILE:O	24:BD:5405:CLA:HBB2	2.16	0.45
4:BD:5337:GLU:O	4:BD:5338:ASN:C	2.55	0.45
10:BK:5011:LEU:HD12	10:BK:5019:ASP:HA	1.98	0.45
12:BM:5033:GLN:HG2	12:BM:5034:LYS:N	2.32	0.45
13:BO:5126:GLY:O	13:BO:5128:ASP:N	2.50	0.45
15:BU:5066:ILE:CG1	15:BU:5072:TYR:CD1	3.00	0.45
16:BV:5124:ALA:HB1	16:BV:5131:ARG:CG	2.47	0.45
20:BZ:5009:LEU:HD13	20:BZ:5054:VAL:HG11	1.98	0.45
1:AA:103:ASP:OD1	31:AA:417:LMG:H342	2.16	0.45
3:AC:249:ILE:O	3:AC:253:LEU:HG	2.17	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
3:AC:472:LEU:HG	4:AD:251:ARG:HH12	1.80	0.45
4:AD:277:THR:HG22	35:AD:405:PL9:H272	1.98	0.45
6:AF:37:ILE:HG22	9:AJ:28:PHE:CE1	2.52	0.45
13:AO:147:THR:O	13:AO:172:PHE:CE2	2.70	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
13:AO:71:LEU:HD23	13:AO:265:PHE:CB	2.47	0.45
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.28	0.45
13:AO:91:PHE:CD1	13:AO:260:LYS:HB2	2.51	0.45
1:BA:5235:TYR:C	1:BA:5237:TYR:H	2.20	0.45
2:BB:5088:PRO:HD2	28:BB:5602:DGD:O4D	2.17	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
4:BD:5067:TYR:CE1	4:BD:5076:VAL:HG11	2.51	0.45
2:BB:5357:ARG:NH2	4:BD:5337:GLU:OE1	2.50	0.45
7:BH:5055:LEU:HB2	7:BH:5058:VAL:CG1	2.46	0.45
13:BO:5056:TYR:O	13:BO:5161:SER:HA	2.17	0.45
1:AA:179:THR:HG22	1:AA:183:MET:CE	2.47	0.45
1:AA:176:ILE:HD12	24:AA:405:CLA:HED3	1.98	0.45
2:AB:345:VAL:HG21	2:AB:402:TYR:HE2	1.82	0.45
2:AB:69:LEU:HD21	24:AB:603:CLA:OBD	2.17	0.45
2:AB:112:CYS:HA	27:AB:617:BCR:H282	1.98	0.45
24:AC:511:CLA:H2	24:AC:511:CLA:H61	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:18:TYR:CD1	7:AH:18:TYR:C	2.89	0.45
8:AI:19:PHE:CE1	8:AI:23:PHE:CE2	3.00	0.45
12:AM:5:GLN:HE22	32:AM:102:LMT:H3'	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:HD12	18:AX:24:LEU:HA	1.69	0.45
2:BB:5008:VAL:HG22	24:BB:5615:CLA:O1A	2.17	0.45
24:BB:5620:CLA:HBB1	24:BB:5620:CLA:HHC	1.99	0.45
3:BC:5256:PRO:HG2	3:BC:5266:TRP:CH2	2.51	0.45
3:BC:5328:VAL:HG23	3:BC:5329:GLY:N	2.31	0.45
18:BX:5043:ILE:O	18:BX:5043:ILE:CG2	2.64	0.45
1:AA:224:ILE:H	1:AA:224:ILE:HG13	1.55	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
2:AB:476:ARG:CZ	2:AB:476:ARG:HB3	2.46	0.45
24:AB:611:CLA:H52	24:AB:614:CLA:HBC2	1.99	0.45
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.31	0.45
3:AC:453:ALA:C	8:AI:34:ARG:HB2	2.38	0.45
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.45
2:BB:5073:GLY:O	2:BB:5093:PHE:CD1	2.70	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
3:BC:5472:LEU:O	3:BC:5473:ASP:O	2.35	0.45
24:BC:5511:CLA:H151	20:BZ:5024:PRO:CG	2.45	0.45
24:BD:5405:CLA:H41	18:BX:5023:LEU:CD1	2.42	0.45
31:BM:5102:LMG:O9	31:BM:5102:LMG:O8	2.35	0.45
20:BZ:5030:PRO:HB3	20:BZ:5033:TRP:CZ3	2.51	0.45
1:AA:187:GLN:HG2	4:AD:183:LEU:HD21	2.00	0.44
1:AA:93:PHE:CE2	24:AA:407:CLA:HBA1	2.52	0.44
2:AB:193:TYR:CD1	2:AB:260:SER:HA	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
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.44
6:AF:31:ILE:HG12	36:AF:101:HEM:HMC2	1.99	0.44
4:AD:70:GLY:O	9:AJ:37:GLY:CA	2.64	0.44
18:AX:12:ILE:CD1	18:AX:16:LEU:HD12	2.47	0.44
1:BA:5271:LEU:CD1	25:BA:5409:MST:H162	2.45	0.44
2:BB:5035:GLY:O	2:BB:5038:ALA:HB3	2.16	0.44
2:BB:5435:GLU:O	2:BB:5436:THR:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:BE:5051:ARG:O	5:BE:5054:SER:N	2.50	0.44
13:BO:5155:THR:HG23	13:BO:5168:PHE:CD2	2.52	0.44
16:BV:5092:ARG:HG3	16:BV:5092:ARG:NH1	2.31	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
6:AF:15:ILE:HG23	36:AF:101:HEM:HAA1	1.98	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
16:AV:121:LEU:CD2	16:AV:138:LEU:HD11	2.47	0.44
1:BA:5011:ALA:O	1:BA:5012:ASN:HB3	2.17	0.44
1:BA:5343:LEU:O	1:BA:5344:ALA:CB	2.64	0.44
2:BB:5173:GLY:N	2:BB:5265:ILE:HD11	2.33	0.44
2:BB:5399:VAL:HG12	2:BB:5417:VAL:HG22	1.99	0.44
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CD2	2.53	0.44
4:BD:5261:PHE:CG	4:BD:5267:LEU:HD12	2.53	0.44
1:BA:5032:TRP:CZ2	8:BI:5022:GLY:HA2	2.52	0.44
13:BO:5184:ASP:OD2	13:BO:5188:ARG:HB2	2.17	0.44
24:BC:5511:CLA:C14	20:BZ:5024:PRO:HG2	2.47	0.44
31:AA:414:LMG:H142	29:AA:415:LHG:H102	1.99	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
4:AD:78:VAL:HG11	4:AD:114:ILE:HD12	1.98	0.44
9:AJ:24:ILE:HG23	9:AJ:25:VAL:N	2.32	0.44
31:AD:408:LMG:HC71	11:AL:15:THR:HG23	1.98	0.44
12:AM:28:GLN:HB3	12:BM:5027:VAL:HG12	1.99	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
1:BA:5042:LEU:HA	1:BA:5042:LEU:HD23	1.76	0.44
1:BA:5051:ALA:HA	27:BA:5411:BCR:H381	1.99	0.44
2:BB:5045:PHE:HE2	2:BB:5047:PRO:HB3	1.83	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
24:BC:5507:CLA:O1D	24:BC:5509:CLA:H101	2.17	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
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
12:BM:5001:MET:CG	12:BM:5002:GLU:N	2.81	0.44
13:BO:5055:ALA:HA	13:BO:5230:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:BB:5334:ASP:HB3	13:BO:5202:GLN:HG3	2.00	0.44
1:BA:5261:GLN:CD	2:BB:5489:GLU:HG3	2.36	0.44
3:BC:5166:ILE:HG13	3:BC:5248:GLY:HA3	1.99	0.44
3:BC:5205:ASP:OD1	3:BC:5207:ARG:HB3	2.17	0.44
4:BD:5126:MET:HE1	4:BD:5147:SER:HA	2.00	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
5:BE:5026:THR:HB	36:BF:5101:HEM:C3B	2.53	0.44
7:BH:5019:GLY:O	7:BH:5021:VAL:CG1	2.66	0.44
5:BE:5015:THR:CG2	9:BJ:5006:GLY:HA2	2.47	0.44
13:BO:5080:GLU:O	13:BO:5089:ALA:CB	2.65	0.44
13:BO:5109:GLY:HA3	13:BO:5122:VAL:O	2.16	0.44
1:AA:113:GLN:HB3	1:AA:117:PHE:CE2	2.52	0.44
1:AA:11:ALA:O	1:AA:12:ASN:HB3	2.18	0.44
1:AA:91:LEU:HD11	1:AA:163:ILE:HA	1.99	0.44
1:AA:59:ASP:OD2	1:AA:62:GLY:HA2	2.17	0.44
2:AB:11:VAL:HG23	11:AL:6:ASN:O	2.18	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:42:LEU:HD21	24:AC:511:CLA:H2A	1.98	0.44
3:AC:438:LEU:HD23	28:AC:517:DGD:HAW2	1.99	0.44
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.44
11:AL:17:LEU:HD12	12:AM:22:LEU:HB3	2.00	0.44
4:AD:195:PRO:HD3	11:AL:34:TYR:CE1	2.52	0.44
15:AU:56:ASP:OD2	15:AU:115:THR:OG1	2.36	0.44
13:AO:210:ARG:HA	15:AU:39:LEU:HD13	1.99	0.44
3:AC:414:ILE:HD11	16:AV:163:TYR:CG	2.53	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
2:BB:5413:ASP:O	2:BB:5414:PRO:C	2.55	0.44
3:BC:5081:MET:HE2	3:BC:5090:PRO:HD3	2.00	0.44
3:BC:5452:ALA:C	3:BC:5454:GLY:N	2.68	0.44
24:BD:5402:CLA:H2	34:BD:5404:PHO:HBB1	2.00	0.44
11:BL:5016:SER:HA	11:BL:5019:LEU:CD1	2.48	0.44
15:BU:5058:ASN:OD1	15:BU:5084:PRO:CA	2.65	0.44
18:BX:5012:ILE:HD13	18:BX:5016:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:41:LEU:HD21	1:AA:122:GLY:HA3	2.00	0.44
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.17	0.44
1:AA:214:MET:CE	4:AD:142:ASN:OD1	2.65	0.44
24:AB:606:CLA:H52	27:AB:619:BCR:H321	2.00	0.44
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.18	0.44
3:AC:344:SER:HB2	3:AC:345:PRO:CD	2.48	0.44
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.44
4:AD:122:LEU:HB3	4:AD:150:ILE:HD11	1.99	0.44
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.18	0.44
4:AD:186:GLN:HB2	24:AD:401:CLA:HBC1	2.00	0.44
6:AF:17:THR:O	6:AF:21:VAL:HG23	2.18	0.44
12:AM:20:VAL:HG11	12:BM:5020:VAL:HG22	2.00	0.44
13:AO:184:ASP:HB2	13:AO:185:PRO:HD2	1.99	0.44
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.18	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
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
28:BB:5602:DGD:C6E	32:BB:5626:LMT:H2'	2.47	0.44
3:BC:5176:VAL:O	3:BC:5180:MET:HG3	2.17	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
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.44
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	2.18	0.44
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.32	0.44
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.53	0.44
3:AC:217:PRO:O	28:AC:517:DGD:HB21	2.17	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
1:BA:5135:TYR:HD2	1:BA:5136:ARG:HH11	1.64	0.44
1:BA:5210:LEU:HD23	1:BA:5210:LEU:C	2.38	0.44
3:BC:5116:VAL:CG2	3:BC:5117:VAL:N	2.81	0.44
3:BC:5053:HIS:ND1	24:BC:5509:CLA:H141	2.33	0.44
3:BC:5053:HIS:HB3	24:BC:5512:CLA:OBD	2.17	0.44
4:BD:5145:ALA:HB2	4:BD:5272:LEU:CD2	2.47	0.44
8:BI:5011:VAL:CG2	32:BI:5102:LMT:H101	2.46	0.44
8:BI:5028:PRO:O	8:BI:5031:ASN:ND2	2.51	0.44
10:BK:5025:LEU:HB2	10:BK:5026:PRO:HD3	2.00	0.44
31:BD:5410:LMG:HC71	11:BL:5015:THR:HG23	1.99	0.44
13:BO:5036:ILE:HG23	13:BO:5041:LEU:HB2	2.00	0.44
20:BZ:5002:THR:O	20:BZ:5005:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:292:THR:HB	28:AC:518:DGD:HAH2	1.99	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
4:AD:161:PRO:CB	4:AD:170:ALA:HB2	2.47	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
13:AO:141:ARG:HH11	13:AO:141:ARG:HG2	1.83	0.44
1:BA:5059:ASP:OD1	1:BA:5064:ARG:N	2.50	0.44
1:BA:5210:LEU:CD2	1:BA:5210:LEU:C	2.86	0.44
1:BA:5304:HIS:CD2	1:BA:5313:VAL:HG11	2.52	0.44
2:BB:5144:PHE:CE1	2:BB:5210:ILE:CG2	3.01	0.44
2:BB:5326:ARG:HD3	2:BB:5442:ILE:HG22	1.98	0.44
3:BC:5264:PHE:CE1	27:BC:5516:BCR:H321	2.49	0.44
4:BD:5126:MET:HE2	4:BD:5146:PHE:HB3	2.00	0.44
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG11	2.53	0.44
2:BB:5363:PHE:CD1	4:BD:5326:ARG:HD2	2.52	0.44
35:BD:5406:PL9:H103	35:BD:5406:PL9:HC72	1.77	0.44
10:BK:5044:GLY:O	10:BK:5045:PHE:C	2.56	0.44
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.44
2:AB:12:LEU:HB2	24:AB:612:CLA:HMC2	1.98	0.44
2:AB:153:PHE:CZ	2:AB:158:LEU:HD21	2.53	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
4:AD:253:TRP:HA	4:AD:256:ILE:CG2	2.48	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
24:BA:5406:CLA:H72	31:BL:5101:LMG:C25	2.47	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
3:BC:5028:GLN:HB2	24:BC:5511:CLA:HED1	1.99	0.44
3:BC:5416:SER:CA	28:BC:5519:DGD:O3E	2.66	0.44
1:BA:5276:ALA:HB2	4:BD:5215:GLY:HA3	2.00	0.44
4:BD:5279:LEU:CD2	24:BD:5402:CLA:HMA2	2.48	0.44
3:BC:5029:GLU:CB	10:BK:5046:ARG:NH1	2.79	0.44
1:BA:5107:TYR:CD1	13:BO:5141:ARG:NH1	2.86	0.44
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA1	2.00	0.43
2:AB:433:ASP:C	2:AB:433:ASP:OD1	2.55	0.43
2:AB:246:PHE:CD2	2:AB:463:PHE:HA	2.53	0.43
24:AB:607:CLA:HMD3	27:BT:5101:BCR:H271	2.00	0.43
30:AB:627:SQD:H45	14:BT:5023:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:BA:5214:MET:O	1:BA:5215:HIS:C	2.54	0.43
2:BB:5091:TRP:CE3	24:BB:5610:CLA:O1A	2.71	0.43
2:BB:5137:LYS:HG3	2:BB:5220:ARG:NH2	2.32	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
4:BD:5183:LEU:HD23	4:BD:5183:LEU:HA	1.87	0.43
4:BD:5253:TRP:HB2	4:BD:5260:ALA:CB	2.48	0.43
4:BD:5039:PRO:HB3	24:BD:5405:CLA:HMC3	2.00	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:CB	2.47	0.43
3:BC:5347:GLY:CA	13:BO:5043:ASN:HB2	2.47	0.43
13:BO:5190:LEU:HB2	13:BO:5214:LYS:HB2	2.00	0.43
1:AA:157:VAL:HG21	24:AA:405:CLA:HMC1	2.00	0.43
1:AA:309:ALA:HB3	16:AV:27:ALA:O	2.17	0.43
2:AB:137:LYS:HG3	2:AB:220:ARG:NH2	2.33	0.43
24:AB:608:CLA:HBA1	30:AB:622:SQD:H102	2.00	0.43
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.81	0.43
3:AC:143:TYR:O	3:AC:144:SER:CB	2.65	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
9:AJ:3:SER:CA	9:AJ:7:ARG:HH22	2.32	0.43
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.40	0.43
1:BA:5093:PHE:CE2	24:BA:5408:CLA:HBA1	2.52	0.43
14:AT:23:PHE:CD1	30:BB:5601:SQD:H45	2.53	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
4:BD:5081:PRO:HB2	4:BD:5085:MET:HG3	1.99	0.43
4:BD:5190:ASN:HB2	4:BD:5296:TYR:CE1	2.53	0.43
5:BE:5008:ARG:NH2	9:BJ:5004:GLU:HB2	2.34	0.43
11:AL:9:PRO:HB3	31:BM:5102:LMG:O2	2.18	0.43
2:AB:247:PHE:O	2:AB:251:VAL:HG23	2.19	0.43
3:AC:185:LEU:HD12	3:AC:230:LEU:HD12	2.00	0.43
3:AC:166:ILE:HG13	3:AC:248:GLY:HA3	2.01	0.43
24:AA:405:CLA:H61	34:AD:402:PHO:HMB3	2.00	0.43
31:AM:101:LMG:H132	24:BB:5618:CLA:H12	2.00	0.43
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.73	0.43
16:AV:54:GLU:O	16:AV:58:LEU:HG	2.18	0.43
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AX:20:PHE:HZ	27:AX:101:BCR:H371	1.84	0.43
1:BA:5010:SER:C	1:BA:5012:ASN:N	2.71	0.43
1:BA:5193:LEU:CD1	4:BD:5179:PHE:HB3	2.47	0.43
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CA	2.30	0.43
2:BB:5024:LEU:HD13	2:BB:5111:ALA:N	2.34	0.43
2:BB:5222:PRO:O	2:BB:5223:GLN:C	2.56	0.43
3:BC:5161:LEU:HD23	3:BC:5251:HIS:HD2	1.84	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
13:BO:5155:THR:HG22	13:BO:5167:ASP:O	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
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.17	0.43
27:AT:101:BCR:H271	24:BB:5611:CLA:HMD3	2.01	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:5179:GLN:NE2	2:BB:5179:GLN:HA	2.22	0.43
2:BB:5260:SER:HG	2:BB:5262:THR:HG22	1.77	0.43
2:BB:5356:VAL:HG22	2:BB:5370:LEU:CD2	2.48	0.43
2:BB:5343:HIS:O	2:BB:5401:PHE:HA	2.18	0.43
2:BB:5476:ARG:CZ	2:BB:5476:ARG:HB3	2.44	0.43
2:BB:5075:TRP:CZ3	28:BB:5602:DGD:HB32	2.54	0.43
3:BC:5407:VAL:HA	28:BC:5519:DGD:O2E	2.18	0.43
5:BE:5007:GLU:O	5:BE:5009:PRO:HD3	2.17	0.43
13:BO:5135:GLN:HE21	13:BO:5135:GLN:HB3	1.53	0.43
13:BO:5168:PHE:O	13:BO:5224:SER:HA	2.18	0.43
1:AA:271:LEU:HD21	25:AA:408:MST:H83	2.00	0.43
2:AB:37:MET:O	2:AB:41:GLU:HG3	2.18	0.43
3:AC:29:GLU:CD	3:AC:29:GLU:N	2.72	0.43
27:AC:514:BCR:H11C	27:AK:102:BCR:H322	2.00	0.43
14:AT:18:PHE:CD1	27:AT:101:BCR:HC8	2.54	0.43
16:AV:148:GLU:N	16:AV:149:PRO:HD2	2.34	0.43
4:AD:17:ILE:CG2	18:AX:42:GLN:HG2	2.42	0.43
2:BB:5348:ASN:O	2:BB:5349:LYS:C	2.56	0.43
24:BB:5607:CLA:HMB1	24:BB:5607:CLA:HAB	1.81	0.43
3:BC:5266:TRP:HB3	3:BC:5271:TYR:OH	2.17	0.43
4:BD:5078:VAL:HG11	4:BD:5114:ILE:HD12	2.01	0.43
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:CD1	2.48	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
1:AA:281:VAL:HG13	1:AA:282:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:230:ARG:H	2:AB:230:ARG:HD2	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
3:AC:377:LEU:CD2	13:AO:126:GLY:HA2	2.48	0.43
3:AC:380:ILE:CA	3:AC:384:ILE:HD11	2.40	0.43
24:AC:510:CLA:H122	24:AC:510:CLA:H161	1.85	0.43
6:AF:15:ILE:HG22	6:AF:16:PHE:CD1	2.50	0.43
14:AT:31:LYS:O	14:AT:32:LYS:HB2	2.18	0.43
13:AO:180:ALA:HB2	15:AU:120:ALA:O	2.18	0.43
1:BA:5013:LEU:HA	1:BA:5016:ARG:NH1	2.33	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
2:BB:5159:THR:OG1	2:BB:5161:LEU:HD13	2.19	0.43
3:BC:5203:THR:O	3:BC:5235:GLY:HA3	2.19	0.43
3:BC:5466:VAL:HA	3:BC:5469:MET:CE	2.48	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
5:BE:5082:GLN:O	5:BE:5083:LEU:C	2.56	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
1:AA:228:THR:CG2	1:AA:229:GLU:N	2.81	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
2:AB:358:ARG:O	2:AB:360:PRO:HD3	2.18	0.43
30:AB:622:SQD:H281	32:AB:624:LMT:H82	2.00	0.43
3:AC:315:MET:HE2	3:AC:365:TRP:HZ3	1.83	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
24:AA:405:CLA:HED2	4:AD:198:MET:SD	2.58	0.43
4:AD:253:TRP:HB2	4:AD:260:ALA:CB	2.49	0.43
4:AD:52:THR:HG22	4:AD:67:TYR:CZ	2.53	0.43
13:AO:127:ILE:H	13:AO:127:ILE:HG12	1.64	0.43
15:AU:66:ILE:HG12	15:AU:72:TYR:CD1	2.54	0.43
24:AC:511:CLA:H141	20:AZ:20:VAL:O	2.18	0.43
1:BA:5214:MET:CE	4:BD:5142:ASN:OD1	2.66	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
3:BC:5071:GLU:OE2	3:BC:5088:LEU:HG	2.19	0.43
3:BC:5324:LEU:HB3	15:BU:5062:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5404:LEU:HD12	3:BC:5404:LEU:HA	1.73	0.43
3:BC:5452:ALA:O	3:BC:5453:ALA:C	2.57	0.43
4:BD:5261:PHE:HE1	4:BD:5266:TRP:CD1	2.37	0.43
1:BA:5342:ASP:HB2	4:BD:5352:LEU:HD21	1.99	0.43
8:BI:5027:ASP:N	8:BI:5028:PRO:HD3	2.33	0.43
11:BL:5024:ILE:HG22	11:BL:5025:LEU:N	2.33	0.43
14:BT:5029:ILE:O	14:BT:5031:LYS:N	2.52	0.43
1:AA:248:ILE:HG12	1:AA:248:ILE:O	2.18	0.43
1:AA:281:VAL:HG11	28:AC:519:DGD:CIA	2.49	0.43
1:AA:325:ASN:HA	1:AA:328:MET:CE	2.31	0.43
2:AB:249:ALA:O	2:AB:252:VAL:HG22	2.19	0.43
2:AB:271:THR:N	2:AB:274:GLN:OE1	2.47	0.43
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.43
4:AD:43:LEU:HD23	4:AD:117:HIS:CE1	2.53	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
5:AE:15:THR:CG2	9:AJ:6:GLY:HA2	2.49	0.43
6:AF:30:THR:HG22	6:AF:34:LEU:CD1	2.48	0.43
1:BA:5013:LEU:HD12	1:BA:5016:ARG:NH1	2.33	0.43
1:BA:5065:GLU:N	1:BA:5066:PRO:HD3	2.34	0.43
1:BA:5299:GLY:O	3:BC:5403:SER:HB2	2.18	0.43
2:BB:5024:LEU:HB3	2:BB:5111:ALA:HB2	2.00	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
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE1	2.53	0.43
5:BE:5057:ALA:H	5:BE:5060:GLN:NE2	2.17	0.43
2:BB:5011:VAL:CG2	11:BL:5007:ARG:HA	2.49	0.43
16:BV:5063:CYS:O	16:BV:5064:ALA:C	2.56	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
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.43
2:AB:354:LEU:HD21	2:AB:378:LYS:CB	2.49	0.43
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
3:AC:466:VAL:HA	3:AC:469:MET:CE	2.48	0.43
24:AC:504:CLA:H141	28:AC:518:DGD:HBT1	2.01	0.43
24:AC:512:CLA:H122	24:AC:512:CLA:H162	1.87	0.43
4:AD:217:THR:O	4:AD:221:THR:HB	2.18	0.43
5:AE:16:SER:HB2	9:AJ:3:SER:O	2.18	0.43
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.43
13:AO:120:THR:HA	13:AO:153:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:130:MET:SD	16:AV:133:LEU:HD22	2.58	0.43
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.73	0.43
1:BA:5113:GLN:HB3	1:BA:5117:PHE:CE2	2.54	0.43
1:BA:5176:ILE:HD12	24:BA:5406:CLA:HED3	2.01	0.43
2:BB:5011:VAL:HG23	11:BL:5007:ARG:HA	2.01	0.43
3:BC:5313:GLN:HB2	3:BC:5313:GLN:HE21	1.54	0.43
3:BC:5415:ASN:O	3:BC:5416:SER:CB	2.63	0.43
3:BC:5438:LEU:HD12	3:BC:5438:LEU:O	2.19	0.43
27:BC:5514:BCR:H11C	27:BK:5102:BCR:H322	2.00	0.43
3:BC:5062:PHE:HZ	10:BK:5028:ILE:CD1	2.29	0.43
13:BO:5147:THR:O	13:BO:5172:PHE:CE2	2.71	0.43
15:BU:5130:ASN:O	15:BU:5132:LEU:HD23	2.18	0.43
16:BV:5071:ILE:CD1	16:BV:5072:THR:N	2.81	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
2:AB:345:VAL:HG21	2:AB:402:TYR:CE2	2.53	0.43
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	2.00	0.43
24:AB:603:CLA:H3A	24:AB:603:CLA:CGA	2.49	0.43
3:AC:232:ASP:OD2	3:AC:232:ASP:N	2.52	0.43
1:AA:295:PHE:HD2	3:AC:291:TRP:CD2	2.37	0.43
3:AC:417:VAL:O	3:AC:417:VAL:HG13	2.19	0.43
4:AD:171:PRO:HG3	4:AD:181:PHE:CE2	2.54	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
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.43
13:AO:32:THR:OG1	13:AO:33:TYR:N	2.52	0.43
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.49	0.43
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.18	0.43
20:AZ:31:GLN:HG3	20:AZ:32:ASP:OD2	2.19	0.43
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.68	0.43
1:BA:5157:VAL:HG21	24:BA:5406:CLA:HMC1	2.00	0.43
1:BA:5207:GLY:HA3	1:BA:5278:TRP:HE1	1.84	0.43
2:BB:5037:MET:O	2:BB:5041:GLU:HG3	2.19	0.43
24:BB:5609:CLA:H143	24:BB:5614:CLA:HBA1	2.01	0.43
3:BC:5366:LEU:HD21	3:BC:5370:ARG:NH2	2.34	0.43
4:BD:5272:LEU:O	4:BD:5276:VAL:HG23	2.19	0.43
5:BE:5035:TRP:C	5:BE:5035:TRP:CD1	2.92	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:HB3	2.00	0.43
1:BA:5032:TRP:HB2	8:BI:5023:PHE:CZ	2.54	0.43
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5239:PHE:HB3	14:BT:5028:ARG:O	2.18	0.43
19:BY:5023:UNK:O	19:BY:5025:UNK:N	2.52	0.43
2:AB:102:VAL:HB	24:AB:606:CLA:H91	2.00	0.42
2:AB:144:PHE:HE1	2:AB:210:ILE:CG2	2.31	0.42
2:AB:250:PHE:HD1	28:AH:101:DGD:HB92	1.83	0.42
2:AB:490:GLN:O	2:AB:491:VAL:O	2.37	0.42
3:AC:404:LEU:HA	3:AC:404:LEU:HD12	1.69	0.42
23:AA:403[A]:CL:CL	4:AD:317:LYS:HD3	2.56	0.42
24:AD:404:CLA:H41	18:AX:23:LEU:CD1	2.43	0.42
16:AV:92:ARG:NH1	16:AV:92:ARG:HG3	2.33	0.42
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CHA	2.48	0.42
2:BB:5135:LEU:HD21	2:BB:5234:ILE:HD13	2.01	0.42
2:BB:5437:LEU:N	2:BB:5437:LEU:HD12	2.34	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
3:BC:5466:VAL:HA	3:BC:5469:MET:HE1	2.01	0.42
3:BC:5042:LEU:CD1	24:BC:5511:CLA:HMA3	2.50	0.42
6:BF:5025:THR:O	6:BF:5029:PRO:HG2	2.18	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
13:BO:5069:LEU:HD12	13:BO:5070:CYS:N	2.33	0.42
13:BO:5127:ILE:H	13:BO:5127:ILE:HG12	1.65	0.42
16:BV:5121:LEU:HD21	16:BV:5138:LEU:HD11	2.01	0.42
19:BY:5021:UNK:O	19:BY:5022:UNK:C	2.66	0.42
1:AA:303:ASN:O	1:AA:304:HIS:HB2	2.20	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
16:AV:90:PRO:O	16:AV:92:ARG:CD	2.67	0.42
10:AK:14:ALA:HB2	20:AZ:61:VAL:HG12	2.01	0.42
1:BA:5259:ILE:N	1:BA:5259:ILE:CD1	2.69	0.42
2:BB:5015:ASP:N	2:BB:5016:PRO:CD	2.81	0.42
2:BB:5137:LYS:HE2	7:BH:5017:GLU:CG	2.49	0.42
2:BB:5358:ARG:O	2:BB:5360:PRO:HD3	2.19	0.42
3:BC:5165:LEU:HD11	24:BC:5506:CLA:CHC	2.48	0.42
3:BC:5426:LEU:HA	3:BC:5426:LEU:HD23	1.86	0.42
29:BA:5413:LHG:HC62	3:BC:5443:TRP:HH2	1.85	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
28:BC:5518:DGD:HBT2	27:BJ:5101:BCR:H342	2.01	0.42
13:BO:5051:THR:OG1	13:BO:5052:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5075:THR:HG21	13:BO:5077:LEU:HD21	2.01	0.42
15:BU:5072:TYR:CG	15:BU:5073:PRO:N	2.84	0.42
1:AA:20:TRP:O	1:AA:23:SER:HB3	2.18	0.42
2:AB:297:THR:OG1	2:AB:298:LEU:N	2.52	0.42
24:AB:614:CLA:HMB1	24:AB:614:CLA:HAB	1.89	0.42
3:AC:304:PRO:HB3	3:AC:395:TYR:CG	2.54	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
3:AC:415:ASN:CB	9:AJ:39:SER:OG	2.67	0.42
1:AA:288:LEU:CD1	3:AC:432:VAL:HG23	2.44	0.42
4:AD:181:PHE:CZ	4:AD:185:PHE:CE1	3.07	0.42
31:AM:101:LMG:O8	31:AM:101:LMG:O9	2.37	0.42
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	2.00	0.42
2:BB:5141:ILE:O	2:BB:5144:PHE:HB3	2.20	0.42
2:BB:5234:ILE:C	2:BB:5236:THR:H	2.23	0.42
2:BB:5345:VAL:HG21	2:BB:5402:TYR:CE2	2.54	0.42
2:BB:5477:ASP:OD2	2:BB:5478:VAL:HG13	2.19	0.42
24:BB:5607:CLA:H203	24:BB:5613:CLA:H92	2.00	0.42
3:BC:5321:ASP:OD2	15:BU:5129:ASN:HB2	2.19	0.42
4:BD:5122:LEU:HD21	24:BD:5402:CLA:C9	2.41	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
30:AB:627:SQD:H45	14:BT:5023:PHE:HD1	1.85	0.42
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.19	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
28:AC:518:DGD:HBT2	27:AJ:101:BCR:H342	2.02	0.42
9:AJ:3:SER:CB	9:AJ:7:ARG:HH22	2.32	0.42
13:AO:57:PRO:HA	13:AO:161:SER:OG	2.19	0.42
1:BA:5042:LEU:HA	1:BA:5045:THR:HG22	2.01	0.42
1:BA:5131:TRP:CZ3	1:BA:5132:GLU:HG3	2.53	0.42
2:BB:5144:PHE:HE1	2:BB:5210:ILE:CG2	2.33	0.42
2:BB:5230:ARG:HD2	2:BB:5230:ARG:H	1.84	0.42
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CE1	2.54	0.42
24:BB:5618:CLA:HAA2	24:BB:5618:CLA:HBD	2.01	0.42
32:BC:5522:LMT:H41	8:BI:5021:PHE:HE1	1.84	0.42
10:BK:5018:PHE:O	10:BK:5019:ASP:C	2.57	0.42
13:BO:5141:ARG:HH11	13:BO:5141:ARG:HG2	1.83	0.42
13:BO:5178:ARG:HG3	13:BO:5178:ARG:NH1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:5056:ASP:HB3	15:BU:5060:THR:H	1.84	0.42
1:AA:257:ARG:NH1	2:AB:489:GLU:OE2	2.52	0.42
2:AB:124:ARG:NH1	2:AB:124:ARG:HG3	2.33	0.42
2:AB:12:LEU:HD13	2:AB:19:LEU:CA	2.38	0.42
2:AB:357:ARG:NH2	4:AD:337:GLU:OE1	2.53	0.42
3:AC:229:ASN:O	3:AC:233:VAL:HG23	2.18	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.19	0.42
13:AO:70:CYS:SG	13:AO:105:ASP:OD1	2.77	0.42
13:AO:73:PRO:HG3	13:AO:146:PHE:CE2	2.54	0.42
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.85	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HG21	2.50	0.42
2:BB:5274:GLN:HG2	2:BB:5279:TYR:CD2	2.54	0.42
3:BC:5217:PRO:O	28:BC:5517:DGD:HB21	2.20	0.42
1:BA:5217:SER:HB2	4:BD:5141:TYR:O	2.19	0.42
5:BE:5069:ARG:CG	5:BE:5070:PHE:N	2.82	0.42
13:BO:5081:GLU:HA	13:BO:5082:PRO:HD3	1.88	0.42
13:BO:5091:PHE:CD1	13:BO:5260:LYS:HB2	2.55	0.42
16:BV:5062:ALA:O	36:BV:5201:HEM:HAB	2.20	0.42
19:BY:5018:UNK:O	19:BY:5022:UNK:N	2.52	0.42
20:BZ:5030:PRO:C	20:BZ:5032:ASP:N	2.72	0.42
2:AB:224:ARG:CZ	32:AB:624:LMT:H2'	2.50	0.42
2:AB:450:TRP:NE1	24:AB:607:CLA:HBA2	2.34	0.42
2:AB:466:HIS:HE1	24:AB:608:CLA:C4D	2.31	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
4:AD:164:GLN:NE2	4:AD:290:ALA:O	2.53	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
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.20	0.42
3:AC:337:LEU:HA	13:AO:131:PRO:HG3	2.01	0.42
14:AT:14:ILE:HD13	14:AT:17:PHE:CD2	2.55	0.42
1:BA:5069:GLY:HA2	1:BA:5075:ASN:HD21	1.83	0.42
2:BB:5246:PHE:CD2	2:BB:5463:PHE:HA	2.54	0.42
2:BB:5238:LEU:CD2	2:BB:5469:HIS:CD2	3.03	0.42
2:BB:5112:CYS:HA	27:BB:5621:BCR:H282	2.01	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
13:BO:5094:THR:HB	13:BO:5135:GLN:O	2.20	0.42
1:AA:259:ILE:N	1:AA:259:ILE:CD1	2.71	0.42
24:AA:405:CLA:H62	34:AD:402:PHO:HMA1	2.01	0.42
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.19	0.42
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	2.02	0.42
13:AO:56:TYR:CD1	13:AO:235:GLY:HA2	2.55	0.42
1:BA:5157:VAL:HG13	1:BA:5172:MET:HB2	2.00	0.42
1:BA:5207:GLY:O	1:BA:5210:LEU:HB3	2.19	0.42
1:BA:5118:HIS:HE1	24:BA:5408:CLA:C1A	2.32	0.42
2:BB:5188:ASP:HA	7:BH:5058:VAL:HG23	2.02	0.42
3:BC:5142:GLU:C	3:BC:5144:SER:H	2.22	0.42
3:BC:5223:TRP:CH2	3:BC:5224:ILE:HD11	2.54	0.42
13:BO:5059:ASP:O	13:BO:5061:SER:N	2.53	0.42
1:AA:149:ALA:HB1	1:AA:283:VAL:CG1	2.49	0.42
1:AA:262:TYR:HE1	31:AA:414:LMG:HO5	1.66	0.42
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.51	0.42
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.42
3:AC:276:LEU:HA	3:AC:276:LEU:HD23	1.76	0.42
3:AC:366:LEU:HD23	3:AC:366:LEU:O	2.20	0.42
1:AA:288:LEU:CD2	3:AC:432:VAL:HG23	2.49	0.42
28:AC:518:DGD:O1B	28:AC:518:DGD:C1G	2.68	0.42
4:AD:68:LEU:HB2	6:AF:40:MET:HE1	2.02	0.42
6:AF:20:TRP:NE1	6:AF:24:HIS:CE1	2.88	0.42
13:AO:141:ARG:NH1	13:AO:141:ARG:HG2	2.35	0.42
1:BA:5240:GLY:HA3	14:BT:5029:ILE:CG2	2.48	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
2:BB:5238:LEU:CA	24:BB:5616:CLA:HMD3	2.50	0.42
3:BC:5318:LEU:C	3:BC:5318:LEU:HD23	2.40	0.42
3:BC:5418:ASN:HB2	28:BC:5519:DGD:O4E	2.20	0.42
4:BD:5014:TRP:CG	4:BD:5015:PHE:N	2.88	0.42
6:BF:5023:VAL:O	6:BF:5027:ALA:HB2	2.20	0.42
7:BH:5019:GLY:O	7:BH:5021:VAL:HG13	2.20	0.42
9:BJ:5021:VAL:HA	9:BJ:5024:ILE:HG22	2.02	0.42
1:AA:254:TYR:OH	4:AD:129:GLN:HB3	2.20	0.42
1:AA:292:THR:HB	28:AC:518:DGD:CDA	2.49	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
2:AB:264:PRO:HG2	2:AB:267:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:356:VAL:HG21	2:AB:424:ALA:CB	2.50	0.42
4:AD:128:ARG:HE	4:AD:128:ARG:HB2	1.66	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
18:AX:16:LEU:HD13	18:AX:16:LEU:C	2.39	0.42
20:AZ:30:PRO:HB3	20:AZ:33:TRP:CZ3	2.54	0.42
1:BA:5200:LEU:HD12	1:BA:5285:PHE:CG	2.54	0.42
1:BA:5286:THR:HG23	24:BA:5405:CLA:HED3	2.02	0.42
32:BB:5603:LMT:H5'	32:BB:5603:LMT:H1B	1.79	0.42
2:BB:5162:PHE:O	24:BB:5610:CLA:HMD3	2.20	0.42
4:BD:5161:PRO:HG3	4:BD:5170:ALA:HB2	2.02	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
20:BZ:5031:GLN:HG3	20:BZ:5032:ASP:OD2	2.18	0.42
1:AA:13:LEU:CA	1:AA:16:ARG:HH11	2.33	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
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
1:AA:281:VAL:HG11	28:AC:519:DGD:HAG3	2.01	0.42
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.20	0.42
5:AE:78:THR:HA	5:AE:81:GLU:CG	2.49	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
14:AT:14:ILE:HD13	14:AT:14:ILE:HA	1.88	0.42
20:AZ:38:GLN:O	20:AZ:42:LEU:HG	2.19	0.42
1:BA:5133:LEU:HD23	4:BD:5252:PHE:HD1	1.81	0.42
1:BA:5147:TYR:CG	1:BA:5147:TYR:O	2.73	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:5450:TRP:NE1	24:BB:5611:CLA:HBA2	2.35	0.42
2:BB:5237:VAL:HB	24:BB:5616:CLA:CMD	2.50	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:5141:GLU:HA	3:BC:5148:GLY:HA3	2.02	0.42
3:BC:5160:ILE:HA	3:BC:5163:PHE:CD2	2.54	0.42
3:BC:5269:GLU:OE1	3:BC:5447:ARG:HD3	2.20	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
1:AA:220:THR:HG23	4:AD:141:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:232:SER:HB3	1:AA:235:TYR:CD2	2.55	0.41
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.85	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
2:AB:187:PRO:HG2	2:AB:188:ASP:N	2.35	0.41
2:AB:390:TYR:HD2	4:AD:344:GLU:OE1	2.02	0.41
24:AB:616:CLA:HHC	24:AB:616:CLA:HBB1	2.01	0.41
32:AB:629:LMT:H51	14:BT:5004:ILE:CG1	2.42	0.41
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.55	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:BA:5032:TRP:CB	8:BI:5023:PHE:CZ	3.03	0.41
1:BA:5191:ASN:ND2	1:BA:5194:MET:HB2	2.35	0.41
24:BB:5606:CLA:H93	7:BH:5046:LEU:HD13	2.02	0.41
2:BB:5152:GLY:C	24:BB:5610:CLA:HMC3	2.40	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
2:BB:5324:LEU:HD13	4:BD:5293:LEU:CD2	2.50	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
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
16:BV:5090:PRO:O	16:BV:5092:ARG:CD	2.67	0.41
20:BZ:5005:PHE:HA	20:BZ:5057:LEU:CD2	2.50	0.41
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.41
1:AA:306:VAL:HG22	1:AA:314:ILE:HB	2.03	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
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.21	0.41
2:AB:348:ASN:O	2:AB:349:LYS:C	2.58	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
3:AC:441:HIS:HD2	3:AC:442:LEU:HD12	1.85	0.41
24:AC:502:CLA:HAA2	24:AC:502:CLA:HBD	2.01	0.41
24:AC:511:CLA:H143	20:AZ:24:PRO:HG2	2.02	0.41
1:AA:140:ARG:HB2	4:AD:220:ASN:HA	2.01	0.41
4:AD:53:THR:HA	4:AD:67:TYR:CD2	2.56	0.41
9:AJ:32:ALA:HA	31:AJ:102:LMG:O3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:114:ASN:HD21	13:AO:120:THR:CG2	2.29	0.41
13:AO:46:PRO:HB2	13:AO:266:TYR:CD2	2.55	0.41
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.20	0.41
1:BA:5239:PHE:O	14:BT:5030:THR:N	2.53	0.41
2:BB:5185:TRP:HD1	24:BB:5606:CLA:HBB2	1.85	0.41
2:BB:5225:LEU:O	2:BB:5226:TYR:C	2.59	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
3:BC:5337:LEU:HD23	3:BC:5342:MET:HE1	2.01	0.41
4:BD:5161:PRO:CB	4:BD:5170:ALA:HB2	2.50	0.41
1:BA:5243:GLU:HA	4:BD:5240:ALA:O	2.20	0.41
7:BH:5017:GLU:CD	7:BH:5017:GLU:N	2.72	0.41
7:BH:5018:TYR:CD1	7:BH:5018:TYR:C	2.94	0.41
3:BC:5062:PHE:CD2	10:BK:5029:PRO:HG3	2.50	0.41
12:BM:5018:PRO:O	12:BM:5021:PHE:HB3	2.20	0.41
13:BO:5106:GLN:HE21	13:BO:5106:GLN:HB3	1.68	0.41
3:BC:5337:LEU:HA	13:BO:5131:PRO:HG3	2.02	0.41
16:BV:5062:ALA:O	36:BV:5201:HEM:CAB	2.68	0.41
2:AB:373:LYS:HG3	2:AB:374:ASN:N	2.35	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
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.41
3:AC:204:LEU:HA	3:AC:204:LEU:HD23	1.79	0.41
4:AD:199:MET:HG2	35:AD:405:PL9:H312	2.03	0.41
5:AE:8:ARG:NH2	9:AJ:4:GLU:HB2	2.35	0.41
13:AO:156:GLN:OE1	13:AO:156:GLN:HA	2.20	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
1:BA:5048:PHE:HA	1:BA:5115:ILE:CD1	2.48	0.41
1:BA:5096:ILE:C	1:BA:5098:GLU:H	2.24	0.41
1:BA:5135:TYR:CE1	3:BC:5449:ARG:HB3	2.55	0.41
1:BA:5321:ILE:HG22	1:BA:5325:ASN:ND2	2.35	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
3:BC:5417:VAL:HG13	3:BC:5417:VAL:O	2.19	0.41
3:BC:5466:VAL:HG21	4:BD:5248:THR:OG1	2.20	0.41
28:BC:5519:DGD:HD3	9:BJ:5032:ALA:O	2.20	0.41
4:BD:5019:ASP:O	4:BD:5020:ASP:C	2.57	0.41
9:BJ:5003:SER:CB	9:BJ:5007:ARG:NH2	2.83	0.41
24:BA:5406:CLA:H72	31:BL:5101:LMG:H241	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BV:5069:GLY:O	16:BV:5156:TRP:O	2.38	0.41
7:BH:5035:MET:SD	27:BX:5101:BCR:H322	2.61	0.41
20:BZ:5022:GLY:O	20:BZ:5023:VAL:C	2.58	0.41
1:AA:36:ILE:HD13	1:AA:36:ILE:HA	1.89	0.41
1:AA:57:PRO:HA	1:AA:68:SER:HA	2.03	0.41
3:AC:367:GLU:OE1	3:AC:367:GLU:HA	2.18	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HD13	2.02	0.41
28:AC:519:DGD:HD3	9:AJ:32:ALA:O	2.20	0.41
4:AD:53:THR:CB	4:AD:67:TYR:HD2	2.34	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
1:BA:5278:TRP:HB3	1:BA:5279:PRO:CD	2.42	0.41
1:BA:5306:VAL:HG22	1:BA:5314:ILE:HB	2.02	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
6:BF:5024:HIS:NE2	36:BF:5101:HEM:NB	2.67	0.41
7:BH:5063:LYS:O	7:BH:5064:ALA:HB3	2.20	0.41
1:BA:5138:GLY:CA	8:BI:5032:PRO:HG2	2.51	0.41
13:BO:5120:THR:HG22	13:BO:5154:SER:CB	2.50	0.41
15:BU:5077:LYS:O	15:BU:5081:LYS:HB2	2.21	0.41
1:AA:200:LEU:HD21	28:AC:519:DGD:CCA	2.50	0.41
2:AB:252:VAL:HG23	2:AB:253:ALA:N	2.35	0.41
2:AB:483:ASP:CB	2:AB:484:PRO:CD	2.94	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
3:AC:42:LEU:CD1	24:AC:511:CLA:HMA3	2.50	0.41
4:AD:218:VAL:HG22	4:AD:244:TYR:CD2	2.54	0.41
7:AH:42:LEU:HD12	7:AH:42:LEU:HA	1.83	0.41
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.24	0.41
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.41
10:AK:21:LEU:HD11	27:AK:102:BCR:HC42	2.03	0.41
3:AC:62:PHE:CD2	10:AK:29:PRO:HG3	2.50	0.41
4:AD:259:ILE:HD13	14:AT:21:ILE:HG12	2.02	0.41
18:AX:12:ILE:CA	27:AX:101:BCR:H401	2.48	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:CZ2	2.38	0.41
1:BA:5172:MET:HA	1:BA:5173:PRO:HD3	1.97	0.41
1:BA:5292:THR:HB	28:BC:5518:DGD:CDA	2.50	0.41
1:BA:5340:PRO:HG3	15:BU:5133:TYR:CD1	2.55	0.41
2:BB:5271:THR:N	2:BB:5274:GLN:OE1	2.45	0.41
2:BB:5298:LEU:HD12	2:BB:5298:LEU:HA	1.89	0.41
2:BB:5026:HIS:HB2	24:BB:5616:CLA:HMB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5244:CYS:HA	24:BC:5506:CLA:CMC	2.51	0.41
4:BD:5272:LEU:HD22	4:BD:5276:VAL:HG21	2.03	0.41
7:BH:5016:SER:C	7:BH:5018:TYR:H	2.23	0.41
9:BJ:5038:SER:OG	9:BJ:5039:SER:N	2.53	0.41
19:BY:5025:UNK:C	19:BY:5027:UNK:N	2.82	0.41
24:AA:405:CLA:H72	31:AB:620:LMG:H241	2.01	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.20	0.41
2:AB:278:SER:HB3	2:AB:281:GLN:NE2	2.32	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
3:AC:149:TYR:HB3	3:AC:156:LYS:HD3	2.02	0.41
3:AC:437:PHE:CD2	24:AC:508:CLA:CMC	3.04	0.41
3:AC:459:ILE:HG21	3:AC:464:GLU:HG3	2.02	0.41
3:AC:466:VAL:HG13	4:AD:251:ARG:CD	2.50	0.41
24:AC:505:CLA:HAA2	24:AC:505:CLA:HBD	2.02	0.41
3:AC:71:GLU:OE2	3:AC:88:LEU:HG	2.21	0.41
1:AA:184:ILE:CD1	4:AD:186:GLN:HG2	2.51	0.41
4:AD:202:ALA:HB3	35:AD:405:PL9:C30	2.49	0.41
4:AD:84:SER:HB3	5:AE:68:ASP:HA	2.03	0.41
13:AO:168:PHE:HB2	13:AO:225:LEU:HB2	2.03	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:5135:LEU:HD23	2:BB:5138:MET:CE	2.50	0.41
2:BB:5193:TYR:CE1	2:BB:5260:SER:HA	2.55	0.41
24:BB:5615:CLA:HBB1	24:BB:5615:CLA:HHC	2.03	0.41
2:BB:5112:CYS:CB	27:BB:5623:BCR:H393	2.51	0.41
2:BB:5489:GLU:CB	5:BE:5003:GLY:N	2.76	0.41
15:BU:5072:TYR:CB	15:BU:5073:PRO:CD	2.98	0.41
20:BZ:5032:ASP:HA	20:BZ:5034:ASP:OD2	2.21	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
2:AB:369:ILE:HD13	4:AD:340:VAL:O	2.21	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
29:AA:412:LHG:C1	3:AC:447:ARG:HE	2.34	0.41
3:AC:48:LYS:HE2	3:AC:138:GLU:OE2	2.20	0.41
3:AC:243:ILE:O	24:AC:506:CLA:HMC1	2.20	0.41
1:AA:278:TRP:CD2	28:AC:519:DGD:CIA	2.96	0.41
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.41
4:AD:261:PHE:CG	4:AD:267:LEU:HD12	2.56	0.41
7:AH:40:VAL:O	7:AH:44:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AJ:101:BCR:H20C	27:AJ:101:BCR:H361	1.91	0.41
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.60	0.41
1:BA:5224:ILE:H	1:BA:5224:ILE:HG13	1.57	0.41
3:BC:5311:GLN:OE1	3:BC:5355:THR:CG2	2.68	0.41
3:BC:5384:ILE:H	3:BC:5384:ILE:HG12	1.75	0.41
3:BC:5038:GLY:HA3	24:BC:5511:CLA:CMD	2.51	0.41
4:BD:5030:VAL:HG12	4:BD:5031:GLY:N	2.35	0.41
1:BA:5129:ARG:NH2	4:BD:5256:ILE:O	2.54	0.41
6:BF:5015:ILE:HG23	36:BF:5101:HEM:HAA1	2.03	0.41
10:BK:5019:ASP:N	10:BK:5020:PRO:CD	2.81	0.41
18:BX:5044:ASP:C	18:BX:5045:LYS:HD3	2.41	0.41
24:AA:404:CLA:H111	34:AD:402:PHO:H3A	2.02	0.41
2:AB:113:TRP:NE1	2:AB:117:TYR:CD1	2.89	0.41
2:AB:324:LEU:HA	4:AD:293:LEU:HD21	1.99	0.41
2:AB:73:GLY:O	2:AB:93:PHE:CD1	2.74	0.41
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.41
3:AC:332:GLN:HG3	13:AO:129:PHE:CE2	2.56	0.41
27:AC:515:BCR:H331	27:AC:515:BCR:H342	2.02	0.41
4:AD:168:PHE:CD2	4:AD:168:PHE:O	2.74	0.41
4:AD:272:LEU:O	4:AD:276:VAL:HG23	2.21	0.41
5:AE:10:PHE:N	5:AE:10:PHE:CD2	2.89	0.41
13:AO:86:ARG:O	13:AO:86:ARG:CG	2.69	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	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:5056:THR:OG1	4:BD:5057:SER:N	2.53	0.41
4:BD:5128:ARG:O	4:BD:5129:GLN:C	2.59	0.41
4:BD:5162:LEU:HD21	4:BD:5167:TRP:CH2	2.56	0.41
3:BC:5466:VAL:HG13	4:BD:5251:ARG:CD	2.51	0.41
7:BH:5018:TYR:CG	7:BH:5019:GLY:N	2.89	0.41
10:BK:5030:VAL:CG1	10:BK:5031:LEU:N	2.84	0.41
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.20	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
3:AC:272:LEU:CA	24:AC:509:CLA:HMD3	2.51	0.41
3:AC:114:VAL:CG2	31:AC:521:LMG:H141	2.50	0.41
4:AD:162:LEU:HD22	28:AH:101:DGD:O1A	2.21	0.41
6:AF:40:MET:O	6:AF:43:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5289:GLY:HA2	1:BA:5292:THR:CG2	2.51	0.41
27:BD:5407:BCR:H392	9:BJ:5025:VAL:HG21	2.03	0.41
10:BK:5043:VAL:CG2	10:BK:5046:ARG:HE	2.34	0.41
13:BO:5162:ILE:O	13:BO:5230:VAL:HG11	2.20	0.41
14:BT:5018:PHE:CD1	27:BT:5101:BCR:HC8	2.56	0.41
19:BY:5021:UNK:HA	19:BY:5024:UNK:CB	2.51	0.41
1:AA:151:LEU:HD21	1:AA:155:PHE:HE2	1.85	0.41
24:AB:607:CLA:HAC2	27:BT:5101:BCR:H393	2.02	0.41
2:AB:329:PRO:CD	24:AB:607:CLA:HED1	2.49	0.41
24:AB:611:CLA:HMD1	31:AD:407:LMG:HC92	2.02	0.41
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: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
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.20	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:HZ2	1.68	0.41
1:BA:5278:TRP:HA	28:BC:5519:DGD:CIA	2.51	0.41
1:BA:5205:VAL:HG21	24:BA:5405:CLA:HMA2	2.03	0.41
2:BB:5137:LYS:HE3	7:BH:5014:LEU:O	2.21	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
3:BC:5455:PHE:C	3:BC:5457:LYS:H	2.24	0.41
4:BD:5179:PHE:HA	4:BD:5182:LEU:HD12	2.03	0.41
4:BD:5214:HIS:HA	35:BD:5406:PL9:O2	2.21	0.41
4:BD:5145:ALA:CB	4:BD:5272:LEU:HD21	2.51	0.41
9:BJ:5036:LEU:C	9:BJ:5038:SER:H	2.22	0.41
13:BO:5078:VAL:HG22	13:BO:5259:VAL:HG22	2.03	0.41
16:BV:5039:ASN:HD21	16:BV:5043:LYS:HB3	1.86	0.41
16:BV:5148:GLU:N	16:BV:5149:PRO:HD2	2.36	0.41
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:CG1	2.51	0.41
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.56	0.41
2:AB:222:PRO:O	2:AB:223:GLN:C	2.58	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:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
3:AC:390:ARG:NE	16:AV:126:ILE:CG2	2.84	0.41
24:AC:504:CLA:H2	28:AC:518:DGD:C2A	2.51	0.41
3:AC:266:TRP:HZ3	24:AC:507:CLA:HBC2	1.86	0.41
4:AD:126:MET:HE2	4:AD:146:PHE:HB3	2.02	0.41
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.33	0.41
8:AI:25:SER:HA	32:AI:103:LMT:H6D	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:30:VAL:CG1	10:AK:31:LEU:N	2.84	0.41
13:AO:55:ALA:HA	13:AO:230:VAL:HG11	2.03	0.41
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.41
1:BA:5258:LEU:HD12	4:BD:5128:ARG:CG	2.51	0.41
29:BA:5415:LHG:H272	10:BK:5045:PHE:CE2	2.56	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:5297:THR:OG1	2:BB:5298:LEU:N	2.54	0.41
2:BB:5328:GLY:O	24:BB:5611:CLA:HBA1	2.21	0.41
2:BB:5348:ASN:O	2:BB:5350:GLU:N	2.54	0.41
2:BB:5377:VAL:HG11	4:BD:5342:PRO:CG	2.51	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
3:BC:5172:ALA:O	3:BC:5176:VAL:HG23	2.21	0.41
3:BC:5305:THR:HG23	3:BC:5307:PRO:HG2	2.03	0.41
3:BC:5472:LEU:HD11	4:BD:5255:GLN:CD	2.40	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
4:BD:5202:ALA:HB3	35:BD:5406:PL9:C30	2.51	0.41
6:BF:5024:HIS:HA	6:BF:5027:ALA:HB3	2.03	0.41
32:BM:5101:LMT:H5'	32:BM:5101:LMT:H1B	1.97	0.41
13:BO:5056:TYR:CD1	13:BO:5235:GLY:HA2	2.55	0.41
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
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
6:AF:29:PRO:O	6:AF:32:PHE:HB3	2.21	0.40
24:AB:602:CLA:H93	7:AH:46:LEU:HD22	2.02	0.40
7:AH:63:LYS:C	7:AH:65:LEU:N	2.73	0.40
8:AI:11:VAL:O	8:AI:15:PHE:HD2	2.04	0.40
9:AJ:10:LEU:HD12	9:AJ:10:LEU:HA	1.86	0.40
1:AA:76:ASN:ND2	11:AL:33:SER:HB3	2.37	0.40
16:AV:71:ILE:CD1	16:AV:72:THR:N	2.82	0.40
1:BA:5012:ASN:O	1:BA:5015:GLU:HB3	2.22	0.40
1:BA:5206:PHE:HD2	1:BA:5206:PHE:HA	1.77	0.40
2:BB:5004:PRO:HB2	2:BB:5006:TYR:CE1	2.56	0.40
2:BB:5172:TYR:O	2:BB:5174:LEU:HG	2.21	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
1:BA:5295:PHE:HD2	3:BC:5291:TRP:CD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5184:ILE:CD1	4:BD:5186:GLN:HG2	2.51	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
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.40
1:AA:278:TRP:HA	28:AC:519:DGD:HAG1	2.02	0.40
2:AB:121:GLU:CG	7:AH:4:ARG:CA	2.94	0.40
3:AC:113:VAL:CG1	31:AC:521:LMG:H132	2.49	0.40
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.51	0.40
6:AF:15:ILE:CG2	6:AF:16:PHE:HD1	2.33	0.40
27:AD:406:BCR:H392	9:AJ:25:VAL:HG21	2.03	0.40
10:AK:15:TYR:OH	20:AZ:58:ASN:ND2	2.52	0.40
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.29	0.40
14:AT:29:ILE:HG22	14:AT:30:THR:H	1.86	0.40
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.89	0.40
15:AU:75:LEU:HA	15:AU:75:LEU:HD23	1.85	0.40
16:AV:121:LEU:HD21	16:AV:138:LEU:HD11	2.02	0.40
1:BA:5029:TYR:HD2	1:BA:5133:LEU:HB2	1.87	0.40
2:BB:5161:LEU:N	2:BB:5161:LEU:CD1	2.84	0.40
28:BB:5602:DGD:HE61	32:BB:5626:LMT:H2'	2.02	0.40
4:BD:5277:THR:HG22	35:BD:5406:PL9:H272	2.02	0.40
9:BJ:5008:ILE:H	9:BJ:5008:ILE:HD12	1.85	0.40
11:BL:5008:GLN:H	11:BL:5008:GLN:HE21	1.68	0.40
13:BO:5032:THR:OG1	13:BO:5033:TYR:N	2.54	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
32:AB:629:LMT:H1B	32:AB:629:LMT:H5'	1.80	0.40
3:AC:161:LEU:HD23	3:AC:251:HIS:HD2	1.85	0.40
4:AD:180:ARG:NH1	4:AD:333:ASP:OD1	2.54	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
10:AK:46:ARG:HB2	10:AK:46:ARG:NH1	2.36	0.40
1:BA:5069:GLY:CA	1:BA:5075:ASN:ND2	2.84	0.40
1:BA:5200:LEU:HD11	28:BC:5519:DGD:CCA	2.27	0.40
2:BB:5151:PHE:CE1	2:BB:5203:ILE:HG23	2.57	0.40
2:BB:5385:ARG:O	2:BB:5386:ALA:C	2.60	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
4:BD:5148:ALA:HB3	4:BD:5149:PRO:CD	2.41	0.40
15:BU:5072:TYR:CD2	15:BU:5073:PRO:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:39:PRO:HG3	27:AA:410:BCR:HC8	2.04	0.40
2:AB:285:ASN:N	2:AB:285:ASN:HD22	2.18	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
24:AC:502:CLA:HBB1	24:AC:502:CLA:HHC	2.03	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
4:AD:313:THR:H	4:AD:316:THR:HG23	1.86	0.40
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
14:AT:30:THR:HB	14:AT:31:LYS:NZ	2.35	0.40
15:AU:51:TYR:HE1	15:AU:60:THR:HG1	1.66	0.40
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.17	0.40
18:AX:30:LEU:HD23	18:AX:30:LEU:HA	1.88	0.40
1:BA:5238:LYS:O	1:BA:5241:GLN:HG3	2.21	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
3:BC:5447:ARG:HG2	3:BC:5447:ARG:HH11	1.86	0.40
8:BI:5007:THR:O	8:BI:5008:VAL:C	2.59	0.40
13:BO:5081:GLU:C	13:BO:5083:LYS:H	2.25	0.40
27:BK:5102:BCR:H332	20:BZ:5017:PHE:CD1	2.56	0.40
1:AA:271:LEU:CD1	25:AA:408:MST:H162	2.48	0.40
2:AB:243:ALA:O	24:AB:608:CLA:HBC3	2.22	0.40
2:AB:283:GLU:O	2:AB:287:ARG:HG3	2.21	0.40
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.02	0.40
3:AC:307:PRO:O	3:AC:311:GLN:HG2	2.21	0.40
24:AC:511:CLA:H151	20:AZ:24:PRO:CG	2.50	0.40
4:AD:24:ARG:NH2	18:AX:44:ASP:O	2.55	0.40
5:AE:38:VAL:HG21	6:AF:36:ALA:O	2.21	0.40
6:AF:21:VAL:HG21	30:AF:102:SQD:H101	2.02	0.40
7:AH:41:PHE:O	7:AH:45:ILE:HG12	2.21	0.40
1:BA:5011:ALA:HB1	1:BA:5015:GLU:OE1	2.21	0.40
1:BA:5296:ASN:HB3	3:BC:5401:LEU:HD13	2.04	0.40
24:BA:5406:CLA:H62	34:BD:5403:PHO:HMA1	2.02	0.40
2:BB:5170:ASP:CB	2:BB:5171:PRO:CD	2.97	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:5095:PRO:HG3	18:BX:5015:SER:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:5020:TRP:NE1	6:BF:5024:HIS:CE1	2.89	0.40
6:BF:5029:PRO:O	6:BF:5032:PHE:HB3	2.22	0.40
12:BM:5016:LEU:HA	12:BM:5016:LEU:HD23	1.78	0.40
13:BO:5065:ARG:CB	13:BO:5065:ARG:NH1	2.85	0.40
13:BO:5132:VAL:HG12	13:BO:5133:THR:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	8	42
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	8	42
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	4	29
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	5	31
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	4	27
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	4	25
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	6	35
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	7	39
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	4	25
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	4	25
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	32
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	32
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	7
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1	12
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	13
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	6
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	6
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	16
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	16
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%)	2	19
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	3	21
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	4	29
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	29
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	2	17
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	23
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	25	68
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	25	68
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0	2
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0	3
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0	3
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	19
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	2	19
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	4	27

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	15	50
1	BA	271/280 (97%)	253 (93%)	18 (7%)	19	57
2	AB	390/407 (96%)	372 (95%)	18 (5%)	31	70
2	BB	390/407 (96%)	374 (96%)	16 (4%)	35	72
3	AC	347/362 (96%)	326 (94%)	21 (6%)	22	61
3	BC	347/362 (96%)	325 (94%)	22 (6%)	21	59
4	AD	275/283 (97%)	249 (90%)	26 (10%)	10	37
4	BD	275/283 (97%)	249 (90%)	26 (10%)	10	37
5	AE	72/73 (99%)	66 (92%)	6 (8%)	13	46
5	BE	72/73 (99%)	66 (92%)	6 (8%)	13	46
6	AF	29/39 (74%)	27 (93%)	2 (7%)	18	55
6	BF	29/39 (74%)	28 (97%)	1 (3%)	42	77
7	AH	53/55 (96%)	42 (79%)	11 (21%)	1	6
7	BH	53/55 (96%)	43 (81%)	10 (19%)	2	9
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	45	79
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	36	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	36	73
10	AK	30/30 (100%)	29 (97%)	1 (3%)	43	78
10	BK	30/30 (100%)	29 (97%)	1 (3%)	43	78
11	AL	35/35 (100%)	33 (94%)	2 (6%)	24	63
11	BL	35/35 (100%)	32 (91%)	3 (9%)	12	43
12	AM	31/33 (94%)	30 (97%)	1 (3%)	44	78
12	BM	31/33 (94%)	29 (94%)	2 (6%)	20	58
13	AO	202/208 (97%)	187 (93%)	15 (7%)	16	52
13	BO	202/208 (97%)	187 (93%)	15 (7%)	16	52
14	AT	29/29 (100%)	28 (97%)	1 (3%)	42	77
14	BT	29/29 (100%)	27 (93%)	2 (7%)	18	55
15	AU	84/89 (94%)	76 (90%)	8 (10%)	10	37
15	BU	84/89 (94%)	76 (90%)	8 (10%)	10	37
16	AV	116/117 (99%)	111 (96%)	5 (4%)	33	71
16	BV	116/117 (99%)	110 (95%)	6 (5%)	27	65
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	1	2
17	By	20/37 (54%)	15 (75%)	5 (25%)	1	2
18	AX	30/34 (88%)	29 (97%)	1 (3%)	43	78
18	BX	30/34 (88%)	29 (97%)	1 (3%)	43	78
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	23	62
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	15	50
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	18	54

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules 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	-	56,73,73	2.37	13 (23%)	65,113,113	1.97	17 (26%)
24	CLA	AA	405	-	56,73,73	2.42	17 (30%)	65,113,113	2.26	20 (30%)
24	CLA	AA	406	-	56,73,73	2.35	15 (26%)	65,113,113	2.21	19 (29%)
24	CLA	AA	407	-	56,73,73	2.37	14 (25%)	65,113,113	2.02	17 (26%)
25	MST	AA	408	-	16,16,16	0.51	0	22,22,22	3.96	9 (40%)
26	OEC	AA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	AA	410	-	41,41,41	1.62	7 (17%)	56,56,56	2.06	21 (37%)
28	DGD	AA	411	-	57,57,67	1.81	14 (24%)	71,71,81	3.72	25 (35%)
29	LHG	AA	412	-	38,38,48	1.94	5 (13%)	39,44,54	1.48	4 (10%)
30	SQD	AA	413	-	50,51,54	2.40	25 (50%)	60,62,65	3.43	23 (38%)
31	LMG	AA	414	-	44,44,55	1.11	3 (6%)	52,52,63	1.53	6 (11%)
29	LHG	AA	415	-	36,36,48	1.06	2 (5%)	37,42,54	1.18	3 (8%)
30	SQD	AA	416	-	53,54,54	2.42	28 (52%)	63,65,65	3.26	23 (36%)
31	LMG	AA	417	-	42,42,55	1.08	5 (11%)	50,50,63	2.38	11 (22%)
24	CLA	AB	601	-	56,73,73	2.84	17 (30%)	65,113,113	1.81	10 (15%)
24	CLA	AB	602	-	56,73,73	2.40	14 (25%)	65,113,113	1.87	13 (20%)
24	CLA	AB	603	-	56,73,73	2.43	14 (25%)	65,113,113	2.35	21 (32%)
24	CLA	AB	604	-	56,73,73	2.45	14 (25%)	65,113,113	1.91	16 (24%)
24	CLA	AB	605	-	56,73,73	2.61	14 (25%)	65,113,113	2.02	19 (29%)
24	CLA	AB	606	-	56,73,73	2.52	16 (28%)	65,113,113	2.00	17 (26%)
24	CLA	AB	607	-	56,73,73	2.42	17 (30%)	65,113,113	2.22	19 (29%)
24	CLA	AB	608	-	56,73,73	2.64	17 (30%)	65,113,113	2.23	18 (27%)
24	CLA	AB	609	-	56,73,73	2.53	14 (25%)	65,113,113	1.91	18 (27%)
24	CLA	AB	610	-	56,73,73	2.41	12 (21%)	65,113,113	1.89	14 (21%)
24	CLA	AB	611	-	56,73,73	2.41	14 (25%)	65,113,113	2.11	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AB	612	-	56,73,73	2.40	13 (23%)	65,113,113	2.13	15 (23%)
24	CLA	AB	613	-	56,73,73	2.24	13 (23%)	65,113,113	1.82	13 (20%)
24	CLA	AB	614	-	56,73,73	2.60	15 (26%)	65,113,113	2.26	16 (24%)
24	CLA	AB	615	-	56,73,73	2.52	13 (23%)	65,113,113	1.91	14 (21%)
24	CLA	AB	616	-	56,73,73	2.52	12 (21%)	65,113,113	1.79	12 (18%)
27	BCR	AB	617	-	41,41,41	1.56	7 (17%)	56,56,56	2.11	21 (37%)
27	BCR	AB	618	-	41,41,41	1.92	7 (17%)	56,56,56	2.07	16 (28%)
27	BCR	AB	619	-	41,41,41	1.85	8 (19%)	56,56,56	1.96	18 (32%)
31	LMG	AB	620	-	51,51,55	1.31	3 (5%)	59,59,63	2.01	13 (22%)
31	LMG	AB	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.93	14 (24%)
30	SQD	AB	622	-	42,43,54	2.58	19 (45%)	52,54,65	3.34	16 (30%)
32	LMT	AB	623	-	36,36,36	1.79	8 (22%)	47,47,47	1.03	2 (4%)
32	LMT	AB	624	-	36,36,36	1.67	9 (25%)	47,47,47	0.96	3 (6%)
33	DMS	AB	625	-	3,3,3	0.72	0	3,3,3	1.43	1 (33%)
33	DMS	AB	626	-	3,3,3	0.67	0	3,3,3	1.04	0
30	SQD	AB	627	-	46,47,54	2.47	23 (50%)	56,58,65	3.21	16 (28%)
28	DGD	AB	628	-	53,53,67	1.46	7 (13%)	67,67,81	2.12	14 (20%)
32	LMT	AB	629	-	36,36,36	1.61	7 (19%)	47,47,47	1.43	7 (14%)
32	LMT	AB	630	-	36,36,36	1.76	9 (25%)	47,47,47	1.04	1 (2%)
24	CLA	AC	501	-	56,73,73	2.54	16 (28%)	65,113,113	2.05	14 (21%)
24	CLA	AC	502	-	56,73,73	2.38	12 (21%)	65,113,113	1.90	14 (21%)
24	CLA	AC	503	-	56,73,73	2.49	13 (23%)	65,113,113	2.11	20 (30%)
24	CLA	AC	504	-	56,73,73	2.35	15 (26%)	65,113,113	2.12	18 (27%)
24	CLA	AC	505	-	56,73,73	2.78	17 (30%)	65,113,113	2.07	15 (23%)
24	CLA	AC	506	-	56,73,73	2.60	15 (26%)	65,113,113	1.93	16 (24%)
24	CLA	AC	507	-	56,73,73	2.33	14 (25%)	65,113,113	1.84	14 (21%)
24	CLA	AC	508	-	56,73,73	2.38	13 (23%)	65,113,113	2.05	18 (27%)
24	CLA	AC	509	-	56,73,73	2.37	12 (21%)	65,113,113	2.10	14 (21%)
24	CLA	AC	510	-	56,73,73	2.44	12 (21%)	65,113,113	1.83	14 (21%)
24	CLA	AC	511	3	56,73,73	2.50	13 (23%)	65,113,113	2.28	19 (29%)
24	CLA	AC	512	-	56,73,73	2.59	13 (23%)	65,113,113	1.86	13 (20%)
24	CLA	AC	513	-	56,73,73	2.56	13 (23%)	65,113,113	2.15	16 (24%)
27	BCR	AC	514	-	41,41,41	1.63	7 (17%)	56,56,56	2.14	23 (41%)
27	BCR	AC	515	-	41,41,41	1.75	7 (17%)	56,56,56	2.24	19 (33%)
27	BCR	AC	516	-	41,41,41	1.64	8 (19%)	56,56,56	2.25	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	AC	517	-	54,54,67	1.36	8 (14%)	68,68,81	2.83	22 (32%)
28	DGD	AC	518	-	63,63,67	1.23	6 (9%)	77,77,81	2.82	26 (33%)
28	DGD	AC	519	-	67,67,67	1.51	13 (19%)	81,81,81	3.42	31 (38%)
31	LMG	AC	520	-	48,48,55	1.05	5 (10%)	56,56,63	1.97	18 (32%)
31	LMG	AC	521	-	45,45,55	1.09	2 (4%)	53,53,63	1.98	14 (26%)
24	CLA	AD	401	-	56,73,73	2.38	14 (25%)	65,113,113	1.92	16 (24%)
34	PHO	AD	402	-	67,69,69	2.16	13 (19%)	87,99,99	1.57	15 (17%)
34	PHO	AD	403	-	67,69,69	2.26	14 (20%)	87,99,99	1.68	17 (19%)
24	CLA	AD	404	-	56,73,73	2.55	15 (26%)	65,113,113	1.99	16 (24%)
35	PL9	AD	405	-	55,55,55	3.71	17 (30%)	69,69,69	2.70	25 (36%)
27	BCR	AD	406	-	41,41,41	1.64	7 (17%)	56,56,56	2.35	23 (41%)
31	LMG	AD	407	-	49,49,55	0.74	2 (4%)	57,57,63	2.73	20 (35%)
31	LMG	AD	408	-	48,48,55	0.96	4 (8%)	56,56,63	2.11	12 (21%)
32	LMT	AD	409	-	32,32,36	1.76	7 (21%)	43,43,47	1.31	3 (6%)
28	DGD	AE	101	-	64,64,67	1.55	13 (20%)	78,78,81	1.47	11 (14%)
36	HEM	AF	101	5,6	28,50,50	3.00	12 (42%)	17,82,82	4.09	8 (47%)
30	SQD	AF	102	-	44,45,54	2.51	20 (45%)	54,56,65	3.53	18 (33%)
28	DGD	AH	101	-	59,59,67	1.33	10 (16%)	73,73,81	2.12	19 (26%)
31	LMG	AI	101	-	43,43,55	1.03	3 (6%)	51,51,63	1.75	7 (13%)
32	LMT	AI	102	-	36,36,36	1.63	8 (22%)	47,47,47	1.04	2 (4%)
32	LMT	AI	103	-	36,36,36	1.46	6 (16%)	47,47,47	1.82	10 (21%)
27	BCR	AJ	101	-	41,41,41	2.46	13 (31%)	56,56,56	3.24	25 (44%)
31	LMG	AJ	102	-	46,46,55	0.96	3 (6%)	54,54,63	2.64	17 (31%)
27	BCR	AK	102	-	41,41,41	1.77	6 (14%)	56,56,56	2.47	25 (44%)
31	LMG	AM	101	-	42,42,55	0.96	3 (7%)	50,50,63	1.71	7 (14%)
32	LMT	AM	102	-	36,36,36	1.77	10 (27%)	47,47,47	0.94	2 (4%)
27	BCR	AT	101	-	41,41,41	1.63	7 (17%)	56,56,56	2.24	24 (42%)
33	DMS	AU	201	-	3,3,3	0.91	0	3,3,3	1.12	0
36	HEM	AV	201	16	28,50,50	2.88	13 (46%)	17,82,82	4.03	10 (58%)
33	DMS	AV	202	-	3,3,3	0.75	0	3,3,3	1.05	0
27	BCR	AX	101	-	41,41,41	1.85	8 (19%)	56,56,56	2.21	22 (39%)
30	SQD	BA	5401	-	53,54,54	2.45	28 (52%)	63,65,65	3.23	24 (38%)
31	LMG	BA	5402	-	42,42,55	1.08	3 (7%)	50,50,63	2.39	11 (22%)
22	BCT	BA	5403	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	BA	5405	-	56,73,73	2.39	13 (23%)	65,113,113	1.92	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BA	5406	-	56,73,73	2.48	15 (26%)	65,113,113	2.28	19 (29%)
24	CLA	BA	5407	-	56,73,73	2.48	16 (28%)	65,113,113	2.22	17 (26%)
24	CLA	BA	5408	-	56,73,73	2.50	14 (25%)	65,113,113	2.01	16 (24%)
25	MST	BA	5409	-	16,16,16	0.48	0	22,22,22	3.89	9 (40%)
26	OEC	BA	5410	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	BA	5411	-	41,41,41	1.68	7 (17%)	56,56,56	2.08	22 (39%)
28	DGD	BA	5412	-	57,57,67	1.84	13 (22%)	71,71,81	3.73	24 (33%)
29	LHG	BA	5413	-	38,38,48	1.93	5 (13%)	39,44,54	1.45	4 (10%)
30	SQD	BA	5414	-	50,51,54	2.48	26 (52%)	60,62,65	3.40	22 (36%)
29	LHG	BA	5415	-	36,36,48	1.07	2 (5%)	37,42,54	1.18	3 (8%)
30	SQD	BB	5601	-	46,47,54	2.46	22 (47%)	56,58,65	3.18	17 (30%)
28	DGD	BB	5602	-	53,53,67	1.50	7 (13%)	67,67,81	2.14	14 (20%)
32	LMT	BB	5603	-	36,36,36	1.61	7 (19%)	47,47,47	1.43	7 (14%)
32	LMT	BB	5604	-	36,36,36	1.73	10 (27%)	47,47,47	1.03	1 (2%)
24	CLA	BB	5605	-	56,73,73	2.82	16 (28%)	65,113,113	1.79	9 (13%)
24	CLA	BB	5606	-	56,73,73	2.42	14 (25%)	65,113,113	1.89	14 (21%)
24	CLA	BB	5607	-	56,73,73	2.37	13 (23%)	65,113,113	2.37	20 (30%)
24	CLA	BB	5608	-	56,73,73	2.42	14 (25%)	65,113,113	1.94	18 (27%)
24	CLA	BB	5609	-	56,73,73	2.50	14 (25%)	65,113,113	2.02	19 (29%)
24	CLA	BB	5610	-	56,73,73	2.55	16 (28%)	65,113,113	2.02	17 (26%)
24	CLA	BB	5611	-	56,73,73	2.36	16 (28%)	65,113,113	2.23	20 (30%)
24	CLA	BB	5612	-	56,73,73	2.60	17 (30%)	65,113,113	2.24	17 (26%)
24	CLA	BB	5613	-	56,73,73	2.50	15 (26%)	65,113,113	1.94	18 (27%)
24	CLA	BB	5614	-	56,73,73	2.39	12 (21%)	65,113,113	1.86	15 (23%)
24	CLA	BB	5615	-	56,73,73	2.46	14 (25%)	65,113,113	2.12	20 (30%)
24	CLA	BB	5616	-	56,73,73	2.46	13 (23%)	65,113,113	2.18	13 (20%)
24	CLA	BB	5617	-	56,73,73	2.26	14 (25%)	65,113,113	1.81	14 (21%)
24	CLA	BB	5618	-	56,73,73	2.59	14 (25%)	65,113,113	2.26	16 (24%)
24	CLA	BB	5619	-	56,73,73	2.46	14 (25%)	65,113,113	1.94	13 (20%)
24	CLA	BB	5620	-	56,73,73	2.55	13 (23%)	65,113,113	1.81	13 (20%)
27	BCR	BB	5621	-	41,41,41	1.50	7 (17%)	56,56,56	2.10	19 (33%)
27	BCR	BB	5622	-	41,41,41	1.88	7 (17%)	56,56,56	2.06	16 (28%)
27	BCR	BB	5623	-	41,41,41	1.72	8 (19%)	56,56,56	1.94	17 (30%)
31	LMG	BB	5624	-	49,49,55	0.81	1 (2%)	57,57,63	1.93	15 (26%)
30	SQD	BB	5625	-	42,43,54	2.60	20 (47%)	52,54,65	3.38	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BB	5626	-	36,36,36	1.79	9 (25%)	47,47,47	1.05	2 (4%)
32	LMT	BB	5627	-	36,36,36	1.64	8 (22%)	47,47,47	0.96	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.70	0	3,3,3	1.13	0
33	DMS	BB	5629	-	3,3,3	0.68	0	3,3,3	1.20	0
24	CLA	BC	5501	-	56,73,73	2.61	15 (26%)	65,113,113	2.04	13 (20%)
24	CLA	BC	5502	-	56,73,73	2.48	14 (25%)	65,113,113	1.96	14 (21%)
24	CLA	BC	5503	-	56,73,73	2.55	14 (25%)	65,113,113	2.04	18 (27%)
24	CLA	BC	5504	-	56,73,73	2.48	15 (26%)	65,113,113	2.11	16 (24%)
24	CLA	BC	5505	-	56,73,73	2.81	18 (32%)	65,113,113	2.04	14 (21%)
24	CLA	BC	5506	-	56,73,73	2.60	15 (26%)	65,113,113	1.93	16 (24%)
24	CLA	BC	5507	-	56,73,73	2.40	14 (25%)	65,113,113	1.86	16 (24%)
24	CLA	BC	5508	-	56,73,73	2.46	13 (23%)	65,113,113	2.06	17 (26%)
24	CLA	BC	5509	-	56,73,73	2.57	15 (26%)	65,113,113	2.04	14 (21%)
24	CLA	BC	5510	-	56,73,73	2.51	12 (21%)	65,113,113	1.82	12 (18%)
24	CLA	BC	5511	3	56,73,73	2.62	15 (26%)	65,113,113	2.28	18 (27%)
24	CLA	BC	5512	-	56,73,73	2.66	15 (26%)	65,113,113	1.85	12 (18%)
24	CLA	BC	5513	-	56,73,73	2.64	14 (25%)	65,113,113	2.14	16 (24%)
27	BCR	BC	5514	-	41,41,41	1.81	6 (14%)	56,56,56	2.10	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.89	8 (19%)	56,56,56	2.24	20 (35%)
27	BCR	BC	5516	-	41,41,41	1.78	7 (17%)	56,56,56	2.21	21 (37%)
28	DGD	BC	5517	-	54,54,67	1.44	8 (14%)	68,68,81	2.83	22 (32%)
28	DGD	BC	5518	-	63,63,67	1.27	6 (9%)	77,77,81	2.80	24 (31%)
28	DGD	BC	5519	-	67,67,67	1.55	13 (19%)	81,81,81	3.41	31 (38%)
31	LMG	BC	5520	-	48,48,55	1.09	3 (6%)	56,56,63	1.93	17 (30%)
31	LMG	BC	5521	-	45,45,55	1.04	2 (4%)	53,53,63	1.97	13 (24%)
32	LMT	BC	5522	-	36,36,36	1.53	7 (19%)	47,47,47	1.81	9 (19%)
24	CLA	BD	5402	-	56,73,73	2.46	15 (26%)	65,113,113	1.94	16 (24%)
34	PHO	BD	5403	-	67,69,69	2.26	13 (19%)	87,99,99	1.58	17 (19%)
34	PHO	BD	5404	-	67,69,69	2.31	14 (20%)	87,99,99	1.72	19 (21%)
24	CLA	BD	5405	-	56,73,73	2.54	14 (25%)	65,113,113	1.96	16 (24%)
35	PL9	BD	5406	-	55,55,55	3.81	18 (32%)	69,69,69	2.70	24 (34%)
27	BCR	BD	5407	-	41,41,41	1.81	9 (21%)	56,56,56	2.33	24 (42%)
31	LMG	BD	5408	-	46,46,55	0.96	3 (6%)	54,54,63	2.63	16 (29%)
31	LMG	BD	5409	-	49,49,55	0.71	0	57,57,63	2.73	20 (35%)
31	LMG	BD	5410	-	48,48,55	0.95	2 (4%)	56,56,63	2.11	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BD	5411	-	32,32,36	1.75	8 (25%)	43,43,47	1.32	2 (4%)
31	LMG	BE	5101	-	44,44,55	1.10	3 (6%)	52,52,63	1.54	6 (11%)
28	DGD	BE	5102	-	64,64,67	1.52	14 (21%)	78,78,81	1.46	9 (11%)
36	HEM	BF	5101	5,6	28,50,50	3.21	12 (42%)	17,82,82	4.10	8 (47%)
30	SQD	BF	5102	-	44,45,54	2.51	20 (45%)	54,56,65	3.54	20 (37%)
28	DGD	BH	5101	-	59,59,67	1.31	8 (13%)	73,73,81	2.13	19 (26%)
31	LMG	BI	5101	-	43,43,55	1.02	3 (6%)	51,51,63	1.73	7 (13%)
32	LMT	BI	5102	-	36,36,36	1.67	8 (22%)	47,47,47	1.03	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.40	14 (34%)	56,56,56	3.22	25 (44%)
27	BCR	BK	5102	-	41,41,41	1.90	8 (19%)	56,56,56	2.43	25 (44%)
31	LMG	BL	5101	-	51,51,55	1.36	3 (5%)	59,59,63	1.99	12 (20%)
32	LMT	BM	5101	-	36,36,36	1.78	9 (25%)	47,47,47	0.94	2 (4%)
31	LMG	BM	5102	-	42,42,55	1.01	3 (7%)	50,50,63	1.71	8 (16%)
27	BCR	BT	5101	-	41,41,41	1.77	6 (14%)	56,56,56	2.24	24 (42%)
36	HEM	BV	5201	16	28,50,50	2.97	14 (50%)	17,82,82	3.99	7 (41%)
33	DMS	BV	5202	-	3,3,3	0.85	0	3,3,3	0.98	0
33	DMS	BV	5203	-	3,3,3	0.83	0	3,3,3	1.17	0
27	BCR	BX	5101	-	41,41,41	1.87	8 (19%)	56,56,56	2.24	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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	405	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	407	-	4/4/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	602	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	603	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	604	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	605	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	616	-	4/4/20/25	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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	505	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	513	-	4/4/20/25	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	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	AD	402	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	AD	403	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	AD	404	-	4/4/20/25	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	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5407	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5408	-	4/4/20/25	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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5616	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5617	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5618	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5619	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5620	-	4/4/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5505	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5513	-	4/4/20/25	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
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	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	BD	5403	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	BD	5404	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	BD	5405	-	4/4/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/6/54/54	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	-	0/6/54/54	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 (1902) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	505	CLA	CAA-C2A	-5.92	1.42	1.54
31	BL	5101	LMG	O7-C8	-5.45	1.32	1.46
31	AB	620	LMG	O7-C8	-5.09	1.33	1.46
35	BD	5406	PL9	C6-C1	-5.09	1.39	1.48
35	AD	405	PL9	C6-C1	-5.01	1.39	1.48
24	BC	5505	CLA	CAA-C2A	-4.95	1.44	1.54
32	BB	5603	LMT	C1B-C2B	-4.49	1.39	1.52
32	BD	5411	LMT	C1B-C2B	-4.49	1.39	1.52
32	AB	624	LMT	C1B-C2B	-4.48	1.39	1.52
32	AB	629	LMT	C1B-C2B	-4.48	1.39	1.52
32	AD	409	LMT	C1B-C2B	-4.47	1.39	1.52
32	AI	103	LMT	C1B-C2B	-4.47	1.39	1.52
32	BB	5627	LMT	C1B-C2B	-4.46	1.39	1.52
32	BB	5604	LMT	C1B-C2B	-4.46	1.39	1.52
32	BM	5101	LMT	C1B-C2B	-4.45	1.39	1.52
32	AI	102	LMT	C1B-C2B	-4.45	1.39	1.52
32	AB	630	LMT	C1B-C2B	-4.45	1.39	1.52
32	BI	5102	LMT	C1B-C2B	-4.45	1.39	1.52
32	AM	102	LMT	C1B-C2B	-4.44	1.39	1.52
32	BB	5626	LMT	C1B-C2B	-4.43	1.39	1.52
32	BC	5522	LMT	C1B-C2B	-4.43	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	623	LMT	C1B-C2B	-4.42	1.39	1.52
28	AC	519	DGD	O5D-C6D	-4.34	1.36	1.43
28	AC	518	DGD	C2A-C1A	-3.95	1.39	1.50
28	BC	5518	DGD	C2A-C1A	-3.94	1.39	1.50
28	BC	5517	DGD	C2A-C1A	-3.90	1.39	1.50
28	AC	519	DGD	C2A-C1A	-3.89	1.39	1.50
28	BH	5101	DGD	C2A-C1A	-3.88	1.39	1.50
28	AC	517	DGD	C2A-C1A	-3.86	1.39	1.50
28	BC	5519	DGD	C2A-C1A	-3.85	1.39	1.50
28	AB	628	DGD	C2A-C1A	-3.84	1.39	1.50
28	AH	101	DGD	C2A-C1A	-3.83	1.39	1.50
28	AE	101	DGD	C2A-C1A	-3.81	1.39	1.50
36	BF	5101	HEM	C4D-ND	-3.80	1.32	1.36
28	BB	5602	DGD	C2A-C1A	-3.80	1.39	1.50
28	BE	5102	DGD	C2A-C1A	-3.79	1.39	1.50
28	AA	411	DGD	C2A-C1A	-3.79	1.39	1.50
28	BA	5412	DGD	C2A-C1A	-3.76	1.39	1.50
32	AM	102	LMT	C6B-C5B	-3.64	1.39	1.51
32	AD	409	LMT	C6B-C5B	-3.63	1.39	1.51
32	BD	5411	LMT	C6B-C5B	-3.63	1.39	1.51
32	AB	623	LMT	C6B-C5B	-3.63	1.39	1.51
32	BB	5604	LMT	C6B-C5B	-3.62	1.39	1.51
32	AI	103	LMT	C6B-C5B	-3.62	1.39	1.51
32	AB	624	LMT	C6B-C5B	-3.61	1.39	1.51
32	BC	5522	LMT	C6B-C5B	-3.61	1.39	1.51
32	AI	102	LMT	C6B-C5B	-3.61	1.39	1.51
32	BB	5603	LMT	C6B-C5B	-3.61	1.39	1.51
32	AB	630	LMT	C6B-C5B	-3.60	1.39	1.51
32	BM	5101	LMT	C6B-C5B	-3.60	1.39	1.51
32	BB	5627	LMT	C6B-C5B	-3.60	1.39	1.51
32	BI	5102	LMT	C6B-C5B	-3.60	1.39	1.51
32	BB	5626	LMT	C6B-C5B	-3.60	1.39	1.51
32	AB	629	LMT	C6B-C5B	-3.58	1.39	1.51
36	BF	5101	HEM	CAD-C3D	-3.56	1.45	1.52
36	AF	101	HEM	C4D-ND	-3.39	1.32	1.36
30	AA	413	SQD	O6-C44	-3.29	1.37	1.43
35	BD	5406	PL9	C37-C38	-3.22	1.39	1.50
36	AF	101	HEM	CAD-C3D	-3.20	1.46	1.52
36	BV	5201	HEM	CAD-C3D	-3.18	1.46	1.52
35	BD	5406	PL9	C32-C33	-3.18	1.39	1.50
35	AD	405	PL9	C32-C33	-3.16	1.39	1.50
28	BC	5519	DGD	O5D-C6D	-3.13	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	505	CLA	CAA-CBA	-3.10	1.42	1.52
28	BA	5412	DGD	O5D-C6D	-3.09	1.38	1.43
35	AD	405	PL9	C37-C38	-3.06	1.40	1.50
36	AV	201	HEM	CAD-C3D	-3.04	1.46	1.52
24	AA	405	CLA	C3D-C2D	-3.00	1.33	1.39
34	AD	402	PHO	C1B-C2B	-2.99	1.39	1.45
28	AA	411	DGD	O5D-C6D	-2.99	1.38	1.43
36	BV	5201	HEM	C3B-CAB	-2.96	1.42	1.47
34	AD	403	PHO	C1B-C2B	-2.95	1.39	1.45
30	BA	5414	SQD	O6-C44	-2.93	1.38	1.43
24	BA	5406	CLA	C3D-C2D	-2.91	1.33	1.39
34	BD	5403	PHO	C1B-C2B	-2.90	1.39	1.45
34	BD	5404	PHO	C1B-C2B	-2.89	1.39	1.45
30	BB	5625	SQD	C12-C11	-2.87	1.35	1.51
24	BC	5505	CLA	CAA-CBA	-2.86	1.43	1.52
28	AC	517	DGD	O3G-C3G	-2.84	1.38	1.43
30	AB	622	SQD	C12-C11	-2.83	1.35	1.51
30	AA	413	SQD	C17-C16	-2.81	1.35	1.51
30	BB	5625	SQD	C11-C10	-2.80	1.35	1.51
30	BB	5601	SQD	C12-C11	-2.80	1.35	1.51
31	AJ	102	LMG	O7-C8	-2.79	1.39	1.46
31	BD	5408	LMG	O7-C8	-2.78	1.39	1.46
30	AB	627	SQD	C15-C14	-2.77	1.35	1.51
30	BB	5601	SQD	C15-C14	-2.76	1.35	1.51
30	BB	5601	SQD	C16-C15	-2.75	1.35	1.51
30	AB	627	SQD	C20-C19	-2.75	1.35	1.51
30	BA	5414	SQD	C17-C16	-2.75	1.35	1.51
30	AA	413	SQD	C15-C14	-2.75	1.35	1.51
30	AB	622	SQD	C11-C10	-2.74	1.35	1.51
30	AB	627	SQD	C16-C15	-2.74	1.36	1.51
30	AB	627	SQD	C12-C11	-2.73	1.36	1.51
30	BF	5102	SQD	C17-C16	-2.72	1.36	1.51
30	BA	5414	SQD	C33-C32	-2.72	1.36	1.51
30	BA	5414	SQD	C15-C14	-2.72	1.36	1.51
30	BB	5601	SQD	C20-C19	-2.72	1.36	1.51
30	AB	627	SQD	C19-C18	-2.70	1.36	1.51
30	BB	5601	SQD	C11-C10	-2.70	1.36	1.51
30	AB	627	SQD	C14-C13	-2.70	1.36	1.51
30	AA	413	SQD	C16-C15	-2.69	1.36	1.51
36	AV	201	HEM	C3B-CAB	-2.69	1.42	1.47
30	BB	5601	SQD	C14-C13	-2.68	1.36	1.51
30	BA	5414	SQD	C16-C15	-2.68	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	413	SQD	C33-C32	-2.68	1.36	1.51
30	BF	5102	SQD	C11-C10	-2.66	1.36	1.51
30	AB	627	SQD	C11-C10	-2.66	1.36	1.51
30	BB	5601	SQD	C17-C16	-2.66	1.36	1.51
27	BB	5621	BCR	C23-C22	-2.66	1.40	1.45
30	BF	5102	SQD	C16-C15	-2.66	1.36	1.51
27	BC	5516	BCR	C19-C18	-2.65	1.40	1.45
24	AB	612	CLA	C2A-C1A	-2.64	1.46	1.52
24	BB	5616	CLA	C2A-C1A	-2.64	1.46	1.52
30	AB	627	SQD	C13-C12	-2.64	1.36	1.51
30	AF	102	SQD	C17-C16	-2.64	1.36	1.51
30	BB	5601	SQD	C19-C18	-2.63	1.36	1.51
30	AF	102	SQD	C11-C10	-2.63	1.36	1.51
30	BA	5414	SQD	C11-C10	-2.63	1.36	1.51
30	AA	416	SQD	C17-C16	-2.63	1.36	1.51
30	BB	5601	SQD	C13-C12	-2.62	1.36	1.51
30	BA	5414	SQD	C12-C11	-2.62	1.36	1.51
30	BA	5414	SQD	C19-C18	-2.60	1.36	1.51
24	AB	608	CLA	CAA-C2A	-2.60	1.49	1.54
30	BF	5102	SQD	C15-C14	-2.59	1.36	1.51
30	AB	627	SQD	C17-C16	-2.59	1.36	1.51
30	AA	413	SQD	C19-C18	-2.59	1.36	1.51
30	BB	5625	SQD	C16-C15	-2.59	1.36	1.51
30	AF	102	SQD	C12-C11	-2.58	1.36	1.51
30	AA	416	SQD	C16-C15	-2.58	1.36	1.51
30	BF	5102	SQD	C12-C11	-2.58	1.36	1.51
24	AB	607	CLA	C3B-CAB	-2.58	1.42	1.47
30	BA	5401	SQD	C36-C35	-2.57	1.36	1.51
30	AA	413	SQD	C12-C11	-2.57	1.36	1.51
30	AB	622	SQD	C16-C15	-2.55	1.37	1.51
30	AA	416	SQD	C19-C18	-2.55	1.37	1.51
30	AA	416	SQD	C12-C11	-2.54	1.37	1.51
30	AF	102	SQD	C15-C14	-2.54	1.37	1.51
30	BA	5401	SQD	C12-C11	-2.53	1.37	1.51
30	AA	413	SQD	C32-C31	-2.53	1.37	1.51
30	AB	622	SQD	C13-C12	-2.53	1.37	1.51
30	AF	102	SQD	C16-C15	-2.52	1.37	1.51
30	BA	5401	SQD	C33-C32	-2.52	1.37	1.51
30	BB	5625	SQD	C13-C12	-2.52	1.37	1.51
30	AA	416	SQD	C36-C35	-2.52	1.37	1.51
30	BA	5414	SQD	C14-C13	-2.52	1.37	1.51
27	AC	516	BCR	C19-C18	-2.51	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5401	SQD	C17-C16	-2.50	1.37	1.51
30	BA	5401	SQD	C15-C14	-2.50	1.37	1.51
30	AA	413	SQD	C14-C13	-2.50	1.37	1.51
30	AA	413	SQD	C11-C10	-2.50	1.37	1.51
27	AB	619	BCR	C23-C22	-2.49	1.40	1.45
30	BA	5401	SQD	C16-C15	-2.49	1.37	1.51
24	BB	5615	CLA	C2A-C1A	-2.49	1.46	1.52
30	AA	413	SQD	C18-C17	-2.49	1.37	1.51
30	AA	413	SQD	C20-C19	-2.48	1.37	1.51
30	BB	5601	SQD	C18-C17	-2.48	1.37	1.51
24	BB	5612	CLA	CAA-C2A	-2.48	1.49	1.54
30	BA	5414	SQD	C20-C19	-2.48	1.37	1.51
27	BC	5515	BCR	C19-C18	-2.47	1.40	1.45
34	BD	5403	PHO	C4D-CHA	-2.46	1.37	1.44
30	AA	416	SQD	C15-C14	-2.46	1.37	1.51
30	AA	416	SQD	C33-C32	-2.46	1.37	1.51
30	BA	5414	SQD	C32-C31	-2.46	1.37	1.51
28	BC	5519	DGD	O3E-C3E	-2.46	1.37	1.43
30	BB	5625	SQD	C15-C14	-2.45	1.37	1.51
30	AB	622	SQD	C15-C14	-2.44	1.37	1.51
30	BA	5401	SQD	C13-C12	-2.44	1.37	1.51
24	BA	5407	CLA	C3D-C2D	-2.44	1.34	1.39
30	BA	5401	SQD	C32-C31	-2.43	1.37	1.51
30	BB	5625	SQD	C14-C13	-2.42	1.37	1.51
30	BA	5414	SQD	C13-C12	-2.42	1.37	1.51
30	BA	5414	SQD	C18-C17	-2.42	1.37	1.51
30	AB	627	SQD	C18-C17	-2.41	1.37	1.51
30	AA	416	SQD	C11-C10	-2.41	1.37	1.51
30	AF	102	SQD	C14-C13	-2.40	1.37	1.51
30	BA	5401	SQD	C34-C33	-2.40	1.37	1.51
30	AB	622	SQD	C14-C13	-2.39	1.37	1.51
30	AA	416	SQD	C20-C19	-2.39	1.37	1.51
30	BA	5401	SQD	C14-C13	-2.39	1.37	1.51
30	AA	413	SQD	C13-C12	-2.39	1.38	1.51
30	AA	416	SQD	C32-C31	-2.39	1.38	1.51
30	AF	102	SQD	C13-C12	-2.38	1.38	1.51
30	BA	5401	SQD	C35-C34	-2.38	1.38	1.51
30	AA	416	SQD	C13-C12	-2.36	1.38	1.51
28	AC	519	DGD	C1E-C2E	-2.35	1.45	1.52
30	BF	5102	SQD	C14-C13	-2.35	1.38	1.51
30	BA	5401	SQD	C19-C18	-2.34	1.38	1.51
30	BA	5401	SQD	C20-C19	-2.34	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	416	SQD	C35-C34	-2.34	1.38	1.51
27	BB	5623	BCR	C23-C22	-2.34	1.40	1.45
30	BF	5102	SQD	C13-C12	-2.33	1.38	1.51
30	BA	5401	SQD	C11-C10	-2.32	1.38	1.51
30	AA	416	SQD	C34-C33	-2.31	1.38	1.51
24	AB	611	CLA	C2A-C1A	-2.31	1.46	1.52
30	AA	416	SQD	C18-C17	-2.31	1.38	1.51
30	AA	416	SQD	C14-C13	-2.31	1.38	1.51
24	AC	507	CLA	C3B-CAB	-2.27	1.43	1.47
30	BB	5625	SQD	C17-C16	-2.27	1.35	1.51
30	AA	416	SQD	O6-C44	-2.26	1.39	1.43
34	AD	402	PHO	C4D-CHA	-2.26	1.37	1.44
30	AB	622	SQD	C17-C16	-2.25	1.35	1.51
24	AB	608	CLA	C2A-C1A	-2.25	1.47	1.52
31	AD	408	LMG	O3-C3	-2.24	1.37	1.43
30	AB	627	SQD	C21-C20	-2.23	1.35	1.51
31	AA	417	LMG	O7-C8	-2.22	1.40	1.46
30	BB	5601	SQD	C21-C20	-2.20	1.36	1.51
27	AC	514	BCR	C23-C22	-2.19	1.41	1.45
24	AC	501	CLA	C3D-CAD	-2.19	1.39	1.46
30	BA	5401	SQD	O6-C44	-2.17	1.39	1.43
27	AC	515	BCR	C19-C18	-2.16	1.41	1.45
31	AD	407	LMG	O7-C8	-2.15	1.41	1.46
28	BC	5519	DGD	C6A-C5A	-2.15	1.39	1.51
28	AC	519	DGD	C6A-C5A	-2.15	1.39	1.51
30	BA	5401	SQD	C18-C17	-2.15	1.39	1.51
32	BB	5603	LMT	C10-C9	-2.14	1.39	1.51
28	AC	518	DGD	C6A-C5A	-2.14	1.39	1.51
28	BC	5518	DGD	C6A-C5A	-2.14	1.39	1.51
32	BB	5604	LMT	C10-C9	-2.14	1.39	1.51
32	AI	102	LMT	C10-C9	-2.13	1.39	1.51
32	AB	629	LMT	C10-C9	-2.13	1.39	1.51
30	AA	416	SQD	C37-C36	-2.13	1.36	1.51
28	BC	5518	DGD	CEB-CDB	-2.13	1.39	1.51
28	AA	411	DGD	C6A-C5A	-2.13	1.39	1.51
28	AH	101	DGD	C6A-C5A	-2.13	1.39	1.51
28	AC	518	DGD	CEB-CDB	-2.13	1.39	1.51
28	BA	5412	DGD	C6A-C5A	-2.13	1.39	1.51
28	BC	5517	DGD	C6A-C5A	-2.13	1.39	1.51
32	AI	103	LMT	C10-C9	-2.13	1.39	1.51
32	BC	5522	LMT	C10-C9	-2.13	1.39	1.51
28	AC	517	DGD	C6A-C5A	-2.12	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AE	101	DGD	CEB-CDB	-2.12	1.39	1.51
28	BH	5101	DGD	C6A-C5A	-2.12	1.39	1.51
28	AB	628	DGD	C6A-C5A	-2.12	1.39	1.51
24	BB	5608	CLA	C2A-C1A	-2.12	1.47	1.52
28	BE	5102	DGD	CEB-CDB	-2.12	1.39	1.51
32	AB	630	LMT	C10-C9	-2.12	1.39	1.51
32	AB	623	LMT	C10-C9	-2.12	1.39	1.51
27	AA	410	BCR	C19-C18	-2.12	1.41	1.45
32	BI	5102	LMT	C10-C9	-2.12	1.39	1.51
28	BB	5602	DGD	C6A-C5A	-2.12	1.39	1.51
32	AB	624	LMT	C10-C9	-2.11	1.39	1.51
32	BB	5626	LMT	C10-C9	-2.11	1.39	1.51
24	BB	5619	CLA	C3D-CAD	-2.11	1.40	1.46
31	BA	5402	LMG	O7-C8	-2.11	1.41	1.46
32	BM	5101	LMT	C10-C9	-2.11	1.39	1.51
32	AM	102	LMT	C10-C9	-2.11	1.39	1.51
28	AE	101	DGD	C6A-C5A	-2.11	1.39	1.51
28	BC	5519	DGD	CEB-CDB	-2.11	1.39	1.51
28	AC	519	DGD	CEB-CDB	-2.11	1.39	1.51
30	BA	5414	SQD	C34-C33	-2.11	1.36	1.51
28	BE	5102	DGD	C6A-C5A	-2.11	1.39	1.51
31	AD	408	LMG	O7-C8	-2.10	1.41	1.46
32	BB	5627	LMT	C10-C9	-2.10	1.39	1.51
28	AA	411	DGD	O2D-C2D	-2.08	1.38	1.43
28	AA	411	DGD	C4D-C3D	-2.07	1.47	1.52
30	AA	413	SQD	C34-C33	-2.07	1.36	1.51
27	BD	5407	BCR	C23-C22	-2.06	1.41	1.45
27	BA	5411	BCR	C19-C18	-2.05	1.41	1.45
28	AC	519	DGD	O3E-C3E	-2.05	1.38	1.43
24	BB	5612	CLA	C2A-C1A	-2.04	1.47	1.52
24	BC	5507	CLA	C3B-CAB	-2.04	1.43	1.47
27	AT	101	BCR	C19-C18	-2.03	1.41	1.45
24	BD	5402	CLA	C3D-C2D	-2.03	1.35	1.39
30	BA	5401	SQD	C37-C36	-2.03	1.37	1.51
30	BA	5414	SQD	C21-C20	-2.03	1.37	1.51
27	AB	617	BCR	C19-C18	-2.02	1.41	1.45
28	AC	517	DGD	C2B-C1B	-2.01	1.44	1.50
24	BC	5501	CLA	C3D-CAD	-2.01	1.40	1.46
24	BB	5607	CLA	C1B-CHB	-2.01	1.34	1.40
24	AB	614	CLA	CAA-C2A	-2.01	1.50	1.54
27	AJ	101	BCR	C4-C5	2.00	1.55	1.51
27	BC	5515	BCR	C38-C26	2.00	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5512	CLA	CHC-C1C	2.00	1.41	1.35
24	BC	5512	CLA	CAC-C3C	2.01	1.56	1.51
32	AB	624	LMT	O1B-C4'	2.01	1.48	1.43
34	AD	403	PHO	C4C-NC	2.01	1.41	1.36
31	BD	5410	LMG	O1-C1	2.02	1.43	1.40
28	BA	5412	DGD	C4E-C3E	2.02	1.57	1.52
30	AB	627	SQD	C8-C7	2.02	1.56	1.50
31	BE	5101	LMG	C3-C2	2.02	1.57	1.52
31	AC	520	LMG	O7-C8	2.02	1.51	1.46
31	AA	414	LMG	O8-C9	2.02	1.49	1.45
32	BD	5411	LMT	C3'-C4'	2.03	1.57	1.52
24	BC	5505	CLA	CAC-C3C	2.03	1.56	1.51
28	BC	5519	DGD	O3G-C3G	2.03	1.47	1.43
28	AH	101	DGD	C3G-C2G	2.03	1.56	1.50
24	BB	5611	CLA	CBD-CHA	2.04	1.62	1.52
31	BI	5101	LMG	C4-C5	2.04	1.57	1.53
31	AD	407	LMG	O6-C1	2.04	1.46	1.41
24	AB	606	CLA	CBA-CGA	2.04	1.56	1.50
30	BF	5102	SQD	C44-C45	2.04	1.56	1.50
28	BE	5102	DGD	O2G-C1B	2.04	1.40	1.34
27	BJ	5101	BCR	C4-C5	2.04	1.55	1.51
24	AB	601	CLA	CBD-CHA	2.04	1.62	1.52
32	AB	624	LMT	C1'-C2'	2.04	1.58	1.52
30	BB	5625	SQD	C8-C7	2.04	1.56	1.50
32	BB	5604	LMT	O5B-C5B	2.05	1.49	1.44
31	AI	101	LMG	C4-C3	2.05	1.57	1.52
31	BC	5520	LMG	O7-C8	2.05	1.51	1.46
36	BV	5201	HEM	C1A-NA	2.05	1.40	1.36
28	AC	519	DGD	C3E-C2E	2.06	1.57	1.52
31	AM	101	LMG	O6-C1	2.06	1.46	1.41
24	AB	603	CLA	C1C-NC	2.06	1.41	1.37
24	BC	5502	CLA	C1C-NC	2.06	1.41	1.37
24	AC	505	CLA	CBD-CHA	2.06	1.62	1.52
27	AC	516	BCR	C33-C5	2.06	1.54	1.51
24	AB	610	CLA	O2A-CGA	2.06	1.39	1.33
24	BB	5606	CLA	CHC-C1C	2.06	1.41	1.35
28	BE	5102	DGD	C4D-C5D	2.06	1.57	1.53
28	AB	628	DGD	O6D-C5D	2.06	1.49	1.44
31	AC	520	LMG	C4-C5	2.06	1.57	1.53
35	AD	405	PL9	C7-C3	2.07	1.53	1.51
27	BJ	5101	BCR	C11-C12	2.07	1.39	1.34
30	AB	622	SQD	C24-C23	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5613	CLA	CHC-C1C	2.07	1.41	1.35
30	BB	5625	SQD	C24-C23	2.07	1.56	1.50
32	AI	102	LMT	O1B-C4'	2.07	1.48	1.43
32	BB	5626	LMT	O5B-C5B	2.07	1.49	1.44
24	AB	609	CLA	CBA-CGA	2.07	1.56	1.50
24	BC	5505	CLA	CBD-CHA	2.07	1.62	1.52
24	AD	404	CLA	CBA-CGA	2.07	1.56	1.50
27	BD	5407	BCR	C14-C13	2.08	1.38	1.35
27	AB	619	BCR	C33-C5	2.08	1.54	1.51
32	AM	102	LMT	O5'-C5'	2.08	1.49	1.44
31	AC	520	LMG	O7-C10	2.08	1.40	1.34
24	BC	5511	CLA	CBA-CGA	2.08	1.56	1.50
27	AB	618	BCR	C33-C5	2.09	1.54	1.51
35	BD	5406	PL9	C7-C3	2.10	1.53	1.51
24	AB	614	CLA	C4C-NC	2.10	1.40	1.37
24	BC	5505	CLA	C1C-NC	2.10	1.41	1.37
32	AD	409	LMT	O5'-C1'	2.10	1.47	1.41
28	AE	101	DGD	C4E-C5E	2.11	1.57	1.53
24	AB	616	CLA	C5-C3	2.11	1.55	1.51
24	BC	5513	CLA	CAC-C3C	2.11	1.56	1.51
36	AV	201	HEM	CMC-C2C	2.11	1.56	1.51
28	AC	517	DGD	C3G-C2G	2.11	1.56	1.50
28	BC	5519	DGD	O4D-C4D	2.11	1.47	1.43
24	BB	5610	CLA	CBA-CGA	2.11	1.56	1.50
24	AB	601	CLA	CBA-CGA	2.12	1.56	1.50
24	AB	613	CLA	CMC-C2C	2.12	1.55	1.50
30	BA	5414	SQD	O6-C1	2.12	1.43	1.40
24	AB	609	CLA	C1C-NC	2.12	1.41	1.37
28	AH	101	DGD	O6D-C5D	2.13	1.49	1.44
34	BD	5404	PHO	C3B-C4B	2.13	1.47	1.43
24	AB	613	CLA	CHC-C1C	2.14	1.41	1.35
24	BB	5619	CLA	C1C-NC	2.14	1.41	1.37
24	AD	401	CLA	O2A-CGA	2.14	1.39	1.33
24	AB	606	CLA	CHC-C1C	2.14	1.41	1.35
36	AV	201	HEM	C1A-NA	2.14	1.40	1.36
32	BM	5101	LMT	O5'-C1'	2.14	1.47	1.41
28	BB	5602	DGD	C3E-C2E	2.15	1.57	1.52
28	AA	411	DGD	C1G-C2G	2.15	1.56	1.50
30	AB	627	SQD	C24-C23	2.15	1.56	1.50
24	BB	5620	CLA	C5-C3	2.15	1.56	1.51
24	BB	5605	CLA	CBD-CGD	2.16	1.59	1.52
24	BC	5511	CLA	C5-C3	2.16	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	407	CLA	CHC-C1C	2.16	1.41	1.35
28	BC	5517	DGD	O6E-C1E	2.16	1.47	1.41
31	AM	101	LMG	O7-C10	2.16	1.40	1.34
32	BB	5627	LMT	O1B-C4'	2.16	1.49	1.43
24	BB	5605	CLA	CBD-CHA	2.17	1.63	1.52
24	AB	601	CLA	CAC-C3C	2.17	1.56	1.51
27	AD	406	BCR	C38-C26	2.18	1.54	1.51
27	BX	5101	BCR	C38-C26	2.18	1.54	1.51
36	BV	5201	HEM	C2A-C3A	2.18	1.44	1.37
24	BC	5509	CLA	OBD-CAD	2.18	1.25	1.22
32	AI	103	LMT	C4'-C5'	2.18	1.58	1.52
27	AX	101	BCR	C14-C13	2.18	1.38	1.35
30	AF	102	SQD	C8-C7	2.18	1.57	1.50
24	AB	606	CLA	CMC-C2C	2.18	1.55	1.50
24	AA	406	CLA	O2A-CGA	2.19	1.39	1.33
24	BB	5605	CLA	CAC-C3C	2.19	1.56	1.51
28	BE	5102	DGD	O6D-C5D	2.19	1.49	1.44
24	AC	513	CLA	C4C-NC	2.19	1.41	1.37
24	AC	508	CLA	C1C-NC	2.19	1.41	1.37
24	BB	5618	CLA	C4C-NC	2.19	1.41	1.37
24	AA	404	CLA	C1C-NC	2.19	1.41	1.37
36	AV	201	HEM	CAA-C2A	2.19	1.55	1.52
24	AA	406	CLA	O1D-CGD	2.20	1.26	1.21
24	AC	505	CLA	C1C-NC	2.20	1.41	1.37
27	AJ	101	BCR	C17-C18	2.20	1.38	1.35
27	BD	5407	BCR	C38-C26	2.20	1.54	1.51
24	BB	5612	CLA	CHC-C1C	2.20	1.41	1.35
27	BJ	5101	BCR	C7-C6	2.20	1.53	1.45
31	AI	101	LMG	O1-C1	2.20	1.44	1.40
28	AC	518	DGD	O2G-C1B	2.20	1.40	1.34
31	AA	417	LMG	C4-C5	2.20	1.57	1.53
24	AC	511	CLA	CMC-C2C	2.20	1.55	1.50
27	AJ	101	BCR	C7-C6	2.21	1.53	1.45
24	AC	504	CLA	C5-C3	2.21	1.56	1.51
24	BB	5610	CLA	CHC-C1C	2.21	1.41	1.35
27	BK	5102	BCR	C38-C26	2.21	1.54	1.51
24	BD	5405	CLA	CHC-C1C	2.21	1.41	1.35
24	BB	5611	CLA	O1D-CGD	2.22	1.26	1.21
24	AD	404	CLA	CAC-C3C	2.22	1.57	1.51
24	BC	5504	CLA	C5-C3	2.22	1.56	1.51
24	BB	5613	CLA	C1C-NC	2.22	1.41	1.37
30	AF	102	SQD	C44-C45	2.23	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BD	5406	PL9	C11-C9	2.23	1.56	1.51
24	BB	5614	CLA	O1D-CGD	2.23	1.26	1.21
28	BC	5517	DGD	C3G-C2G	2.23	1.57	1.50
24	AC	501	CLA	C1C-NC	2.23	1.41	1.37
32	BC	5522	LMT	O1'-C1'	2.24	1.44	1.40
31	AA	417	LMG	O8-C9	2.24	1.50	1.45
24	BB	5615	CLA	C1C-NC	2.24	1.41	1.37
24	BB	5613	CLA	CBA-CGA	2.24	1.57	1.50
32	BI	5102	LMT	O1B-C4'	2.25	1.49	1.43
30	AA	413	SQD	O6-C1	2.25	1.44	1.40
24	AC	506	CLA	CHC-C1C	2.25	1.41	1.35
24	AB	613	CLA	C4C-NC	2.26	1.41	1.37
28	AC	519	DGD	O5D-C1E	2.26	1.44	1.40
36	BV	5201	HEM	CAA-C2A	2.26	1.55	1.52
27	AA	410	BCR	C5-C6	2.26	1.38	1.34
32	AB	623	LMT	C4'-C5'	2.26	1.59	1.52
28	BC	5519	DGD	C6E-C5E	2.26	1.59	1.51
36	AF	101	HEM	C1B-NB	2.27	1.39	1.36
27	BB	5623	BCR	C33-C5	2.27	1.54	1.51
24	AB	601	CLA	CBD-CGD	2.27	1.59	1.52
24	AC	502	CLA	CHC-C1C	2.27	1.41	1.35
34	BD	5404	PHO	C4C-NC	2.27	1.42	1.36
31	AJ	102	LMG	O6-C1	2.27	1.47	1.41
24	AC	511	CLA	C4C-NC	2.27	1.41	1.37
24	BC	5509	CLA	C1C-NC	2.28	1.41	1.37
32	AM	102	LMT	O5'-C1'	2.28	1.47	1.41
24	AC	501	CLA	C4C-NC	2.28	1.41	1.37
24	AB	602	CLA	CHC-C1C	2.28	1.41	1.35
32	BC	5522	LMT	O1B-C1B	2.28	1.47	1.41
28	AH	101	DGD	O3G-C1D	2.29	1.44	1.40
24	BC	5509	CLA	C4C-NC	2.29	1.41	1.37
24	BB	5609	CLA	CHC-C1C	2.29	1.41	1.35
28	AC	519	DGD	O4D-C4D	2.29	1.48	1.43
24	BB	5618	CLA	C1C-NC	2.29	1.41	1.37
31	BI	5101	LMG	O1-C1	2.29	1.44	1.40
27	AT	101	BCR	C26-C25	2.29	1.38	1.34
32	AI	102	LMT	O1B-C1B	2.29	1.47	1.41
24	AB	611	CLA	C1C-NC	2.30	1.41	1.37
30	BB	5601	SQD	C24-C23	2.30	1.57	1.50
30	BF	5102	SQD	C8-C7	2.30	1.57	1.50
32	BD	5411	LMT	O5'-C1'	2.31	1.47	1.41
28	BH	5101	DGD	O3G-C1D	2.31	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5404	PHO	O1D-CGD	2.31	1.27	1.21
28	BA	5412	DGD	C1G-C2G	2.32	1.57	1.50
28	AC	519	DGD	C6E-C5E	2.32	1.59	1.51
35	AD	405	PL9	C27-C28	2.32	1.58	1.50
34	AD	403	PHO	O2A-CGA	2.32	1.40	1.33
24	AC	507	CLA	CMC-C2C	2.32	1.55	1.50
24	BB	5614	CLA	C1C-NC	2.32	1.41	1.37
28	BC	5517	DGD	O6D-C5D	2.33	1.50	1.44
24	BC	5511	CLA	CMC-C2C	2.33	1.55	1.50
24	BC	5513	CLA	CMC-C2C	2.33	1.55	1.50
32	AM	102	LMT	O1B-C1B	2.33	1.47	1.41
32	AI	102	LMT	O5'-C1'	2.33	1.47	1.41
24	AC	504	CLA	C1C-NC	2.33	1.41	1.37
24	BB	5620	CLA	C1C-NC	2.33	1.41	1.37
24	BC	5505	CLA	CHC-C1C	2.33	1.42	1.35
28	BA	5412	DGD	O3G-C1D	2.34	1.44	1.40
24	AC	512	CLA	O2A-CGA	2.34	1.40	1.33
24	BA	5408	CLA	O2A-CGA	2.34	1.40	1.33
31	AC	520	LMG	O1-C1	2.34	1.44	1.40
24	BB	5611	CLA	C1C-NC	2.35	1.41	1.37
28	BE	5102	DGD	O2G-C2G	2.35	1.52	1.46
24	AC	507	CLA	C1C-NC	2.35	1.41	1.37
31	AA	417	LMG	O1-C1	2.35	1.44	1.40
24	AC	508	CLA	O1D-CGD	2.35	1.27	1.21
32	BB	5626	LMT	O1B-C1B	2.35	1.48	1.41
24	AA	406	CLA	CMC-C2C	2.35	1.56	1.50
27	BC	5514	BCR	C5-C6	2.35	1.38	1.34
24	AB	609	CLA	CMC-C2C	2.35	1.56	1.50
24	BC	5502	CLA	CHC-C1C	2.35	1.42	1.35
31	BM	5102	LMG	O6-C1	2.35	1.47	1.41
32	AB	629	LMT	O1B-C4'	2.35	1.49	1.43
24	AA	406	CLA	C4C-NC	2.36	1.41	1.37
24	BB	5615	CLA	CHC-C1C	2.36	1.42	1.35
36	BV	5201	HEM	C4C-NC	2.36	1.39	1.36
24	AC	505	CLA	O1D-CGD	2.36	1.27	1.21
24	AC	504	CLA	O1D-CGD	2.36	1.27	1.21
27	BK	5102	BCR	C14-C13	2.36	1.38	1.35
24	AC	510	CLA	CMC-C2C	2.36	1.56	1.50
24	BC	5503	CLA	OBD-CAD	2.37	1.25	1.22
30	AF	102	SQD	O8-S	2.37	1.55	1.47
27	AX	101	BCR	C38-C26	2.37	1.55	1.51
24	AC	505	CLA	CHC-C1C	2.37	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AD	409	LMT	C4'-C5'	2.38	1.59	1.52
24	BB	5609	CLA	C1C-NC	2.38	1.41	1.37
36	BV	5201	HEM	C4B-NB	2.38	1.41	1.36
35	BD	5406	PL9	C27-C28	2.38	1.58	1.50
36	AV	201	HEM	C1B-NB	2.38	1.39	1.36
34	AD	403	PHO	O1D-CGD	2.38	1.27	1.21
24	BC	5508	CLA	O2A-CGA	2.39	1.40	1.33
24	AA	407	CLA	O2A-CGA	2.39	1.40	1.33
24	BB	5611	CLA	CHC-C1C	2.39	1.42	1.35
32	BB	5627	LMT	O5'-C1'	2.39	1.47	1.41
32	AI	103	LMT	O1B-C1B	2.39	1.48	1.41
24	AC	509	CLA	CHC-C1C	2.39	1.42	1.35
24	BB	5611	CLA	CMC-C2C	2.39	1.56	1.50
28	AE	101	DGD	O2G-C2G	2.39	1.52	1.46
30	BB	5625	SQD	C44-C45	2.39	1.57	1.50
27	BJ	5101	BCR	C24-C23	2.40	1.40	1.33
24	AA	404	CLA	C4C-NC	2.40	1.41	1.37
32	BB	5604	LMT	C4'-C5'	2.40	1.59	1.52
28	BC	5517	DGD	O3G-C1D	2.40	1.44	1.40
36	AF	101	HEM	CMC-C2C	2.40	1.56	1.51
24	AC	501	CLA	CBA-CGA	2.40	1.57	1.50
27	BX	5101	BCR	C14-C13	2.40	1.39	1.35
27	AC	514	BCR	C5-C6	2.40	1.38	1.34
24	BB	5617	CLA	CHC-C1C	2.41	1.42	1.35
24	AA	406	CLA	C1C-NC	2.41	1.41	1.37
24	BB	5606	CLA	O1D-CGD	2.41	1.27	1.21
27	AJ	101	BCR	C24-C23	2.41	1.40	1.33
24	AB	614	CLA	CMC-C2C	2.41	1.56	1.50
31	BM	5102	LMG	O7-C10	2.41	1.41	1.34
27	BJ	5101	BCR	C17-C18	2.41	1.39	1.35
24	BC	5506	CLA	CHC-C1C	2.41	1.42	1.35
24	BB	5616	CLA	CMC-C2C	2.41	1.56	1.50
32	AB	624	LMT	C4'-C5'	2.42	1.59	1.52
24	AB	608	CLA	CHC-C1C	2.42	1.42	1.35
24	AC	513	CLA	CMC-C2C	2.42	1.56	1.50
24	AC	506	CLA	CBA-CGA	2.42	1.57	1.50
27	AD	406	BCR	C5-C6	2.42	1.38	1.34
24	BC	5506	CLA	CBA-CGA	2.42	1.57	1.50
24	BC	5508	CLA	C1C-NC	2.42	1.41	1.37
24	BB	5605	CLA	C1C-NC	2.42	1.41	1.37
32	BB	5604	LMT	O5'-C1'	2.42	1.47	1.41
28	BC	5518	DGD	O2G-C1B	2.42	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5608	CLA	CHC-C1C	2.42	1.42	1.35
24	BC	5507	CLA	CMC-C2C	2.42	1.56	1.50
24	AC	507	CLA	O1D-CGD	2.42	1.27	1.21
24	AB	604	CLA	O1D-CGD	2.42	1.27	1.21
32	AB	630	LMT	C4'-C5'	2.43	1.59	1.52
24	BB	5610	CLA	OBD-CAD	2.43	1.25	1.22
24	AC	509	CLA	O2A-CGA	2.43	1.40	1.33
24	AB	610	CLA	O1D-CGD	2.44	1.27	1.21
24	AC	506	CLA	CMC-C2C	2.44	1.56	1.50
28	AC	519	DGD	C4E-C3E	2.45	1.58	1.52
34	BD	5403	PHO	O2A-CGA	2.45	1.40	1.33
30	AA	416	SQD	C8-C7	2.45	1.57	1.50
34	AD	403	PHO	CHC-C1C	2.45	1.43	1.38
24	BB	5617	CLA	CMC-C2C	2.45	1.56	1.50
24	AB	607	CLA	CMC-C2C	2.45	1.56	1.50
24	AB	614	CLA	O1D-CGD	2.46	1.27	1.21
24	AC	504	CLA	CMC-C2C	2.46	1.56	1.50
24	AB	611	CLA	CHC-C1C	2.46	1.42	1.35
28	BE	5102	DGD	O6E-C5E	2.46	1.50	1.44
30	AF	102	SQD	C24-C23	2.46	1.57	1.50
24	BC	5501	CLA	C1C-NC	2.47	1.41	1.37
34	AD	403	PHO	CMC-C2C	2.47	1.56	1.50
24	BC	5513	CLA	C4C-NC	2.47	1.41	1.37
24	AB	603	CLA	CMC-C2C	2.47	1.56	1.50
24	BB	5608	CLA	CMC-C2C	2.47	1.56	1.50
30	BF	5102	SQD	C24-C23	2.47	1.57	1.50
24	BC	5507	CLA	C1C-NC	2.48	1.41	1.37
24	BB	5607	CLA	CMC-C2C	2.48	1.56	1.50
24	BD	5405	CLA	C1C-NC	2.48	1.41	1.37
32	BI	5102	LMT	O5'-C1'	2.49	1.48	1.41
28	AA	411	DGD	C4E-C3E	2.49	1.58	1.52
24	BD	5402	CLA	O1D-CGD	2.49	1.27	1.21
24	BC	5504	CLA	O1D-CGD	2.49	1.27	1.21
32	BB	5627	LMT	C4'-C5'	2.49	1.59	1.52
24	BC	5511	CLA	C4C-NC	2.49	1.41	1.37
24	BC	5502	CLA	CMC-C2C	2.50	1.56	1.50
32	BC	5522	LMT	C4'-C5'	2.50	1.59	1.52
24	AA	405	CLA	CHC-C1C	2.50	1.42	1.35
24	AC	501	CLA	C5-C3	2.50	1.56	1.51
24	AC	501	CLA	O1D-CGD	2.50	1.27	1.21
24	AB	602	CLA	O2A-CGA	2.50	1.40	1.33
24	BB	5610	CLA	CMC-C2C	2.50	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	405	CLA	OBD-CAD	2.50	1.26	1.22
31	AM	101	LMG	O1-C1	2.51	1.44	1.40
32	BB	5626	LMT	C4'-C5'	2.51	1.59	1.52
24	AA	404	CLA	CHC-C1C	2.51	1.42	1.35
24	AC	503	CLA	C1C-NC	2.52	1.41	1.37
30	AB	627	SQD	O6-C1	2.52	1.44	1.40
24	BB	5617	CLA	O2A-CGA	2.52	1.40	1.33
32	AI	102	LMT	O1'-C1'	2.52	1.44	1.40
24	AB	614	CLA	C1C-NC	2.52	1.41	1.37
24	BB	5613	CLA	CMC-C2C	2.53	1.56	1.50
24	BB	5610	CLA	C1C-NC	2.53	1.41	1.37
24	AB	602	CLA	O1D-CGD	2.53	1.27	1.21
31	BM	5102	LMG	O1-C1	2.53	1.44	1.40
24	AC	508	CLA	O2A-CGA	2.53	1.40	1.33
24	BC	5510	CLA	C1C-NC	2.53	1.41	1.37
28	AE	101	DGD	C1G-C2G	2.54	1.57	1.50
24	BB	5609	CLA	C4C-NC	2.54	1.41	1.37
30	BA	5414	SQD	C8-C7	2.54	1.58	1.50
34	BD	5404	PHO	CHC-C1C	2.55	1.43	1.38
32	BD	5411	LMT	C4'-C5'	2.55	1.59	1.52
24	BA	5407	CLA	O2A-CGA	2.55	1.40	1.33
31	BD	5408	LMG	O6-C1	2.55	1.48	1.41
24	BC	5507	CLA	O1D-CGD	2.55	1.27	1.21
32	AB	623	LMT	O1B-C1B	2.55	1.48	1.41
24	AD	404	CLA	O2A-CGA	2.55	1.40	1.33
24	AB	607	CLA	O1D-CGD	2.56	1.27	1.21
24	BA	5405	CLA	CHC-C1C	2.56	1.42	1.35
24	BA	5406	CLA	O2A-CGA	2.56	1.40	1.33
24	AD	401	CLA	O1D-CGD	2.57	1.27	1.21
24	AB	608	CLA	O1D-CGD	2.57	1.27	1.21
24	AB	604	CLA	CHC-C1C	2.57	1.42	1.35
24	BC	5512	CLA	O2A-CGA	2.57	1.40	1.33
30	BA	5401	SQD	C8-C7	2.57	1.58	1.50
35	AD	405	PL9	C38-C39	2.57	1.39	1.33
31	AC	520	LMG	O6-C1	2.58	1.48	1.41
24	AC	506	CLA	C1C-NC	2.58	1.41	1.37
24	AC	504	CLA	O2A-CGA	2.58	1.40	1.33
24	BB	5617	CLA	C4C-NC	2.59	1.41	1.37
24	AB	613	CLA	C1C-NC	2.59	1.41	1.37
34	BD	5404	PHO	CMC-C2C	2.59	1.56	1.50
36	BF	5101	HEM	CAA-C2A	2.59	1.56	1.52
28	BE	5102	DGD	C1G-C2G	2.59	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	612	CLA	O1D-CGD	2.59	1.27	1.21
24	BB	5609	CLA	CMC-C2C	2.59	1.56	1.50
35	AD	405	PL9	C3-C4	2.59	1.53	1.49
24	BB	5612	CLA	C1C-NC	2.59	1.41	1.37
24	AC	503	CLA	O1D-CGD	2.59	1.27	1.21
24	AB	615	CLA	O1D-CGD	2.59	1.27	1.21
24	BC	5508	CLA	O1D-CGD	2.59	1.27	1.21
30	BA	5401	SQD	O8-S	2.59	1.56	1.47
24	BB	5619	CLA	CMC-C2C	2.59	1.56	1.50
27	AX	101	BCR	C5-C6	2.60	1.38	1.34
24	BC	5510	CLA	CMC-C2C	2.60	1.56	1.50
24	AA	407	CLA	CMC-C2C	2.60	1.56	1.50
24	BA	5407	CLA	C1C-NC	2.61	1.41	1.37
35	AD	405	PL9	C18-C19	2.61	1.39	1.33
28	BH	5101	DGD	O6E-C1E	2.61	1.48	1.41
24	AB	606	CLA	OBD-CAD	2.61	1.26	1.22
35	BD	5406	PL9	C18-C19	2.62	1.39	1.33
24	BB	5606	CLA	O2A-CGA	2.62	1.41	1.33
24	BB	5610	CLA	O2A-CGA	2.62	1.41	1.33
31	BC	5520	LMG	O1-C1	2.63	1.44	1.40
32	BB	5626	LMT	O5'-C1'	2.63	1.48	1.41
24	BA	5406	CLA	O1D-CGD	2.63	1.27	1.21
28	AE	101	DGD	O6D-C5D	2.63	1.50	1.44
24	BA	5407	CLA	CHC-C1C	2.63	1.42	1.35
24	AB	611	CLA	O1D-CGD	2.63	1.27	1.21
24	BB	5618	CLA	O1D-CGD	2.64	1.27	1.21
24	AB	612	CLA	CMC-C2C	2.64	1.56	1.50
24	AB	606	CLA	C1C-NC	2.64	1.42	1.37
36	BV	5201	HEM	CMC-C2C	2.64	1.57	1.51
24	BB	5612	CLA	O1D-CGD	2.64	1.27	1.21
31	AD	408	LMG	O6-C1	2.65	1.48	1.41
32	AB	630	LMT	O5'-C1'	2.65	1.48	1.41
24	BD	5402	CLA	O2A-CGA	2.65	1.41	1.33
30	BB	5601	SQD	O5-C1	2.65	1.48	1.41
32	BB	5604	LMT	O1'-C1'	2.65	1.44	1.40
24	BB	5608	CLA	O2A-CGA	2.65	1.41	1.33
27	AC	516	BCR	C29-C30	2.66	1.60	1.54
28	BA	5412	DGD	O6D-C5D	2.66	1.50	1.44
32	BB	5603	LMT	O1B-C4'	2.66	1.50	1.43
24	AB	601	CLA	CMC-C2C	2.66	1.56	1.50
27	BB	5623	BCR	C26-C25	2.66	1.39	1.34
24	AB	603	CLA	C4C-NC	2.66	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5403	PHO	CMC-C2C	2.66	1.56	1.50
24	BB	5619	CLA	C4C-NC	2.66	1.41	1.37
31	AD	408	LMG	O1-C1	2.66	1.44	1.40
32	BD	5411	LMT	O1B-C1B	2.66	1.48	1.41
28	AH	101	DGD	O6E-C1E	2.67	1.48	1.41
24	AB	607	CLA	CHC-C1C	2.67	1.43	1.35
31	AB	621	LMG	O6-C1	2.67	1.48	1.41
30	AB	627	SQD	O5-C1	2.67	1.48	1.41
24	BB	5611	CLA	CBA-CGA	2.67	1.58	1.50
35	BD	5406	PL9	C38-C39	2.67	1.39	1.33
32	AB	630	LMT	O1'-C1'	2.67	1.44	1.40
24	AB	605	CLA	CHC-C1C	2.68	1.43	1.35
24	BB	5605	CLA	CMC-C2C	2.68	1.56	1.50
28	BA	5412	DGD	C3G-C2G	2.68	1.58	1.50
24	BB	5616	CLA	CHC-C1C	2.69	1.43	1.35
24	BC	5503	CLA	C1C-NC	2.69	1.42	1.37
24	BC	5509	CLA	CHC-C1C	2.69	1.43	1.35
24	BB	5618	CLA	CMC-C2C	2.69	1.56	1.50
30	AB	622	SQD	C44-C45	2.69	1.58	1.50
24	AB	602	CLA	CMC-C2C	2.69	1.56	1.50
24	AC	504	CLA	CHC-C1C	2.69	1.43	1.35
27	BT	5101	BCR	C26-C25	2.70	1.39	1.34
24	BA	5408	CLA	CHC-C1C	2.70	1.43	1.35
28	AC	519	DGD	O3G-C3G	2.70	1.48	1.43
28	AH	101	DGD	C1G-C2G	2.70	1.58	1.50
28	AC	517	DGD	O6D-C5D	2.70	1.50	1.44
24	AB	613	CLA	O1D-CGD	2.71	1.28	1.21
32	BM	5101	LMT	O1B-C1B	2.71	1.48	1.41
24	BC	5503	CLA	CMC-C2C	2.71	1.56	1.50
24	AD	404	CLA	C1C-NC	2.71	1.42	1.37
30	AB	622	SQD	O5-C1	2.71	1.48	1.41
31	BE	5101	LMG	O1-C1	2.71	1.44	1.40
24	BA	5406	CLA	C4C-C3C	2.71	1.49	1.45
24	AB	612	CLA	O2A-CGA	2.71	1.41	1.33
24	AA	407	CLA	O1D-CGD	2.72	1.28	1.21
24	AB	615	CLA	CMC-C2C	2.72	1.56	1.50
32	AB	624	LMT	O5'-C1'	2.72	1.48	1.41
24	AB	607	CLA	CBA-CGA	2.72	1.58	1.50
24	AB	605	CLA	C4C-NC	2.72	1.41	1.37
24	AC	512	CLA	CMC-C2C	2.72	1.56	1.50
36	BF	5101	HEM	CMC-C2C	2.72	1.57	1.51
30	BB	5625	SQD	O5-C1	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	416	SQD	O8-S	2.73	1.56	1.47
24	BC	5501	CLA	CBA-CGA	2.73	1.58	1.50
24	AC	508	CLA	CHC-C1C	2.73	1.43	1.35
32	BI	5102	LMT	O1B-C1B	2.73	1.49	1.41
24	BC	5504	CLA	CMC-C2C	2.74	1.56	1.50
24	AB	608	CLA	CMC-C2C	2.74	1.56	1.50
24	BD	5402	CLA	CHC-C1C	2.74	1.43	1.35
31	AI	101	LMG	O6-C1	2.74	1.48	1.41
31	BD	5410	LMG	O6-C1	2.74	1.48	1.41
24	AC	512	CLA	O1D-CGD	2.74	1.28	1.21
28	AE	101	DGD	O6E-C5E	2.74	1.51	1.44
28	AE	101	DGD	C3G-C2G	2.74	1.58	1.50
24	AB	604	CLA	O2A-CGA	2.74	1.41	1.33
24	AC	505	CLA	C4C-NC	2.74	1.41	1.37
27	BB	5622	BCR	C14-C13	2.74	1.39	1.35
24	AC	512	CLA	C1C-NC	2.75	1.42	1.37
24	BA	5408	CLA	O1D-CGD	2.75	1.28	1.21
32	AB	623	LMT	O5'-C1'	2.75	1.48	1.41
32	AB	630	LMT	O1B-C1B	2.75	1.49	1.41
28	AE	101	DGD	O6D-C1D	2.75	1.48	1.41
32	BI	5102	LMT	O1'-C1'	2.76	1.45	1.40
24	BC	5503	CLA	O1D-CGD	2.76	1.28	1.21
31	BA	5402	LMG	O1-C1	2.76	1.45	1.40
24	BC	5507	CLA	C4C-NC	2.76	1.42	1.37
24	BB	5619	CLA	O1D-CGD	2.76	1.28	1.21
24	BB	5608	CLA	O1D-CGD	2.76	1.28	1.21
27	AB	617	BCR	C1-C6	2.77	1.57	1.53
24	BD	5405	CLA	O2A-CGA	2.77	1.41	1.33
24	BB	5612	CLA	CBA-CGA	2.77	1.58	1.50
24	BB	5607	CLA	O1D-CGD	2.77	1.28	1.21
27	BB	5622	BCR	C5-C6	2.77	1.39	1.34
24	BB	5615	CLA	O2A-CGA	2.77	1.41	1.33
31	BB	5624	LMG	O6-C1	2.77	1.48	1.41
28	BH	5101	DGD	C1G-C2G	2.77	1.58	1.50
27	BB	5621	BCR	C30-C25	2.78	1.57	1.53
28	BE	5102	DGD	O6D-C1D	2.78	1.48	1.41
24	AB	607	CLA	C4C-NC	2.78	1.42	1.37
28	BC	5519	DGD	O5D-C1E	2.78	1.45	1.40
24	AD	401	CLA	CHC-C1C	2.78	1.43	1.35
24	BB	5620	CLA	O2A-CGA	2.78	1.41	1.33
24	AB	605	CLA	C1C-NC	2.78	1.42	1.37
24	AB	603	CLA	O1D-CGD	2.79	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	5407	CLA	C4C-NC	2.79	1.42	1.37
24	AB	608	CLA	CBA-CGA	2.79	1.58	1.50
24	AB	605	CLA	CMC-C2C	2.79	1.56	1.50
24	AB	615	CLA	O2A-CGA	2.80	1.41	1.33
28	AA	411	DGD	C3G-C2G	2.80	1.58	1.50
27	BB	5621	BCR	C1-C6	2.80	1.57	1.53
24	BB	5613	CLA	C4C-NC	2.80	1.42	1.37
30	AA	413	SQD	C8-C7	2.80	1.58	1.50
35	BD	5406	PL9	C3-C4	2.80	1.54	1.49
24	BC	5506	CLA	CMC-C2C	2.80	1.57	1.50
36	AF	101	HEM	CAA-C2A	2.81	1.56	1.52
24	BB	5610	CLA	O1D-CGD	2.81	1.28	1.21
32	BM	5101	LMT	C4'-C5'	2.81	1.60	1.52
24	BC	5509	CLA	O2A-CGA	2.81	1.41	1.33
31	BI	5101	LMG	O6-C1	2.81	1.48	1.41
24	BA	5406	CLA	C1C-NC	2.81	1.42	1.37
32	AD	409	LMT	O1B-C1B	2.82	1.49	1.41
36	BF	5101	HEM	C1B-NB	2.82	1.40	1.36
28	AA	411	DGD	O6D-C5D	2.82	1.51	1.44
24	AA	405	CLA	C4C-NC	2.82	1.42	1.37
24	AA	406	CLA	CHB-C4A	2.82	1.37	1.33
30	BB	5601	SQD	O6-C1	2.82	1.45	1.40
31	AA	417	LMG	O6-C1	2.83	1.48	1.41
24	BB	5609	CLA	O1D-CGD	2.83	1.28	1.21
24	BB	5606	CLA	CMC-C2C	2.83	1.57	1.50
24	AC	511	CLA	O1D-CGD	2.83	1.28	1.21
24	AB	604	CLA	C1C-NC	2.83	1.42	1.37
32	BB	5604	LMT	O1B-C1B	2.84	1.49	1.41
32	BD	5411	LMT	O1'-C1'	2.84	1.45	1.40
24	BC	5504	CLA	CHC-C1C	2.84	1.43	1.35
30	BF	5102	SQD	O8-S	2.84	1.57	1.47
24	AB	608	CLA	C1C-NC	2.84	1.42	1.37
24	BC	5505	CLA	C4C-NC	2.84	1.42	1.37
24	AB	603	CLA	CBA-CGA	2.84	1.58	1.50
24	BB	5606	CLA	C1C-NC	2.84	1.42	1.37
28	BC	5519	DGD	O6E-C1E	2.84	1.48	1.41
24	AC	503	CLA	CMC-C2C	2.84	1.57	1.50
24	BA	5405	CLA	CMC-C2C	2.84	1.57	1.50
24	BC	5509	CLA	CMC-C2C	2.84	1.57	1.50
32	AB	629	LMT	O5'-C1'	2.85	1.48	1.41
24	AC	509	CLA	CMC-C2C	2.85	1.57	1.50
24	AC	510	CLA	O1D-CGD	2.85	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5506	CLA	C1C-NC	2.85	1.42	1.37
24	BB	5610	CLA	C4C-NC	2.85	1.42	1.37
24	AC	506	CLA	O1D-CGD	2.85	1.28	1.21
24	AB	607	CLA	CBB-CAB	2.85	1.49	1.28
27	AK	102	BCR	C2-C1	2.86	1.60	1.54
24	AA	407	CLA	C4C-NC	2.86	1.42	1.37
24	BC	5506	CLA	O1D-CGD	2.86	1.28	1.21
30	BB	5601	SQD	O3-C3	2.86	1.49	1.43
24	AA	405	CLA	C1C-NC	2.86	1.42	1.37
24	BB	5607	CLA	CBA-CGA	2.86	1.59	1.50
24	BA	5407	CLA	CMC-C2C	2.86	1.57	1.50
28	BE	5102	DGD	C3G-C2G	2.86	1.58	1.50
24	AA	405	CLA	O1D-CGD	2.86	1.28	1.21
27	AC	516	BCR	C26-C25	2.87	1.39	1.34
24	BC	5501	CLA	CMC-C2C	2.87	1.57	1.50
24	BB	5619	CLA	O2A-CGA	2.87	1.41	1.33
34	AD	402	PHO	O2A-CGA	2.88	1.41	1.33
24	BD	5402	CLA	CMC-C2C	2.88	1.57	1.50
28	BE	5102	DGD	O6E-C1E	2.88	1.49	1.41
24	AC	510	CLA	C1C-NC	2.88	1.42	1.37
24	AA	406	CLA	CHC-C1C	2.89	1.43	1.35
24	AD	404	CLA	O1D-CGD	2.89	1.28	1.21
31	BC	5520	LMG	O6-C1	2.89	1.49	1.41
27	BA	5411	BCR	C5-C6	2.89	1.39	1.34
31	BA	5402	LMG	O6-C1	2.89	1.49	1.41
24	BB	5611	CLA	CBB-CAB	2.89	1.49	1.28
24	AC	502	CLA	O1D-CGD	2.90	1.28	1.21
24	AA	405	CLA	O2A-CGA	2.90	1.41	1.33
24	BB	5612	CLA	CMC-C2C	2.90	1.57	1.50
27	AC	514	BCR	C2-C1	2.90	1.60	1.54
24	BC	5512	CLA	CMC-C2C	2.91	1.57	1.50
24	AB	607	CLA	C1C-NC	2.91	1.42	1.37
27	AX	101	BCR	C2-C1	2.91	1.60	1.54
27	BD	5407	BCR	C5-C6	2.91	1.39	1.34
30	AB	627	SQD	O8-S	2.91	1.57	1.47
30	BA	5414	SQD	O8-S	2.91	1.57	1.47
24	BA	5405	CLA	O1D-CGD	2.92	1.28	1.21
30	BF	5102	SQD	O3-C3	2.92	1.49	1.43
30	AA	413	SQD	O8-S	2.92	1.57	1.47
24	BC	5513	CLA	CHC-C1C	2.92	1.43	1.35
24	BC	5508	CLA	CHC-C1C	2.93	1.43	1.35
27	BC	5514	BCR	C26-C25	2.93	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	615	CLA	C4C-NC	2.93	1.42	1.37
24	BB	5615	CLA	C4C-C3C	2.93	1.50	1.45
34	AD	402	PHO	CMC-C2C	2.93	1.57	1.50
27	BC	5516	BCR	C29-C30	2.93	1.60	1.54
31	BC	5521	LMG	O6-C1	2.93	1.49	1.41
24	BC	5501	CLA	C4C-NC	2.94	1.42	1.37
27	BA	5411	BCR	C2-C1	2.94	1.60	1.54
24	BB	5617	CLA	CBB-CAB	2.94	1.49	1.28
24	BC	5502	CLA	O1D-CGD	2.94	1.28	1.21
27	BC	5515	BCR	C2-C1	2.94	1.61	1.54
24	AB	601	CLA	C1C-NC	2.94	1.42	1.37
27	BC	5516	BCR	C26-C25	2.95	1.39	1.34
24	AB	603	CLA	CHC-C1C	2.95	1.43	1.35
31	AB	620	LMG	O6-C1	2.95	1.49	1.41
24	AB	610	CLA	CMC-C2C	2.96	1.57	1.50
24	AC	507	CLA	O2A-CGA	2.96	1.42	1.33
24	AA	405	CLA	C4C-C3C	2.96	1.50	1.45
24	BB	5612	CLA	C4C-NC	2.96	1.42	1.37
32	AM	102	LMT	C4'-C5'	2.96	1.60	1.52
24	BC	5504	CLA	C1C-NC	2.97	1.42	1.37
24	AB	611	CLA	O2A-CGA	2.97	1.42	1.33
24	AB	613	CLA	CBB-CAB	2.97	1.49	1.28
24	AC	507	CLA	C4C-NC	2.97	1.42	1.37
24	AB	602	CLA	C1C-NC	2.97	1.42	1.37
24	BB	5613	CLA	O1D-CGD	2.97	1.28	1.21
31	BC	5521	LMG	O1-C1	2.97	1.45	1.40
24	BC	5510	CLA	O1D-CGD	2.97	1.28	1.21
27	AD	406	BCR	C1-C6	2.98	1.57	1.53
24	AC	501	CLA	CMC-C2C	2.98	1.57	1.50
24	AC	513	CLA	O1D-CGD	2.98	1.28	1.21
24	BB	5615	CLA	O1D-CGD	2.98	1.28	1.21
24	AB	615	CLA	C1C-NC	2.98	1.42	1.37
24	AB	612	CLA	CHC-C1C	2.98	1.44	1.35
28	BH	5101	DGD	O6D-C1D	2.99	1.49	1.41
34	AD	402	PHO	O1D-CGD	2.99	1.28	1.21
30	AA	413	SQD	O5-C1	2.99	1.49	1.41
24	BB	5616	CLA	CHB-C4A	3.00	1.37	1.33
28	AE	101	DGD	O6E-C1E	3.00	1.49	1.41
24	AB	606	CLA	C4C-NC	3.00	1.42	1.37
24	BB	5617	CLA	O1D-CGD	3.00	1.28	1.21
24	AC	508	CLA	C4C-C3C	3.00	1.50	1.45
32	BB	5603	LMT	O5'-C1'	3.00	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5504	CLA	O2A-CGA	3.00	1.42	1.33
27	AB	619	BCR	C26-C25	3.00	1.39	1.34
24	AB	616	CLA	O2A-CGA	3.01	1.42	1.33
24	AA	404	CLA	O1D-CGD	3.01	1.28	1.21
24	BC	5507	CLA	O2A-CGA	3.01	1.42	1.33
24	BB	5614	CLA	CMC-C2C	3.01	1.57	1.50
30	AF	102	SQD	O3-C3	3.01	1.49	1.43
24	BB	5611	CLA	CHB-C4A	3.01	1.37	1.33
32	AM	102	LMT	O1'-C1'	3.01	1.45	1.40
30	BB	5601	SQD	O8-S	3.02	1.57	1.47
24	BA	5408	CLA	CMC-C2C	3.02	1.57	1.50
24	BC	5508	CLA	C4C-C3C	3.02	1.50	1.45
24	AC	511	CLA	CBB-CAB	3.02	1.50	1.28
24	AB	606	CLA	O2A-CGA	3.02	1.42	1.33
24	AB	604	CLA	CMC-C2C	3.03	1.57	1.50
32	BM	5101	LMT	O1'-C1'	3.03	1.45	1.40
24	AB	609	CLA	O1D-CGD	3.03	1.28	1.21
24	BC	5501	CLA	O1D-CGD	3.03	1.28	1.21
24	AB	614	CLA	CBB-CAB	3.03	1.50	1.28
32	AB	624	LMT	O5B-C1B	3.04	1.49	1.41
27	AA	410	BCR	C2-C1	3.04	1.61	1.54
24	AB	606	CLA	O1D-CGD	3.04	1.28	1.21
24	BB	5614	CLA	C4C-NC	3.04	1.42	1.37
24	AA	407	CLA	CBB-CAB	3.04	1.50	1.28
24	AC	513	CLA	CHC-C1C	3.05	1.44	1.35
27	BB	5623	BCR	C5-C6	3.05	1.39	1.34
27	BB	5621	BCR	C29-C30	3.05	1.61	1.54
24	AC	513	CLA	O2A-CGA	3.05	1.42	1.33
27	BX	5101	BCR	C5-C6	3.05	1.39	1.34
24	AB	610	CLA	C4C-NC	3.05	1.42	1.37
32	BB	5627	LMT	O1'-C1'	3.05	1.45	1.40
32	AB	630	LMT	O1B-C4'	3.05	1.51	1.43
31	BE	5101	LMG	O6-C1	3.05	1.49	1.41
24	AC	511	CLA	O2A-CGA	3.05	1.42	1.33
28	BA	5412	DGD	O1G-C1A	3.05	1.42	1.33
24	AB	605	CLA	O1D-CGD	3.06	1.28	1.21
28	BC	5519	DGD	C4E-C3E	3.06	1.60	1.52
24	BB	5607	CLA	CBB-CAB	3.06	1.50	1.28
24	BC	5511	CLA	CBB-CAB	3.06	1.50	1.28
24	AC	502	CLA	C4C-C3C	3.06	1.50	1.45
24	AA	404	CLA	CMC-C2C	3.06	1.57	1.50
24	BB	5618	CLA	CBB-CAB	3.06	1.50	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	AA	414	LMG	O6-C1	3.07	1.49	1.41
24	AA	407	CLA	C1C-NC	3.07	1.42	1.37
32	AD	409	LMT	O1'-C1'	3.07	1.45	1.40
30	AB	627	SQD	O3-C3	3.07	1.50	1.43
30	BA	5414	SQD	O3-C3	3.07	1.50	1.43
24	BC	5511	CLA	O2A-CGA	3.07	1.42	1.33
28	AH	101	DGD	O6D-C1D	3.08	1.49	1.41
24	BB	5611	CLA	C5-C3	3.08	1.58	1.51
24	BA	5408	CLA	CBB-CAB	3.09	1.50	1.28
27	AA	410	BCR	C29-C30	3.09	1.61	1.54
24	BA	5406	CLA	CMC-C2C	3.09	1.57	1.50
24	BC	5509	CLA	O1D-CGD	3.10	1.29	1.21
24	AC	504	CLA	CBB-CAB	3.10	1.50	1.28
27	BA	5411	BCR	C29-C30	3.10	1.61	1.54
27	AD	406	BCR	C2-C1	3.10	1.61	1.54
24	BD	5402	CLA	C4C-NC	3.11	1.42	1.37
24	BC	5512	CLA	O1D-CGD	3.11	1.29	1.21
24	BB	5607	CLA	CHC-C1C	3.11	1.44	1.35
24	AA	405	CLA	CMC-C2C	3.11	1.57	1.50
24	BA	5406	CLA	C4C-NC	3.11	1.42	1.37
24	BC	5504	CLA	CBB-CAB	3.11	1.50	1.28
31	BD	5408	LMG	O1-C1	3.12	1.45	1.40
32	BB	5627	LMT	O5B-C1B	3.12	1.49	1.41
24	BB	5613	CLA	O2A-CGA	3.12	1.42	1.33
27	BJ	5101	BCR	C21-C22	3.13	1.39	1.35
24	AC	510	CLA	C4C-NC	3.13	1.42	1.37
24	BD	5405	CLA	CMC-C2C	3.13	1.57	1.50
30	BA	5401	SQD	O3-C3	3.13	1.50	1.43
30	BB	5625	SQD	O8-S	3.14	1.58	1.47
24	BB	5611	CLA	O2A-CGA	3.14	1.42	1.33
24	AB	608	CLA	C4C-C3C	3.14	1.50	1.45
29	AA	412	LHG	O7-C7	3.14	1.43	1.34
30	AA	413	SQD	O3-C3	3.15	1.50	1.43
24	BB	5616	CLA	O2A-CGA	3.15	1.42	1.33
27	BD	5407	BCR	C1-C6	3.15	1.58	1.53
24	BA	5407	CLA	CHB-C4A	3.15	1.37	1.33
27	AB	617	BCR	C29-C30	3.15	1.61	1.54
24	BD	5405	CLA	O1D-CGD	3.15	1.29	1.21
24	AB	612	CLA	CBB-CAB	3.15	1.51	1.28
28	AA	411	DGD	O1G-C1A	3.15	1.42	1.33
24	AC	501	CLA	O2A-CGA	3.15	1.42	1.33
24	AC	504	CLA	C4C-NC	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AD	402	PHO	C3D-C4D	3.15	1.52	1.43
24	AB	611	CLA	CBB-CAB	3.16	1.51	1.28
24	BC	5513	CLA	O2A-CGA	3.16	1.42	1.33
28	AB	628	DGD	O6E-C1E	3.16	1.49	1.41
30	AA	416	SQD	O5-C1	3.16	1.49	1.41
30	BA	5414	SQD	O5-C1	3.16	1.49	1.41
31	AA	414	LMG	O1-C1	3.16	1.45	1.40
30	BB	5625	SQD	O6-C1	3.17	1.45	1.40
27	BK	5102	BCR	C2-C1	3.17	1.61	1.54
24	AA	407	CLA	C4C-C3C	3.18	1.50	1.45
24	BB	5616	CLA	O1D-CGD	3.18	1.29	1.21
24	BB	5608	CLA	C4C-NC	3.18	1.42	1.37
24	AB	603	CLA	CBB-CAB	3.18	1.51	1.28
34	AD	403	PHO	C3D-C4D	3.18	1.52	1.43
28	BB	5602	DGD	O6E-C1E	3.18	1.49	1.41
24	AC	503	CLA	O2A-CGA	3.18	1.42	1.33
24	BC	5505	CLA	O1D-CGD	3.19	1.29	1.21
24	BB	5612	CLA	C4C-C3C	3.19	1.50	1.45
24	AB	616	CLA	C4C-NC	3.19	1.42	1.37
31	BL	5101	LMG	O6-C1	3.19	1.49	1.41
27	AC	514	BCR	C26-C25	3.19	1.39	1.34
24	BA	5405	CLA	C1C-NC	3.19	1.42	1.37
27	BB	5621	BCR	C5-C6	3.19	1.39	1.34
27	AB	617	BCR	C30-C25	3.20	1.58	1.53
27	AC	515	BCR	C2-C1	3.20	1.61	1.54
24	AD	401	CLA	CMC-C2C	3.20	1.57	1.50
27	AJ	101	BCR	C21-C22	3.20	1.40	1.35
29	BA	5413	LHG	O8-C23	3.21	1.42	1.33
34	BD	5403	PHO	C3D-C4D	3.21	1.53	1.43
24	BC	5509	CLA	CBB-CAB	3.21	1.51	1.28
27	AT	101	BCR	C2-C1	3.21	1.61	1.54
24	BB	5616	CLA	CBB-CAB	3.21	1.51	1.28
24	AB	612	CLA	CHB-C4A	3.21	1.37	1.33
27	BD	5407	BCR	C2-C1	3.22	1.61	1.54
34	BD	5403	PHO	O1D-CGD	3.22	1.29	1.21
27	AC	514	BCR	C29-C30	3.22	1.61	1.54
24	AB	607	CLA	C5-C3	3.22	1.58	1.51
34	BD	5404	PHO	C3D-C4D	3.22	1.53	1.43
27	AB	619	BCR	C5-C6	3.22	1.40	1.34
24	AD	404	CLA	CBB-CAB	3.22	1.51	1.28
24	BA	5406	CLA	OBD-CAD	3.22	1.27	1.22
24	AA	406	CLA	CBA-CGA	3.23	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BD	5405	CLA	CBB-CAB	3.23	1.51	1.28
24	AD	401	CLA	C1C-NC	3.23	1.42	1.37
27	BC	5514	BCR	C2-C1	3.23	1.61	1.54
24	BB	5615	CLA	CBB-CAB	3.23	1.51	1.28
24	AD	401	CLA	C4C-NC	3.23	1.42	1.37
31	AC	521	LMG	O1-C1	3.23	1.45	1.40
24	BC	5503	CLA	O2A-CGA	3.24	1.42	1.33
28	BH	5101	DGD	O2G-C2G	3.24	1.55	1.46
27	BT	5101	BCR	C29-C30	3.24	1.61	1.54
24	AB	609	CLA	C4C-NC	3.24	1.42	1.37
30	AB	622	SQD	O8-S	3.25	1.58	1.47
27	BA	5411	BCR	C26-C25	3.25	1.40	1.34
24	BC	5508	CLA	CBB-CAB	3.25	1.51	1.28
30	AA	413	SQD	O48-C23	3.26	1.42	1.33
27	AC	516	BCR	C2-C1	3.26	1.61	1.54
32	AB	624	LMT	O1'-C1'	3.27	1.45	1.40
24	AB	607	CLA	O2A-CGA	3.27	1.42	1.33
30	AA	416	SQD	O3-C3	3.27	1.50	1.43
27	AB	618	BCR	C5-C6	3.27	1.40	1.34
24	BB	5609	CLA	C4C-C3C	3.27	1.50	1.45
24	AA	404	CLA	CBB-CAB	3.27	1.51	1.28
28	AH	101	DGD	O2G-C2G	3.27	1.55	1.46
24	BC	5513	CLA	O1D-CGD	3.27	1.29	1.21
36	AV	201	HEM	CBB-CAB	3.27	1.51	1.28
24	BD	5402	CLA	CBB-CAB	3.28	1.51	1.28
24	AC	505	CLA	CMC-C2C	3.28	1.58	1.50
24	BB	5610	CLA	CBB-CAB	3.28	1.52	1.28
30	BA	5401	SQD	O5-C1	3.29	1.50	1.41
24	AB	616	CLA	O1D-CGD	3.29	1.29	1.21
24	BC	5502	CLA	O2A-CGA	3.29	1.43	1.33
24	AC	502	CLA	CBB-CAB	3.29	1.52	1.28
24	BB	5617	CLA	C1C-NC	3.29	1.43	1.37
24	AC	509	CLA	CBB-CAB	3.29	1.52	1.28
32	AB	629	LMT	O1B-C1B	3.30	1.50	1.41
24	AC	508	CLA	CBB-CAB	3.30	1.52	1.28
24	AB	607	CLA	CHB-C4A	3.30	1.37	1.33
24	BA	5408	CLA	C4C-NC	3.31	1.42	1.37
24	AC	506	CLA	O2A-CGA	3.31	1.43	1.33
34	AD	402	PHO	C4C-C3C	3.31	1.51	1.45
27	AC	515	BCR	C29-C30	3.31	1.61	1.54
24	BC	5512	CLA	C1C-NC	3.31	1.43	1.37
24	AC	503	CLA	CBB-CAB	3.31	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BJ	5101	BCR	C2-C1	3.32	1.61	1.54
27	BK	5102	BCR	C29-C30	3.32	1.61	1.54
24	AB	605	CLA	C4C-C3C	3.32	1.50	1.45
24	AA	406	CLA	O2D-CGD	3.32	1.41	1.33
24	BB	5620	CLA	O1D-CGD	3.32	1.29	1.21
32	AM	102	LMT	O1B-C4'	3.32	1.51	1.43
24	AB	606	CLA	CBB-CAB	3.33	1.52	1.28
24	AC	511	CLA	CHC-C1C	3.33	1.45	1.35
24	BB	5609	CLA	O2A-CGA	3.33	1.43	1.33
32	BB	5603	LMT	O1B-C1B	3.34	1.50	1.41
30	AA	413	SQD	O7-S	3.34	1.54	1.45
27	BX	5101	BCR	C2-C1	3.34	1.61	1.54
24	AB	610	CLA	CBB-CAB	3.34	1.52	1.28
24	BA	5407	CLA	CBA-CGA	3.34	1.60	1.50
30	BF	5102	SQD	O5-C1	3.34	1.50	1.41
27	AB	617	BCR	C2-C1	3.34	1.61	1.54
24	BC	5507	CLA	CBB-CAB	3.34	1.52	1.28
24	AC	507	CLA	CBB-CAB	3.35	1.52	1.28
24	AD	401	CLA	CBB-CAB	3.35	1.52	1.28
31	AC	521	LMG	O6-C1	3.35	1.50	1.41
27	AC	515	BCR	C5-C6	3.35	1.40	1.34
24	BC	5511	CLA	O1D-CGD	3.35	1.29	1.21
32	AI	103	LMT	O5B-C1B	3.36	1.50	1.41
24	BB	5614	CLA	CBB-CAB	3.36	1.52	1.28
27	AT	101	BCR	C29-C30	3.36	1.61	1.54
27	BB	5622	BCR	C29-C30	3.36	1.61	1.54
27	BC	5514	BCR	C29-C30	3.36	1.61	1.54
36	AF	101	HEM	C1C-NC	3.36	1.40	1.36
30	AA	416	SQD	O6-C1	3.36	1.46	1.40
24	BB	5620	CLA	CBB-CAB	3.36	1.52	1.28
24	BB	5619	CLA	C4C-C3C	3.37	1.51	1.45
24	BC	5501	CLA	O2A-CGA	3.37	1.43	1.33
24	AB	605	CLA	O2A-CGA	3.37	1.43	1.33
24	BA	5405	CLA	CBB-CAB	3.37	1.52	1.28
27	AJ	101	BCR	C2-C1	3.38	1.62	1.54
24	BC	5511	CLA	CHC-C1C	3.38	1.45	1.35
24	AB	608	CLA	C4C-NC	3.38	1.42	1.37
27	AC	516	BCR	C30-C25	3.39	1.58	1.53
24	AC	512	CLA	CBB-CAB	3.39	1.52	1.28
24	BC	5512	CLA	CBB-CAB	3.39	1.52	1.28
24	BB	5606	CLA	CBB-CAB	3.39	1.52	1.28
24	BC	5510	CLA	CBB-CAB	3.39	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BB	5602	DGD	O3G-C1D	3.39	1.46	1.40
24	AC	510	CLA	CBB-CAB	3.39	1.52	1.28
24	BD	5405	CLA	C4C-NC	3.39	1.42	1.37
24	BB	5608	CLA	CBB-CAB	3.39	1.52	1.28
24	AB	609	CLA	O2A-CGA	3.40	1.43	1.33
24	AD	404	CLA	CMC-C2C	3.40	1.58	1.50
24	BC	5506	CLA	CBB-CAB	3.40	1.52	1.28
32	BB	5604	LMT	O1B-C4'	3.40	1.52	1.43
27	BB	5621	BCR	C2-C1	3.40	1.62	1.54
24	BC	5502	CLA	CBB-CAB	3.40	1.52	1.28
32	BM	5101	LMT	O1B-C4'	3.41	1.52	1.43
24	AC	506	CLA	CBB-CAB	3.41	1.52	1.28
30	BA	5401	SQD	O6-C1	3.41	1.46	1.40
30	BB	5601	SQD	O48-C23	3.41	1.43	1.33
24	AB	609	CLA	CBB-CAB	3.41	1.52	1.28
24	AC	509	CLA	O1D-CGD	3.41	1.29	1.21
36	AF	101	HEM	CBC-CAC	3.41	1.52	1.28
24	BC	5505	CLA	CMC-C2C	3.41	1.58	1.50
24	AB	604	CLA	C4C-NC	3.41	1.43	1.37
30	BA	5414	SQD	O48-C23	3.41	1.43	1.33
24	AA	405	CLA	CBA-CGA	3.41	1.60	1.50
30	AB	622	SQD	O3-C3	3.42	1.50	1.43
24	AC	512	CLA	C4C-NC	3.42	1.43	1.37
24	AB	608	CLA	CBB-CAB	3.42	1.52	1.28
24	BC	5505	CLA	C4C-C3C	3.42	1.51	1.45
27	AB	619	BCR	C2-C1	3.42	1.62	1.54
27	BB	5623	BCR	C29-C30	3.42	1.62	1.54
24	AC	513	CLA	CBB-CAB	3.42	1.53	1.28
24	BC	5503	CLA	CBB-CAB	3.42	1.53	1.28
27	BT	5101	BCR	C2-C1	3.43	1.62	1.54
24	AB	602	CLA	CBB-CAB	3.44	1.53	1.28
27	AD	406	BCR	C29-C30	3.44	1.62	1.54
24	AB	601	CLA	O2A-CGA	3.45	1.43	1.33
24	BC	5504	CLA	CHB-C4A	3.45	1.37	1.33
24	AC	503	CLA	C4C-NC	3.46	1.43	1.37
27	BJ	5101	BCR	C10-C9	3.46	1.40	1.35
24	BB	5612	CLA	CBB-CAB	3.46	1.53	1.28
34	AD	402	PHO	C1C-C2C	3.46	1.53	1.45
24	AB	616	CLA	CBB-CAB	3.46	1.53	1.28
24	AA	406	CLA	CBB-CAB	3.46	1.53	1.28
32	AM	102	LMT	O5B-C1B	3.46	1.50	1.41
27	AB	618	BCR	C29-C30	3.46	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	504	CLA	C4C-C3C	3.47	1.51	1.45
24	BA	5406	CLA	O2D-CGD	3.47	1.42	1.33
24	AB	602	CLA	C4C-NC	3.48	1.43	1.37
24	BC	5513	CLA	CBB-CAB	3.48	1.53	1.28
24	BA	5406	CLA	CBB-CAB	3.48	1.53	1.28
30	AA	416	SQD	O48-C23	3.48	1.43	1.33
24	AC	504	CLA	CHB-C4A	3.48	1.38	1.33
24	AB	615	CLA	CBB-CAB	3.49	1.53	1.28
24	BB	5605	CLA	O1D-CGD	3.49	1.30	1.21
27	AB	619	BCR	C29-C30	3.49	1.62	1.54
27	AK	102	BCR	C1-C6	3.49	1.58	1.53
30	AB	622	SQD	O6-C1	3.49	1.46	1.40
24	BB	5619	CLA	CBB-CAB	3.49	1.53	1.28
36	BV	5201	HEM	CBB-CAB	3.50	1.53	1.28
27	AB	617	BCR	C5-C6	3.50	1.40	1.34
24	BA	5406	CLA	CBA-CGA	3.50	1.60	1.50
36	AF	101	HEM	CBB-CAB	3.50	1.53	1.28
32	BD	5411	LMT	O5B-C1B	3.50	1.50	1.41
24	BA	5407	CLA	O1D-CGD	3.51	1.30	1.21
27	AA	410	BCR	C26-C25	3.51	1.40	1.34
30	AA	416	SQD	O7-S	3.51	1.55	1.45
24	BC	5506	CLA	O2A-CGA	3.51	1.43	1.33
27	BB	5623	BCR	C2-C1	3.51	1.62	1.54
24	BC	5502	CLA	C4C-C3C	3.51	1.51	1.45
32	BB	5626	LMT	O1'-C1'	3.51	1.46	1.40
24	AC	501	CLA	CBB-CAB	3.51	1.53	1.28
34	BD	5403	PHO	C1C-C2C	3.51	1.53	1.45
30	BB	5625	SQD	O3-C3	3.51	1.51	1.43
34	BD	5404	PHO	C1C-C2C	3.51	1.53	1.45
32	BB	5603	LMT	O5B-C1B	3.51	1.50	1.41
24	BA	5407	CLA	O2D-CGD	3.51	1.42	1.33
28	BA	5412	DGD	O2G-C1B	3.52	1.44	1.34
27	BC	5515	BCR	C29-C30	3.52	1.62	1.54
24	BA	5407	CLA	CBB-CAB	3.52	1.53	1.28
24	AC	508	CLA	C4C-NC	3.53	1.43	1.37
24	AB	604	CLA	CBB-CAB	3.53	1.53	1.28
30	AF	102	SQD	O5-C1	3.53	1.50	1.41
36	BF	5101	HEM	CBC-CAC	3.54	1.53	1.28
24	BB	5613	CLA	CBB-CAB	3.54	1.53	1.28
24	BB	5609	CLA	CBB-CAB	3.54	1.53	1.28
28	AA	411	DGD	O2G-C1B	3.54	1.44	1.34
36	AV	201	HEM	C1C-NC	3.55	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AD	403	PHO	C1C-C2C	3.55	1.53	1.45
32	BC	5522	LMT	O5B-C1B	3.55	1.50	1.41
24	AB	611	CLA	C4C-C3C	3.56	1.51	1.45
24	BB	5605	CLA	CBB-CAB	3.56	1.53	1.28
36	BF	5101	HEM	CBB-CAB	3.56	1.53	1.28
24	AB	605	CLA	CBB-CAB	3.56	1.54	1.28
31	AJ	102	LMG	O1-C1	3.57	1.46	1.40
24	BB	5605	CLA	O2A-CGA	3.57	1.43	1.33
24	BC	5510	CLA	C4C-NC	3.57	1.43	1.37
24	BC	5501	CLA	CBB-CAB	3.57	1.54	1.28
28	BC	5518	DGD	O5D-C1E	3.58	1.46	1.40
24	AC	502	CLA	C4C-NC	3.58	1.43	1.37
24	AC	502	CLA	CHB-C4A	3.58	1.38	1.33
24	AA	405	CLA	CBB-CAB	3.59	1.54	1.28
24	AD	404	CLA	C4C-NC	3.59	1.43	1.37
32	AB	629	LMT	O5B-C1B	3.59	1.50	1.41
28	AC	518	DGD	O5D-C1E	3.59	1.46	1.40
30	BB	5601	SQD	O47-C7	3.59	1.44	1.34
24	BB	5611	CLA	O2D-CGD	3.60	1.42	1.33
30	AB	627	SQD	O47-C7	3.61	1.44	1.34
27	AB	618	BCR	C2-C1	3.61	1.62	1.54
24	BA	5405	CLA	CHB-C4A	3.61	1.38	1.33
24	BB	5617	CLA	C4C-C3C	3.62	1.51	1.45
36	BV	5201	HEM	CBC-CAC	3.62	1.54	1.28
30	AA	413	SQD	O5-C5	3.62	1.53	1.44
24	BB	5620	CLA	C4C-NC	3.62	1.43	1.37
24	AC	513	CLA	CHB-C4A	3.62	1.38	1.33
36	AV	201	HEM	CBC-CAC	3.62	1.54	1.28
27	AK	102	BCR	C29-C30	3.63	1.62	1.54
24	AB	601	CLA	CBB-CAB	3.63	1.54	1.28
24	BA	5408	CLA	C4C-C3C	3.64	1.51	1.45
24	AC	505	CLA	CBB-CAB	3.64	1.54	1.28
30	BF	5102	SQD	O7-S	3.64	1.55	1.45
24	BC	5505	CLA	CBB-CAB	3.65	1.54	1.28
24	BB	5618	CLA	O2A-CGA	3.65	1.44	1.33
27	BB	5621	BCR	C26-C25	3.65	1.40	1.34
24	BB	5605	CLA	C4C-NC	3.66	1.43	1.37
32	BI	5102	LMT	O5B-C1B	3.66	1.50	1.41
24	BB	5606	CLA	C4C-NC	3.66	1.43	1.37
28	BB	5602	DGD	O6D-C1D	3.66	1.50	1.41
32	BM	5101	LMT	O5B-C1B	3.67	1.50	1.41
24	AC	505	CLA	C4C-C3C	3.67	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	413	SQD	C1-C2	3.67	1.63	1.52
27	AC	516	BCR	C5-C6	3.68	1.40	1.34
24	AA	404	CLA	CHB-C4A	3.68	1.38	1.33
24	AC	502	CLA	O2A-CGA	3.69	1.44	1.33
24	AB	601	CLA	O1D-CGD	3.69	1.30	1.21
24	BC	5504	CLA	C4C-NC	3.69	1.43	1.37
24	AB	607	CLA	C4C-C3C	3.69	1.51	1.45
28	AB	628	DGD	O6D-C1D	3.69	1.51	1.41
24	BC	5513	CLA	CHB-C4A	3.69	1.38	1.33
30	BA	5401	SQD	O48-C23	3.69	1.44	1.33
27	BC	5516	BCR	C2-C1	3.70	1.62	1.54
29	BA	5413	LHG	O7-C7	3.70	1.45	1.34
24	BC	5512	CLA	C4C-NC	3.70	1.43	1.37
32	BB	5604	LMT	O5B-C1B	3.70	1.51	1.41
24	AC	511	CLA	C4C-C3C	3.71	1.51	1.45
24	AB	604	CLA	O2D-CGD	3.72	1.42	1.33
28	BE	5102	DGD	O5D-C1E	3.72	1.46	1.40
24	BA	5407	CLA	C4C-C3C	3.72	1.51	1.45
24	BB	5612	CLA	O2D-CGD	3.72	1.42	1.33
24	AB	613	CLA	O2D-CGD	3.73	1.42	1.33
30	AB	627	SQD	O48-C23	3.73	1.44	1.33
24	BB	5618	CLA	CHC-C1C	3.73	1.46	1.35
32	AD	409	LMT	O5B-C1B	3.73	1.51	1.41
27	AK	102	BCR	C26-C25	3.74	1.40	1.34
24	BC	5502	CLA	C4C-NC	3.74	1.43	1.37
30	BA	5401	SQD	O7-S	3.74	1.56	1.45
29	BA	5413	LHG	P-O6	3.75	1.75	1.59
24	BB	5607	CLA	C4C-C3C	3.75	1.51	1.45
27	BB	5622	BCR	C2-C1	3.75	1.62	1.54
24	AB	614	CLA	O2A-CGA	3.76	1.44	1.33
30	BB	5625	SQD	O7-S	3.76	1.56	1.45
24	AB	614	CLA	CHC-C1C	3.76	1.46	1.35
30	AF	102	SQD	O7-S	3.76	1.56	1.45
24	AC	511	CLA	CHB-C4A	3.76	1.38	1.33
36	BF	5101	HEM	C4C-NC	3.76	1.41	1.36
24	AC	501	CLA	C4C-C3C	3.76	1.51	1.45
27	AJ	101	BCR	C10-C9	3.77	1.40	1.35
32	AB	623	LMT	O1'-C1'	3.77	1.46	1.40
24	BA	5405	CLA	C4C-NC	3.78	1.43	1.37
24	BB	5608	CLA	C4C-C3C	3.78	1.51	1.45
32	AI	102	LMT	O5B-C1B	3.78	1.51	1.41
36	BV	5201	HEM	C1C-NC	3.78	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	617	BCR	C26-C25	3.78	1.41	1.34
29	AA	412	LHG	O8-C23	3.78	1.44	1.33
27	BK	5102	BCR	C26-C25	3.78	1.41	1.34
28	BC	5519	DGD	C3E-C2E	3.79	1.62	1.52
30	BA	5414	SQD	C1-C2	3.79	1.63	1.52
24	AA	407	CLA	CHB-C4A	3.80	1.38	1.33
24	AB	607	CLA	O2D-CGD	3.81	1.42	1.33
28	AC	517	DGD	O5D-C1E	3.81	1.46	1.40
27	AC	516	BCR	C1-C6	3.82	1.59	1.53
24	BA	5408	CLA	C1C-NC	3.82	1.43	1.37
30	BA	5401	SQD	C1-C2	3.82	1.63	1.52
24	BC	5503	CLA	C4C-NC	3.83	1.43	1.37
24	AC	509	CLA	C4C-C3C	3.83	1.51	1.45
30	BF	5102	SQD	O6-C1	3.84	1.46	1.40
24	AA	406	CLA	C4C-C3C	3.84	1.51	1.45
24	AB	612	CLA	O2D-CGD	3.85	1.43	1.33
24	AB	608	CLA	O2D-CGD	3.85	1.43	1.33
24	AB	612	CLA	C4C-C3C	3.86	1.51	1.45
24	AB	601	CLA	C4C-NC	3.86	1.43	1.37
30	BB	5625	SQD	O48-C23	3.86	1.44	1.33
27	BD	5407	BCR	C29-C30	3.87	1.63	1.54
24	BC	5511	CLA	C4C-C3C	3.87	1.51	1.45
30	AA	416	SQD	C1-C2	3.87	1.63	1.52
27	AT	101	BCR	C5-C6	3.88	1.41	1.34
27	BX	5101	BCR	C29-C30	3.88	1.63	1.54
28	AB	628	DGD	O3G-C1D	3.88	1.47	1.40
24	BB	5614	CLA	O2D-CGD	3.89	1.43	1.33
24	AB	603	CLA	C4C-C3C	3.89	1.51	1.45
24	AB	609	CLA	C4C-C3C	3.90	1.51	1.45
24	AA	405	CLA	CHB-C4A	3.90	1.38	1.33
24	AA	405	CLA	O2D-CGD	3.90	1.43	1.33
32	BB	5626	LMT	O5B-C1B	3.90	1.51	1.41
27	BB	5622	BCR	C26-C25	3.90	1.41	1.34
24	BC	5508	CLA	CHB-C4A	3.92	1.38	1.33
24	AC	505	CLA	O2D-CGD	3.92	1.43	1.33
24	BC	5506	CLA	C4C-NC	3.92	1.43	1.37
28	AB	628	DGD	O5D-C1E	3.93	1.47	1.40
30	AF	102	SQD	O6-C1	3.93	1.47	1.40
28	AE	101	DGD	O5D-C1E	3.94	1.47	1.40
28	BA	5412	DGD	O6E-C1E	3.94	1.51	1.41
24	BC	5506	CLA	CHB-C4A	3.94	1.38	1.33
30	BF	5102	SQD	O48-C23	3.95	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BC	5515	BCR	C5-C6	3.95	1.41	1.34
24	BB	5611	CLA	C4C-C3C	3.95	1.52	1.45
36	AF	101	HEM	C4C-NC	3.95	1.41	1.36
24	BC	5508	CLA	C4C-NC	3.96	1.43	1.37
24	BC	5510	CLA	C4C-C3C	3.96	1.52	1.45
24	AD	401	CLA	O2D-CGD	3.96	1.43	1.33
24	AB	611	CLA	C4C-NC	3.96	1.43	1.37
29	AA	415	LHG	O7-C7	3.96	1.45	1.34
28	AH	101	DGD	O5D-C1E	3.96	1.47	1.40
27	AK	102	BCR	C5-C6	3.97	1.41	1.34
30	BA	5414	SQD	O5-C5	3.97	1.54	1.44
24	BD	5402	CLA	C1C-NC	3.97	1.44	1.37
24	BD	5405	CLA	C4C-C3C	3.97	1.52	1.45
27	BJ	5101	BCR	C29-C30	3.98	1.63	1.54
36	AV	201	HEM	C4C-NC	3.98	1.41	1.36
27	AC	515	BCR	C26-C25	3.98	1.41	1.34
24	BB	5617	CLA	O2D-CGD	3.98	1.43	1.33
24	BC	5506	CLA	C4C-C3C	3.98	1.52	1.45
24	AD	404	CLA	O2D-CGD	3.98	1.43	1.33
24	BB	5613	CLA	CHB-C4A	3.98	1.38	1.33
24	AC	504	CLA	O2D-CGD	3.99	1.43	1.33
24	AC	503	CLA	C4C-C3C	3.99	1.52	1.45
24	AC	506	CLA	C4C-NC	3.99	1.43	1.37
24	AB	615	CLA	C4C-C3C	4.00	1.52	1.45
27	BC	5516	BCR	C30-C25	4.00	1.59	1.53
24	BB	5613	CLA	C4C-C3C	4.01	1.52	1.45
24	BC	5505	CLA	O2A-CGA	4.01	1.45	1.33
24	AB	604	CLA	C4C-C3C	4.01	1.52	1.45
24	BC	5504	CLA	C4C-C3C	4.01	1.52	1.45
24	AB	616	CLA	C4C-C3C	4.01	1.52	1.45
29	BA	5415	LHG	O7-C7	4.01	1.45	1.34
24	BC	5502	CLA	CHB-C4A	4.01	1.38	1.33
24	AC	503	CLA	O2D-CGD	4.02	1.43	1.33
27	BC	5515	BCR	C26-C25	4.02	1.41	1.34
30	AB	627	SQD	O7-S	4.04	1.56	1.45
27	BK	5102	BCR	C1-C6	4.04	1.59	1.53
27	AX	101	BCR	C29-C30	4.04	1.63	1.54
34	BD	5404	PHO	C4C-C3C	4.05	1.52	1.45
32	AB	630	LMT	O5B-C1B	4.06	1.51	1.41
28	AE	101	DGD	O3G-C1D	4.06	1.47	1.40
24	BC	5509	CLA	C4C-C3C	4.06	1.52	1.45
27	AC	515	BCR	C1-C6	4.06	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	627	SQD	O5-C5	4.08	1.54	1.44
30	AB	622	SQD	O48-C23	4.08	1.45	1.33
30	AB	627	SQD	C1-C2	4.09	1.64	1.52
24	BC	5503	CLA	C4C-C3C	4.09	1.52	1.45
27	BJ	5101	BCR	C26-C25	4.09	1.41	1.34
24	AD	401	CLA	C4C-C3C	4.10	1.52	1.45
24	AC	508	CLA	CHB-C4A	4.10	1.38	1.33
28	BH	5101	DGD	O5D-C1E	4.10	1.47	1.40
30	AB	622	SQD	O7-S	4.10	1.57	1.45
24	BB	5610	CLA	CHB-C4A	4.11	1.38	1.33
27	AJ	101	BCR	C26-C25	4.11	1.41	1.34
27	AJ	101	BCR	C29-C30	4.11	1.63	1.54
27	AT	101	BCR	C30-C25	4.11	1.59	1.53
34	AD	402	PHO	O2D-CGD	4.12	1.43	1.33
30	AB	622	SQD	C1-C2	4.13	1.64	1.52
24	BB	5605	CLA	C4C-C3C	4.13	1.52	1.45
32	AB	623	LMT	O5B-C1B	4.13	1.52	1.41
30	AF	102	SQD	O47-C7	4.13	1.46	1.34
24	BC	5501	CLA	C4C-C3C	4.13	1.52	1.45
24	AD	404	CLA	C4C-C3C	4.13	1.52	1.45
30	BA	5414	SQD	O7-S	4.14	1.57	1.45
30	AA	416	SQD	O47-C7	4.14	1.46	1.34
30	BB	5601	SQD	O7-S	4.14	1.57	1.45
24	AB	615	CLA	O2D-CGD	4.14	1.43	1.33
30	BB	5601	SQD	C1-C2	4.14	1.64	1.52
30	AF	102	SQD	O48-C23	4.15	1.45	1.33
24	AC	505	CLA	O2A-CGA	4.15	1.45	1.33
28	AA	411	DGD	O6E-C1E	4.15	1.52	1.41
24	AC	501	CLA	O2D-CGD	4.16	1.43	1.33
30	BF	5102	SQD	C1-C2	4.16	1.64	1.52
24	BB	5620	CLA	C4C-C3C	4.17	1.52	1.45
24	BA	5408	CLA	O2D-CGD	4.17	1.43	1.33
24	BB	5616	CLA	O2D-CGD	4.18	1.43	1.33
24	AC	513	CLA	C4C-C3C	4.19	1.52	1.45
24	AA	407	CLA	O2D-CGD	4.19	1.43	1.33
30	AB	622	SQD	O47-C7	4.20	1.46	1.34
24	BB	5619	CLA	O2D-CGD	4.20	1.43	1.33
24	AA	404	CLA	C4C-C3C	4.20	1.52	1.45
24	AB	604	CLA	CHB-C4A	4.21	1.38	1.33
24	AB	603	CLA	O2D-CGD	4.22	1.43	1.33
24	AB	611	CLA	CHB-C4A	4.22	1.38	1.33
24	BB	5615	CLA	C4C-NC	4.22	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	606	CLA	CHB-C4A	4.23	1.38	1.33
24	AC	511	CLA	O2D-CGD	4.23	1.43	1.33
24	AC	506	CLA	C4C-C3C	4.23	1.52	1.45
24	BB	5608	CLA	O2D-CGD	4.24	1.43	1.33
30	BB	5625	SQD	C1-C2	4.24	1.64	1.52
29	BA	5415	LHG	O8-C23	4.24	1.45	1.33
34	BD	5403	PHO	C4C-C3C	4.24	1.52	1.45
30	BB	5601	SQD	O5-C5	4.24	1.54	1.44
24	BB	5606	CLA	C4C-C3C	4.24	1.52	1.45
24	BB	5607	CLA	O2A-CGA	4.24	1.45	1.33
29	AA	412	LHG	P-O6	4.25	1.77	1.59
36	BF	5101	HEM	C1C-NC	4.25	1.41	1.36
24	AB	614	CLA	C4C-C3C	4.25	1.52	1.45
27	BJ	5101	BCR	C14-C13	4.26	1.41	1.35
24	AC	512	CLA	O2D-CGD	4.26	1.44	1.33
30	AA	416	SQD	O5-C5	4.27	1.54	1.44
24	AB	613	CLA	C4C-C3C	4.27	1.52	1.45
24	AC	507	CLA	CHB-C4A	4.27	1.39	1.33
24	BC	5507	CLA	CHB-C4A	4.27	1.39	1.33
29	AA	415	LHG	O8-C23	4.27	1.45	1.33
24	AB	611	CLA	O2D-CGD	4.29	1.44	1.33
30	AB	622	SQD	O5-C5	4.29	1.54	1.44
27	AA	410	BCR	C30-C25	4.29	1.59	1.53
30	BB	5625	SQD	O5-C5	4.30	1.54	1.44
24	BC	5503	CLA	O2D-CGD	4.30	1.44	1.33
24	AD	401	CLA	CHB-C4A	4.31	1.39	1.33
24	AB	602	CLA	O2D-CGD	4.31	1.44	1.33
24	AC	510	CLA	O2D-CGD	4.32	1.44	1.33
24	AC	507	CLA	O2D-CGD	4.32	1.44	1.33
24	BC	5512	CLA	O2D-CGD	4.32	1.44	1.33
30	AA	413	SQD	O47-C7	4.32	1.46	1.34
24	BC	5505	CLA	O2D-CGD	4.32	1.44	1.33
24	BC	5513	CLA	C4C-C3C	4.34	1.52	1.45
24	AC	510	CLA	C4C-C3C	4.35	1.52	1.45
24	BB	5618	CLA	C4C-C3C	4.36	1.52	1.45
24	BD	5402	CLA	O2D-CGD	4.36	1.44	1.33
24	BC	5511	CLA	CHB-C4A	4.36	1.39	1.33
24	BD	5402	CLA	CHB-C4A	4.36	1.39	1.33
27	BC	5516	BCR	C5-C6	4.36	1.42	1.34
24	AB	606	CLA	C4C-C3C	4.37	1.52	1.45
24	BB	5606	CLA	O2D-CGD	4.37	1.44	1.33
24	BB	5615	CLA	CHB-C4A	4.37	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	512	CLA	C4C-C3C	4.37	1.52	1.45
24	BC	5507	CLA	C4C-C3C	4.38	1.52	1.45
27	AD	406	BCR	C30-C25	4.38	1.59	1.53
27	AD	406	BCR	C26-C25	4.38	1.42	1.34
30	BA	5401	SQD	O47-C7	4.38	1.47	1.34
24	BC	5504	CLA	O2D-CGD	4.38	1.44	1.33
27	BX	5101	BCR	C1-C6	4.39	1.59	1.53
27	BT	5101	BCR	C30-C25	4.39	1.59	1.53
24	BB	5610	CLA	C4C-C3C	4.39	1.52	1.45
24	AB	601	CLA	C4C-C3C	4.39	1.52	1.45
34	AD	403	PHO	CBB-CAB	4.40	1.52	1.30
34	AD	403	PHO	C4C-C3C	4.42	1.53	1.45
34	AD	402	PHO	CBB-CAB	4.42	1.52	1.30
34	BD	5404	PHO	O2D-CGD	4.42	1.44	1.33
34	BD	5403	PHO	CBB-CAB	4.42	1.52	1.30
36	AV	201	HEM	C3C-CAC	4.42	1.56	1.47
28	AC	517	DGD	O6D-C1D	4.44	1.52	1.41
24	AC	502	CLA	O2D-CGD	4.44	1.44	1.33
27	AC	514	BCR	C1-C6	4.44	1.59	1.53
24	AB	603	CLA	O2A-CGA	4.45	1.46	1.33
30	AF	102	SQD	C1-C2	4.45	1.65	1.52
30	BA	5414	SQD	O47-C7	4.46	1.47	1.34
27	BT	5101	BCR	C5-C6	4.47	1.42	1.34
30	BF	5102	SQD	O47-C7	4.47	1.47	1.34
24	BB	5616	CLA	C4C-C3C	4.48	1.52	1.45
28	AA	411	DGD	O6D-C1D	4.48	1.53	1.41
24	BB	5620	CLA	C1C-C2C	4.49	1.53	1.44
24	BD	5402	CLA	C4C-C3C	4.49	1.53	1.45
24	AB	602	CLA	C4C-C3C	4.49	1.53	1.45
24	AC	502	CLA	C1C-C2C	4.49	1.53	1.44
24	BB	5614	CLA	CHB-C4A	4.50	1.39	1.33
24	BA	5405	CLA	C4C-C3C	4.51	1.53	1.45
24	BB	5610	CLA	C1C-C2C	4.51	1.53	1.44
24	AB	610	CLA	C4C-C3C	4.51	1.53	1.45
24	BB	5615	CLA	C1C-C2C	4.51	1.53	1.44
27	AB	618	BCR	C26-C25	4.52	1.42	1.34
34	BD	5404	PHO	CBB-CAB	4.52	1.53	1.30
30	AF	102	SQD	O5-C5	4.52	1.55	1.44
24	AB	608	CLA	CHB-C4A	4.52	1.39	1.33
24	AB	606	CLA	C1C-C2C	4.52	1.53	1.44
24	AC	508	CLA	O2D-CGD	4.52	1.44	1.33
24	BA	5405	CLA	O2D-CGD	4.52	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5401	SQD	O5-C5	4.53	1.55	1.44
24	BB	5605	CLA	C1C-C2C	4.53	1.53	1.44
24	AC	504	CLA	C1C-C2C	4.53	1.53	1.44
24	BC	5501	CLA	C1C-C2C	4.53	1.53	1.44
27	BA	5411	BCR	C30-C25	4.54	1.60	1.53
24	BD	5405	CLA	C1C-C2C	4.54	1.53	1.44
34	AD	403	PHO	O2D-CGD	4.54	1.44	1.33
24	BB	5619	CLA	C1C-C2C	4.54	1.53	1.44
27	BB	5623	BCR	C30-C25	4.55	1.60	1.53
24	BB	5609	CLA	C1C-C2C	4.55	1.53	1.44
24	BB	5614	CLA	C1C-C2C	4.55	1.53	1.44
24	AC	501	CLA	C1C-C2C	4.55	1.53	1.44
24	AC	512	CLA	C1C-C2C	4.55	1.53	1.44
24	BB	5606	CLA	C1C-C2C	4.55	1.53	1.44
30	BF	5102	SQD	O5-C5	4.56	1.55	1.44
24	BB	5608	CLA	C1C-C2C	4.56	1.53	1.44
24	BA	5407	CLA	C1C-C2C	4.56	1.53	1.44
24	AB	615	CLA	C1C-C2C	4.56	1.53	1.44
24	BB	5617	CLA	C1C-C2C	4.56	1.53	1.44
24	BC	5512	CLA	C1C-C2C	4.56	1.53	1.44
24	AB	616	CLA	C1C-C2C	4.56	1.53	1.44
28	BE	5102	DGD	O3G-C1D	4.57	1.48	1.40
24	AB	610	CLA	C1C-C2C	4.57	1.53	1.44
24	BD	5405	CLA	O2D-CGD	4.57	1.44	1.33
24	BB	5606	CLA	CHB-C4A	4.57	1.39	1.33
24	AB	601	CLA	C1C-C2C	4.57	1.53	1.44
24	BC	5503	CLA	C1C-C2C	4.57	1.53	1.44
24	AC	507	CLA	C1C-C2C	4.57	1.53	1.44
24	AB	612	CLA	C1C-C2C	4.57	1.53	1.44
24	BC	5509	CLA	C1C-C2C	4.57	1.53	1.44
24	AC	510	CLA	C1C-C2C	4.58	1.53	1.44
24	BC	5507	CLA	C1C-C2C	4.58	1.53	1.44
24	BB	5607	CLA	C1C-C2C	4.58	1.53	1.44
24	AB	609	CLA	C1C-C2C	4.58	1.53	1.44
24	AC	508	CLA	C1C-C2C	4.58	1.53	1.44
24	BB	5612	CLA	C1C-C2C	4.58	1.53	1.44
24	AB	611	CLA	C1C-C2C	4.58	1.53	1.44
24	AB	602	CLA	C1C-C2C	4.58	1.53	1.44
24	BC	5512	CLA	C4C-C3C	4.58	1.53	1.45
24	BC	5502	CLA	C1C-C2C	4.58	1.53	1.44
24	BB	5616	CLA	C1C-C2C	4.58	1.53	1.44
24	AB	603	CLA	C1C-C2C	4.58	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	406	CLA	C1C-C2C	4.59	1.53	1.44
24	AC	506	CLA	CHB-C4A	4.59	1.39	1.33
24	AB	613	CLA	C1C-C2C	4.59	1.53	1.44
24	BB	5613	CLA	C1C-C2C	4.59	1.53	1.44
24	AC	503	CLA	C1C-C2C	4.59	1.53	1.44
24	AD	404	CLA	C1C-C2C	4.59	1.53	1.44
36	BF	5101	HEM	C3C-CAC	4.59	1.56	1.47
24	BC	5508	CLA	C1C-C2C	4.59	1.53	1.44
24	AB	605	CLA	C1C-C2C	4.59	1.53	1.44
24	AC	511	CLA	C1C-C2C	4.60	1.53	1.44
27	BK	5102	BCR	C5-C6	4.60	1.42	1.34
24	BB	5618	CLA	CHB-C4A	4.60	1.39	1.33
28	AC	518	DGD	O6D-C1D	4.60	1.53	1.41
24	BC	5511	CLA	O2D-CGD	4.60	1.44	1.33
24	AA	404	CLA	C1C-C2C	4.60	1.53	1.44
24	AA	407	CLA	C1C-C2C	4.60	1.53	1.44
30	BB	5625	SQD	O47-C7	4.60	1.47	1.34
24	BC	5504	CLA	C1C-C2C	4.60	1.53	1.44
24	AB	607	CLA	C1C-C2C	4.61	1.53	1.44
24	BC	5509	CLA	O2D-CGD	4.61	1.44	1.33
24	AB	608	CLA	C1C-C2C	4.61	1.53	1.44
24	AC	509	CLA	C1C-C2C	4.61	1.53	1.44
24	BB	5611	CLA	C1C-C2C	4.61	1.53	1.44
27	BD	5407	BCR	C26-C25	4.62	1.42	1.34
29	AA	412	LHG	P-O3	4.62	1.78	1.59
24	BC	5510	CLA	O2D-CGD	4.62	1.44	1.33
24	BB	5610	CLA	O2D-CGD	4.62	1.44	1.33
24	AC	513	CLA	C1C-C2C	4.62	1.53	1.44
24	BC	5511	CLA	C1C-C2C	4.62	1.53	1.44
24	AC	509	CLA	CHB-C4A	4.63	1.39	1.33
24	AB	604	CLA	C1C-C2C	4.63	1.53	1.44
24	AB	603	CLA	C3B-C2B	4.63	1.46	1.40
24	BC	5510	CLA	C1C-C2C	4.63	1.53	1.44
24	BC	5505	CLA	C1C-C2C	4.63	1.53	1.44
24	AA	405	CLA	C1C-C2C	4.64	1.53	1.44
24	AC	506	CLA	C1C-C2C	4.65	1.53	1.44
24	BC	5502	CLA	O2D-CGD	4.65	1.45	1.33
24	BC	5506	CLA	C1C-C2C	4.65	1.53	1.44
24	BA	5408	CLA	C1C-C2C	4.66	1.53	1.44
24	AB	614	CLA	C1C-C2C	4.66	1.53	1.44
24	BC	5513	CLA	C1C-C2C	4.66	1.53	1.44
24	BB	5612	CLA	CHB-C4A	4.66	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	5406	CLA	C1C-C2C	4.67	1.53	1.44
24	AB	614	CLA	O2D-CGD	4.67	1.45	1.33
24	BB	5618	CLA	C1C-C2C	4.68	1.53	1.44
24	BB	5615	CLA	O2D-CGD	4.68	1.45	1.33
24	BA	5405	CLA	C1C-C2C	4.68	1.53	1.44
24	BB	5614	CLA	C4C-C3C	4.68	1.53	1.45
24	AC	505	CLA	C1C-C2C	4.69	1.53	1.44
24	AD	401	CLA	C1C-C2C	4.71	1.53	1.44
36	AF	101	HEM	C3C-CAC	4.73	1.57	1.47
24	AB	610	CLA	CHB-C4A	4.74	1.39	1.33
24	BB	5613	CLA	O2D-CGD	4.74	1.45	1.33
27	AX	101	BCR	C1-C6	4.74	1.60	1.53
24	BD	5402	CLA	C1C-C2C	4.74	1.53	1.44
29	BA	5413	LHG	P-O3	4.74	1.79	1.59
24	BB	5607	CLA	O2D-CGD	4.74	1.45	1.33
27	AJ	101	BCR	C14-C13	4.75	1.42	1.35
24	BC	5501	CLA	O2D-CGD	4.75	1.45	1.33
24	AB	616	CLA	O2D-CGD	4.76	1.45	1.33
28	BC	5517	DGD	O6D-C1D	4.77	1.53	1.41
24	AB	608	CLA	O2A-CGA	4.80	1.47	1.33
24	AB	609	CLA	O2D-CGD	4.81	1.45	1.33
24	BB	5609	CLA	CHB-C4A	4.81	1.39	1.33
24	AB	610	CLA	O2D-CGD	4.81	1.45	1.33
34	BD	5403	PHO	O2D-CGD	4.82	1.45	1.33
28	BC	5518	DGD	O6D-C1D	4.82	1.53	1.41
27	AA	410	BCR	C1-C6	4.83	1.60	1.53
24	BB	5612	CLA	O2A-CGA	4.83	1.47	1.33
24	BB	5611	CLA	C3C-C2C	4.83	1.47	1.36
24	AC	507	CLA	C4C-C3C	4.84	1.53	1.45
24	AA	404	CLA	O2D-CGD	4.85	1.45	1.33
24	BB	5617	CLA	CHB-C4A	4.86	1.39	1.33
28	BC	5517	DGD	O5D-C1E	4.87	1.48	1.40
24	BB	5608	CLA	CHB-C4A	4.87	1.39	1.33
24	AB	606	CLA	O2D-CGD	4.87	1.45	1.33
24	BB	5607	CLA	C3B-C2B	4.87	1.46	1.40
24	BC	5507	CLA	O2D-CGD	4.89	1.45	1.33
27	AX	101	BCR	C26-C25	4.90	1.42	1.34
27	AT	101	BCR	C1-C6	4.90	1.60	1.53
28	BB	5602	DGD	O5D-C1E	4.90	1.48	1.40
24	BB	5620	CLA	O2D-CGD	4.91	1.45	1.33
24	BB	5609	CLA	O2D-CGD	4.91	1.45	1.33
24	AB	602	CLA	CHB-C4A	4.93	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5618	CLA	O2D-CGD	4.94	1.45	1.33
28	BC	5519	DGD	O6D-C1D	4.95	1.54	1.41
24	AB	614	CLA	CHB-C4A	4.95	1.39	1.33
27	BX	5101	BCR	C26-C25	4.96	1.43	1.34
27	BC	5516	BCR	C1-C6	4.97	1.60	1.53
24	AB	613	CLA	CHB-C4A	5.00	1.39	1.33
27	AX	101	BCR	C30-C25	5.00	1.60	1.53
27	BJ	5101	BCR	C1-C6	5.02	1.60	1.53
24	BA	5408	CLA	CHB-C4A	5.03	1.39	1.33
28	AC	519	DGD	O6D-C1D	5.04	1.54	1.41
24	AB	609	CLA	CHB-C4A	5.05	1.40	1.33
24	AC	513	CLA	O2D-CGD	5.06	1.46	1.33
27	BB	5623	BCR	C1-C6	5.06	1.60	1.53
24	BD	5405	CLA	CHB-C4A	5.07	1.40	1.33
24	AC	509	CLA	O2D-CGD	5.07	1.46	1.33
24	AC	506	CLA	O2D-CGD	5.08	1.46	1.33
27	BB	5622	BCR	C30-C25	5.08	1.60	1.53
27	AB	618	BCR	C30-C25	5.09	1.60	1.53
24	BC	5503	CLA	CHB-C4A	5.10	1.40	1.33
28	BA	5412	DGD	O6D-C1D	5.13	1.54	1.41
24	BC	5506	CLA	O2D-CGD	5.13	1.46	1.33
36	BV	5201	HEM	C3C-CAC	5.14	1.58	1.47
24	AB	607	CLA	C3B-C2B	5.15	1.47	1.40
24	BC	5509	CLA	CHB-C4A	5.16	1.40	1.33
27	AC	514	BCR	C30-C25	5.16	1.60	1.53
24	BB	5617	CLA	C3B-C2B	5.17	1.47	1.40
27	AJ	101	BCR	C5-C6	5.20	1.43	1.34
24	AA	405	CLA	C3C-C2C	5.20	1.47	1.36
24	AB	616	CLA	C3C-C2C	5.24	1.48	1.36
27	BX	5101	BCR	C30-C25	5.25	1.61	1.53
24	BB	5609	CLA	C3C-C2C	5.27	1.48	1.36
27	BC	5515	BCR	C1-C6	5.27	1.61	1.53
24	BC	5513	CLA	O2D-CGD	5.29	1.46	1.33
24	BC	5507	CLA	C3C-C2C	5.29	1.48	1.36
24	AB	605	CLA	O2D-CGD	5.30	1.46	1.33
27	AJ	101	BCR	C1-C6	5.32	1.61	1.53
27	BJ	5101	BCR	C5-C6	5.32	1.43	1.34
27	BA	5411	BCR	C1-C6	5.33	1.61	1.53
24	AC	507	CLA	C3C-C2C	5.36	1.48	1.36
31	AB	620	LMG	O1-C1	5.37	1.49	1.40
24	AB	611	CLA	C3C-C2C	5.39	1.48	1.36
27	AC	515	BCR	C30-C25	5.43	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	619	BCR	C1-C6	5.47	1.61	1.53
27	BD	5407	BCR	C30-C25	5.47	1.61	1.53
24	AC	502	CLA	C3C-C2C	5.48	1.48	1.36
24	AB	616	CLA	CHB-C4A	5.49	1.40	1.33
24	BB	5605	CLA	O2D-CGD	5.50	1.47	1.33
24	AB	605	CLA	C3C-C2C	5.50	1.48	1.36
27	AK	102	BCR	C30-C25	5.51	1.61	1.53
24	BB	5613	CLA	C3C-C2C	5.52	1.48	1.36
24	BB	5620	CLA	C3C-C2C	5.52	1.48	1.36
27	BC	5515	BCR	C30-C25	5.52	1.61	1.53
24	AC	503	CLA	CHB-C4A	5.52	1.40	1.33
24	AA	406	CLA	C3C-C2C	5.53	1.48	1.36
24	BC	5508	CLA	O2D-CGD	5.53	1.47	1.33
31	BL	5101	LMG	O1-C1	5.55	1.49	1.40
27	BT	5101	BCR	C1-C6	5.57	1.61	1.53
24	AB	613	CLA	C3C-C2C	5.57	1.48	1.36
24	BB	5617	CLA	C3C-C2C	5.59	1.48	1.36
27	AB	618	BCR	C1-C6	5.60	1.61	1.53
24	AC	510	CLA	C3C-C2C	5.61	1.48	1.36
27	BC	5514	BCR	C30-C25	5.61	1.61	1.53
24	AD	404	CLA	CHB-C4A	5.66	1.40	1.33
24	BC	5501	CLA	CHB-C4A	5.69	1.40	1.33
24	BB	5615	CLA	C3C-C2C	5.70	1.49	1.36
24	BB	5619	CLA	C3C-C2C	5.72	1.49	1.36
24	AB	601	CLA	O2D-CGD	5.72	1.47	1.33
24	AB	613	CLA	C3B-C2B	5.73	1.47	1.40
24	AB	609	CLA	C3C-C2C	5.76	1.49	1.36
27	BK	5102	BCR	C30-C25	5.76	1.61	1.53
27	BB	5622	BCR	C1-C6	5.76	1.61	1.53
24	AB	607	CLA	C3C-C2C	5.78	1.49	1.36
34	BD	5403	PHO	C3C-C2C	5.78	1.49	1.36
24	BC	5508	CLA	C3C-C2C	5.79	1.49	1.36
24	AB	605	CLA	CHB-C4A	5.81	1.40	1.33
27	AB	619	BCR	C30-C25	5.82	1.61	1.53
24	BB	5608	CLA	C3C-C2C	5.84	1.49	1.36
24	BC	5505	CLA	CHB-C4A	5.85	1.41	1.33
28	AA	411	DGD	O5D-C1E	5.86	1.50	1.40
24	BA	5406	CLA	C3C-C2C	5.86	1.49	1.36
24	AC	501	CLA	C3C-C2C	5.86	1.49	1.36
24	AB	614	CLA	C3C-C2C	5.89	1.49	1.36
24	AC	508	CLA	C3C-C2C	5.89	1.49	1.36
27	BC	5514	BCR	C1-C6	5.93	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	503	CLA	C3C-C2C	5.93	1.49	1.36
24	BB	5620	CLA	CHB-C4A	5.94	1.41	1.33
24	AB	606	CLA	C3C-C2C	5.94	1.49	1.36
24	AC	505	CLA	CHB-C4A	5.96	1.41	1.33
24	AC	506	CLA	C3C-C2C	5.97	1.49	1.36
24	AC	509	CLA	C3C-C2C	5.97	1.49	1.36
24	BC	5503	CLA	C3C-C2C	5.98	1.49	1.36
24	AB	602	CLA	C3C-C2C	5.99	1.49	1.36
24	BC	5510	CLA	C3C-C2C	5.99	1.49	1.36
34	AD	402	PHO	C3C-C2C	6.00	1.49	1.36
24	AC	510	CLA	CHB-C4A	6.02	1.41	1.33
28	BA	5412	DGD	O5D-C1E	6.04	1.50	1.40
24	AC	512	CLA	C3C-C2C	6.08	1.49	1.36
24	AD	401	CLA	C3C-C2C	6.09	1.49	1.36
24	BB	5606	CLA	C3C-C2C	6.10	1.49	1.36
24	AB	610	CLA	C3C-C2C	6.16	1.50	1.36
24	BC	5501	CLA	C3C-C2C	6.16	1.50	1.36
24	BB	5610	CLA	C3C-C2C	6.16	1.50	1.36
24	BB	5614	CLA	C3C-C2C	6.17	1.50	1.36
24	BA	5407	CLA	C3C-C2C	6.17	1.50	1.36
34	AD	403	PHO	C3C-C2C	6.18	1.50	1.36
24	AA	407	CLA	C3C-C2C	6.18	1.50	1.36
24	BD	5402	CLA	C3C-C2C	6.19	1.50	1.36
24	AB	612	CLA	C3C-C2C	6.21	1.50	1.36
24	AB	608	CLA	C3C-C2C	6.21	1.50	1.36
24	AC	504	CLA	C3C-C2C	6.23	1.50	1.36
24	BC	5506	CLA	C3C-C2C	6.23	1.50	1.36
24	BB	5618	CLA	C3C-C2C	6.23	1.50	1.36
24	AB	615	CLA	C3C-C2C	6.25	1.50	1.36
24	BB	5607	CLA	C3C-C2C	6.29	1.50	1.36
24	BC	5510	CLA	CHB-C4A	6.30	1.41	1.33
24	AC	505	CLA	C3C-C2C	6.36	1.50	1.36
24	AC	501	CLA	CHB-C4A	6.38	1.41	1.33
24	BC	5505	CLA	C3C-C2C	6.38	1.50	1.36
24	BB	5619	CLA	CHB-C4A	6.39	1.41	1.33
24	BB	5616	CLA	C3C-C2C	6.40	1.50	1.36
24	BC	5502	CLA	C3C-C2C	6.41	1.50	1.36
24	BB	5612	CLA	C3C-C2C	6.41	1.50	1.36
24	AA	404	CLA	C3C-C2C	6.43	1.50	1.36
24	BA	5408	CLA	C3C-C2C	6.44	1.50	1.36
24	BC	5512	CLA	C3C-C2C	6.45	1.50	1.36
24	BB	5611	CLA	C3B-C2B	6.45	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	5405	CLA	C3C-C2C	6.45	1.50	1.36
24	BB	5605	CLA	CHB-C4A	6.47	1.41	1.33
24	AB	606	CLA	C3B-C2B	6.49	1.48	1.40
24	AC	511	CLA	C3C-C2C	6.52	1.50	1.36
24	BC	5509	CLA	C3C-C2C	6.53	1.50	1.36
24	AB	604	CLA	C3C-C2C	6.56	1.50	1.36
24	BD	5405	CLA	C3C-C2C	6.61	1.50	1.36
24	AC	513	CLA	C3C-C2C	6.63	1.51	1.36
34	BD	5404	PHO	C3C-C2C	6.65	1.51	1.36
24	AA	405	CLA	C3B-C2B	6.68	1.49	1.40
24	BC	5511	CLA	C3C-C2C	6.71	1.51	1.36
24	BC	5512	CLA	CHB-C4A	6.72	1.42	1.33
24	AB	603	CLA	C3C-C2C	6.74	1.51	1.36
24	AC	507	CLA	C3B-C2B	6.74	1.49	1.40
24	BC	5513	CLA	C3C-C2C	6.76	1.51	1.36
27	BJ	5101	BCR	C30-C25	6.76	1.63	1.53
24	AB	601	CLA	CHB-C4A	6.78	1.42	1.33
24	AB	615	CLA	CHB-C4A	6.78	1.42	1.33
24	AC	512	CLA	CHB-C4A	6.83	1.42	1.33
24	BB	5612	CLA	C3B-C2B	6.84	1.49	1.40
24	BC	5504	CLA	C3C-C2C	6.85	1.51	1.36
24	AD	404	CLA	C3C-C2C	6.86	1.51	1.36
24	AC	508	CLA	C3B-C2B	6.86	1.49	1.40
34	AD	402	PHO	C3B-C2B	6.87	1.50	1.37
24	AB	602	CLA	C3B-C2B	6.97	1.49	1.40
24	BB	5605	CLA	C3C-C2C	6.98	1.51	1.36
35	AD	405	PL9	O2-C1	7.00	1.43	1.24
35	BD	5406	PL9	O2-C1	7.03	1.43	1.24
24	AD	401	CLA	C3B-C2B	7.05	1.49	1.40
24	AB	601	CLA	C3C-C2C	7.06	1.51	1.36
24	BC	5504	CLA	C3B-C2B	7.09	1.49	1.40
24	AA	404	CLA	C3B-C2B	7.12	1.49	1.40
24	AC	504	CLA	C3B-C2B	7.14	1.49	1.40
27	AJ	101	BCR	C30-C25	7.14	1.63	1.53
30	AA	413	SQD	C4-C3	7.20	1.70	1.52
24	AA	407	CLA	C3B-C2B	7.20	1.49	1.40
24	AC	502	CLA	C3B-C2B	7.21	1.49	1.40
24	BC	5508	CLA	C3B-C2B	7.23	1.49	1.40
34	AD	403	PHO	C3B-C2B	7.25	1.50	1.37
24	BB	5610	CLA	C3B-C2B	7.27	1.50	1.40
36	AV	201	HEM	C3B-C2B	7.28	1.50	1.40
24	BB	5606	CLA	C3B-C2B	7.28	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	509	CLA	C3B-C2B	7.31	1.50	1.40
24	BA	5408	CLA	C3B-C2B	7.32	1.50	1.40
36	BV	5201	HEM	C3C-C2C	7.33	1.50	1.40
24	BB	5616	CLA	C3B-C2B	7.34	1.50	1.40
24	BD	5402	CLA	C3B-C2B	7.39	1.50	1.40
24	AB	611	CLA	C3B-C2B	7.42	1.50	1.40
36	AV	201	HEM	C3C-C2C	7.42	1.50	1.40
24	AB	608	CLA	C3B-C2B	7.42	1.50	1.40
30	AF	102	SQD	C4-C3	7.43	1.71	1.52
24	AB	612	CLA	C3B-C2B	7.45	1.50	1.40
24	BB	5620	CLA	C3B-C2B	7.47	1.50	1.40
24	BA	5405	CLA	C3B-C2B	7.47	1.50	1.40
24	BA	5405	CLA	C2-C3	7.48	1.51	1.33
24	AC	501	CLA	C3B-C2B	7.52	1.50	1.40
29	BA	5413	LHG	P-O5	7.53	1.79	1.50
36	AF	101	HEM	C3C-C2C	7.56	1.50	1.40
24	BD	5405	CLA	C3B-C2B	7.57	1.50	1.40
30	BF	5102	SQD	C4-C3	7.57	1.71	1.52
34	BD	5403	PHO	C3B-C2B	7.58	1.51	1.37
29	AA	412	LHG	P-O5	7.59	1.79	1.50
24	BB	5608	CLA	C3B-C2B	7.60	1.50	1.40
24	AD	404	CLA	C3B-C2B	7.61	1.50	1.40
24	AB	610	CLA	C3B-C2B	7.64	1.50	1.40
24	BC	5507	CLA	C3B-C2B	7.64	1.50	1.40
24	BB	5615	CLA	C3B-C2B	7.64	1.50	1.40
24	BB	5618	CLA	C3B-C2B	7.65	1.50	1.40
24	AB	604	CLA	C3B-C2B	7.66	1.50	1.40
24	AB	614	CLA	C3B-C2B	7.67	1.50	1.40
30	AA	416	SQD	C4-C3	7.72	1.72	1.52
36	BV	5201	HEM	C3B-C2B	7.73	1.50	1.40
24	AC	510	CLA	C3B-C2B	7.73	1.50	1.40
30	BB	5601	SQD	C4-C3	7.76	1.72	1.52
35	AD	405	PL9	C48-C49	7.76	1.55	1.32
24	AA	406	CLA	C3B-C2B	7.77	1.50	1.40
24	AC	511	CLA	C3B-C2B	7.80	1.50	1.40
30	BA	5414	SQD	C4-C3	7.82	1.72	1.52
36	AF	101	HEM	C3B-C2B	7.83	1.50	1.40
24	BC	5502	CLA	C3B-C2B	7.86	1.50	1.40
24	AC	503	CLA	C3B-C2B	7.89	1.50	1.40
30	BA	5401	SQD	C4-C3	7.91	1.72	1.52
24	AB	615	CLA	C3B-C2B	7.93	1.50	1.40
35	BD	5406	PL9	C48-C49	7.96	1.55	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	627	SQD	C4-C3	7.97	1.72	1.52
24	BB	5614	CLA	C3B-C2B	7.99	1.50	1.40
34	BD	5404	PHO	C3B-C2B	7.99	1.52	1.37
24	AB	616	CLA	C3B-C2B	8.07	1.51	1.40
24	BC	5510	CLA	C3B-C2B	8.07	1.51	1.40
24	AB	609	CLA	C3B-C2B	8.16	1.51	1.40
24	BC	5506	CLA	C3B-C2B	8.16	1.51	1.40
24	BA	5407	CLA	C3B-C2B	8.16	1.51	1.40
24	AC	513	CLA	C3B-C2B	8.18	1.51	1.40
24	BB	5613	CLA	C3B-C2B	8.20	1.51	1.40
24	BC	5511	CLA	C3B-C2B	8.20	1.51	1.40
35	AD	405	PL9	C23-C24	8.21	1.53	1.33
24	BB	5619	CLA	C2-C3	8.22	1.53	1.33
36	BF	5101	HEM	C3B-C2B	8.24	1.51	1.40
24	BB	5619	CLA	C3B-C2B	8.24	1.51	1.40
24	BB	5614	CLA	C2-C3	8.27	1.53	1.33
24	BB	5609	CLA	C3B-C2B	8.27	1.51	1.40
24	AB	615	CLA	C2-C3	8.28	1.53	1.33
24	AC	506	CLA	C3B-C2B	8.30	1.51	1.40
24	AC	507	CLA	C2-C3	8.32	1.53	1.33
30	AB	622	SQD	C4-C3	8.34	1.73	1.52
35	AD	405	PL9	C2-C3	8.35	1.57	1.34
24	BC	5501	CLA	C3B-C2B	8.37	1.51	1.40
24	AC	509	CLA	C2-C3	8.38	1.54	1.33
24	BC	5503	CLA	C3B-C2B	8.39	1.51	1.40
24	AB	610	CLA	C2-C3	8.39	1.54	1.33
24	AA	404	CLA	C2-C3	8.40	1.54	1.33
35	BD	5406	PL9	C2-C3	8.45	1.57	1.34
24	AB	613	CLA	C2-C3	8.45	1.54	1.33
24	AB	605	CLA	C3B-C2B	8.45	1.51	1.40
24	AC	504	CLA	C2-C3	8.46	1.54	1.33
24	BB	5608	CLA	C2-C3	8.49	1.54	1.33
24	AD	401	CLA	C2-C3	8.49	1.54	1.33
24	BB	5617	CLA	C2-C3	8.49	1.54	1.33
24	AC	512	CLA	C3B-C2B	8.50	1.51	1.40
24	BC	5510	CLA	C2-C3	8.53	1.54	1.33
30	BB	5625	SQD	C4-C3	8.54	1.74	1.52
35	AD	405	PL9	C43-C44	8.56	1.54	1.33
24	AC	512	CLA	C2-C3	8.56	1.54	1.33
24	AB	604	CLA	C2-C3	8.57	1.54	1.33
24	AB	602	CLA	C2-C3	8.58	1.54	1.33
35	AD	405	PL9	C8-C9	8.58	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	510	CLA	C2-C3	8.61	1.54	1.33
24	BA	5407	CLA	C2-C3	8.61	1.54	1.33
24	BC	5509	CLA	C3B-C2B	8.62	1.51	1.40
24	BC	5512	CLA	C2-C3	8.62	1.54	1.33
36	BF	5101	HEM	C3C-C2C	8.63	1.51	1.40
24	AD	404	CLA	C2-C3	8.63	1.54	1.33
24	BC	5507	CLA	C2-C3	8.64	1.54	1.33
24	BD	5402	CLA	C2-C3	8.65	1.54	1.33
24	AC	503	CLA	C2-C3	8.65	1.54	1.33
24	BB	5616	CLA	C2-C3	8.68	1.54	1.33
24	BC	5513	CLA	C3B-C2B	8.68	1.51	1.40
35	BD	5406	PL9	C8-C9	8.68	1.54	1.33
24	BC	5503	CLA	C2-C3	8.68	1.54	1.33
24	AA	407	CLA	C2-C3	8.69	1.54	1.33
24	BC	5512	CLA	C3B-C2B	8.71	1.51	1.40
24	BB	5606	CLA	C2-C3	8.71	1.54	1.33
24	BC	5504	CLA	C2-C3	8.73	1.54	1.33
24	BA	5406	CLA	C3B-C2B	8.78	1.51	1.40
24	AB	612	CLA	C2-C3	8.78	1.55	1.33
24	BC	5502	CLA	C2-C3	8.79	1.55	1.33
24	AA	406	CLA	C2-C3	8.80	1.55	1.33
35	AD	405	PL9	C33-C34	8.80	1.55	1.33
24	AC	508	CLA	C2-C3	8.81	1.55	1.33
35	BD	5406	PL9	C43-C44	8.85	1.55	1.33
34	AD	402	PHO	C2-C3	8.89	1.55	1.33
24	AB	611	CLA	C2-C3	8.90	1.55	1.33
24	BA	5406	CLA	C2-C3	8.90	1.55	1.33
24	AA	405	CLA	C2-C3	8.92	1.55	1.33
24	BC	5508	CLA	C2-C3	8.93	1.55	1.33
24	BC	5509	CLA	C2-C3	8.95	1.55	1.33
24	BA	5408	CLA	C2-C3	8.96	1.55	1.33
24	BC	5501	CLA	C2-C3	9.01	1.55	1.33
24	AB	601	CLA	C2-C3	9.03	1.55	1.33
24	BB	5609	CLA	C2-C3	9.04	1.55	1.33
24	AC	502	CLA	C2-C3	9.05	1.55	1.33
24	BD	5405	CLA	C2-C3	9.06	1.55	1.33
35	BD	5406	PL9	C33-C34	9.07	1.55	1.33
24	AC	501	CLA	C2-C3	9.09	1.55	1.33
24	BC	5513	CLA	C2-C3	9.10	1.55	1.33
24	AC	505	CLA	C3B-C2B	9.11	1.52	1.40
24	AC	513	CLA	C2-C3	9.12	1.55	1.33
24	AB	605	CLA	C2-C3	9.12	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5403	PHO	C2-C3	9.16	1.55	1.33
24	AC	505	CLA	C2-C3	9.16	1.55	1.33
34	BD	5404	PHO	C2-C3	9.16	1.55	1.33
35	AD	405	PL9	C13-C14	9.17	1.55	1.33
35	BD	5406	PL9	C23-C24	9.19	1.56	1.33
24	AB	601	CLA	C3B-C2B	9.20	1.52	1.40
24	BB	5618	CLA	C2-C3	9.20	1.56	1.33
35	BD	5406	PL9	C28-C29	9.21	1.56	1.33
24	BB	5605	CLA	C2-C3	9.22	1.56	1.33
24	BB	5611	CLA	C2-C3	9.22	1.56	1.33
24	BB	5615	CLA	C2-C3	9.23	1.56	1.33
24	AC	506	CLA	C2-C3	9.23	1.56	1.33
34	AD	403	PHO	C2-C3	9.25	1.56	1.33
35	BD	5406	PL9	C13-C14	9.28	1.56	1.33
24	BB	5607	CLA	C2-C3	9.31	1.56	1.33
24	BC	5506	CLA	C2-C3	9.32	1.56	1.33
24	AB	609	CLA	C2-C3	9.34	1.56	1.33
35	AD	405	PL9	C28-C29	9.35	1.56	1.33
24	BC	5505	CLA	C2-C3	9.38	1.56	1.33
24	BC	5505	CLA	C3B-C2B	9.42	1.52	1.40
24	AB	603	CLA	C2-C3	9.48	1.56	1.33
24	AC	511	CLA	C2-C3	9.53	1.56	1.33
24	AB	616	CLA	C2-C3	9.53	1.56	1.33
24	BB	5613	CLA	C2-C3	9.54	1.56	1.33
24	AB	614	CLA	C2-C3	9.55	1.56	1.33
24	BB	5605	CLA	C3B-C2B	9.70	1.53	1.40
24	BC	5511	CLA	C2-C3	9.73	1.57	1.33
24	BB	5620	CLA	C2-C3	9.75	1.57	1.33
24	AB	607	CLA	C2-C3	9.75	1.57	1.33
24	BB	5610	CLA	C2-C3	10.03	1.58	1.33
24	AB	606	CLA	C2-C3	10.04	1.58	1.33
24	BB	5612	CLA	C2-C3	10.05	1.58	1.33
24	AB	608	CLA	C2-C3	10.06	1.58	1.33

All (2638) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	519	DGD	C3G-O3G-C1D	-10.00	93.25	113.76
27	BJ	5101	BCR	C32-C1-C6	-9.99	94.11	110.31
27	AJ	101	BCR	C32-C1-C6	-9.93	94.20	110.31
28	BC	5519	DGD	C3G-O3G-C1D	-9.83	93.61	113.76
27	BJ	5101	BCR	C32-C1-C31	-9.42	79.64	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AJ	101	BCR	C32-C1-C31	-9.38	79.78	108.50
36	BF	5101	HEM	CMA-C3A-C2A	-9.33	107.34	124.94
36	AF	101	HEM	CMA-C3A-C2A	-9.14	107.71	124.94
36	AV	201	HEM	CMA-C3A-C2A	-9.00	107.97	124.94
36	BV	5201	HEM	CMA-C3A-C2A	-8.97	108.03	124.94
24	AC	503	CLA	C1-C2-C3	-8.62	110.08	125.96
28	AA	411	DGD	C6D-C5D-C4D	-8.59	93.70	112.00
35	AD	405	PL9	C7-C8-C9	-8.57	112.38	126.71
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
35	BD	5406	PL9	C7-C8-C9	-8.50	112.50	126.71
28	BA	5412	DGD	C6D-C5D-C4D	-8.49	93.92	112.00
24	BC	5503	CLA	C1-C2-C3	-8.45	110.38	125.96
24	AB	611	CLA	C1-C2-C3	-7.99	111.24	125.96
24	BB	5615	CLA	C1-C2-C3	-7.98	111.26	125.96
24	BC	5501	CLA	C1-C2-C3	-7.77	111.64	125.96
24	BB	5619	CLA	C1-C2-C3	-7.75	111.68	125.96
24	BA	5405	CLA	C1-C2-C3	-7.72	111.74	125.96
28	BA	5412	DGD	O3G-C1D-C2D	-7.70	95.67	108.23
24	AC	501	CLA	C1-C2-C3	-7.70	111.77	125.96
28	BC	5519	DGD	C6D-O5D-C1E	-7.67	98.02	113.76
24	AB	615	CLA	C1-C2-C3	-7.67	111.83	125.96
24	BB	5608	CLA	C1-C2-C3	-7.65	111.86	125.96
28	AA	411	DGD	O3G-C1D-C2D	-7.62	95.80	108.23
24	AB	604	CLA	C1-C2-C3	-7.58	111.99	125.96
24	BB	5614	CLA	C1-C2-C3	-7.55	112.05	125.96
24	BC	5512	CLA	C1-C2-C3	-7.55	112.05	125.96
24	AA	404	CLA	C1-C2-C3	-7.53	112.08	125.96
24	BD	5402	CLA	C1-C2-C3	-7.52	112.11	125.96
31	AD	407	LMG	C19-C18-C17	-7.51	75.76	114.45
31	BD	5409	LMG	C19-C18-C17	-7.48	75.90	114.45
36	AF	101	HEM	C4A-C3A-C2A	-7.48	101.79	107.00
24	AC	512	CLA	C1-C2-C3	-7.44	112.25	125.96
24	AC	508	CLA	C1-C2-C3	-7.44	112.26	125.96
34	BD	5403	PHO	C1-C2-C3	-7.40	112.33	125.96
24	AB	610	CLA	C1-C2-C3	-7.36	112.39	125.96
24	BC	5510	CLA	C1-C2-C3	-7.36	112.39	125.96
24	BC	5508	CLA	C1-C2-C3	-7.33	112.45	125.96
24	AC	509	CLA	C1-C2-C3	-7.33	112.46	125.96
36	BF	5101	HEM	C4A-C3A-C2A	-7.32	101.90	107.00
24	AC	510	CLA	C1-C2-C3	-7.32	112.46	125.96
24	AD	401	CLA	C1-C2-C3	-7.31	112.48	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	C1-C2-C3	-7.28	112.55	125.96
34	AD	402	PHO	C1-C2-C3	-7.25	112.60	125.96
24	BA	5408	CLA	C1-C2-C3	-7.24	112.62	125.96
24	BC	5504	CLA	C1-C2-C3	-7.24	112.62	125.96
24	BA	5407	CLA	C1-C2-C3	-7.23	112.63	125.96
24	AB	612	CLA	C1-C2-C3	-7.22	112.65	125.96
24	BB	5616	CLA	C1-C2-C3	-7.21	112.67	125.96
24	AA	407	CLA	C1-C2-C3	-7.21	112.67	125.96
28	AC	519	DGD	C6D-O5D-C1E	-7.20	98.99	113.76
24	AC	504	CLA	C1-C2-C3	-7.18	112.73	125.96
24	AC	506	CLA	C1-C2-C3	-7.17	112.75	125.96
34	BD	5404	PHO	C1-C2-C3	-7.16	112.77	125.96
24	BC	5509	CLA	C1-C2-C3	-7.12	112.83	125.96
24	BB	5606	CLA	C1-C2-C3	-7.12	112.84	125.96
24	BB	5609	CLA	C1-C2-C3	-7.10	112.88	125.96
24	AA	406	CLA	C1-C2-C3	-7.08	112.91	125.96
24	BC	5506	CLA	C1-C2-C3	-7.08	112.91	125.96
24	BB	5617	CLA	C1-C2-C3	-7.07	112.94	125.96
24	AB	613	CLA	C1-C2-C3	-7.06	112.94	125.96
24	BC	5502	CLA	C1-C2-C3	-7.06	112.95	125.96
24	AD	404	CLA	C1-C2-C3	-7.06	112.96	125.96
24	BB	5612	CLA	C1-C2-C3	-7.05	112.96	125.96
24	BC	5505	CLA	C1-C2-C3	-7.05	112.96	125.96
24	AB	601	CLA	C1-C2-C3	-7.05	112.97	125.96
24	BC	5513	CLA	C1-C2-C3	-7.03	113.00	125.96
24	AB	608	CLA	C1-C2-C3	-7.03	113.01	125.96
30	AA	413	SQD	O8-S-C6	-7.02	97.44	106.01
30	AA	416	SQD	O8-S-C6	-7.01	97.45	106.01
27	AJ	101	BCR	C32-C1-C2	-7.01	81.14	108.80
28	BA	5412	DGD	C6D-O5D-C1E	-7.00	99.41	113.76
24	AC	505	CLA	C1-C2-C3	-6.98	113.09	125.96
24	AB	616	CLA	C1-C2-C3	-6.97	113.11	125.96
30	AF	102	SQD	O8-S-C6	-6.97	97.50	106.01
24	AB	602	CLA	C1-C2-C3	-6.97	113.11	125.96
24	AC	513	CLA	C1-C2-C3	-6.96	113.13	125.96
24	BD	5405	CLA	C1-C2-C3	-6.95	113.15	125.96
24	AB	605	CLA	C1-C2-C3	-6.93	113.19	125.96
28	AA	411	DGD	C6D-O5D-C1E	-6.90	99.60	113.76
24	BB	5605	CLA	C1-C2-C3	-6.89	113.26	125.96
27	BJ	5101	BCR	C32-C1-C2	-6.89	81.62	108.80
30	BF	5102	SQD	O8-S-C6	-6.89	97.60	106.01
24	BB	5613	CLA	C1-C2-C3	-6.88	113.28	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5620	CLA	C1-C2-C3	-6.86	113.31	125.96
24	AB	609	CLA	C1-C2-C3	-6.86	113.32	125.96
24	AA	405	CLA	C1-C2-C3	-6.85	113.34	125.96
30	BA	5401	SQD	O8-S-C6	-6.85	97.65	106.01
24	BA	5406	CLA	C1-C2-C3	-6.84	113.36	125.96
24	AC	502	CLA	C1-C2-C3	-6.84	113.36	125.96
31	BL	5101	LMG	C7-O1-C1	-6.82	99.77	113.76
24	AC	507	CLA	C1-C2-C3	-6.77	113.48	125.96
28	AC	517	DGD	O1G-C1G-C2G	-6.76	91.68	108.66
24	BC	5507	CLA	C1-C2-C3	-6.76	113.51	125.96
31	AD	408	LMG	C13-C12-C11	-6.75	88.49	113.24
31	BD	5410	LMG	C13-C12-C11	-6.75	88.49	113.24
36	BV	5201	HEM	C4A-C3A-C2A	-6.72	102.32	107.00
31	AB	620	LMG	C7-O1-C1	-6.71	99.99	113.76
24	BB	5618	CLA	C1-C2-C3	-6.71	113.60	125.96
24	BB	5607	CLA	C1-C2-C3	-6.67	113.68	125.96
24	AB	614	CLA	C1-C2-C3	-6.65	113.70	125.96
36	AV	201	HEM	C4A-C3A-C2A	-6.60	102.40	107.00
24	AB	606	CLA	C1-C2-C3	-6.60	113.79	125.96
24	BB	5610	CLA	C1-C2-C3	-6.59	113.82	125.96
31	AA	417	LMG	C7-O1-C1	-6.59	100.25	113.76
24	AB	603	CLA	C1-C2-C3	-6.59	113.83	125.96
28	BC	5517	DGD	O1G-C1G-C2G	-6.57	92.14	108.66
31	BD	5408	LMG	C7-O1-C1	-6.56	100.31	113.76
25	AA	408	MST	C10-N9-C4	-6.48	120.93	128.02
31	AJ	102	LMG	C13-C12-C11	-6.46	89.56	113.24
31	BA	5402	LMG	C7-O1-C1	-6.44	100.56	113.76
31	AB	620	LMG	C13-C12-C11	-6.42	89.70	113.24
31	BD	5408	LMG	C13-C12-C11	-6.41	89.73	113.24
31	AJ	102	LMG	C7-O1-C1	-6.40	100.63	113.76
31	BL	5101	LMG	C13-C12-C11	-6.37	89.90	113.24
30	AB	627	SQD	O8-S-C6	-6.34	98.26	106.01
32	BC	5522	LMT	C1B-O1B-C4'	-6.34	102.55	118.00
31	BA	5402	LMG	C13-C12-C11	-6.29	90.20	113.24
31	AA	417	LMG	C13-C12-C11	-6.27	90.26	113.24
28	AC	519	DGD	C6D-C5D-C4D	-6.22	98.75	112.00
28	AA	411	DGD	C1D-O6D-C5D	-6.20	102.04	113.72
28	BC	5519	DGD	C4B-C3B-C2B	-6.19	90.56	113.24
35	BD	5406	PL9	C32-C33-C34	-6.16	112.22	127.68
28	AC	518	DGD	C4A-C3A-C2A	-6.15	90.70	113.24
32	AI	103	LMT	C1B-O1B-C4'	-6.13	103.06	118.00
25	BA	5409	MST	C10-N9-C4	-6.11	121.33	128.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	5602	DGD	C3G-O3G-C1D	-6.11	101.22	113.76
28	BA	5412	DGD	C1D-O6D-C5D	-6.09	102.23	113.72
28	BC	5517	DGD	C6D-O5D-C1E	-6.08	101.29	113.76
35	AD	405	PL9	C32-C33-C34	-6.06	112.45	127.68
24	BC	5511	CLA	C1-C2-C3	-6.06	114.80	125.96
30	BA	5414	SQD	O8-S-C6	-6.06	98.61	106.01
24	BB	5611	CLA	C1-C2-C3	-6.04	114.83	125.96
28	AB	628	DGD	C3G-O3G-C1D	-6.03	101.39	113.76
30	AB	622	SQD	O8-S-C6	-6.02	98.66	106.01
24	AC	511	CLA	C1-C2-C3	-6.01	114.89	125.96
28	AC	519	DGD	C4B-C3B-C2B	-6.01	91.23	113.24
31	BD	5409	LMG	C13-C12-C11	-5.98	91.32	113.24
28	AC	517	DGD	C4B-C3B-C2B	-5.97	91.35	113.24
24	AB	607	CLA	C1-C2-C3	-5.97	114.96	125.96
28	BC	5518	DGD	C4A-C3A-C2A	-5.97	91.37	113.24
28	BC	5517	DGD	C4B-C3B-C2B	-5.96	91.39	113.24
31	AD	407	LMG	C13-C12-C11	-5.92	91.53	113.24
28	AC	518	DGD	C3G-O3G-C1D	-5.90	101.66	113.76
30	BB	5601	SQD	O8-S-C6	-5.89	98.81	106.01
28	BC	5518	DGD	C6D-O5D-C1E	-5.87	101.72	113.76
24	AA	405	CLA	CAA-C2A-C1A	-5.85	92.81	111.97
30	BB	5625	SQD	O8-S-C6	-5.83	98.90	106.01
24	BA	5406	CLA	CAA-C2A-C1A	-5.82	92.90	111.97
28	BC	5518	DGD	C3G-O3G-C1D	-5.81	101.84	113.76
28	AC	517	DGD	C6D-O5D-C1E	-5.78	101.91	113.76
32	BD	5411	LMT	C1B-O1B-C4'	-5.72	104.06	118.00
35	AD	405	PL9	C10-C9-C8	-5.69	108.51	123.69
28	BC	5519	DGD	C6D-C5D-C4D	-5.67	99.91	112.00
31	BD	5409	LMG	C17-C16-C15	-5.66	85.27	114.45
28	AC	517	DGD	C6D-C5D-C4D	-5.61	100.05	112.00
31	AD	407	LMG	C17-C16-C15	-5.59	85.67	114.45
28	AC	518	DGD	C6D-O5D-C1E	-5.57	102.33	113.76
28	BC	5517	DGD	C6D-C5D-C4D	-5.54	100.20	112.00
32	AD	409	LMT	C1B-O1B-C4'	-5.53	104.52	118.00
35	BD	5406	PL9	C10-C9-C8	-5.46	109.11	123.69
24	BB	5612	CLA	CAA-C2A-C1A	-5.45	94.13	111.97
24	AB	608	CLA	CAA-C2A-C1A	-5.42	94.20	111.97
35	AD	405	PL9	C22-C23-C24	-5.31	114.33	127.68
24	BA	5407	CLA	CAA-C2A-C1A	-5.27	94.72	111.97
30	BB	5625	SQD	O9-S-C6	-5.26	102.33	106.83
24	AC	505	CLA	CAA-CBA-CGA	-5.22	97.64	113.35
24	BC	5505	CLA	CAA-CBA-CGA	-5.20	97.68	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BV	5201	HEM	CBD-CAD-C3D	-5.18	102.58	112.47
35	BD	5406	PL9	C22-C23-C24	-5.14	114.77	127.68
24	BB	5611	CLA	CAA-C2A-C1A	-5.14	95.14	111.97
28	BH	5101	DGD	C6D-O5D-C1E	-5.12	103.26	113.76
28	BH	5101	DGD	C6D-C5D-C4D	-5.11	101.12	112.00
24	AB	607	CLA	CAA-C2A-C1A	-5.07	95.36	111.97
28	AC	518	DGD	C6D-C5D-C4D	-5.05	101.24	112.00
28	AH	101	DGD	C6D-C5D-C4D	-5.04	101.26	112.00
30	BB	5601	SQD	O9-S-C6	-5.04	102.52	106.83
36	AV	201	HEM	CBD-CAD-C3D	-5.04	102.86	112.47
24	AA	406	CLA	CAA-C2A-C1A	-5.03	95.48	111.97
31	BD	5409	LMG	C9-C8-C7	-5.03	100.51	111.86
31	AD	407	LMG	C9-C8-C7	-5.00	100.58	111.86
28	BC	5519	DGD	O2G-C2G-C1G	-4.96	90.41	108.44
28	BC	5518	DGD	C6D-C5D-C4D	-4.90	101.56	112.00
28	AH	101	DGD	C6D-O5D-C1E	-4.89	103.73	113.76
27	AJ	101	BCR	C1-C6-C5	-4.87	115.75	122.59
28	BC	5519	DGD	C1D-O6D-C5D	-4.84	104.59	113.72
28	AH	101	DGD	O3G-C3G-C2G	-4.83	99.50	110.99
27	BJ	5101	BCR	C1-C6-C5	-4.83	115.81	122.59
31	AC	521	LMG	C7-O1-C1	-4.83	103.86	113.76
30	BF	5102	SQD	O9-S-C6	-4.81	102.72	106.83
31	BC	5521	LMG	C7-O1-C1	-4.81	103.90	113.76
31	BD	5408	LMG	O8-C9-C8	-4.80	96.59	108.66
31	BC	5521	LMG	C13-C12-C11	-4.79	95.69	113.24
31	AC	521	LMG	C13-C12-C11	-4.78	95.72	113.24
30	AF	102	SQD	O9-S-C6	-4.77	102.75	106.83
35	BD	5406	PL9	C12-C13-C14	-4.76	115.73	127.68
28	BC	5519	DGD	C1E-C2E-C3E	-4.75	101.15	109.98
31	BE	5101	LMG	C7-O1-C1	-4.73	104.06	113.76
30	AB	622	SQD	O9-S-C6	-4.73	102.79	106.83
30	AB	627	SQD	O9-S-C6	-4.72	102.79	106.83
31	AA	414	LMG	C7-O1-C1	-4.72	104.08	113.76
30	BA	5414	SQD	O9-S-C6	-4.70	102.81	106.83
30	AA	416	SQD	O9-S-C6	-4.70	102.81	106.83
28	BC	5518	DGD	C1D-O6D-C5D	-4.69	104.88	113.72
28	BC	5517	DGD	C4A-C3A-C2A	-4.67	96.12	113.24
31	AJ	102	LMG	O8-C9-C8	-4.67	96.92	108.66
28	AC	519	DGD	O2G-C2G-C1G	-4.66	91.50	108.44
28	AC	519	DGD	C1D-O6D-C5D	-4.65	104.95	113.72
30	BA	5401	SQD	O9-S-C6	-4.64	102.86	106.83
35	AD	405	PL9	C12-C13-C14	-4.63	116.06	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BH	5101	DGD	O3G-C3G-C2G	-4.61	100.01	110.99
36	AF	101	HEM	CBD-CAD-C3D	-4.60	103.69	112.47
36	BF	5101	HEM	CBD-CAD-C3D	-4.58	103.74	112.47
24	AB	614	CLA	C2C-C1C-NC	-4.55	107.10	110.22
28	AC	518	DGD	C1D-O6D-C5D	-4.54	105.16	113.72
24	BC	5511	CLA	C2C-C1C-NC	-4.54	107.10	110.22
27	AD	406	BCR	C38-C26-C27	-4.52	104.87	113.45
28	AC	517	DGD	C4A-C3A-C2A	-4.50	96.74	113.24
24	AC	511	CLA	C2C-C1C-NC	-4.49	107.14	110.22
28	AC	519	DGD	C1E-C2E-C3E	-4.47	101.68	109.98
24	AB	608	CLA	CAA-CBA-CGA	-4.45	99.96	113.35
25	AA	408	MST	N5-C6-N1	-4.41	119.57	126.23
24	AC	504	CLA	CAA-C2A-C1A	-4.40	97.56	111.97
27	AJ	101	BCR	C38-C26-C27	-4.38	105.14	113.45
25	BA	5409	MST	N5-C6-N1	-4.38	119.61	126.23
24	BB	5618	CLA	C2C-C1C-NC	-4.35	107.24	110.22
27	AK	102	BCR	C33-C5-C4	-4.34	105.21	113.45
27	BD	5407	BCR	C38-C26-C27	-4.31	105.28	113.45
24	BC	5504	CLA	CAA-C2A-C1A	-4.29	97.90	111.97
31	AD	407	LMG	C15-C14-C13	-4.27	92.47	114.45
31	BA	5402	LMG	O8-C9-C8	-4.26	97.96	108.66
31	BD	5409	LMG	C15-C14-C13	-4.25	92.55	114.45
24	BB	5612	CLA	CAA-CBA-CGA	-4.24	100.59	113.35
28	AH	101	DGD	C5B-C4B-C3B	-4.23	92.68	114.45
28	AA	411	DGD	C1G-O1G-C1A	-4.23	104.42	117.13
28	BA	5412	DGD	C1G-O1G-C1A	-4.22	104.43	117.13
27	BJ	5101	BCR	C38-C26-C27	-4.22	105.45	113.45
27	AB	618	BCR	C38-C26-C27	-4.21	105.47	113.45
28	BH	5101	DGD	C5B-C4B-C3B	-4.19	92.85	114.45
32	BB	5626	LMT	C1B-O1B-C4'	-4.16	107.85	118.00
27	BB	5622	BCR	C38-C26-C27	-4.16	105.56	113.45
31	AI	101	LMG	C9-C8-C7	-4.15	102.50	111.86
28	BE	5102	DGD	C6D-O5D-C1E	-4.15	105.25	113.76
24	BB	5607	CLA	C2C-C1C-NC	-4.15	107.38	110.22
28	BH	5101	DGD	O3G-C1D-C2D	-4.14	101.48	108.23
28	AB	628	DGD	C4B-C3B-C2B	-4.13	98.10	113.24
28	AC	519	DGD	C8A-C7A-C6A	-4.13	93.20	114.45
27	BX	5101	BCR	C38-C26-C27	-4.11	105.66	113.45
27	BK	5102	BCR	C33-C5-C4	-4.10	105.67	113.45
25	AA	408	MST	N5-C4-N3	-4.10	120.03	126.23
27	BC	5516	BCR	C33-C5-C4	-4.09	105.69	113.45
28	BC	5519	DGD	C8A-C7A-C6A	-4.09	93.40	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	5602	DGD	C4B-C3B-C2B	-4.09	98.26	113.24
27	BB	5621	BCR	C38-C26-C27	-4.08	105.71	113.45
28	AH	101	DGD	C3B-C2B-C1B	-4.07	98.73	113.58
28	AH	101	DGD	O3G-C1D-C2D	-4.06	101.60	108.23
28	AC	517	DGD	C1D-O6D-C5D	-4.06	106.07	113.72
28	BB	5602	DGD	O1G-C1G-C2G	-4.06	98.46	108.66
27	BT	5101	BCR	C33-C5-C4	-4.04	105.79	113.45
28	BH	5101	DGD	C3B-C2B-C1B	-4.04	98.84	113.58
27	AX	101	BCR	C38-C26-C27	-4.03	105.80	113.45
31	BC	5520	LMG	C12-C11-C10	-4.03	98.87	113.58
28	BC	5517	DGD	C1D-O6D-C5D	-4.03	106.13	113.72
27	AT	101	BCR	C33-C5-C4	-4.03	105.81	113.45
31	BD	5410	LMG	C19-C18-C17	-4.02	93.72	114.45
32	AB	629	LMT	C1-O1'-C1'	-4.02	106.96	113.87
31	AA	417	LMG	O8-C9-C8	-4.01	98.58	108.66
25	BA	5409	MST	N5-C4-N3	-4.00	120.19	126.23
28	AE	101	DGD	C6D-O5D-C1E	-4.00	105.56	113.76
28	BC	5518	DGD	C8A-C7A-C6A	-4.00	93.86	114.45
32	AB	623	LMT	C1B-O1B-C4'	-4.00	108.26	118.00
28	AB	628	DGD	O1G-C1G-C2G	-3.99	98.63	108.66
31	AD	408	LMG	C19-C18-C17	-3.98	93.94	114.45
28	AC	518	DGD	C8A-C7A-C6A	-3.98	93.96	114.45
27	AJ	101	BCR	C30-C25-C26	-3.97	117.00	122.59
31	BI	5101	LMG	C9-C8-C7	-3.97	102.89	111.86
31	AD	408	LMG	C7-O1-C1	-3.97	105.61	113.76
24	AC	513	CLA	C2C-C1C-NC	-3.97	107.50	110.22
27	AC	514	BCR	C38-C26-C27	-3.97	105.93	113.45
31	AC	520	LMG	C12-C11-C10	-3.96	99.12	113.58
24	AB	603	CLA	C2C-C1C-NC	-3.96	107.50	110.22
27	AB	617	BCR	C38-C26-C27	-3.96	105.94	113.45
27	AC	515	BCR	C38-C26-C27	-3.95	105.96	113.45
31	BD	5410	LMG	C7-O1-C1	-3.94	105.68	113.76
27	AC	516	BCR	C33-C5-C4	-3.93	105.99	113.45
24	BC	5508	CLA	CAA-C2A-C1A	-3.93	99.09	111.97
28	AC	518	DGD	C3G-C2G-C1G	-3.93	103.00	111.86
24	BC	5505	CLA	CAA-C2A-C1A	-3.92	99.12	111.97
27	BC	5515	BCR	C33-C5-C4	-3.92	106.02	113.45
27	BB	5621	BCR	C33-C5-C4	-3.91	106.04	113.45
28	BC	5519	DGD	O1G-C1G-C2G	-3.90	98.84	108.66
27	BJ	5101	BCR	C30-C25-C26	-3.90	117.11	122.59
28	BC	5518	DGD	C3G-C2G-C1G	-3.90	103.06	111.86
28	AC	517	DGD	O3G-C1D-C2D	-3.90	101.87	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	515	BCR	C33-C5-C4	-3.90	106.05	113.45
32	BB	5603	LMT	C1-O1'-C1'	-3.90	107.17	113.87
24	AC	505	CLA	CAA-C2A-C1A	-3.87	99.30	111.97
27	BT	5101	BCR	C38-C26-C27	-3.86	106.12	113.45
27	AC	516	BCR	C38-C26-C27	-3.86	106.13	113.45
24	BC	5513	CLA	C2C-C1C-NC	-3.85	107.58	110.22
27	BJ	5101	BCR	C33-C5-C4	-3.84	106.17	113.45
28	AC	519	DGD	C6B-C5B-C4B	-3.83	94.73	114.45
27	AT	101	BCR	C38-C26-C27	-3.81	106.22	113.45
24	AC	508	CLA	CAA-C2A-C1A	-3.80	99.52	111.97
27	AK	102	BCR	C38-C26-C27	-3.80	106.25	113.45
27	BC	5515	BCR	C38-C26-C27	-3.80	106.25	113.45
27	AJ	101	BCR	C33-C5-C4	-3.79	106.26	113.45
32	BC	5522	LMT	O1'-C1-C2	-3.78	96.18	109.68
31	AB	621	LMG	C14-C13-C12	-3.77	95.02	114.45
32	AI	103	LMT	O1'-C1-C2	-3.76	96.26	109.68
28	BC	5519	DGD	C6B-C5B-C4B	-3.76	95.10	114.45
31	BB	5624	LMG	C14-C13-C12	-3.75	95.11	114.45
31	AB	621	LMG	C37-C36-C35	-3.73	95.23	114.45
25	AA	408	MST	N3-C2-N1	-3.73	120.15	126.82
35	BD	5406	PL9	C11-C9-C8	-3.72	113.48	121.10
31	BB	5624	LMG	C37-C36-C35	-3.72	95.28	114.45
27	BC	5516	BCR	C38-C26-C27	-3.72	106.40	113.45
35	AD	405	PL9	C20-C19-C18	-3.72	113.77	123.69
28	BC	5517	DGD	O3G-C1D-C2D	-3.71	102.17	108.23
27	BK	5102	BCR	C38-C26-C27	-3.70	106.43	113.45
27	AD	406	BCR	C30-C25-C26	-3.68	117.42	122.59
28	AC	519	DGD	O1G-C1G-C2G	-3.68	99.42	108.66
27	BD	5407	BCR	C30-C25-C26	-3.68	117.43	122.59
30	AA	413	SQD	O9-S-C6	-3.67	103.69	106.83
27	AB	617	BCR	C33-C5-C4	-3.65	106.52	113.45
25	BA	5409	MST	N3-C2-N1	-3.64	120.32	126.82
27	BA	5411	BCR	C38-C26-C27	-3.63	106.56	113.45
27	AX	101	BCR	C30-C25-C26	-3.62	117.50	122.59
32	BB	5603	LMT	C1B-O1B-C4'	-3.62	109.18	118.00
24	AB	612	CLA	C2C-C1C-NC	-3.62	107.74	110.22
28	BA	5412	DGD	C3A-C2A-C1A	-3.62	100.38	113.58
27	AC	514	BCR	C33-C5-C4	-3.61	106.59	113.45
27	BB	5623	BCR	C38-C26-C27	-3.61	106.60	113.45
27	BC	5514	BCR	C38-C26-C27	-3.61	106.61	113.45
32	AB	629	LMT	C1B-O1B-C4'	-3.60	109.23	118.00
24	AC	501	CLA	CAA-C2A-C1A	-3.59	100.20	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	516	BCR	C1-C6-C5	-3.58	117.56	122.59
24	BC	5501	CLA	CAA-C2A-C1A	-3.58	100.24	111.97
27	AA	410	BCR	C38-C26-C27	-3.58	106.66	113.45
27	BA	5411	BCR	C33-C5-C4	-3.58	106.66	113.45
27	BT	5101	BCR	C30-C25-C26	-3.58	117.56	122.59
28	AA	411	DGD	C3A-C2A-C1A	-3.57	100.54	113.58
27	AK	102	BCR	C1-C6-C5	-3.57	117.58	122.59
35	AD	405	PL9	C11-C9-C8	-3.56	113.81	121.10
27	AT	101	BCR	C30-C25-C26	-3.56	117.59	122.59
28	BA	5412	DGD	O1G-C1A-O1A	-3.55	114.75	123.55
28	AA	411	DGD	O1G-C1A-O1A	-3.53	114.78	123.55
27	BK	5102	BCR	C1-C6-C5	-3.53	117.63	122.59
24	BC	5508	CLA	C2C-C1C-NC	-3.53	107.80	110.22
35	BD	5406	PL9	C20-C19-C18	-3.52	114.29	123.69
31	AB	621	LMG	C12-C11-C10	-3.50	100.80	113.58
27	AK	102	BCR	C30-C25-C26	-3.49	117.68	122.59
27	BX	5101	BCR	C30-C25-C26	-3.48	117.70	122.59
27	AB	619	BCR	C38-C26-C27	-3.48	106.86	113.45
27	BX	5101	BCR	C33-C5-C4	-3.47	106.86	113.45
27	BD	5407	BCR	C33-C5-C4	-3.47	106.87	113.45
27	AB	618	BCR	C30-C25-C26	-3.46	117.72	122.59
27	AA	410	BCR	C33-C5-C4	-3.46	106.89	113.45
31	BB	5624	LMG	C33-C32-C31	-3.46	96.64	114.45
27	BK	5102	BCR	C8-C9-C10	-3.45	113.64	118.94
31	BB	5624	LMG	C12-C11-C10	-3.44	101.01	113.58
24	BC	5511	CLA	CAA-C2A-C1A	-3.44	100.70	111.97
27	BB	5622	BCR	C30-C25-C26	-3.43	117.77	122.59
31	AI	101	LMG	C12-C11-C10	-3.43	101.06	113.58
24	AB	605	CLA	CAA-C2A-C1A	-3.43	100.74	111.97
31	BI	5101	LMG	C12-C11-C10	-3.42	101.09	113.58
31	AI	101	LMG	C7-O1-C1	-3.42	106.74	113.76
27	AX	101	BCR	C33-C5-C4	-3.42	106.97	113.45
24	BB	5615	CLA	C2C-C1C-NC	-3.39	107.89	110.22
27	AC	516	BCR	C30-C25-C26	-3.39	117.82	122.59
24	BB	5618	CLA	CAA-CBA-CGA	-3.38	103.15	113.35
27	AB	618	BCR	C33-C5-C4	-3.37	107.05	113.45
31	BI	5101	LMG	C7-O1-C1	-3.37	106.84	113.76
24	AC	511	CLA	CAA-C2A-C1A	-3.37	100.92	111.97
24	BB	5609	CLA	CAA-C2A-C1A	-3.37	100.93	111.97
31	AB	621	LMG	C33-C32-C31	-3.37	97.09	114.45
27	BC	5516	BCR	C1-C6-C5	-3.36	117.86	122.59
35	BD	5406	PL9	C50-C49-C48	-3.36	112.51	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5502	CLA	CAA-C2A-C1A	-3.36	100.97	111.97
24	AC	508	CLA	C2C-C1C-NC	-3.36	107.92	110.22
28	BH	5101	DGD	C1D-O6D-C5D	-3.35	107.40	113.72
27	AD	406	BCR	C33-C5-C4	-3.35	107.09	113.45
31	BD	5409	LMG	O1-C7-C8	-3.35	103.02	110.99
28	BC	5517	DGD	C6B-C5B-C4B	-3.35	97.20	114.45
28	AC	517	DGD	C6B-C5B-C4B	-3.34	97.22	114.45
27	AB	619	BCR	C33-C5-C4	-3.34	107.12	113.45
31	BD	5408	LMG	O7-C10-C11	-3.32	104.65	111.55
27	AC	515	BCR	C30-C25-C26	-3.32	117.92	122.59
24	AB	614	CLA	CAA-CBA-CGA	-3.32	103.35	113.35
27	BC	5515	BCR	C1-C6-C5	-3.31	117.94	122.59
31	AC	521	LMG	O8-C9-C8	-3.31	100.35	108.66
27	AK	102	BCR	C8-C9-C10	-3.30	113.87	118.94
35	AD	405	PL9	C50-C49-C48	-3.28	112.74	122.65
27	BB	5621	BCR	C30-C25-C26	-3.28	117.98	122.59
24	BB	5615	CLA	CAA-C2A-C1A	-3.28	101.23	111.97
27	BC	5514	BCR	C33-C5-C4	-3.27	107.26	113.45
31	AD	408	LMG	C17-C16-C15	-3.26	97.65	114.45
27	BK	5102	BCR	C30-C25-C26	-3.26	118.01	122.59
24	AC	501	CLA	CAA-CBA-CGA	-3.26	103.53	113.35
27	AC	515	BCR	C1-C6-C5	-3.26	118.01	122.59
31	AM	101	LMG	C12-C11-C10	-3.25	101.71	113.58
24	AB	614	CLA	CAA-C2A-C1A	-3.25	101.34	111.97
31	BC	5521	LMG	O8-C9-C8	-3.25	100.50	108.66
27	AC	514	BCR	C1-C6-C5	-3.24	118.03	122.59
27	BB	5623	BCR	C33-C5-C4	-3.24	107.31	113.45
27	BX	5101	BCR	C1-C6-C5	-3.24	118.04	122.59
24	AA	406	CLA	O2A-CGA-O1A	-3.24	115.52	123.55
27	BK	5102	BCR	C12-C13-C14	-3.23	113.98	118.94
24	BB	5616	CLA	C2C-C1C-NC	-3.23	108.00	110.22
28	AC	519	DGD	C1D-C2D-C3D	-3.23	103.98	109.98
24	AC	504	CLA	C2C-C1C-NC	-3.23	108.01	110.22
34	BD	5404	PHO	CBD-CHA-C4D	-3.23	104.91	108.54
24	AC	503	CLA	C7-C6-C5	-3.23	104.15	113.11
24	BB	5611	CLA	CAA-CBA-CGA	-3.22	103.64	113.35
27	BC	5516	BCR	C30-C25-C26	-3.22	118.07	122.59
24	BC	5508	CLA	O1D-CGD-CBD	-3.22	118.82	124.60
24	BA	5406	CLA	C3D-CAD-CBD	-3.21	103.05	107.60
24	BB	5618	CLA	CAA-C2A-C1A	-3.21	101.44	111.97
28	AH	101	DGD	C1D-O6D-C5D	-3.21	107.66	113.72
27	AB	617	BCR	C30-C25-C26	-3.21	118.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	502	CLA	CAA-C2A-C1A	-3.21	101.47	111.97
27	BC	5515	BCR	C30-C25-C26	-3.21	118.09	122.59
31	AC	520	LMG	C14-C13-C12	-3.20	97.94	114.45
31	BD	5410	LMG	C17-C16-C15	-3.20	97.98	114.45
28	BH	5101	DGD	C3G-C2G-C1G	-3.19	104.65	111.86
31	AD	407	LMG	O1-C7-C8	-3.19	103.41	110.99
24	AB	611	CLA	C2C-C1C-NC	-3.17	108.04	110.22
24	BC	5501	CLA	CAA-CBA-CGA	-3.17	103.79	113.35
35	BD	5406	PL9	C35-C34-C33	-3.16	115.25	123.69
24	BA	5407	CLA	O2A-CGA-O1A	-3.16	115.70	123.55
27	BB	5622	BCR	C33-C5-C4	-3.16	107.46	113.45
24	BA	5406	CLA	O2A-CGA-O1A	-3.15	115.73	123.55
31	BC	5520	LMG	C14-C13-C12	-3.14	98.27	114.45
24	AB	607	CLA	C2C-C1C-NC	-3.14	108.07	110.22
35	AD	405	PL9	C35-C34-C33	-3.13	115.35	123.69
31	BD	5408	LMG	C15-C14-C13	-3.12	98.37	114.45
31	AC	520	LMG	C9-C8-C7	-3.12	104.82	111.86
24	BB	5610	CLA	C3D-CAD-CBD	-3.12	103.19	107.60
31	BM	5102	LMG	C12-C11-C10	-3.11	102.21	113.58
31	AJ	102	LMG	C15-C14-C13	-3.11	98.41	114.45
28	BC	5519	DGD	CBA-CAA-C9A	-3.10	98.49	114.45
27	AA	410	BCR	C30-C25-C26	-3.10	118.24	122.59
28	AC	517	DGD	C3G-O3G-C1D	-3.09	107.41	113.76
27	BX	5101	BCR	C12-C13-C14	-3.09	114.20	118.94
31	BD	5408	LMG	O7-C8-C9	-3.09	97.20	108.44
24	BB	5611	CLA	C2C-C1C-NC	-3.09	108.10	110.22
24	AA	405	CLA	CAA-CBA-CGA	-3.08	104.07	113.35
28	AH	101	DGD	C3G-C2G-C1G	-3.08	104.91	111.86
31	BB	5624	LMG	O7-C10-O9	-3.08	116.00	123.68
31	BC	5520	LMG	C9-C8-C7	-3.07	104.93	111.86
31	AJ	102	LMG	O7-C10-C11	-3.07	105.19	111.55
24	BD	5405	CLA	CAA-C2A-C1A	-3.06	101.94	111.97
27	BC	5514	BCR	C1-C6-C5	-3.06	118.29	122.59
24	AB	611	CLA	CAA-C2A-C1A	-3.06	101.94	111.97
24	BC	5503	CLA	C7-C6-C5	-3.06	104.61	113.11
24	BC	5503	CLA	O1D-CGD-CBD	-3.06	119.11	124.60
24	AC	511	CLA	C6-C7-C8	-3.06	105.70	115.73
24	BA	5407	CLA	C2C-C1C-NC	-3.05	108.13	110.22
27	AK	102	BCR	C12-C13-C14	-3.05	114.26	118.94
31	AJ	102	LMG	O7-C8-C9	-3.04	97.37	108.44
32	BC	5522	LMT	C4-C3-C2	-3.04	98.77	114.45
24	AD	404	CLA	CAA-C2A-C1A	-3.04	102.00	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	5411	BCR	C30-C25-C26	-3.04	118.32	122.59
27	BC	5515	BCR	C12-C13-C14	-3.04	114.28	118.94
27	AX	101	BCR	C12-C13-C14	-3.04	114.28	118.94
30	AB	622	SQD	C3-C4-C5	-3.04	104.87	110.22
24	AA	405	CLA	C3D-CAD-CBD	-3.03	103.31	107.60
32	AI	103	LMT	C4-C3-C2	-3.03	98.87	114.45
34	BD	5404	PHO	CAB-C3B-C2B	-3.02	118.44	128.56
27	BB	5623	BCR	C30-C25-C26	-3.02	118.35	122.59
24	BC	5510	CLA	O1D-CGD-CBD	-3.02	119.18	124.60
28	BC	5517	DGD	C3G-O3G-C1D	-3.02	107.57	113.76
24	BA	5406	CLA	CAA-CBA-CGA	-3.01	104.28	113.35
31	AB	621	LMG	O7-C10-O9	-3.01	116.17	123.68
27	AB	619	BCR	C30-C25-C26	-3.00	118.37	122.59
32	BB	5603	LMT	C9-C8-C7	-3.00	98.99	114.45
28	AC	519	DGD	CBA-CAA-C9A	-3.00	99.00	114.45
28	AA	411	DGD	O6D-C1D-C2D	-3.00	104.51	110.30
27	AC	514	BCR	C30-C25-C26	-3.00	118.38	122.59
24	AA	405	CLA	O2A-CGA-O1A	-3.00	116.11	123.55
34	AD	403	PHO	CAB-C3B-C2B	-2.99	118.54	128.56
32	AB	629	LMT	C9-C8-C7	-2.99	99.06	114.45
24	AB	606	CLA	C3D-CAD-CBD	-2.98	103.38	107.60
27	AT	101	BCR	C1-C6-C5	-2.98	118.40	122.59
24	AB	608	CLA	C2C-C1C-NC	-2.98	108.18	110.22
34	AD	402	PHO	CAB-C3B-C2B	-2.98	118.58	128.56
24	BC	5511	CLA	C6-C7-C8	-2.98	105.95	115.73
27	AD	406	BCR	C12-C13-C14	-2.97	114.38	118.94
24	BC	5507	CLA	C7-C6-C5	-2.97	104.84	113.11
30	BB	5625	SQD	C3-C4-C5	-2.97	104.98	110.22
27	AC	515	BCR	C12-C13-C14	-2.97	114.38	118.94
24	BC	5509	CLA	C2C-C1C-NC	-2.97	108.19	110.22
32	BB	5604	LMT	C4-C3-C2	-2.97	99.16	114.45
24	AB	607	CLA	CAA-CBA-CGA	-2.97	104.41	113.35
27	AX	101	BCR	C1-C6-C5	-2.97	118.42	122.59
24	AC	506	CLA	CAA-C2A-C1A	-2.97	102.26	111.97
27	BT	5101	BCR	C1-C6-C5	-2.97	118.42	122.59
24	BB	5617	CLA	C2C-C1C-NC	-2.96	108.19	110.22
24	BC	5504	CLA	C2C-C1C-NC	-2.96	108.19	110.22
24	AC	509	CLA	C2C-C1C-NC	-2.96	108.19	110.22
28	BC	5519	DGD	C8B-C7B-C6B	-2.96	99.21	114.45
28	BA	5412	DGD	O6D-C1D-C2D	-2.95	104.60	110.30
24	AC	504	CLA	CAA-CBA-CGA	-2.95	104.47	113.35
32	AB	630	LMT	C4-C3-C2	-2.95	99.27	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AH	101	DGD	C7B-C6B-C5B	-2.95	99.28	114.45
35	BD	5406	PL9	C15-C14-C13	-2.94	115.83	123.69
34	AD	403	PHO	CBD-CHA-C4D	-2.94	105.22	108.54
24	BC	5504	CLA	CAA-CBA-CGA	-2.94	104.50	113.35
28	AC	519	DGD	C8B-C7B-C6B	-2.93	99.34	114.45
24	AB	603	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
24	BC	5506	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
24	BC	5503	CLA	C3D-CAD-CBD	-2.93	103.46	107.60
24	AB	603	CLA	C7-C6-C5	-2.92	105.00	113.11
24	AA	407	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
27	AD	406	BCR	C23-C22-C21	-2.91	114.48	118.94
24	AB	607	CLA	CAA-C2A-C3A	-2.91	104.84	112.81
32	BB	5603	LMT	C4-C3-C2	-2.90	99.51	114.45
25	BA	5409	MST	C15-N14-C6	-2.90	120.03	123.69
28	BH	5101	DGD	C7B-C6B-C5B	-2.90	99.53	114.45
27	BC	5514	BCR	C23-C22-C21	-2.89	114.50	118.94
31	BI	5101	LMG	C14-C13-C12	-2.89	99.56	114.45
31	BD	5410	LMG	C32-C31-C30	-2.89	99.56	114.45
30	AA	416	SQD	C3-C4-C5	-2.89	105.13	110.22
35	AD	405	PL9	C25-C24-C23	-2.88	116.01	123.69
24	AB	605	CLA	C2C-C1C-NC	-2.87	108.25	110.22
34	BD	5403	PHO	CAB-C3B-C2B	-2.87	118.94	128.56
24	AC	507	CLA	C7-C6-C5	-2.87	105.14	113.11
30	BA	5401	SQD	C3-C4-C5	-2.86	105.17	110.22
24	AA	407	CLA	C2C-C1C-NC	-2.86	108.26	110.22
24	BB	5611	CLA	O2A-CGA-O1A	-2.86	116.45	123.55
31	AD	408	LMG	C32-C31-C30	-2.86	99.73	114.45
24	BB	5610	CLA	O2A-CGA-O1A	-2.86	116.46	123.55
24	AB	603	CLA	CAA-C2A-C3A	-2.85	104.98	112.81
24	BC	5508	CLA	C3D-CAD-CBD	-2.85	103.57	107.60
24	BB	5616	CLA	O1D-CGD-CBD	-2.84	119.49	124.60
24	BB	5610	CLA	CAA-C2A-C1A	-2.84	102.67	111.97
31	BB	5624	LMG	C16-C15-C14	-2.83	99.86	114.45
24	AC	508	CLA	C3D-CAD-CBD	-2.83	103.60	107.60
24	BC	5502	CLA	C3D-CAD-CBD	-2.82	103.61	107.60
34	BD	5404	PHO	C2A-C1A-NA	-2.82	108.48	111.91
27	BB	5622	BCR	C1-C6-C5	-2.82	118.63	122.59
24	BA	5408	CLA	C2C-C1C-NC	-2.82	108.29	110.22
31	BL	5101	LMG	C15-C14-C13	-2.81	99.95	114.45
31	AI	101	LMG	C14-C13-C12	-2.81	99.95	114.45
24	AC	502	CLA	C2C-C1C-NC	-2.81	108.29	110.22
35	AD	405	PL9	C15-C14-C13	-2.81	116.20	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AD	406	BCR	C1-C6-C5	-2.81	118.65	122.59
24	BB	5607	CLA	CAA-C2A-C1A	-2.81	102.78	111.97
31	AB	621	LMG	C16-C15-C14	-2.80	100.03	114.45
24	BC	5510	CLA	C3D-CAD-CBD	-2.80	103.64	107.60
27	AC	514	BCR	C23-C22-C21	-2.79	114.66	118.94
27	AA	410	BCR	C1-C6-C5	-2.79	118.67	122.59
27	BD	5407	BCR	C1-C6-C5	-2.78	118.68	122.59
24	BB	5607	CLA	CAA-C2A-C3A	-2.78	105.18	112.81
24	AA	406	CLA	C2C-C1C-NC	-2.78	108.31	110.22
24	BA	5405	CLA	C3D-CAD-CBD	-2.78	103.66	107.60
24	BB	5611	CLA	CAA-C2A-C3A	-2.78	105.19	112.81
32	AB	629	LMT	C4-C3-C2	-2.78	100.14	114.45
36	AF	101	HEM	C4C-C3C-C2C	-2.78	104.96	106.90
31	AB	620	LMG	C15-C14-C13	-2.78	100.14	114.45
27	BB	5623	BCR	C1-C6-C5	-2.77	118.69	122.59
24	AB	612	CLA	O1D-CGD-CBD	-2.76	119.65	124.60
24	BB	5607	CLA	C7-C6-C5	-2.76	105.45	113.11
24	BA	5408	CLA	CAA-C2A-C1A	-2.75	102.96	111.97
27	BD	5407	BCR	C23-C22-C21	-2.75	114.72	118.94
24	BC	5501	CLA	O2A-CGA-O1A	-2.75	116.73	123.55
35	BD	5406	PL9	C25-C24-C23	-2.74	116.38	123.69
27	BC	5516	BCR	C40-C30-C29	-2.73	98.02	108.80
34	BD	5404	PHO	O1D-CGD-CBD	-2.72	119.71	124.60
31	BD	5410	LMG	C15-C14-C13	-2.72	100.43	114.45
24	AB	606	CLA	CAA-C2A-C1A	-2.72	103.06	111.97
24	AC	503	CLA	O1D-CGD-CBD	-2.72	119.72	124.60
34	AD	403	PHO	O1D-CGD-CBD	-2.71	119.73	124.60
35	BD	5406	PL9	C7-C3-C2	-2.71	119.37	123.23
24	AB	607	CLA	O2A-CGA-O1A	-2.71	116.82	123.55
32	BI	5102	LMT	C4-C3-C2	-2.70	100.52	114.45
24	AA	405	CLA	C2C-C1C-NC	-2.70	108.37	110.22
24	AB	611	CLA	O1D-CGD-CBD	-2.70	119.76	124.60
32	AI	102	LMT	C4-C3-C2	-2.69	100.59	114.45
24	AA	406	CLA	O1D-CGD-CBD	-2.69	119.77	124.60
28	BC	5519	DGD	C1D-C2D-C3D	-2.69	104.98	109.98
24	AC	508	CLA	O1D-CGD-CBD	-2.69	119.77	124.60
27	BT	5101	BCR	C8-C9-C10	-2.68	114.83	118.94
24	AC	510	CLA	O1D-CGD-CBD	-2.68	119.79	124.60
27	BC	5514	BCR	C30-C25-C26	-2.68	118.83	122.59
24	AA	406	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
27	AC	516	BCR	C40-C30-C29	-2.68	98.25	108.80
27	AB	618	BCR	C1-C6-C5	-2.67	118.83	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	619	BCR	C1-C6-C5	-2.67	118.84	122.59
24	BA	5408	CLA	O1D-CGD-CBD	-2.66	119.83	124.60
27	BB	5621	BCR	C1-C6-C5	-2.65	118.86	122.59
24	BB	5609	CLA	C2C-C1C-NC	-2.65	108.40	110.22
24	BB	5606	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
24	BB	5612	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
24	BC	5505	CLA	C3D-CAD-CBD	-2.64	103.87	107.60
24	AB	611	CLA	C7-C6-C5	-2.64	105.78	113.11
31	AM	101	LMG	O7-C10-O9	-2.63	117.11	123.68
24	AC	503	CLA	C3D-CAD-CBD	-2.63	103.88	107.60
24	BB	5612	CLA	C2C-C1C-NC	-2.63	108.42	110.22
27	BT	5101	BCR	C19-C18-C17	-2.62	114.92	118.94
27	AT	101	BCR	C8-C9-C10	-2.62	114.92	118.94
27	AT	101	BCR	C19-C18-C17	-2.62	114.92	118.94
27	AT	101	BCR	C23-C22-C21	-2.62	114.92	118.94
24	AA	404	CLA	C3D-CAD-CBD	-2.62	103.89	107.60
28	AC	517	DGD	C8A-C7A-C6A	-2.62	100.97	114.45
24	AB	606	CLA	O2A-CGA-O1A	-2.62	117.05	123.55
24	BB	5615	CLA	C7-C6-C5	-2.62	105.84	113.11
28	AC	519	DGD	O6D-C1D-C2D	-2.61	105.25	110.30
31	AA	417	LMG	C15-C14-C13	-2.61	101.00	114.45
30	BA	5414	SQD	O8-S-O9	-2.61	105.38	111.37
24	BB	5615	CLA	C3D-CAD-CBD	-2.61	103.91	107.60
24	BB	5607	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
31	AD	408	LMG	C15-C14-C13	-2.60	101.05	114.45
30	BB	5601	SQD	C3-C4-C5	-2.60	105.63	110.22
24	BB	5607	CLA	CAA-CBA-CGA	-2.60	105.51	113.35
27	BC	5515	BCR	C19-C18-C17	-2.60	114.95	118.94
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	AC	515	BCR	C19-C18-C17	-2.60	114.96	118.94
36	BF	5101	HEM	C4C-C3C-C2C	-2.60	105.08	106.90
24	AB	602	CLA	C3D-CAD-CBD	-2.59	103.93	107.60
24	AB	610	CLA	O1D-CGD-CBD	-2.59	119.94	124.60
31	BA	5402	LMG	C15-C14-C13	-2.59	101.12	114.45
27	AB	617	BCR	C8-C9-C10	-2.59	114.97	118.94
34	BD	5403	PHO	O1D-CGD-CBD	-2.59	119.95	124.60
24	BB	5607	CLA	O1D-CGD-CBD	-2.59	119.96	124.60
31	AC	520	LMG	C32-C31-C30	-2.58	101.14	114.45
24	BB	5608	CLA	O2A-CGA-O1A	-2.58	117.15	123.55
34	AD	403	PHO	C6-C7-C8	-2.58	107.27	115.73
31	BM	5102	LMG	O7-C10-O9	-2.58	117.25	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5502	CLA	O1D-CGD-CBD	-2.57	119.98	124.60
24	BB	5615	CLA	O1D-CGD-CBD	-2.57	119.98	124.60
24	BA	5406	CLA	C2C-C1C-NC	-2.57	108.46	110.22
29	BA	5415	LHG	C5-O7-C7	-2.57	111.81	117.88
27	BD	5407	BCR	C12-C13-C14	-2.56	115.01	118.94
24	BC	5504	CLA	O1D-CGD-CBD	-2.56	120.00	124.60
29	AA	415	LHG	C5-O7-C7	-2.56	111.83	117.88
24	BB	5608	CLA	C3D-CAD-CBD	-2.56	103.98	107.60
24	AD	401	CLA	O2A-CGA-O1A	-2.56	117.20	123.55
24	AD	401	CLA	O1D-CGD-CBD	-2.56	120.01	124.60
24	AA	405	CLA	O1D-CGD-CBD	-2.55	120.02	124.60
24	AA	405	CLA	CMB-C2B-C1B	-2.54	124.55	128.46
24	AB	603	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
34	AD	403	PHO	C2A-C1A-NA	-2.53	108.83	111.91
35	AD	405	PL9	C7-C3-C2	-2.53	119.63	123.23
24	AC	508	CLA	O2A-CGA-O1A	-2.53	117.26	123.55
27	BC	5514	BCR	C12-C13-C14	-2.53	115.06	118.94
31	AA	417	LMG	C32-C31-C30	-2.53	101.42	114.45
31	BC	5520	LMG	C32-C31-C30	-2.53	101.42	114.45
24	AB	613	CLA	C6-C7-C8	-2.53	107.43	115.73
24	AC	503	CLA	CAA-C2A-C1A	-2.52	103.71	111.97
27	BA	5411	BCR	C1-C6-C5	-2.52	119.05	122.59
24	AB	613	CLA	C3D-CAD-CBD	-2.52	104.03	107.60
24	BC	5506	CLA	C3D-CAD-CBD	-2.52	104.04	107.60
36	AV	201	HEM	C4C-C3C-C2C	-2.51	105.14	106.90
24	AA	406	CLA	CAA-CBA-CGA	-2.51	105.77	113.35
24	BD	5402	CLA	O1D-CGD-CBD	-2.51	120.09	124.60
28	AA	411	DGD	C5A-C4A-C3A	-2.51	101.53	114.45
30	AB	627	SQD	C3-C4-C5	-2.51	105.80	110.22
31	BA	5402	LMG	C32-C31-C30	-2.50	101.56	114.45
24	BB	5619	CLA	C2C-C1C-NC	-2.50	108.51	110.22
31	AJ	102	LMG	C32-C31-C30	-2.50	101.58	114.45
24	BC	5512	CLA	C3D-CAD-CBD	-2.50	104.07	107.60
27	BB	5621	BCR	C12-C13-C14	-2.50	115.11	118.94
24	BB	5619	CLA	O1D-CGD-CBD	-2.50	120.12	124.60
24	AA	407	CLA	O1D-CGD-CBD	-2.50	120.12	124.60
28	BC	5517	DGD	C8A-C7A-C6A	-2.49	101.60	114.45
24	AB	605	CLA	O1D-CGD-CBD	-2.49	120.12	124.60
27	BT	5101	BCR	C23-C22-C21	-2.49	115.12	118.94
24	AC	501	CLA	O2A-CGA-O1A	-2.49	117.36	123.55
28	BA	5412	DGD	C5A-C4A-C3A	-2.49	101.62	114.45
24	BC	5503	CLA	CAA-C2A-C1A	-2.49	103.82	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	504	CLA	C3D-CAD-CBD	-2.49	104.08	107.60
24	BB	5609	CLA	O1D-CGD-CBD	-2.49	120.13	124.60
28	BC	5519	DGD	O1G-C1A-O1A	-2.48	117.38	123.55
24	AB	605	CLA	CAA-CBA-CGA	-2.48	105.86	113.35
24	BA	5405	CLA	C2C-C1C-NC	-2.48	108.52	110.22
27	AB	617	BCR	C1-C6-C5	-2.48	119.11	122.59
24	AB	610	CLA	C3D-CAD-CBD	-2.48	104.10	107.60
31	AB	621	LMG	C7-O1-C1	-2.47	108.68	113.76
24	BC	5508	CLA	O2A-CGA-O1A	-2.47	117.41	123.55
24	BA	5406	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
32	BC	5522	LMT	O1'-C1'-C2'	-2.47	104.20	108.23
24	AC	510	CLA	O2A-CGA-O1A	-2.47	117.42	123.55
27	BB	5621	BCR	C19-C18-C17	-2.47	115.15	118.94
24	BD	5405	CLA	O1D-CGD-CBD	-2.46	120.17	124.60
24	BB	5614	CLA	C3D-CAD-CBD	-2.46	104.11	107.60
27	BD	5407	BCR	C8-C9-C10	-2.46	115.16	118.94
24	BC	5507	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
24	AB	605	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	BB	5615	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
27	BA	5411	BCR	C12-C13-C14	-2.46	115.17	118.94
31	BD	5408	LMG	C36-C35-C34	-2.46	101.78	114.45
34	AD	402	PHO	C3A-C4A-NA	-2.46	108.82	113.06
24	BB	5613	CLA	O2A-CGA-O1A	-2.46	117.45	123.55
24	AB	607	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
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	AC	502	CLA	O1D-CGD-CBD	-2.45	120.19	124.60
24	BB	5608	CLA	C6-C7-C8	-2.45	107.68	115.73
24	AB	603	CLA	CAA-CBA-CGA	-2.45	105.97	113.35
27	BC	5516	BCR	C23-C22-C21	-2.45	115.18	118.94
24	BB	5609	CLA	C3D-CAD-CBD	-2.45	104.14	107.60
24	AB	610	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
30	AB	622	SQD	O8-S-O9	-2.45	105.76	111.37
30	BB	5625	SQD	O8-S-O9	-2.44	105.77	111.37
24	BC	5508	CLA	CAA-CBA-CGA	-2.44	105.98	113.35
24	BB	5614	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
27	AC	514	BCR	C12-C13-C14	-2.44	115.19	118.94
28	AB	628	DGD	C4A-C3A-C2A	-2.44	104.30	113.24
24	AC	502	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
24	BC	5502	CLA	C2C-C1C-NC	-2.44	108.55	110.22
24	AC	506	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
24	BB	5608	CLA	C2C-C1C-NC	-2.44	108.55	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BD	5403	PHO	C3A-C4A-NA	-2.43	108.86	113.06
30	BF	5102	SQD	C3-C4-C5	-2.43	105.93	110.22
31	BD	5408	LMG	C32-C31-C30	-2.43	101.92	114.45
24	BB	5610	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
28	AC	517	DGD	O2G-C2G-C1G	-2.43	99.61	108.44
24	AD	401	CLA	C6-C7-C8	-2.43	107.76	115.73
32	AI	103	LMT	O1'-C1'-C2'	-2.43	104.27	108.23
31	AC	521	LMG	C15-C14-C13	-2.43	101.95	114.45
27	AB	617	BCR	C12-C13-C14	-2.43	115.22	118.94
24	AC	505	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
24	BC	5513	CLA	C3D-CAD-CBD	-2.42	104.17	107.60
32	BB	5627	LMT	C4-C3-C2	-2.42	101.98	114.45
34	AD	402	PHO	O1D-CGD-CBD	-2.42	120.25	124.60
36	BV	5201	HEM	C4C-C3C-C2C	-2.42	105.21	106.90
24	BB	5616	CLA	C3D-CAD-CBD	-2.42	104.18	107.60
24	AD	401	CLA	CMB-C2B-C1B	-2.41	124.75	128.46
25	AA	408	MST	C15-N14-C6	-2.41	120.65	123.69
28	AC	518	DGD	CBA-CAA-C9A	-2.41	102.03	114.45
24	AB	601	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
24	AC	511	CLA	O1D-CGD-CBD	-2.41	120.27	124.60
24	BB	5609	CLA	CAA-CBA-CGA	-2.41	106.09	113.35
24	BB	5605	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
28	BC	5518	DGD	CBA-CAA-C9A	-2.41	102.05	114.45
31	BC	5521	LMG	C15-C14-C13	-2.41	102.05	114.45
28	BH	5101	DGD	O2G-C1B-O1B	-2.41	117.67	123.68
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
31	AD	408	LMG	O7-C8-C9	-2.40	99.70	108.44
31	BB	5624	LMG	C40-C39-C38	-2.40	102.10	114.45
31	AC	520	LMG	O7-C10-O9	-2.39	117.70	123.68
24	BD	5402	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
24	BA	5406	CLA	O1D-CGD-CBD	-2.39	120.31	124.60
24	BD	5402	CLA	C6-C7-C8	-2.39	107.88	115.73
24	AB	604	CLA	O2A-CGA-O1A	-2.39	117.62	123.55
32	AB	624	LMT	C4-C3-C2	-2.39	102.15	114.45
24	AA	407	CLA	O2A-CGA-O1A	-2.39	117.63	123.55
24	AC	508	CLA	CAA-CBA-CGA	-2.38	106.17	113.35
24	AB	611	CLA	CAA-CBA-CGA	-2.38	106.17	113.35
31	AB	621	LMG	C40-C39-C38	-2.38	102.18	114.45
24	BC	5505	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
24	AB	612	CLA	C3D-CAD-CBD	-2.38	104.23	107.60
31	AD	408	LMG	O8-C9-C8	-2.38	102.68	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BC	5517	DGD	CBA-CAA-C9A	-2.38	102.21	114.45
31	AB	620	LMG	O7-C8-C9	-2.37	99.81	108.44
24	AC	509	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
24	BC	5511	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
24	AA	406	CLA	C3D-CAD-CBD	-2.37	104.25	107.60
31	BD	5410	LMG	O8-C9-C8	-2.37	102.71	108.66
28	AC	517	DGD	CBA-CAA-C9A	-2.36	102.29	114.45
28	BB	5602	DGD	C4A-C3A-C2A	-2.36	104.59	113.24
24	BB	5608	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
27	AB	617	BCR	C19-C18-C17	-2.36	115.32	118.94
24	AB	613	CLA	C2C-C1C-NC	-2.36	108.60	110.22
24	BB	5616	CLA	CAA-CBA-CGA	-2.36	106.25	113.35
24	BA	5407	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
24	AB	604	CLA	C2C-C1C-NC	-2.35	108.61	110.22
24	AB	604	CLA	C6-C7-C8	-2.35	108.00	115.73
24	AB	616	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
31	BM	5102	LMG	C14-C13-C12	-2.35	102.33	114.45
24	BC	5511	CLA	C3D-CAD-CBD	-2.35	104.27	107.60
31	BC	5520	LMG	O1-C7-C8	-2.35	105.40	110.99
27	BB	5621	BCR	C8-C9-C10	-2.35	115.33	118.94
24	AC	511	CLA	C3D-CAD-CBD	-2.35	104.28	107.60
24	BA	5408	CLA	O2A-CGA-O1A	-2.35	117.73	123.55
31	BB	5624	LMG	C7-O1-C1	-2.35	108.95	113.76
24	BA	5407	CLA	CAA-CBA-CGA	-2.34	106.29	113.35
24	AB	612	CLA	CAA-CBA-CGA	-2.34	106.29	113.35
24	BC	5509	CLA	C3D-CAD-CBD	-2.34	104.28	107.60
31	BL	5101	LMG	O7-C8-C9	-2.34	99.92	108.44
24	AB	604	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
28	AB	628	DGD	C6B-C5B-C4B	-2.33	102.44	114.45
24	BD	5402	CLA	O2A-CGA-O1A	-2.33	117.76	123.55
31	AM	101	LMG	C14-C13-C12	-2.33	102.44	114.45
24	BB	5611	CLA	C3D-CAD-CBD	-2.33	104.30	107.60
31	AJ	102	LMG	C36-C35-C34	-2.33	102.47	114.45
28	AH	101	DGD	O2G-C1B-O1B	-2.33	117.87	123.68
24	BB	5611	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
31	AC	521	LMG	C19-C18-C17	-2.32	102.48	114.45
31	BD	5410	LMG	O7-C8-C9	-2.32	99.99	108.44
24	BB	5613	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
30	AF	102	SQD	C3-C4-C5	-2.32	106.13	110.22
28	BE	5102	DGD	C5B-C4B-C3B	-2.32	102.52	114.45
24	BC	5510	CLA	O2A-CGA-O1A	-2.32	117.80	123.55
34	BD	5404	PHO	C6-C7-C8	-2.31	108.14	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5614	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
24	AC	504	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
24	BA	5405	CLA	CAA-C2A-C3A	-2.31	106.48	112.81
24	AA	407	CLA	C3D-CAD-CBD	-2.31	104.33	107.60
27	BC	5516	BCR	C19-C18-C17	-2.30	115.42	118.94
24	BA	5408	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
24	AA	404	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
28	BC	5517	DGD	O2G-C2G-C1G	-2.29	100.10	108.44
24	BA	5406	CLA	C12-C11-C10	-2.29	102.16	113.25
27	AA	410	BCR	C8-C9-C10	-2.29	115.42	118.94
28	BB	5602	DGD	C6B-C5B-C4B	-2.29	102.64	114.45
24	AB	615	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
27	AK	102	BCR	C32-C1-C2	-2.29	99.78	108.80
24	AB	606	CLA	CAA-C2A-C3A	-2.28	106.55	112.81
24	BB	5610	CLA	C2C-C1C-NC	-2.28	108.66	110.22
31	AD	407	LMG	O1-C1-C2	-2.28	104.51	108.23
24	AB	604	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
24	BC	5504	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
31	BD	5409	LMG	C32-C31-C30	-2.28	102.70	114.45
28	AE	101	DGD	C5B-C4B-C3B	-2.28	102.71	114.45
31	AC	520	LMG	O9-C10-C11	-2.27	114.69	123.68
31	BC	5520	LMG	O9-C10-C11	-2.27	114.70	123.68
24	AA	404	CLA	CAA-C2A-C3A	-2.27	106.58	112.81
27	AC	516	BCR	C23-C22-C21	-2.27	115.45	118.94
30	BF	5102	SQD	O8-S-O9	-2.27	106.17	111.37
27	BA	5411	BCR	C8-C9-C10	-2.27	115.46	118.94
31	BD	5409	LMG	C6-C5-C4	-2.27	107.70	113.00
31	BD	5409	LMG	C1-O6-C5	-2.26	109.45	113.72
24	BC	5511	CLA	CAA-CBA-CGA	-2.26	106.53	113.35
27	AB	618	BCR	C23-C22-C21	-2.26	115.47	118.94
24	AD	404	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
24	AB	611	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
24	BA	5407	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
24	AB	602	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
27	AB	619	BCR	C12-C13-C14	-2.26	115.48	118.94
31	BL	5101	LMG	C19-C18-C17	-2.26	102.83	114.45
24	AB	606	CLA	C2C-C1C-NC	-2.26	108.67	110.22
24	AA	404	CLA	C2C-C1C-NC	-2.25	108.68	110.22
24	AC	511	CLA	CAA-CBA-CGA	-2.25	106.56	113.35
24	BA	5407	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
27	AD	406	BCR	C8-C9-C10	-2.25	115.49	118.94
31	AC	520	LMG	O1-C7-C8	-2.25	105.64	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	AI	103	LMT	C3'-C4'-C5'	-2.25	106.11	110.88
31	AD	407	LMG	C32-C31-C30	-2.24	102.89	114.45
31	BD	5409	LMG	O1-C1-C2	-2.24	104.58	108.23
24	AB	611	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
24	AC	509	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
24	AC	505	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
24	BB	5617	CLA	C6-C7-C8	-2.23	108.40	115.73
27	AD	406	BCR	C19-C18-C17	-2.23	115.51	118.94
24	BD	5405	CLA	CAA-CBA-CGA	-2.23	106.62	113.35
27	AA	410	BCR	C12-C13-C14	-2.23	115.52	118.94
35	BD	5406	PL9	C42-C41-C39	-2.23	105.38	112.93
24	AC	507	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
24	BC	5509	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
24	BB	5610	CLA	CAA-C2A-C3A	-2.23	106.70	112.81
27	BT	5101	BCR	C40-C30-C29	-2.23	100.02	108.80
24	BB	5620	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
24	AB	611	CLA	C3D-CAD-CBD	-2.23	104.45	107.60
24	AC	513	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
24	AB	609	CLA	C6-C7-C8	-2.23	108.43	115.73
27	BK	5102	BCR	C32-C1-C2	-2.22	100.04	108.80
28	AC	518	DGD	CDB-CCB-CBB	-2.22	103.01	114.45
34	BD	5404	PHO	C3A-C4A-NA	-2.22	109.23	113.06
31	BC	5520	LMG	O7-C10-O9	-2.22	118.14	123.68
24	AA	404	CLA	C6-C7-C8	-2.22	108.45	115.73
24	AB	603	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
31	BC	5521	LMG	C19-C18-C17	-2.21	103.07	114.45
24	BC	5507	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
24	AB	609	CLA	O2A-CGA-O1A	-2.21	118.07	123.55
31	AB	620	LMG	C19-C18-C17	-2.21	103.08	114.45
28	BC	5518	DGD	CDB-CCB-CBB	-2.21	103.09	114.45
24	AB	609	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
28	AC	518	DGD	C8B-C7B-C6B	-2.20	103.11	114.45
24	AC	503	CLA	C2C-C1C-NC	-2.20	108.71	110.22
27	BD	5407	BCR	C19-C18-C17	-2.20	115.56	118.94
24	AB	611	CLA	O2A-CGA-O1A	-2.20	118.09	123.55
24	BA	5405	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
24	AC	506	CLA	C2C-C1C-NC	-2.20	108.71	110.22
24	BC	5506	CLA	O2A-CGA-O1A	-2.20	118.10	123.55
24	BC	5513	CLA	O2A-CGA-O1A	-2.20	118.10	123.55
31	AB	620	LMG	C17-C16-C15	-2.19	103.15	114.45
24	BA	5405	CLA	C7-C6-C5	-2.19	107.02	113.11
36	AV	201	HEM	CMD-C2D-C1D	-2.19	125.10	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BC	5518	DGD	C8B-C7B-C6B	-2.19	103.17	114.45
24	BB	5615	CLA	O2A-CGA-O1A	-2.19	118.12	123.55
24	AC	513	CLA	O2A-CGA-O1A	-2.18	118.13	123.55
24	BB	5615	CLA	C4-C3-C5	-2.18	111.50	115.29
24	BB	5613	CLA	C6-C7-C8	-2.18	108.56	115.73
24	BB	5618	CLA	C3D-CAD-CBD	-2.18	104.51	107.60
24	BC	5503	CLA	CAA-CBA-CGA	-2.18	106.78	113.35
24	BC	5513	CLA	O1D-CGD-CBD	-2.18	120.69	124.60
24	AB	614	CLA	C3D-CAD-CBD	-2.18	104.52	107.60
27	BK	5102	BCR	C23-C22-C21	-2.18	115.60	118.94
24	AB	609	CLA	C2C-C1C-NC	-2.18	108.73	110.22
24	BB	5613	CLA	CAA-C2A-C1A	-2.18	104.85	111.97
24	AC	503	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
31	BL	5101	LMG	C17-C16-C15	-2.17	103.25	114.45
24	AB	615	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
24	AC	506	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
24	BC	5506	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
24	BB	5615	CLA	CAA-CBA-CGA	-2.17	106.81	113.35
30	AA	413	SQD	O8-S-O9	-2.17	106.40	111.37
31	BM	5102	LMG	C6-C5-C4	-2.17	107.93	113.00
24	AC	502	CLA	CAA-CBA-CGA	-2.17	106.82	113.35
24	AB	608	CLA	C4-C3-C5	-2.17	111.53	115.29
31	AM	101	LMG	C6-C5-C4	-2.16	107.94	113.00
24	BB	5613	CLA	C3D-CAD-CBD	-2.16	104.54	107.60
24	AD	404	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
24	AA	405	CLA	C12-C11-C10	-2.16	102.80	113.25
24	AB	615	CLA	C2C-C1C-NC	-2.16	108.74	110.22
31	BC	5521	LMG	C17-C16-C15	-2.16	103.31	114.45
30	AF	102	SQD	O8-S-O9	-2.16	106.41	111.37
27	AB	619	BCR	C23-C22-C21	-2.16	115.62	118.94
24	BC	5506	CLA	C2C-C1C-NC	-2.16	108.74	110.22
35	AD	405	PL9	C42-C41-C39	-2.16	105.62	112.93
24	AB	609	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
24	AA	406	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
32	AB	624	LMT	C1'-O5'-C5'	-2.16	109.65	113.72
24	AC	506	CLA	O2A-CGA-O1A	-2.16	118.20	123.55
24	AC	510	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
34	BD	5404	PHO	O2A-CGA-O1A	-2.15	118.20	123.55
24	BD	5405	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
28	AE	101	DGD	C6D-C5D-C4D	-2.15	107.41	112.00
24	AD	404	CLA	O1D-CGD-CBD	-2.15	120.74	124.60
24	BC	5506	CLA	O1D-CGD-CBD	-2.15	120.74	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5622	BCR	C23-C22-C21	-2.15	115.64	118.94
24	BB	5609	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
24	AC	512	CLA	CHA-C1A-NA	-2.15	121.19	126.18
24	BD	5402	CLA	C3D-CAD-CBD	-2.15	104.56	107.60
31	BC	5520	LMG	C6-C5-C4	-2.15	107.98	113.00
24	BA	5407	CLA	OBD-CAD-CBD	-2.14	122.70	125.94
30	BB	5601	SQD	O48-C23-O10	-2.14	118.23	123.55
24	AC	509	CLA	CHA-C1A-NA	-2.14	121.22	126.18
28	BA	5412	DGD	O1A-C1A-C2A	-2.13	115.25	123.68
24	AC	507	CLA	C3D-CAD-CBD	-2.13	104.58	107.60
24	AC	503	CLA	CAA-CBA-CGA	-2.13	106.93	113.35
24	BB	5612	CLA	C4-C3-C5	-2.13	111.59	115.29
27	AT	101	BCR	C40-C30-C29	-2.13	100.41	108.80
24	BA	5406	CLA	CBC-CAC-C3C	-2.13	106.37	112.41
24	AA	407	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
24	AB	603	CLA	C3C-C4C-NC	-2.13	108.06	110.21
24	BA	5406	CLA	C4-C3-C5	-2.12	111.60	115.29
24	AC	506	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
24	BB	5614	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
27	AC	516	BCR	C19-C18-C17	-2.12	115.69	118.94
30	BF	5102	SQD	O3-C3-C2	-2.11	105.75	110.36
32	AB	629	LMT	C6'-C5'-C4'	-2.11	107.47	113.24
27	BC	5514	BCR	C8-C9-C10	-2.11	115.70	118.94
28	AC	519	DGD	O1G-C1A-O1A	-2.11	118.31	123.55
24	BB	5613	CLA	OBD-CAD-CBD	-2.11	122.75	125.94
24	BB	5620	CLA	C2C-C1C-NC	-2.11	108.78	110.22
24	BB	5613	CLA	C2C-C1C-NC	-2.11	108.78	110.22
28	BE	5102	DGD	C6E-C5E-C4E	-2.11	108.07	113.00
24	BB	5606	CLA	CAA-CBA-CGA	-2.11	107.00	113.35
32	BC	5522	LMT	C3'-C4'-C5'	-2.11	106.41	110.88
27	BC	5515	BCR	C8-C9-C10	-2.11	115.71	118.94
24	AD	404	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
24	BB	5617	CLA	O1D-CGD-CBD	-2.10	120.82	124.60
24	AB	607	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
24	AA	405	CLA	CBC-CAC-C3C	-2.10	106.45	112.41
24	BB	5618	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
30	BA	5414	SQD	C3-C4-C5	-2.10	106.52	110.22
24	AA	404	CLA	C7-C6-C5	-2.09	107.29	113.11
24	AC	513	CLA	C3C-C4C-NC	-2.09	108.09	110.21
24	BB	5607	CLA	C3C-C4C-NC	-2.09	108.09	110.21
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BB	5627	LMT	C1'-O5'-C5'	-2.09	109.78	113.72
34	AD	402	PHO	CBD-CHA-C4D	-2.09	106.19	108.54
28	AA	411	DGD	O1A-C1A-C2A	-2.09	115.43	123.68
31	AC	521	LMG	C17-C16-C15	-2.09	103.69	114.45
24	BB	5620	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
27	AC	516	BCR	C12-C13-C14	-2.09	115.74	118.94
24	AB	616	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
34	BD	5403	PHO	CBD-CHA-C4D	-2.09	106.19	108.54
34	AD	403	PHO	C3A-C4A-NA	-2.09	109.47	113.06
27	AA	410	BCR	C19-C18-C17	-2.08	115.74	118.94
31	AD	407	LMG	C6-C5-C4	-2.08	108.13	113.00
24	BB	5606	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
31	AD	407	LMG	C1-O6-C5	-2.08	109.79	113.72
31	BD	5408	LMG	C17-C16-C15	-2.08	103.73	114.45
30	BF	5102	SQD	O48-C23-O10	-2.08	118.39	123.55
24	AC	511	CLA	C12-C11-C10	-2.08	103.20	113.25
27	BB	5623	BCR	C23-C22-C21	-2.08	115.75	118.94
24	BB	5608	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
24	AB	601	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
24	AC	512	CLA	O2A-CGA-O1A	-2.08	118.40	123.55
27	BC	5514	BCR	C32-C1-C2	-2.08	100.62	108.80
30	BA	5414	SQD	O3-C3-C2	-2.08	105.84	110.36
31	AC	521	LMG	O7-C8-C9	-2.07	100.89	108.44
24	AB	605	CLA	CAA-C2A-C3A	-2.07	107.12	112.81
24	AC	513	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
24	AB	609	CLA	C3D-CAD-CBD	-2.07	104.67	107.60
27	AK	102	BCR	C19-C18-C17	-2.07	115.77	118.94
32	BB	5603	LMT	C6'-C5'-C4'	-2.07	107.59	113.24
24	BC	5513	CLA	C3C-C4C-NC	-2.07	108.12	110.21
28	BA	5412	DGD	O1B-C1B-C2B	-2.07	115.52	123.68
24	BC	5507	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
30	BA	5401	SQD	O3-C3-C2	-2.06	105.87	110.36
30	AA	413	SQD	O6-C44-C45	-2.06	106.08	110.99
31	AB	620	LMG	O7-C10-C11	-2.06	107.27	111.55
24	AB	614	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
30	AA	416	SQD	O3-C3-C2	-2.06	105.87	110.36
24	AB	612	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	AC	508	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	AC	511	CLA	C3C-C4C-NC	-2.06	108.12	110.21
30	AA	413	SQD	C3-C4-C5	-2.06	106.59	110.22
24	BC	5509	CLA	CHA-C1A-NA	-2.06	121.40	126.18
24	BC	5512	CLA	CHA-C1A-NA	-2.06	121.40	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5513	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
24	BB	5609	CLA	CAA-C2A-C3A	-2.05	107.18	112.81
24	AC	504	CLA	O2A-CGA-O1A	-2.05	118.45	123.55
34	BD	5404	PHO	C12-C11-C10	-2.05	103.32	113.25
24	AA	404	CLA	O2A-CGA-O1A	-2.05	118.45	123.55
24	AB	608	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
24	BD	5405	CLA	C2C-C1C-NC	-2.05	108.81	110.22
24	BC	5508	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
24	AC	503	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
24	AD	401	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
24	AB	611	CLA	C12-C11-C10	-2.05	103.34	113.25
24	AB	609	CLA	O1D-CGD-CBD	-2.05	120.92	124.60
27	BK	5102	BCR	C19-C18-C17	-2.05	115.80	118.94
28	BC	5519	DGD	O6D-C1D-C2D	-2.05	106.35	110.30
32	BI	5102	LMT	C9-C8-C7	-2.04	103.92	114.45
24	BC	5503	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
24	AC	505	CLA	C2C-C1C-NC	-2.04	108.82	110.22
28	AE	101	DGD	C4A-C3A-C2A	-2.04	105.75	113.24
24	AB	615	CLA	CHA-C1A-NA	-2.04	121.43	126.18
28	BC	5517	DGD	C4E-C3E-C2E	-2.04	107.23	110.84
28	AA	411	DGD	O1B-C1B-C2B	-2.04	115.62	123.68
31	AC	520	LMG	C36-C35-C34	-2.04	103.94	114.45
34	BD	5403	PHO	C6-C7-C8	-2.04	109.04	115.73
35	BD	5406	PL9	C31-C29-C28	-2.04	116.93	121.10
24	AD	404	CLA	CAA-CBA-CGA	-2.04	107.21	113.35
24	AC	511	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
24	AB	605	CLA	CMB-C2B-C1B	-2.04	125.34	128.46
27	BA	5411	BCR	C19-C18-C17	-2.03	115.82	118.94
24	BC	5504	CLA	C6-C7-C8	-2.03	109.06	115.73
35	AD	405	PL9	C31-C29-C28	-2.03	116.94	121.10
24	BB	5609	CLA	CBC-CAC-C3C	-2.03	106.64	112.41
24	BB	5606	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
31	BB	5624	LMG	C6-C5-C4	-2.03	108.25	113.00
31	BC	5521	LMG	O7-C8-C9	-2.03	101.06	108.44
24	AA	405	CLA	CAA-C2A-C3A	-2.03	107.25	112.81
24	BB	5619	CLA	C3D-CAD-CBD	-2.02	104.73	107.60
28	AE	101	DGD	C6E-C5E-C4E	-2.02	108.27	113.00
30	BA	5401	SQD	O48-C23-O10	-2.02	118.53	123.55
24	AB	605	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
28	AH	101	DGD	O1B-C1B-C2B	-2.02	115.69	123.68
34	AD	403	PHO	C12-C11-C10	-2.02	103.47	113.25
24	AC	504	CLA	CMB-C2B-C1B	-2.02	125.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5502	CLA	CAA-CBA-CGA	-2.02	107.26	113.35
24	AB	602	CLA	CAA-CBA-CGA	-2.02	107.26	113.35
24	BB	5608	CLA	CAA-CBA-CGA	-2.02	107.26	113.35
31	AC	520	LMG	C6-C5-C4	-2.02	108.28	113.00
27	BC	5516	BCR	C32-C1-C2	-2.02	100.84	108.80
24	BB	5619	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
30	BB	5601	SQD	O8-S-O9	-2.01	106.75	111.37
24	BC	5511	CLA	C12-C11-C10	-2.01	103.52	113.25
24	BC	5507	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
24	BA	5405	CLA	C6-C7-C8	-2.01	109.13	115.73
24	BB	5608	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
35	AD	405	PL9	C2-C3-C4	-2.01	116.02	118.81
24	AB	616	CLA	C3D-CAD-CBD	-2.01	104.75	107.60
24	AC	504	CLA	C6-C7-C8	-2.01	109.14	115.73
28	AC	519	DGD	C3E-C4E-C5E	-2.00	106.68	110.22
24	BC	5511	CLA	C3C-C4C-NC	-2.00	108.18	110.21
24	BA	5405	CLA	O2A-CGA-O1A	-2.00	118.57	123.55
24	BB	5620	CLA	C3D-CAD-CBD	-2.00	104.76	107.60
31	AJ	102	LMG	C6-C5-C4	-2.00	108.31	113.00
32	AI	102	LMT	C9-C8-C7	-2.00	104.14	114.45
27	BC	5516	BCR	C12-C13-C14	-2.00	115.87	118.94
31	AJ	102	LMG	C17-C16-C15	-2.00	104.15	114.45
27	BK	5102	BCR	C11-C12-C13	2.00	132.04	126.42
30	BA	5401	SQD	O8-S-O7	2.00	115.96	111.37
27	AB	617	BCR	C7-C8-C9	2.00	129.22	126.21
30	AA	413	SQD	O47-C45-C44	2.00	115.72	108.44
30	AA	413	SQD	C13-C12-C11	2.00	124.79	114.45
24	AB	603	CLA	CMA-C3A-C4A	2.01	117.16	111.77
30	AB	627	SQD	C17-C16-C15	2.01	124.79	114.45
24	AB	607	CLA	CED-O2D-CGD	2.01	120.68	115.97
24	AC	501	CLA	OBD-CAD-C3D	2.01	131.73	128.03
27	BJ	5101	BCR	C30-C25-C24	2.01	121.38	115.73
30	BA	5401	SQD	C13-C12-C11	2.01	124.83	114.45
24	BB	5606	CLA	C1D-CHD-C4C	2.02	125.24	122.48
30	AA	416	SQD	C13-C12-C11	2.02	124.85	114.45
24	AB	611	CLA	C5-C3-C2	2.02	125.24	121.10
24	BB	5618	CLA	C2A-C1A-CHA	2.02	127.50	123.92
24	BA	5406	CLA	C2A-C1A-CHA	2.02	127.50	123.92
28	AH	101	DGD	O1G-C1A-C2A	2.02	117.78	111.90
32	AB	624	LMT	O1B-C1B-C2B	2.02	112.66	108.11
27	AX	101	BCR	C37-C22-C23	2.02	121.32	118.10
28	BC	5518	DGD	C1G-O1G-C1A	2.02	123.21	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	518	DGD	C1G-O1G-C1A	2.02	123.21	117.13
27	AC	516	BCR	C7-C8-C9	2.02	129.25	126.21
24	BB	5611	CLA	CMC-C2C-C1C	2.03	128.09	125.02
27	BA	5411	BCR	C32-C1-C6	2.03	113.60	110.31
24	AB	604	CLA	C2A-C1A-CHA	2.03	127.52	123.92
24	AA	404	CLA	O2D-CGD-CBD	2.03	114.93	111.30
27	AK	102	BCR	C36-C18-C19	2.03	121.33	118.10
32	BB	5603	LMT	C6B-C5B-C4B	2.03	117.76	113.00
30	BA	5414	SQD	C13-C12-C11	2.03	124.93	114.45
24	AB	612	CLA	CED-O2D-CGD	2.03	120.73	115.97
31	BM	5102	LMG	C34-C33-C32	2.03	124.93	114.45
27	BB	5623	BCR	C30-C25-C24	2.03	121.45	115.73
27	AC	514	BCR	C30-C25-C24	2.04	121.45	115.73
28	AC	518	DGD	O3D-C3D-C2D	2.04	114.79	110.36
33	AB	625	DMS	O-S-C1	2.04	117.29	106.54
32	AI	103	LMT	C3-C2-C1	2.04	122.64	113.48
27	BT	5101	BCR	C28-C27-C26	2.04	117.29	113.78
30	BF	5102	SQD	C17-C16-C15	2.04	124.96	114.45
24	BC	5513	CLA	C2A-C1A-CHA	2.04	127.53	123.92
24	AC	504	CLA	CED-O2D-CGD	2.04	120.75	115.97
27	BB	5623	BCR	C36-C18-C19	2.04	121.35	118.10
27	BD	5407	BCR	C15-C14-C13	2.04	130.23	127.31
34	BD	5403	PHO	C1B-NB-C4B	2.04	110.57	106.52
27	AJ	101	BCR	C30-C25-C24	2.05	121.49	115.73
24	BB	5611	CLA	CED-O2D-CGD	2.05	120.78	115.97
24	AB	610	CLA	CMB-C2B-C3B	2.05	128.70	124.89
24	BB	5608	CLA	C2A-C1A-CHA	2.05	127.56	123.92
24	AD	404	CLA	C1D-CHD-C4C	2.05	125.29	122.48
24	AB	616	CLA	OBD-CAD-C3D	2.05	131.81	128.03
24	BB	5614	CLA	C1D-CHD-C4C	2.05	125.29	122.48
24	BB	5609	CLA	OBD-CAD-C3D	2.06	131.82	128.03
24	BB	5607	CLA	OBD-CAD-C3D	2.06	131.82	128.03
27	AB	619	BCR	C40-C30-C25	2.06	113.65	110.31
30	AB	627	SQD	C15-C14-C13	2.06	125.07	114.45
27	AX	101	BCR	C34-C9-C8	2.06	121.39	118.10
24	AC	513	CLA	C2A-C1A-CHA	2.06	127.58	123.92
24	AC	510	CLA	C2A-C3A-C4A	2.06	105.20	101.87
24	AA	406	CLA	CED-O2D-CGD	2.06	120.81	115.97
27	AC	514	BCR	C28-C27-C26	2.07	117.34	113.78
27	AT	101	BCR	C28-C27-C26	2.07	117.35	113.78
27	AD	406	BCR	C34-C9-C8	2.07	121.40	118.10
31	BC	5520	LMG	O8-C28-C29	2.07	117.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	613	CLA	CED-O2D-CGD	2.08	120.84	115.97
27	AK	102	BCR	C11-C12-C13	2.08	132.25	126.42
30	AA	416	SQD	C17-C16-C15	2.08	125.15	114.45
32	AD	409	LMT	C6B-C5B-C4B	2.08	117.86	113.00
30	AF	102	SQD	C17-C16-C15	2.08	125.16	114.45
27	BC	5514	BCR	C34-C9-C8	2.08	121.41	118.10
32	AB	629	LMT	C6B-C5B-C4B	2.08	117.87	113.00
27	AB	617	BCR	C34-C9-C8	2.08	121.42	118.10
30	AF	102	SQD	C32-C31-C30	2.08	129.67	113.42
24	BC	5510	CLA	OBD-CAD-C3D	2.08	131.86	128.03
31	AC	521	LMG	O1-C7-C8	2.08	115.94	110.99
24	AC	508	CLA	C1D-CHD-C4C	2.08	125.33	122.48
30	BA	5414	SQD	O47-C7-C8	2.08	115.88	111.55
28	BA	5412	DGD	O3D-C3D-C2D	2.08	114.89	110.36
27	AB	619	BCR	C30-C25-C24	2.08	121.59	115.73
30	AA	413	SQD	C17-C16-C15	2.09	125.21	114.45
27	AJ	101	BCR	C16-C17-C18	2.09	130.29	127.31
28	AA	411	DGD	O3D-C3D-C2D	2.09	114.91	110.36
30	BB	5601	SQD	C15-C14-C13	2.09	125.23	114.45
24	AC	507	CLA	OBD-CAD-C3D	2.09	131.88	128.03
28	AB	628	DGD	O5D-C1E-C2E	2.09	111.65	108.23
24	AD	401	CLA	C1D-CHD-C4C	2.10	125.35	122.48
28	AC	519	DGD	C4D-C3D-C2D	2.10	114.53	110.84
24	BB	5613	CLA	C1D-CHD-C4C	2.10	125.35	122.48
32	AI	103	LMT	C6B-C5B-C4B	2.10	117.91	113.00
24	BA	5405	CLA	C1D-CHD-C4C	2.10	125.35	122.48
34	AD	402	PHO	CBD-CHA-C1A	2.10	131.30	126.36
30	BF	5102	SQD	C32-C31-C30	2.10	129.81	113.42
31	BD	5408	LMG	C35-C34-C33	2.10	125.28	114.45
27	AT	101	BCR	C34-C9-C8	2.10	121.45	118.10
24	BC	5507	CLA	OBD-CAD-C3D	2.10	131.90	128.03
31	AJ	102	LMG	C35-C34-C33	2.10	125.29	114.45
24	BA	5408	CLA	C1D-CHD-C4C	2.10	125.36	122.48
28	AB	628	DGD	O5D-C6D-C5D	2.10	112.46	108.94
24	AC	503	CLA	C1D-CHD-C4C	2.11	125.36	122.48
27	BB	5621	BCR	C24-C23-C22	2.11	129.38	126.21
27	BC	5515	BCR	C7-C8-C9	2.11	129.38	126.21
27	AB	618	BCR	C37-C22-C23	2.11	121.46	118.10
32	AM	102	LMT	C6B-C5B-C4B	2.11	117.94	113.00
27	BC	5514	BCR	C36-C18-C19	2.11	121.46	118.10
24	AB	602	CLA	C1D-CHD-C4C	2.11	125.37	122.48
24	BC	5503	CLA	C1D-CHD-C4C	2.11	125.37	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5614	CLA	CED-O2D-CGD	2.11	120.93	115.97
28	BC	5519	DGD	O3G-C3G-C2G	2.11	116.02	110.99
30	BA	5414	SQD	O8-S-O7	2.11	116.22	111.37
24	AB	608	CLA	C1D-CHD-C4C	2.12	125.38	122.48
28	AC	518	DGD	O6E-C5E-C4E	2.12	113.56	109.66
27	BC	5514	BCR	C30-C25-C24	2.12	121.68	115.73
27	BX	5101	BCR	C34-C9-C8	2.12	121.47	118.10
27	BX	5101	BCR	C37-C22-C23	2.12	121.48	118.10
30	AA	416	SQD	O8-S-O7	2.12	116.23	111.37
24	BB	5614	CLA	CMB-C2B-C3B	2.12	128.83	124.89
28	AC	518	DGD	O2G-C2G-C1G	2.12	116.16	108.44
27	AT	101	BCR	C40-C30-C25	2.12	113.75	110.31
27	BA	5411	BCR	C1-C6-C7	2.13	121.70	115.73
24	BB	5620	CLA	OBD-CAD-C3D	2.13	131.94	128.03
27	BT	5101	BCR	C34-C9-C8	2.13	121.49	118.10
24	AC	510	CLA	OBD-CAD-C3D	2.13	131.94	128.03
24	AB	610	CLA	C1D-CHD-C4C	2.13	125.39	122.48
28	BH	5101	DGD	O1G-C1A-C2A	2.13	118.09	111.90
27	BB	5621	BCR	C34-C9-C8	2.13	121.49	118.10
24	BC	5509	CLA	OBD-CAD-C3D	2.13	131.95	128.03
34	BD	5403	PHO	CBD-CHA-C1A	2.13	131.38	126.36
30	BA	5414	SQD	C17-C16-C15	2.13	125.44	114.45
27	BC	5515	BCR	C24-C23-C22	2.13	129.42	126.21
24	BC	5503	CLA	C2A-C1A-CHA	2.13	127.70	123.92
24	BB	5617	CLA	O2D-CGD-CBD	2.14	115.11	111.30
27	BB	5623	BCR	C37-C22-C23	2.14	121.50	118.10
24	BB	5608	CLA	C1D-CHD-C4C	2.14	125.41	122.48
24	BA	5405	CLA	O2D-CGD-CBD	2.14	115.12	111.30
24	AA	405	CLA	C2A-C1A-CHA	2.14	127.72	123.92
34	AD	402	PHO	CED-O2D-CGD	2.14	121.00	115.97
34	BD	5404	PHO	C1B-NB-C4B	2.14	110.77	106.52
27	BB	5621	BCR	C11-C10-C9	2.14	130.37	127.31
31	BC	5520	LMG	O7-C8-C9	2.14	116.23	108.44
27	AC	514	BCR	C23-C24-C25	2.15	133.26	127.25
24	AA	405	CLA	CMB-C2B-C3B	2.15	128.88	124.89
27	BC	5514	BCR	C23-C24-C25	2.15	133.27	127.25
24	AC	505	CLA	OBD-CAD-C3D	2.15	131.99	128.03
27	AC	514	BCR	C36-C18-C19	2.15	121.53	118.10
24	BA	5406	CLA	CMB-C2B-C3B	2.15	128.89	124.89
28	AC	518	DGD	O6E-C1E-C2E	2.16	114.45	110.30
24	AA	406	CLA	CMB-C2B-C3B	2.16	128.90	124.89
28	BH	5101	DGD	C1G-O1G-C1A	2.16	123.63	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	5411	BCR	C34-C9-C8	2.16	121.54	118.10
32	BM	5101	LMT	C6B-C5B-C4B	2.16	118.06	113.00
27	BJ	5101	BCR	C3-C4-C5	2.16	117.50	113.78
31	AC	520	LMG	O7-C8-C9	2.16	116.30	108.44
24	AB	614	CLA	C2A-C1A-CHA	2.16	127.75	123.92
30	BA	5401	SQD	C17-C16-C15	2.17	125.61	114.45
28	BH	5101	DGD	O2G-C2G-C3G	2.17	116.31	108.44
27	BJ	5101	BCR	C28-C27-C26	2.17	117.51	113.78
27	AX	101	BCR	C7-C8-C9	2.17	129.47	126.21
24	BB	5607	CLA	CBA-CAA-C2A	2.17	120.29	113.80
28	AH	101	DGD	O2G-C2G-C3G	2.17	116.33	108.44
28	AC	518	DGD	C7A-C6A-C5A	2.17	125.64	114.45
31	BD	5409	LMG	C14-C13-C12	2.17	125.65	114.45
28	AC	517	DGD	O2G-C2G-C3G	2.17	116.34	108.44
27	BX	5101	BCR	C1-C6-C7	2.18	121.85	115.73
24	AB	605	CLA	C1D-CHD-C4C	2.18	125.47	122.48
32	BC	5522	LMT	C6B-C5B-C4B	2.18	118.11	113.00
24	AB	609	CLA	C1D-CHD-C4C	2.18	125.47	122.48
27	AA	410	BCR	C34-C9-C8	2.19	121.58	118.10
24	BC	5505	CLA	OBD-CAD-C3D	2.19	132.06	128.03
27	AC	516	BCR	C36-C18-C19	2.19	121.58	118.10
28	AA	411	DGD	C3G-C2G-C1G	2.19	116.79	111.86
30	BA	5401	SQD	C34-C33-C32	2.19	125.74	114.45
24	BB	5606	CLA	CED-O2D-CGD	2.19	121.11	115.97
31	BL	5101	LMG	C34-C33-C32	2.19	125.75	114.45
27	BJ	5101	BCR	C40-C30-C25	2.19	113.86	110.31
30	AA	413	SQD	O47-C7-C8	2.19	116.11	111.55
34	BD	5404	PHO	CED-O2D-CGD	2.20	121.12	115.97
24	AB	607	CLA	C11-C12-C13	2.20	122.94	115.73
24	AA	406	CLA	C1D-CHD-C4C	2.20	125.49	122.48
27	BB	5622	BCR	C37-C22-C23	2.20	121.60	118.10
31	AC	520	LMG	O8-C28-C29	2.20	118.29	111.90
24	BB	5611	CLA	C11-C12-C13	2.20	122.94	115.73
24	BB	5612	CLA	CED-O2D-CGD	2.20	121.12	115.97
24	BB	5614	CLA	OBD-CAD-C3D	2.20	132.07	128.03
24	AC	509	CLA	OBD-CAD-C3D	2.20	132.08	128.03
27	BB	5622	BCR	C16-C17-C18	2.20	130.45	127.31
27	BX	5101	BCR	C7-C8-C9	2.20	129.52	126.21
27	BC	5516	BCR	C16-C17-C18	2.20	130.46	127.31
27	AB	618	BCR	C16-C17-C18	2.21	130.46	127.31
24	AC	507	CLA	C11-C12-C13	2.21	122.98	115.73
28	BB	5602	DGD	O5D-C6D-C5D	2.21	112.64	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BX	5101	BCR	C36-C18-C19	2.21	121.62	118.10
31	BC	5520	LMG	C39-C38-C37	2.21	125.84	114.45
24	BC	5511	CLA	OBD-CAD-C3D	2.21	132.10	128.03
31	AD	407	LMG	C14-C13-C12	2.21	125.84	114.45
27	AB	618	BCR	C1-C6-C7	2.21	121.95	115.73
34	AD	403	PHO	CED-O2D-CGD	2.21	121.16	115.97
28	BB	5602	DGD	O5D-C1E-C2E	2.22	111.85	108.23
24	AA	407	CLA	CED-O2D-CGD	2.22	121.17	115.97
27	AA	410	BCR	C1-C6-C7	2.22	121.97	115.73
28	BC	5518	DGD	C7A-C6A-C5A	2.22	125.89	114.45
28	BC	5518	DGD	O6E-C1E-C2E	2.22	114.58	110.30
24	AD	401	CLA	OBD-CAD-C3D	2.22	132.12	128.03
28	AE	101	DGD	C3G-C2G-C1G	2.22	116.86	111.86
30	AA	416	SQD	C34-C33-C32	2.22	125.90	114.45
24	BD	5402	CLA	OBD-CAD-C3D	2.22	132.12	128.03
28	BC	5518	DGD	O2G-C2G-C1G	2.23	116.53	108.44
27	AD	406	BCR	C15-C14-C13	2.23	130.49	127.31
27	AJ	101	BCR	C28-C27-C26	2.23	117.61	113.78
28	BC	5519	DGD	C5B-C4B-C3B	2.23	125.94	114.45
32	BM	5101	LMT	O1B-C1B-C2B	2.23	113.13	108.11
24	BD	5405	CLA	OBD-CAD-C3D	2.23	132.13	128.03
27	AC	515	BCR	C37-C22-C23	2.23	121.65	118.10
36	AV	201	HEM	CMB-C2B-C3B	2.23	129.03	124.89
27	BJ	5101	BCR	C31-C1-C2	2.23	117.60	108.80
24	BD	5402	CLA	CED-O2D-CGD	2.23	121.21	115.97
30	BF	5102	SQD	C15-C14-C13	2.23	125.97	114.45
28	BC	5518	DGD	O6D-C1D-O3G	2.23	115.33	110.02
27	AJ	101	BCR	C31-C1-C2	2.24	117.62	108.80
24	AB	609	CLA	OBD-CAD-C3D	2.24	132.15	128.03
24	BA	5407	CLA	C1D-CHD-C4C	2.24	125.54	122.48
24	AB	602	CLA	CED-O2D-CGD	2.24	121.22	115.97
27	AJ	101	BCR	C3-C4-C5	2.24	117.64	113.78
24	AB	615	CLA	OBD-CAD-C3D	2.24	132.16	128.03
30	AF	102	SQD	C15-C14-C13	2.24	126.01	114.45
27	AB	619	BCR	C24-C23-C22	2.24	129.58	126.21
30	BA	5401	SQD	C15-C14-C13	2.24	126.02	114.45
24	AB	603	CLA	CBA-CAA-C2A	2.25	120.53	113.80
24	BB	5609	CLA	C1D-CHD-C4C	2.25	125.56	122.48
27	AC	514	BCR	C15-C14-C13	2.25	130.53	127.31
27	BT	5101	BCR	C20-C21-C22	2.25	130.53	127.31
31	AB	620	LMG	C34-C33-C32	2.25	126.07	114.45
27	AX	101	BCR	C1-C6-C7	2.26	122.07	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	603	CLA	CED-O2D-CGD	2.26	121.26	115.97
24	BB	5615	CLA	C5-C3-C2	2.26	125.73	121.10
24	BA	5408	CLA	CED-O2D-CGD	2.26	121.27	115.97
34	AD	403	PHO	CBD-CHA-C1A	2.26	131.69	126.36
24	BC	5513	CLA	OBD-CAD-C3D	2.26	132.20	128.03
24	AB	604	CLA	C1D-CHD-C4C	2.26	125.58	122.48
35	AD	405	PL9	C45-C44-C46	2.27	119.22	115.29
24	BC	5503	CLA	CED-O2D-CGD	2.27	121.29	115.97
27	AK	102	BCR	C15-C14-C13	2.27	130.55	127.31
24	BD	5402	CLA	C1D-CHD-C4C	2.27	125.59	122.48
28	BC	5519	DGD	O2E-C2E-C3E	2.27	115.30	110.36
24	AC	512	CLA	OBD-CAD-C3D	2.27	132.22	128.03
32	AM	102	LMT	O1B-C1B-C2B	2.27	113.23	108.11
28	AC	519	DGD	C5B-C4B-C3B	2.28	126.19	114.45
24	BD	5405	CLA	C1D-CHD-C4C	2.28	125.60	122.48
24	BC	5511	CLA	CED-O2D-CGD	2.28	121.32	115.97
27	AA	410	BCR	C30-C25-C24	2.28	122.14	115.73
27	AC	515	BCR	C15-C14-C13	2.28	130.57	127.31
24	BB	5619	CLA	CED-O2D-CGD	2.28	121.32	115.97
27	BD	5407	BCR	C36-C18-C19	2.28	121.74	118.10
24	AB	608	CLA	CED-O2D-CGD	2.28	121.32	115.97
24	BC	5507	CLA	C1D-CHD-C4C	2.29	125.61	122.48
27	AB	619	BCR	C37-C22-C23	2.29	121.74	118.10
27	BA	5411	BCR	C30-C25-C24	2.29	122.15	115.73
24	BC	5507	CLA	C11-C12-C13	2.29	123.25	115.73
30	AA	413	SQD	O8-S-O7	2.29	116.62	111.37
27	AA	410	BCR	C36-C18-C19	2.29	121.75	118.10
24	BA	5408	CLA	OBD-CAD-C3D	2.29	132.24	128.03
30	BB	5601	SQD	O47-C7-C8	2.29	116.31	111.55
27	BC	5516	BCR	C36-C18-C19	2.29	121.75	118.10
24	BC	5512	CLA	OBD-CAD-C3D	2.29	132.25	128.03
31	AC	520	LMG	C39-C38-C37	2.29	126.26	114.45
24	AD	404	CLA	OBD-CAD-C3D	2.30	132.25	128.03
27	AC	515	BCR	C34-C9-C8	2.30	121.76	118.10
27	AA	410	BCR	C37-C22-C23	2.30	121.76	118.10
24	AC	508	CLA	C2A-C1A-CHA	2.30	127.99	123.92
27	BC	5515	BCR	C37-C22-C23	2.30	121.76	118.10
24	AB	606	CLA	CBA-CAA-C2A	2.30	120.68	113.80
27	AJ	101	BCR	C40-C30-C25	2.30	114.04	110.31
27	BB	5623	BCR	C35-C13-C12	2.30	121.77	118.10
27	BB	5621	BCR	C8-C7-C6	2.31	133.71	127.25
27	BT	5101	BCR	C40-C30-C25	2.31	114.05	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5610	CLA	O2D-CGD-CBD	2.31	115.42	111.30
24	AC	504	CLA	C1D-CHD-C4C	2.31	125.64	122.48
24	BC	5503	CLA	C6-C5-C3	2.31	117.90	112.66
24	AC	510	CLA	C1D-CHD-C4C	2.31	125.65	122.48
24	BB	5612	CLA	C1D-CHD-C4C	2.31	125.65	122.48
24	BC	5508	CLA	C2A-C1A-CHA	2.31	128.02	123.92
24	AB	603	CLA	OBD-CAD-C3D	2.31	132.29	128.03
24	BC	5504	CLA	C1D-CHD-C4C	2.31	125.65	122.48
24	AB	605	CLA	OBD-CAD-C3D	2.31	132.29	128.03
24	BA	5405	CLA	C2A-C1A-CHA	2.32	128.02	123.92
30	AB	627	SQD	O47-C7-C8	2.32	116.36	111.55
27	BC	5515	BCR	C34-C9-C8	2.32	121.80	118.10
27	AX	101	BCR	C36-C18-C19	2.32	121.80	118.10
27	AB	619	BCR	C1-C6-C7	2.32	122.26	115.73
24	AC	511	CLA	CED-O2D-CGD	2.32	121.42	115.97
24	AC	503	CLA	CED-O2D-CGD	2.32	121.42	115.97
30	AA	416	SQD	C15-C14-C13	2.33	126.44	114.45
28	AC	519	DGD	O3G-C3G-C2G	2.33	116.53	110.99
24	AA	404	CLA	C1D-CHD-C4C	2.33	125.67	122.48
27	AT	101	BCR	C37-C22-C23	2.33	121.81	118.10
27	BJ	5101	BCR	C16-C17-C18	2.33	130.63	127.31
24	BC	5505	CLA	C1D-CHD-C4C	2.33	125.67	122.48
24	BC	5508	CLA	OBD-CAD-C3D	2.33	132.32	128.03
24	AB	602	CLA	C2A-C1A-CHA	2.33	128.05	123.92
27	BA	5411	BCR	C37-C22-C23	2.34	121.82	118.10
27	AC	516	BCR	C30-C25-C24	2.34	122.30	115.73
27	AB	617	BCR	C8-C7-C6	2.34	133.80	127.25
24	BB	5606	CLA	C2A-C1A-CHA	2.34	128.06	123.92
24	AD	401	CLA	CBA-CAA-C2A	2.34	120.80	113.80
24	BB	5606	CLA	OBD-CAD-C3D	2.34	132.34	128.03
24	BB	5618	CLA	OBD-CAD-C3D	2.34	132.34	128.03
24	AB	613	CLA	OBD-CAD-C3D	2.34	132.34	128.03
24	AC	507	CLA	C1D-CHD-C4C	2.34	125.69	122.48
24	AD	401	CLA	CED-O2D-CGD	2.34	121.46	115.97
27	AT	101	BCR	C8-C7-C6	2.34	133.82	127.25
28	BB	5602	DGD	O2G-C2G-C3G	2.35	116.96	108.44
27	BA	5411	BCR	C16-C17-C18	2.35	130.66	127.31
31	BC	5520	LMG	C13-C12-C11	2.35	121.84	113.24
27	BA	5411	BCR	C36-C18-C19	2.35	121.84	118.10
27	BX	5101	BCR	C28-C27-C26	2.35	117.83	113.78
24	AC	503	CLA	C6-C5-C3	2.35	117.99	112.66
27	BK	5102	BCR	C15-C14-C13	2.36	130.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BD	5407	BCR	C28-C27-C26	2.36	117.84	113.78
27	BC	5516	BCR	C30-C25-C24	2.36	122.36	115.73
31	AC	521	LMG	C34-C33-C32	2.36	126.62	114.45
24	BB	5617	CLA	C3A-C2A-C1A	2.36	104.88	101.34
27	BT	5101	BCR	C8-C7-C6	2.37	133.88	127.25
34	BD	5404	PHO	CBD-CHA-C1A	2.37	131.94	126.36
24	AB	612	CLA	OBD-CAD-C3D	2.37	132.39	128.03
24	AB	608	CLA	C2A-C1A-CHA	2.37	128.12	123.92
24	BC	5503	CLA	OBD-CAD-C3D	2.37	132.40	128.03
24	BB	5605	CLA	C3A-C2A-C1A	2.37	104.90	101.34
24	BC	5505	CLA	C2A-C1A-CHA	2.38	128.13	123.92
30	AA	413	SQD	C15-C14-C13	2.38	126.72	114.45
27	BT	5101	BCR	C37-C22-C23	2.38	121.89	118.10
27	AB	618	BCR	C32-C1-C6	2.38	114.17	110.31
24	BC	5512	CLA	C1D-CHD-C4C	2.38	125.75	122.48
24	AC	503	CLA	C2A-C1A-CHA	2.38	128.15	123.92
24	BC	5512	CLA	O2D-CGD-CBD	2.39	115.56	111.30
24	AB	610	CLA	OBD-CAD-C3D	2.39	132.43	128.03
31	AB	621	LMG	C13-C12-C11	2.39	122.00	113.24
31	BD	5409	LMG	C39-C38-C37	2.39	126.77	114.45
27	BB	5623	BCR	C1-C6-C7	2.39	122.45	115.73
24	AC	503	CLA	OBD-CAD-C3D	2.39	132.43	128.03
31	BC	5521	LMG	C34-C33-C32	2.39	126.78	114.45
24	AD	404	CLA	C2A-C1A-CHA	2.39	128.16	123.92
31	AD	407	LMG	O8-C28-C29	2.39	118.86	111.90
24	AB	614	CLA	OBD-CAD-C3D	2.39	132.44	128.03
24	AB	613	CLA	O2D-CGD-CBD	2.39	115.58	111.30
24	AB	615	CLA	CED-O2D-CGD	2.40	121.59	115.97
30	AA	416	SQD	O47-C7-C8	2.40	116.53	111.55
24	AB	606	CLA	OBD-CAD-C3D	2.40	132.45	128.03
27	AC	516	BCR	C24-C23-C22	2.40	129.82	126.21
28	BE	5102	DGD	C3G-C2G-C1G	2.40	117.28	111.86
27	AD	406	BCR	C36-C18-C19	2.41	121.93	118.10
30	BA	5414	SQD	C15-C14-C13	2.41	126.86	114.45
27	BC	5515	BCR	C36-C18-C19	2.41	121.94	118.10
27	BD	5407	BCR	C34-C9-C8	2.41	121.94	118.10
24	BD	5402	CLA	CBA-CAA-C2A	2.41	121.02	113.80
24	AB	605	CLA	C2A-C1A-CHA	2.41	128.19	123.92
28	AB	628	DGD	O2G-C2G-C3G	2.41	117.21	108.44
31	AD	407	LMG	C39-C38-C37	2.42	126.90	114.45
31	BB	5624	LMG	C13-C12-C11	2.42	122.10	113.24
24	AC	502	CLA	OBD-CAD-C3D	2.42	132.49	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	508	CLA	OBD-CAD-C3D	2.42	132.49	128.03
24	BD	5405	CLA	C2A-C1A-CHA	2.42	128.21	123.92
24	BB	5612	CLA	C2A-C1A-CHA	2.43	128.22	123.92
24	AB	606	CLA	O2D-CGD-CBD	2.43	115.63	111.30
27	AB	617	BCR	C11-C10-C9	2.43	130.77	127.31
24	BB	5610	CLA	CBA-CAA-C2A	2.43	121.06	113.80
27	AB	617	BCR	C37-C22-C23	2.43	121.97	118.10
27	BX	5101	BCR	C16-C17-C18	2.43	130.78	127.31
24	AB	610	CLA	CED-O2D-CGD	2.43	121.66	115.97
27	BB	5622	BCR	C1-C6-C7	2.43	122.56	115.73
24	BC	5507	CLA	C3A-C2A-C1A	2.43	104.98	101.34
31	AC	521	LMG	C9-C8-C7	2.43	117.35	111.86
24	AC	505	CLA	C1D-CHD-C4C	2.44	125.81	122.48
27	AC	515	BCR	C24-C23-C22	2.44	129.87	126.21
24	AB	608	CLA	OBD-CAD-C3D	2.44	132.52	128.03
28	BC	5519	DGD	C1E-O6E-C5E	2.44	118.31	113.72
27	BB	5622	BCR	C32-C1-C6	2.44	114.27	110.31
28	AC	518	DGD	O6D-C1D-O3G	2.44	115.82	110.02
24	AB	604	CLA	CBA-CAA-C2A	2.44	121.11	113.80
24	BB	5609	CLA	C2A-C1A-CHA	2.44	128.25	123.92
30	BF	5102	SQD	C45-O47-C7	2.44	123.65	117.88
24	AB	602	CLA	OBD-CAD-C3D	2.45	132.53	128.03
24	AC	507	CLA	CED-O2D-CGD	2.45	121.72	115.97
31	AC	520	LMG	C13-C12-C11	2.45	122.22	113.24
27	AC	514	BCR	C32-C1-C6	2.45	114.28	110.31
27	BB	5623	BCR	C24-C23-C22	2.45	129.90	126.21
24	BB	5617	CLA	OBD-CAD-C3D	2.45	132.55	128.03
24	AC	511	CLA	OBD-CAD-C3D	2.45	132.55	128.03
24	BA	5405	CLA	CED-O2D-CGD	2.45	121.72	115.97
27	BC	5514	BCR	C32-C1-C6	2.46	114.29	110.31
34	BD	5403	PHO	CED-O2D-CGD	2.46	121.73	115.97
35	BD	5406	PL9	C45-C44-C46	2.46	119.55	115.29
31	BD	5409	LMG	O8-C28-C29	2.46	119.05	111.90
24	AC	510	CLA	C3A-C2A-C1A	2.46	105.02	101.34
27	AC	515	BCR	C36-C18-C19	2.46	122.02	118.10
24	BC	5510	CLA	CED-O2D-CGD	2.46	121.74	115.97
24	AC	512	CLA	C1D-CHD-C4C	2.46	125.85	122.48
24	BB	5617	CLA	CED-O2D-CGD	2.46	121.74	115.97
30	BA	5401	SQD	O47-C7-C8	2.46	116.67	111.55
24	AC	512	CLA	C3A-C2A-C1A	2.46	105.03	101.34
24	AC	513	CLA	OBD-CAD-C3D	2.46	132.57	128.03
30	BA	5401	SQD	C36-C35-C34	2.47	127.17	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5502	CLA	OBD-CAD-C3D	2.47	132.57	128.03
24	BC	5502	CLA	CED-O2D-CGD	2.47	121.77	115.97
24	AC	511	CLA	C3A-C2A-C1A	2.47	105.04	101.34
24	BC	5503	CLA	CBA-CAA-C2A	2.47	121.20	113.80
24	AC	513	CLA	C3A-C2A-C1A	2.47	105.05	101.34
24	AC	510	CLA	CED-O2D-CGD	2.48	121.78	115.97
24	BC	5501	CLA	C1D-CHD-C4C	2.48	125.87	122.48
24	AA	405	CLA	OBD-CAD-C3D	2.48	132.59	128.03
24	AB	606	CLA	C1D-CHD-C4C	2.48	125.88	122.48
27	AK	102	BCR	C30-C25-C24	2.48	122.71	115.73
27	AC	516	BCR	C37-C22-C23	2.49	122.06	118.10
27	AX	101	BCR	C28-C27-C26	2.49	118.06	113.78
30	AB	622	SQD	C15-C14-C13	2.49	127.27	114.45
27	BC	5514	BCR	C40-C30-C25	2.49	114.34	110.31
24	BC	5506	CLA	OBD-CAD-C3D	2.49	132.62	128.03
24	BB	5615	CLA	CED-O2D-CGD	2.49	121.81	115.97
28	BC	5518	DGD	C5A-C4A-C3A	2.49	127.31	114.45
24	BB	5612	CLA	OBD-CAD-C3D	2.49	132.62	128.03
31	BC	5521	LMG	C12-C11-C10	2.50	122.69	113.58
28	AC	518	DGD	C5A-C4A-C3A	2.50	127.32	114.45
24	AC	503	CLA	CBA-CAA-C2A	2.50	121.27	113.80
24	BC	5513	CLA	C3A-C2A-C1A	2.50	105.08	101.34
27	AA	410	BCR	C35-C13-C12	2.50	122.08	118.10
27	BC	5514	BCR	C7-C8-C9	2.50	129.97	126.21
30	AF	102	SQD	O47-C7-C8	2.50	116.75	111.55
24	AC	507	CLA	C3A-C2A-C1A	2.50	105.09	101.34
27	BT	5101	BCR	C36-C18-C19	2.50	122.09	118.10
30	BB	5625	SQD	C15-C14-C13	2.50	127.36	114.45
24	BC	5507	CLA	CED-O2D-CGD	2.51	121.84	115.97
24	BD	5402	CLA	C3A-C2A-C1A	2.51	105.09	101.34
24	AB	601	CLA	C3A-C2A-C1A	2.51	105.09	101.34
27	AA	410	BCR	C24-C23-C22	2.51	129.98	126.21
27	BJ	5101	BCR	C11-C10-C9	2.51	130.89	127.31
24	AC	505	CLA	C2A-C1A-CHA	2.51	128.37	123.92
24	AD	401	CLA	C3A-C2A-C1A	2.51	105.10	101.34
27	AC	514	BCR	C1-C6-C7	2.51	122.80	115.73
34	AD	402	PHO	C1C-NC-C4C	2.52	111.50	106.52
27	AC	516	BCR	C16-C17-C18	2.52	130.91	127.31
30	BB	5601	SQD	C31-C30-C29	2.52	133.12	113.42
27	AB	619	BCR	C35-C13-C12	2.53	122.12	118.10
24	AC	506	CLA	OBD-CAD-C3D	2.53	132.68	128.03
24	BB	5617	CLA	C1D-CHD-C4C	2.53	125.94	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BD	5403	PHO	C1C-NC-C4C	2.53	111.52	106.52
24	AC	512	CLA	O2D-CGD-CBD	2.53	115.81	111.30
24	BB	5610	CLA	OBD-CAD-C3D	2.53	132.68	128.03
24	BC	5511	CLA	C3A-C2A-C1A	2.53	105.13	101.34
27	BK	5102	BCR	C37-C22-C23	2.53	122.13	118.10
30	AB	627	SQD	C31-C30-C29	2.54	133.21	113.42
27	BK	5102	BCR	C30-C25-C24	2.54	122.85	115.73
24	BB	5613	CLA	CED-O2D-CGD	2.54	121.91	115.97
24	AA	406	CLA	C3A-C2A-C1A	2.54	105.14	101.34
24	BB	5616	CLA	OBD-CAD-C3D	2.54	132.70	128.03
30	AA	416	SQD	C36-C35-C34	2.54	127.54	114.45
24	BB	5613	CLA	OBD-CAD-C3D	2.54	132.71	128.03
24	AB	611	CLA	CED-O2D-CGD	2.54	121.93	115.97
32	AI	103	LMT	C1B-C2B-C3B	2.54	114.70	109.98
27	AK	102	BCR	C37-C22-C23	2.54	122.15	118.10
24	BC	5509	CLA	CED-O2D-CGD	2.54	121.93	115.97
24	AB	609	CLA	C2A-C1A-CHA	2.54	128.43	123.92
34	AD	402	PHO	O2A-CGA-CBA	2.54	119.30	111.90
24	AC	512	CLA	CED-O2D-CGD	2.54	121.93	115.97
30	AB	622	SQD	C31-C30-C29	2.54	133.28	113.42
27	AJ	101	BCR	C1-C6-C7	2.55	122.88	115.73
24	BB	5608	CLA	CBA-CAA-C2A	2.55	121.44	113.80
27	AB	617	BCR	C24-C23-C22	2.55	130.05	126.21
24	AC	502	CLA	CED-O2D-CGD	2.56	121.96	115.97
27	AC	514	BCR	C8-C7-C6	2.56	134.41	127.25
27	BJ	5101	BCR	C1-C6-C7	2.56	122.92	115.73
27	AC	516	BCR	C35-C13-C12	2.56	122.17	118.10
24	AB	616	CLA	CED-O2D-CGD	2.56	121.97	115.97
24	BB	5608	CLA	O2D-CGD-CBD	2.56	115.88	111.30
24	AA	404	CLA	C2A-C1A-CHA	2.56	128.46	123.92
28	BC	5517	DGD	C3A-C2A-C1A	2.56	122.94	113.58
27	BD	5407	BCR	C35-C13-C12	2.57	122.19	118.10
27	BK	5102	BCR	C34-C9-C8	2.57	122.19	118.10
30	BB	5625	SQD	C31-C30-C29	2.57	133.50	113.42
27	BC	5516	BCR	C24-C23-C22	2.57	130.08	126.21
31	AC	521	LMG	C12-C11-C10	2.57	122.98	113.58
32	BC	5522	LMT	C1B-C2B-C3B	2.58	114.77	109.98
24	AA	407	CLA	C1D-CHD-C4C	2.58	126.01	122.48
30	AA	416	SQD	C45-O47-C7	2.58	123.97	117.88
24	AC	501	CLA	CED-O2D-CGD	2.58	122.03	115.97
28	AC	518	DGD	O6D-C5D-C4D	2.58	114.42	109.66
30	BF	5102	SQD	O47-C7-C8	2.59	116.92	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AV	201	HEM	C1D-C2D-C3D	2.59	108.80	107.00
24	BC	5501	CLA	CED-O2D-CGD	2.59	122.03	115.97
24	AB	609	CLA	CED-O2D-CGD	2.59	122.04	115.97
27	BD	5407	BCR	C37-C22-C23	2.59	122.22	118.10
24	BB	5607	CLA	CED-O2D-CGD	2.59	122.05	115.97
27	BC	5514	BCR	C8-C7-C6	2.59	134.51	127.25
24	AC	502	CLA	C3A-C2A-C1A	2.59	105.22	101.34
27	AC	514	BCR	C40-C30-C25	2.59	114.51	110.31
28	BC	5519	DGD	C3G-C2G-C1G	2.59	117.70	111.86
24	BC	5506	CLA	C2A-C1A-CHA	2.59	128.51	123.92
34	BD	5403	PHO	O2A-CGA-CBA	2.60	119.45	111.90
27	BC	5516	BCR	C37-C22-C23	2.60	122.24	118.10
24	BB	5613	CLA	C2A-C1A-CHA	2.60	128.53	123.92
24	AB	607	CLA	C1D-CHD-C4C	2.60	126.04	122.48
27	AT	101	BCR	C20-C21-C22	2.60	131.03	127.31
34	AD	403	PHO	C1C-NC-C4C	2.60	111.68	106.52
27	AX	101	BCR	C15-C14-C13	2.61	131.03	127.31
24	BC	5512	CLA	CED-O2D-CGD	2.61	122.08	115.97
34	BD	5403	PHO	C3A-C4A-CHB	2.61	126.17	121.75
24	BB	5619	CLA	C1D-CHD-C4C	2.61	126.05	122.48
27	AB	617	BCR	C16-C17-C18	2.61	131.04	127.31
31	AB	621	LMG	O7-C8-C7	2.61	117.93	108.44
24	AC	506	CLA	O2D-CGD-CBD	2.62	115.97	111.30
24	AB	615	CLA	C1D-CHD-C4C	2.62	126.06	122.48
30	AF	102	SQD	C45-O47-C7	2.62	124.07	117.88
27	AX	101	BCR	C16-C17-C18	2.62	131.05	127.31
27	BT	5101	BCR	C23-C24-C25	2.62	134.59	127.25
24	BB	5610	CLA	C1D-CHD-C4C	2.62	126.07	122.48
27	AD	406	BCR	C37-C22-C23	2.63	122.28	118.10
27	BA	5411	BCR	C2-C1-C6	2.63	114.58	110.48
36	BF	5101	HEM	CAD-C3D-C2D	2.63	136.50	129.00
27	AD	406	BCR	C35-C13-C12	2.63	122.28	118.10
24	BB	5615	CLA	OBD-CAD-C3D	2.63	132.87	128.03
27	AC	514	BCR	C37-C22-C23	2.63	122.29	118.10
24	AC	506	CLA	C2A-C1A-CHA	2.63	128.58	123.92
32	BB	5626	LMT	O1B-C1B-C2B	2.63	114.04	108.11
24	BA	5405	CLA	OBD-CAD-C3D	2.63	132.88	128.03
31	BC	5521	LMG	C9-C8-C7	2.63	117.80	111.86
30	BA	5401	SQD	C45-O47-C7	2.63	124.10	117.88
24	AC	501	CLA	C1D-CHD-C4C	2.63	126.09	122.48
24	BB	5606	CLA	C3A-C2A-C1A	2.63	105.28	101.34
24	BB	5618	CLA	C3A-C2A-C1A	2.64	105.29	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BC	5520	LMG	O7-C8-C7	2.64	118.02	108.44
27	BC	5514	BCR	C37-C22-C23	2.64	122.30	118.10
27	AT	101	BCR	C36-C18-C19	2.64	122.31	118.10
24	BA	5407	CLA	OBD-CAD-C3D	2.64	132.89	128.03
24	AB	604	CLA	O2D-CGD-CBD	2.64	116.02	111.30
27	AA	410	BCR	C16-C17-C18	2.65	131.09	127.31
24	BB	5611	CLA	O2D-CGD-CBD	2.65	116.03	111.30
28	AC	517	DGD	C3A-C2A-C1A	2.65	123.25	113.58
27	BB	5621	BCR	C36-C18-C19	2.65	122.32	118.10
31	AC	520	LMG	O7-C8-C7	2.65	118.07	108.44
24	AC	504	CLA	OBD-CAD-C3D	2.66	132.92	128.03
36	BV	5201	HEM	CAA-CBA-CGA	2.66	117.20	112.66
28	AC	519	DGD	O3D-C3D-C2D	2.66	116.14	110.36
24	AB	601	CLA	CED-O2D-CGD	2.66	122.20	115.97
31	AB	620	LMG	C12-C11-C10	2.66	123.29	113.58
24	AA	407	CLA	OBD-CAD-C3D	2.66	132.94	128.03
28	AC	518	DGD	C3A-C2A-C1A	2.67	123.31	113.58
27	BC	5514	BCR	C1-C6-C7	2.67	123.22	115.73
34	BD	5403	PHO	CAB-C3B-C4B	2.67	136.38	126.11
31	BB	5624	LMG	O7-C8-C7	2.67	118.13	108.44
36	AF	101	HEM	CAD-C3D-C2D	2.67	136.62	129.00
27	AT	101	BCR	C32-C1-C6	2.67	114.64	110.31
28	BC	5518	DGD	C3A-C2A-C1A	2.67	123.33	113.58
28	AB	628	DGD	O6E-C1E-O5D	2.67	116.36	110.02
27	AC	514	BCR	C7-C8-C9	2.67	130.23	126.21
29	BA	5413	LHG	O8-C6-C5	2.67	115.37	108.66
28	AC	519	DGD	C3G-C2G-C1G	2.67	117.89	111.86
27	BX	5101	BCR	C11-C10-C9	2.68	131.13	127.31
27	BB	5621	BCR	C16-C17-C18	2.68	131.14	127.31
24	AB	607	CLA	O2D-CGD-CBD	2.68	116.09	111.30
27	BX	5101	BCR	C15-C14-C13	2.69	131.15	127.31
24	AB	611	CLA	OBD-CAD-C3D	2.70	132.99	128.03
28	AC	519	DGD	O6E-C5E-C4E	2.70	114.63	109.66
24	AA	404	CLA	OBD-CAD-C3D	2.70	133.00	128.03
31	BL	5101	LMG	C12-C11-C10	2.70	123.43	113.58
24	BB	5610	CLA	CED-O2D-CGD	2.70	122.30	115.97
24	AB	613	CLA	C3A-C2A-C1A	2.70	105.39	101.34
31	AA	414	LMG	O8-C9-C8	2.70	115.44	108.66
34	AD	403	PHO	CAB-C3B-C4B	2.70	136.51	126.11
34	BD	5404	PHO	CAB-C3B-C4B	2.71	136.54	126.11
27	AT	101	BCR	C23-C24-C25	2.71	134.84	127.25
24	BA	5405	CLA	C3A-C2A-C1A	2.72	105.41	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	614	CLA	C3A-C2A-C1A	2.72	105.41	101.34
24	AC	509	CLA	CED-O2D-CGD	2.72	122.34	115.97
24	AC	509	CLA	C3A-C2A-C1A	2.72	105.41	101.34
27	BA	5411	BCR	C35-C13-C12	2.72	122.43	118.10
27	AJ	101	BCR	C21-C20-C19	2.72	131.58	123.23
28	BC	5519	DGD	O3D-C3D-C2D	2.72	116.28	110.36
28	BH	5101	DGD	O6D-C1D-O3G	2.72	116.48	110.02
24	BB	5605	CLA	CED-O2D-CGD	2.72	122.36	115.97
36	AV	201	HEM	CAA-CBA-CGA	2.73	117.32	112.66
24	AC	509	CLA	O2D-CGD-CBD	2.73	116.17	111.30
24	BC	5513	CLA	CED-O2D-CGD	2.73	122.37	115.97
31	BB	5624	LMG	O8-C28-C29	2.73	119.84	111.90
24	BB	5620	CLA	CED-O2D-CGD	2.73	122.37	115.97
24	AA	406	CLA	OBD-CAD-C3D	2.73	133.06	128.03
32	AB	623	LMT	O1B-C1B-C2B	2.74	114.28	108.11
24	BC	5512	CLA	C3A-C2A-C1A	2.74	105.44	101.34
24	BC	5504	CLA	OBD-CAD-C3D	2.74	133.07	128.03
27	AC	515	BCR	C35-C13-C12	2.74	122.47	118.10
24	AB	612	CLA	C2A-C1A-CHA	2.74	128.78	123.92
27	AJ	101	BCR	C11-C10-C9	2.74	131.23	127.31
24	BB	5612	CLA	C11-C12-C13	2.74	124.74	115.73
24	AB	602	CLA	C3A-C2A-C1A	2.75	105.46	101.34
27	AX	101	BCR	C11-C10-C9	2.75	131.24	127.31
24	AB	607	CLA	OBD-CAD-C3D	2.75	133.10	128.03
27	BB	5621	BCR	C35-C13-C12	2.75	122.49	118.10
24	BB	5608	CLA	OBD-CAD-C3D	2.76	133.11	128.03
24	AB	614	CLA	CED-O2D-CGD	2.76	122.44	115.97
31	BE	5101	LMG	O8-C9-C8	2.76	115.60	108.66
35	AD	405	PL9	C26-C27-C28	2.76	121.44	111.97
28	BC	5518	DGD	O6D-C5D-C4D	2.76	114.75	109.66
24	AC	510	CLA	C2A-C1A-CHA	2.76	128.82	123.92
28	AH	101	DGD	O6D-C1D-O3G	2.76	116.58	110.02
35	BD	5406	PL9	C30-C29-C31	2.77	120.09	115.29
31	BD	5410	LMG	O7-C8-C7	2.77	118.49	108.44
27	BC	5516	BCR	C35-C13-C12	2.77	122.51	118.10
24	BC	5506	CLA	O2D-CGD-CBD	2.77	116.25	111.30
28	BB	5602	DGD	O6E-C1E-O5D	2.77	116.60	110.02
24	BA	5408	CLA	C2A-C1A-CHA	2.77	128.83	123.92
24	BC	5509	CLA	O2D-CGD-CBD	2.77	116.26	111.30
24	AB	608	CLA	C11-C12-C13	2.78	124.84	115.73
27	BJ	5101	BCR	C16-C15-C14	2.78	129.39	123.46
27	AC	514	BCR	C35-C13-C12	2.78	122.52	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	613	CLA	C1D-CHD-C4C	2.78	126.29	122.48
34	AD	402	PHO	C3A-C4A-CHB	2.78	126.46	121.75
24	BC	5509	CLA	C1D-CHD-C4C	2.79	126.29	122.48
27	AK	102	BCR	C34-C9-C8	2.79	122.54	118.10
24	AA	407	CLA	CBA-CAA-C2A	2.79	122.14	113.80
24	AB	613	CLA	O2A-CGA-CBA	2.79	120.02	111.90
27	BC	5515	BCR	C16-C17-C18	2.79	131.29	127.31
24	BC	5501	CLA	O2D-CGD-CBD	2.79	116.29	111.30
27	BA	5411	BCR	C24-C23-C22	2.79	130.41	126.21
24	BB	5617	CLA	C2A-C1A-CHA	2.79	128.87	123.92
27	BB	5623	BCR	C23-C24-C25	2.80	135.08	127.25
34	AD	402	PHO	CAB-C3B-C4B	2.80	136.88	126.11
35	AD	405	PL9	C30-C29-C31	2.80	120.14	115.29
27	AX	101	BCR	C35-C13-C12	2.80	122.56	118.10
31	BE	5101	LMG	C34-C33-C32	2.80	128.90	114.45
27	AJ	101	BCR	C16-C15-C14	2.81	129.46	123.46
24	BA	5407	CLA	C3A-C2A-C1A	2.82	105.56	101.34
24	AD	401	CLA	C2A-C1A-CHA	2.82	128.92	123.92
24	AA	404	CLA	C3A-C2A-C1A	2.82	105.56	101.34
27	BK	5102	BCR	C35-C13-C12	2.82	122.59	118.10
27	BJ	5101	BCR	C21-C20-C19	2.82	131.90	123.23
31	AD	408	LMG	O7-C8-C7	2.83	118.71	108.44
27	AB	617	BCR	C36-C18-C19	2.83	122.61	118.10
24	AC	506	CLA	CED-O2D-CGD	2.83	122.61	115.97
31	AA	414	LMG	C34-C33-C32	2.83	129.06	114.45
27	BT	5101	BCR	C32-C1-C6	2.84	114.91	110.31
24	BB	5611	CLA	OBD-CAD-C3D	2.84	133.25	128.03
29	AA	415	LHG	O8-C23-C24	2.84	120.16	111.90
24	AA	404	CLA	CED-O2D-CGD	2.84	122.63	115.97
27	AB	617	BCR	C35-C13-C12	2.84	122.63	118.10
34	BD	5404	PHO	C1C-NC-C4C	2.84	112.15	106.52
34	AD	402	PHO	C3A-C2A-C1A	2.84	105.03	101.68
24	BC	5506	CLA	CED-O2D-CGD	2.85	122.64	115.97
28	BC	5517	DGD	C3G-C2G-C1G	2.85	118.28	111.86
24	BB	5618	CLA	CED-O2D-CGD	2.85	122.64	115.97
27	AD	406	BCR	C7-C8-C9	2.85	130.49	126.21
24	BB	5605	CLA	C2A-C1A-CHA	2.85	128.97	123.92
27	AK	102	BCR	C16-C17-C18	2.85	131.38	127.31
28	AC	517	DGD	C3G-C2G-C1G	2.85	118.29	111.86
27	AK	102	BCR	C35-C13-C12	2.85	122.65	118.10
29	BA	5415	LHG	O8-C23-C24	2.86	120.21	111.90
24	AB	611	CLA	CBA-CAA-C2A	2.86	122.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AB	622	SQD	C45-O47-C7	2.86	124.63	117.88
24	BB	5615	CLA	C6-C5-C3	2.86	119.14	112.66
24	AB	606	CLA	CED-O2D-CGD	2.86	122.68	115.97
24	AB	616	CLA	O2A-CGA-CBA	2.86	120.23	111.90
28	BC	5519	DGD	O1G-C1A-C2A	2.87	120.25	111.90
28	AC	517	DGD	O6D-C1D-O3G	2.87	116.84	110.02
27	BT	5101	BCR	C2-C1-C6	2.87	114.97	110.48
27	BB	5623	BCR	C8-C7-C6	2.88	135.32	127.25
24	BC	5510	CLA	C2A-C1A-CHA	2.88	129.03	123.92
27	AB	619	BCR	C8-C7-C6	2.88	135.33	127.25
31	AB	621	LMG	O8-C28-C29	2.89	120.30	111.90
35	BD	5406	PL9	C26-C27-C28	2.89	121.89	111.97
24	AB	604	CLA	C3A-C2A-C1A	2.89	105.67	101.34
24	BB	5616	CLA	C2A-C1A-CHA	2.89	129.05	123.92
27	BK	5102	BCR	C16-C17-C18	2.90	131.44	127.31
27	AT	101	BCR	C2-C1-C6	2.90	115.01	110.48
28	BH	5101	DGD	C3G-O3G-C1D	2.90	119.71	113.76
24	AB	604	CLA	OBD-CAD-C3D	2.90	133.38	128.03
24	AC	508	CLA	CED-O2D-CGD	2.90	122.78	115.97
24	BB	5618	CLA	O2A-CGA-CBA	2.90	120.35	111.90
24	BC	5508	CLA	CED-O2D-CGD	2.91	122.78	115.97
28	BC	5517	DGD	O6D-C1D-O3G	2.91	116.92	110.02
27	BT	5101	BCR	C7-C8-C9	2.91	130.58	126.21
24	AA	407	CLA	C2A-C1A-CHA	2.91	129.08	123.92
27	BX	5101	BCR	C35-C13-C12	2.91	122.74	118.10
24	BC	5502	CLA	C3A-C2A-C1A	2.92	105.71	101.34
28	AH	101	DGD	C3G-O3G-C1D	2.92	119.75	113.76
24	AC	513	CLA	CED-O2D-CGD	2.92	122.82	115.97
24	BB	5615	CLA	CBA-CAA-C2A	2.92	122.54	113.80
24	BB	5609	CLA	O2D-CGD-CBD	2.92	116.52	111.30
27	BK	5102	BCR	C8-C7-C6	2.92	135.44	127.25
28	AC	519	DGD	O1G-C1A-C2A	2.93	120.42	111.90
27	AD	406	BCR	C11-C10-C9	2.93	131.49	127.31
24	BC	5510	CLA	C3A-C2A-C1A	2.93	105.73	101.34
27	BD	5407	BCR	C11-C10-C9	2.93	131.49	127.31
24	BB	5614	CLA	C2A-C1A-CHA	2.93	129.11	123.92
29	AA	412	LHG	O7-C7-C8	2.93	117.64	111.55
24	AB	605	CLA	CED-O2D-CGD	2.93	122.84	115.97
24	BB	5613	CLA	C3A-C2A-C1A	2.93	105.73	101.34
31	BE	5101	LMG	O8-C28-C29	2.93	120.43	111.90
24	BB	5620	CLA	C3A-C2A-C1A	2.93	105.73	101.34
24	AB	613	CLA	C2A-C1A-CHA	2.93	129.12	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AA	414	LMG	O8-C28-C29	2.94	120.44	111.90
32	AB	629	LMT	O1B-C1B-C2B	2.94	114.73	108.11
29	BA	5413	LHG	O7-C7-C8	2.94	117.66	111.55
27	BJ	5101	BCR	C8-C7-C6	2.94	135.49	127.25
32	BB	5603	LMT	O1B-C1B-C2B	2.95	114.75	108.11
24	BB	5617	CLA	O2A-CGA-CBA	2.95	120.47	111.90
27	BC	5514	BCR	C35-C13-C12	2.95	122.80	118.10
24	BB	5620	CLA	O2A-CGA-CBA	2.95	120.48	111.90
28	AA	411	DGD	C4A-C3A-C2A	2.96	124.07	113.24
28	BC	5519	DGD	O6E-C5E-C4E	2.96	115.11	109.66
24	AB	610	CLA	C2A-C1A-CHA	2.96	129.16	123.92
24	BA	5406	CLA	C3A-C2A-C1A	2.96	105.77	101.34
27	AA	410	BCR	C2-C1-C6	2.96	115.11	110.48
24	AB	611	CLA	C6-C5-C3	2.97	119.38	112.66
24	BD	5402	CLA	C2A-C1A-CHA	2.97	129.18	123.92
24	AD	404	CLA	C3A-C2A-C1A	2.97	105.79	101.34
24	AB	614	CLA	O2D-CGD-CBD	2.97	116.61	111.30
27	AB	619	BCR	C23-C24-C25	2.97	135.57	127.25
24	BC	5509	CLA	C3A-C2A-C1A	2.97	105.79	101.34
24	AB	609	CLA	O2D-CGD-CBD	2.98	116.62	111.30
24	BB	5614	CLA	C3A-C2A-C1A	2.98	105.80	101.34
24	BC	5507	CLA	C2A-C1A-CHA	2.98	129.20	123.92
24	AB	609	CLA	C3A-C2A-C1A	2.98	105.81	101.34
24	AB	601	CLA	C2A-C1A-CHA	2.98	129.20	123.92
24	AB	616	CLA	C3A-C2A-C1A	2.99	105.81	101.34
28	BA	5412	DGD	C4A-C3A-C2A	2.99	124.19	113.24
27	BB	5621	BCR	C2-C1-C6	2.99	115.15	110.48
24	AC	501	CLA	O2D-CGD-CBD	2.99	116.64	111.30
28	AE	101	DGD	O5D-C6D-C5D	3.00	113.96	108.94
27	AA	410	BCR	C23-C24-C25	3.00	135.66	127.25
28	BE	5102	DGD	O5D-C6D-C5D	3.00	113.97	108.94
31	BL	5101	LMG	C9-O8-C28	3.01	126.17	117.13
27	AB	619	BCR	C2-C1-C6	3.01	115.18	110.48
24	BB	5608	CLA	C3A-C2A-C1A	3.01	105.85	101.34
24	BA	5408	CLA	CBA-CAA-C2A	3.01	122.81	113.80
24	BB	5609	CLA	CED-O2D-CGD	3.01	123.03	115.97
27	AB	617	BCR	C2-C1-C6	3.01	115.19	110.48
24	AB	603	CLA	C1D-CHD-C4C	3.01	126.61	122.48
27	BD	5407	BCR	C16-C17-C18	3.01	131.61	127.31
24	AC	507	CLA	C2A-C1A-CHA	3.01	129.26	123.92
24	BB	5611	CLA	C1D-CHD-C4C	3.01	126.61	122.48
27	AC	515	BCR	C16-C17-C18	3.02	131.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5611	CLA	C2A-C1A-CHA	3.02	129.27	123.92
31	AA	414	LMG	O7-C10-C11	3.02	117.82	111.55
27	BC	5515	BCR	C8-C7-C6	3.02	135.71	127.25
28	BC	5519	DGD	O6E-C1E-C2E	3.02	116.13	110.30
24	AB	610	CLA	C3A-C2A-C1A	3.03	105.87	101.34
24	BB	5607	CLA	C6-C5-C3	3.03	119.52	112.66
30	AA	413	SQD	C32-C31-C30	3.03	130.06	114.45
27	BA	5411	BCR	C23-C24-C25	3.03	135.74	127.25
27	AC	515	BCR	C8-C7-C6	3.03	135.75	127.25
31	AB	620	LMG	C9-O8-C28	3.04	126.27	117.13
27	AJ	101	BCR	C8-C7-C6	3.04	135.76	127.25
31	BD	5409	LMG	C16-C15-C14	3.04	130.13	114.45
27	AT	101	BCR	C16-C17-C18	3.05	131.66	127.31
24	AB	614	CLA	O2A-CGA-CBA	3.05	120.76	111.90
27	AK	102	BCR	C8-C7-C6	3.05	135.80	127.25
24	BD	5405	CLA	C3A-C2A-C1A	3.06	105.92	101.34
31	BE	5101	LMG	O7-C10-C11	3.07	117.92	111.55
27	AC	514	BCR	C2-C1-C6	3.07	115.28	110.48
31	AM	101	LMG	O7-C8-C7	3.07	119.61	108.44
29	AA	412	LHG	O8-C6-C5	3.07	116.38	108.66
24	BD	5405	CLA	O2A-CGA-CBA	3.07	120.84	111.90
24	AC	511	CLA	C1D-CHD-C4C	3.08	126.69	122.48
31	AD	407	LMG	C16-C15-C14	3.08	130.31	114.45
30	BB	5601	SQD	C44-O6-C1	3.08	120.08	113.76
28	BA	5412	DGD	O2G-C2G-C3G	3.08	119.64	108.44
24	BB	5615	CLA	O2D-CGD-CBD	3.08	116.81	111.30
28	BE	5102	DGD	O5D-C1E-C2E	3.08	113.27	108.23
24	AB	612	CLA	O2A-CGA-CBA	3.08	120.87	111.90
30	AB	627	SQD	C44-O6-C1	3.09	120.08	113.76
31	AA	417	LMG	C12-C11-C10	3.09	124.84	113.58
24	AB	607	CLA	C2A-C1A-CHA	3.09	129.39	123.92
24	AB	615	CLA	O2A-CGA-CBA	3.09	120.90	111.90
27	BB	5622	BCR	C24-C23-C22	3.10	130.87	126.21
27	BC	5515	BCR	C35-C13-C12	3.10	123.03	118.10
27	AX	101	BCR	C8-C7-C6	3.10	135.93	127.25
24	AB	609	CLA	CBA-CAA-C2A	3.10	123.08	113.80
30	BA	5414	SQD	C32-C31-C30	3.11	130.46	114.45
28	AA	411	DGD	O2G-C2G-C3G	3.11	119.72	108.44
27	BX	5101	BCR	C8-C7-C6	3.11	135.95	127.25
24	BB	5619	CLA	O2A-CGA-CBA	3.12	120.97	111.90
31	BM	5102	LMG	O7-C8-C7	3.12	119.78	108.44
31	BA	5402	LMG	O1-C7-C8	3.12	118.41	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	405	CLA	C3A-C2A-C1A	3.12	106.02	101.34
27	BD	5407	BCR	C7-C8-C9	3.13	130.91	126.21
28	AC	519	DGD	O6E-C1E-C2E	3.13	116.33	110.30
24	BB	5613	CLA	CBA-CAA-C2A	3.13	123.17	113.80
27	AD	406	BCR	C16-C17-C18	3.13	131.78	127.31
34	BD	5403	PHO	C4A-NA-C1A	3.14	110.70	108.16
34	BD	5403	PHO	C3A-C2A-C1A	3.14	105.38	101.68
31	BD	5409	LMG	C12-C11-C10	3.14	125.03	113.58
31	BA	5402	LMG	C12-C11-C10	3.14	125.05	113.58
24	BB	5607	CLA	C1D-CHD-C4C	3.14	126.78	122.48
24	AB	603	CLA	C6-C5-C3	3.15	119.79	112.66
27	BD	5407	BCR	C2-C1-C6	3.15	115.40	110.48
24	BC	5511	CLA	C1D-CHD-C4C	3.15	126.79	122.48
28	BC	5518	DGD	O2G-C2G-C3G	3.15	119.88	108.44
24	BB	5613	CLA	O2D-CGD-CBD	3.16	116.94	111.30
24	BC	5505	CLA	O2D-CGD-CBD	3.16	116.94	111.30
28	AC	518	DGD	O2G-C2G-C3G	3.16	119.92	108.44
34	AD	402	PHO	C4A-NA-C1A	3.16	110.72	108.16
24	AC	509	CLA	C1D-CHD-C4C	3.16	126.81	122.48
31	AD	407	LMG	C12-C11-C10	3.16	125.13	113.58
28	AH	101	DGD	C4B-C3B-C2B	3.17	124.84	113.24
24	AB	602	CLA	O2D-CGD-CBD	3.17	116.96	111.30
27	AB	618	BCR	C24-C23-C22	3.17	130.98	126.21
28	BB	5602	DGD	C3B-C2B-C1B	3.18	125.18	113.58
24	AC	506	CLA	C3A-C2A-C1A	3.18	106.10	101.34
28	AB	628	DGD	C3B-C2B-C1B	3.18	125.19	113.58
24	AB	612	CLA	C1D-CHD-C4C	3.19	126.84	122.48
31	BC	5520	LMG	C8-O7-C10	3.19	125.41	117.88
27	BC	5514	BCR	C29-C30-C25	3.19	115.47	110.48
27	AT	101	BCR	C7-C8-C9	3.19	131.01	126.21
24	BC	5506	CLA	C3A-C2A-C1A	3.19	106.12	101.34
31	BC	5520	LMG	C9-O8-C28	3.19	126.74	117.13
30	BB	5625	SQD	C45-O47-C7	3.20	125.43	117.88
24	AB	615	CLA	C3A-C2A-C1A	3.20	106.13	101.34
24	BC	5502	CLA	O2D-CGD-CBD	3.20	117.01	111.30
27	BK	5102	BCR	C24-C23-C22	3.20	131.02	126.21
27	AK	102	BCR	C24-C23-C22	3.20	131.02	126.21
24	BB	5619	CLA	O2D-CGD-CBD	3.20	117.02	111.30
35	BD	5406	PL9	C51-C49-C50	3.20	122.08	114.60
27	BT	5101	BCR	C24-C23-C22	3.21	131.03	126.21
27	AB	618	BCR	C8-C7-C6	3.22	136.26	127.25
31	AC	520	LMG	O8-C9-C8	3.22	116.76	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	5602	DGD	O3G-C3G-C2G	3.23	118.66	110.99
31	AC	520	LMG	C9-O8-C28	3.23	126.84	117.13
24	AD	401	CLA	O2D-CGD-CBD	3.23	117.06	111.30
24	BB	5610	CLA	C2A-C1A-CHA	3.23	129.65	123.92
24	AC	513	CLA	O2D-CGD-CBD	3.23	117.08	111.30
24	AB	606	CLA	C2A-C1A-CHA	3.24	129.66	123.92
27	BC	5514	BCR	C2-C1-C6	3.24	115.54	110.48
28	BB	5602	DGD	O6D-C5D-C6D	3.24	113.10	106.64
24	BC	5503	CLA	C3A-C2A-C1A	3.24	106.19	101.34
24	AC	502	CLA	O2D-CGD-CBD	3.24	117.09	111.30
24	BB	5619	CLA	C3A-C2A-C1A	3.24	106.20	101.34
28	BH	5101	DGD	C4B-C3B-C2B	3.24	125.12	113.24
24	AB	603	CLA	O2D-CGD-CBD	3.25	117.10	111.30
24	AC	501	CLA	CBA-CAA-C2A	3.25	123.52	113.80
24	BC	5505	CLA	O2A-CGA-CBA	3.25	121.36	111.90
31	AA	417	LMG	O1-C7-C8	3.25	118.72	110.99
28	AC	517	DGD	C3B-C2B-C1B	3.25	125.45	113.58
27	AB	618	BCR	C23-C24-C25	3.25	136.35	127.25
24	AB	605	CLA	O2D-CGD-CBD	3.26	117.11	111.30
28	AC	519	DGD	C3B-C2B-C1B	3.26	125.48	113.58
31	BC	5520	LMG	O8-C9-C8	3.26	116.85	108.66
24	BB	5607	CLA	O2D-CGD-CBD	3.27	117.14	111.30
28	AE	101	DGD	O5D-C1E-C2E	3.27	113.58	108.23
24	AC	513	CLA	C1D-CHD-C4C	3.28	126.97	122.48
27	AD	406	BCR	C2-C1-C6	3.28	115.61	110.48
24	AD	404	CLA	O2A-CGA-CBA	3.28	121.45	111.90
31	AC	520	LMG	C8-O7-C10	3.29	125.64	117.88
24	AB	611	CLA	C3A-C2A-C1A	3.29	106.26	101.34
27	AX	101	BCR	C24-C23-C22	3.29	131.15	126.21
31	AI	101	LMG	C8-O7-C10	3.29	125.65	117.88
27	BB	5622	BCR	C8-C7-C6	3.29	136.47	127.25
28	AB	628	DGD	O6D-C5D-C6D	3.29	113.22	106.64
30	BA	5401	SQD	C32-C31-C30	3.30	131.44	114.45
24	BB	5618	CLA	O2D-CGD-CBD	3.30	117.19	111.30
24	BB	5616	CLA	C1D-CHD-C4C	3.30	126.99	122.48
24	AB	616	CLA	C2A-C1A-CHA	3.30	129.76	123.92
24	AA	407	CLA	C3A-C2A-C1A	3.30	106.28	101.34
35	AD	405	PL9	C51-C49-C50	3.30	122.30	114.60
24	AB	608	CLA	O2A-CGA-CBA	3.31	121.53	111.90
27	AA	410	BCR	C29-C30-C25	3.31	115.65	110.48
28	AC	518	DGD	O6E-C1E-O5D	3.31	117.88	110.02
27	AT	101	BCR	C24-C23-C22	3.31	131.19	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BT	5101	BCR	C16-C17-C18	3.32	132.04	127.31
24	BB	5616	CLA	O2A-CGA-CBA	3.32	121.55	111.90
24	BB	5620	CLA	C2A-C1A-CHA	3.32	129.80	123.92
24	AC	505	CLA	O2A-CGA-CBA	3.32	121.56	111.90
27	AX	101	BCR	C23-C24-C25	3.33	136.56	127.25
27	BX	5101	BCR	C23-C24-C25	3.33	136.58	127.25
27	BB	5623	BCR	C2-C1-C6	3.33	115.69	110.48
30	AA	416	SQD	C32-C31-C30	3.33	131.63	114.45
27	AB	618	BCR	C2-C1-C6	3.34	115.70	110.48
24	BC	5513	CLA	O2D-CGD-CBD	3.34	117.27	111.30
27	BC	5516	BCR	C8-C7-C6	3.34	136.61	127.25
24	BB	5612	CLA	O2A-CGA-CBA	3.34	121.63	111.90
24	BC	5513	CLA	C1D-CHD-C4C	3.35	127.06	122.48
29	BA	5413	LHG	O8-C23-C24	3.35	121.64	111.90
27	BD	5407	BCR	C8-C7-C6	3.35	136.64	127.25
31	AB	621	LMG	C39-C38-C37	3.35	131.74	114.45
24	AC	503	CLA	C3A-C2A-C1A	3.36	106.37	101.34
27	AC	514	BCR	C29-C30-C25	3.36	115.73	110.48
27	AD	406	BCR	C8-C7-C6	3.37	136.68	127.25
24	AC	508	CLA	O2D-CGD-CBD	3.37	117.32	111.30
27	BX	5101	BCR	C24-C23-C22	3.37	131.28	126.21
24	BC	5504	CLA	O2A-CGA-CBA	3.38	121.72	111.90
27	BB	5622	BCR	C29-C30-C25	3.38	115.76	110.48
24	AB	611	CLA	O2D-CGD-CBD	3.38	117.33	111.30
24	BD	5405	CLA	CBA-CAA-C2A	3.39	123.94	113.80
28	BC	5518	DGD	O6E-C1E-O5D	3.39	118.08	110.02
27	BB	5623	BCR	C29-C30-C25	3.40	115.79	110.48
27	BB	5622	BCR	C2-C1-C6	3.40	115.79	110.48
24	BC	5501	CLA	CBA-CAA-C2A	3.40	123.97	113.80
24	BC	5504	CLA	C3A-C2A-C1A	3.40	106.44	101.34
27	AC	515	BCR	C29-C30-C25	3.40	115.80	110.48
24	AB	615	CLA	O2D-CGD-CBD	3.41	117.39	111.30
28	BE	5102	DGD	C2G-O2G-C1B	3.41	125.93	117.88
31	BI	5101	LMG	C8-O7-C10	3.41	125.93	117.88
31	BB	5624	LMG	C39-C38-C37	3.41	132.03	114.45
24	BB	5606	CLA	O2D-CGD-CBD	3.41	117.39	111.30
27	BB	5622	BCR	C23-C24-C25	3.41	136.80	127.25
27	AB	618	BCR	C29-C30-C25	3.41	115.81	110.48
24	AC	501	CLA	C2A-C1A-CHA	3.41	129.97	123.92
24	AC	504	CLA	C3A-C2A-C1A	3.41	106.45	101.34
24	BC	5501	CLA	C2A-C1A-CHA	3.42	129.98	123.92
24	AC	508	CLA	C3A-C2A-C1A	3.42	106.47	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	C1D-CHD-C4C	3.43	127.17	122.48
28	AB	628	DGD	O3G-C3G-C2G	3.43	119.14	110.99
24	AB	610	CLA	O2A-CGA-CBA	3.44	121.89	111.90
31	BD	5410	LMG	C12-C11-C10	3.44	126.15	113.58
27	BC	5515	BCR	C2-C1-C6	3.45	115.86	110.48
28	AE	101	DGD	C2G-O2G-C1B	3.45	126.02	117.88
28	BC	5517	DGD	C3B-C2B-C1B	3.45	126.16	113.58
24	AB	616	CLA	O2D-CGD-CBD	3.45	117.46	111.30
24	AB	608	CLA	O2D-CGD-CBD	3.45	117.47	111.30
27	BA	5411	BCR	C29-C30-C25	3.45	115.88	110.48
27	AC	516	BCR	C8-C7-C6	3.46	136.94	127.25
27	BC	5516	BCR	C2-C1-C6	3.46	115.89	110.48
24	BB	5605	CLA	O2A-CGA-CBA	3.46	121.98	111.90
27	BC	5516	BCR	C23-C24-C25	3.47	136.96	127.25
27	BK	5102	BCR	C29-C30-C25	3.47	115.90	110.48
24	BA	5408	CLA	C3A-C2A-C1A	3.47	106.53	101.34
24	AC	506	CLA	CBA-CAA-C2A	3.48	124.20	113.80
36	BF	5101	HEM	CAA-CBA-CGA	3.48	118.61	112.66
24	BB	5614	CLA	O2A-CGA-CBA	3.49	122.05	111.90
31	AD	408	LMG	C12-C11-C10	3.49	126.33	113.58
35	BD	5406	PL9	C25-C24-C26	3.50	121.36	115.29
24	BC	5512	CLA	O2A-CGA-CBA	3.50	122.08	111.90
24	BB	5615	CLA	C3A-C2A-C1A	3.50	106.58	101.34
24	BC	5509	CLA	C2A-C1A-CHA	3.50	130.13	123.92
24	AB	605	CLA	C3A-C2A-C1A	3.50	106.59	101.34
27	AC	515	BCR	C2-C1-C6	3.51	115.97	110.48
28	BC	5519	DGD	C3B-C2B-C1B	3.51	126.39	113.58
34	AD	402	PHO	C4D-C3D-CAD	3.51	111.92	105.41
24	BC	5511	CLA	O2D-CGD-CBD	3.51	117.58	111.30
24	BB	5612	CLA	O2D-CGD-CBD	3.52	117.58	111.30
24	BB	5616	CLA	C3A-C2A-C1A	3.52	106.61	101.34
24	BD	5402	CLA	O2D-CGD-CBD	3.52	117.59	111.30
27	BD	5407	BCR	C23-C24-C25	3.52	137.11	127.25
27	AK	102	BCR	C29-C30-C25	3.52	115.99	110.48
24	BB	5609	CLA	O2A-CGA-CBA	3.53	122.16	111.90
27	BB	5621	BCR	C23-C24-C25	3.53	137.12	127.25
24	BB	5605	CLA	O2D-CGD-CBD	3.53	117.60	111.30
24	BC	5510	CLA	O2A-CGA-CBA	3.53	122.16	111.90
27	AC	516	BCR	C23-C24-C25	3.53	137.14	127.25
24	BC	5508	CLA	C3A-C2A-C1A	3.53	106.63	101.34
24	AB	614	CLA	C1D-CHD-C4C	3.54	127.32	122.48
27	AB	619	BCR	C29-C30-C25	3.54	116.02	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	610	CLA	O2D-CGD-CBD	3.54	117.63	111.30
24	AC	512	CLA	C2A-C1A-CHA	3.54	130.20	123.92
34	BD	5404	PHO	C4D-C3D-CAD	3.55	112.00	105.41
24	AC	511	CLA	O2A-CGA-CBA	3.55	122.23	111.90
34	AD	403	PHO	O2D-CGD-CBD	3.55	117.65	111.30
24	AB	601	CLA	O2A-CGA-CBA	3.55	122.24	111.90
34	BD	5403	PHO	C4D-C3D-CAD	3.56	112.01	105.41
24	BC	5506	CLA	CBA-CAA-C2A	3.56	124.44	113.80
27	AX	101	BCR	C2-C1-C6	3.56	116.04	110.48
24	AD	404	CLA	CBA-CAA-C2A	3.56	124.45	113.80
34	AD	403	PHO	C4D-C3D-CAD	3.56	112.02	105.41
24	AC	501	CLA	O2A-CGA-CBA	3.57	122.28	111.90
27	BC	5515	BCR	C29-C30-C25	3.57	116.06	110.48
24	BC	5508	CLA	O2D-CGD-CBD	3.57	117.68	111.30
27	AB	617	BCR	C29-C30-C25	3.57	116.06	110.48
27	AK	102	BCR	C23-C24-C25	3.58	137.28	127.25
27	AD	406	BCR	C23-C24-C25	3.59	137.29	127.25
35	AD	405	PL9	C2-C1-C6	3.59	123.84	117.82
27	BK	5102	BCR	C23-C24-C25	3.59	137.30	127.25
24	BB	5620	CLA	O2D-CGD-CBD	3.59	117.72	111.30
24	BC	5512	CLA	C2A-C1A-CHA	3.59	130.29	123.92
30	AB	627	SQD	C11-C10-C9	3.60	132.99	114.45
24	AB	612	CLA	C3A-C2A-C1A	3.60	106.73	101.34
24	BC	5511	CLA	O2A-CGA-CBA	3.60	122.37	111.90
27	BJ	5101	BCR	C29-C30-C25	3.60	116.11	110.48
24	AC	509	CLA	C2A-C1A-CHA	3.60	130.30	123.92
24	AA	404	CLA	O2A-CGA-CBA	3.60	122.38	111.90
36	AF	101	HEM	CAA-CBA-CGA	3.60	118.82	112.66
24	BB	5614	CLA	O2D-CGD-CBD	3.60	117.74	111.30
31	BD	5408	LMG	C12-C11-C10	3.61	126.75	113.58
24	BC	5509	CLA	O2A-CGA-CBA	3.61	122.40	111.90
24	BA	5405	CLA	O2A-CGA-CBA	3.61	122.40	111.90
24	AC	504	CLA	O2A-CGA-CBA	3.61	122.41	111.90
24	AC	507	CLA	O2D-CGD-CBD	3.61	117.75	111.30
29	AA	412	LHG	O8-C23-C24	3.61	122.42	111.90
35	BD	5406	PL9	C2-C1-C6	3.62	123.90	117.82
24	AB	615	CLA	C2A-C1A-CHA	3.62	130.34	123.92
24	AB	605	CLA	O2A-CGA-CBA	3.63	122.45	111.90
34	AD	402	PHO	O2D-CGD-CBD	3.63	117.79	111.30
24	AB	607	CLA	C3A-C2A-C1A	3.64	106.78	101.34
34	BD	5403	PHO	O2D-CGD-CBD	3.64	117.80	111.30
27	BJ	5101	BCR	C7-C8-C9	3.64	131.68	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	601	CLA	O2D-CGD-CBD	3.64	117.80	111.30
30	AA	413	SQD	O48-C23-C24	3.64	122.49	111.90
35	AD	405	PL9	C25-C24-C26	3.65	121.62	115.29
24	AA	407	CLA	O2A-CGA-CBA	3.65	122.52	111.90
34	BD	5404	PHO	O2A-CGA-CBA	3.65	122.52	111.90
31	AJ	102	LMG	O1-C7-C8	3.65	119.67	110.99
30	BB	5601	SQD	C11-C10-C9	3.66	133.29	114.45
30	BA	5414	SQD	O48-C23-C24	3.66	122.54	111.90
24	BB	5619	CLA	C2A-C1A-CHA	3.66	130.40	123.92
27	AJ	101	BCR	C29-C30-C25	3.67	116.21	110.48
24	BC	5502	CLA	O2A-CGA-CBA	3.67	122.58	111.90
35	AD	405	PL9	C15-C14-C16	3.67	121.66	115.29
30	BA	5414	SQD	C11-C10-C9	3.67	133.37	114.45
30	AA	413	SQD	C11-C10-C9	3.67	133.38	114.45
24	BC	5510	CLA	O2D-CGD-CBD	3.67	117.86	111.30
34	BD	5404	PHO	O2D-CGD-CBD	3.68	117.87	111.30
24	BC	5505	CLA	C3A-C2A-C1A	3.68	106.85	101.34
24	AC	510	CLA	O2A-CGA-CBA	3.68	122.61	111.90
24	AC	512	CLA	O2A-CGA-CBA	3.68	122.61	111.90
30	BF	5102	SQD	C11-C10-C9	3.69	133.46	114.45
27	AB	617	BCR	C23-C24-C25	3.69	137.59	127.25
24	BC	5502	CLA	CBA-CAA-C2A	3.69	124.85	113.80
24	AC	502	CLA	O2A-CGA-CBA	3.70	122.66	111.90
30	AF	102	SQD	C11-C10-C9	3.70	133.51	114.45
34	AD	403	PHO	O2A-CGA-CBA	3.70	122.66	111.90
24	BB	5609	CLA	C3A-C2A-C1A	3.70	106.88	101.34
24	BA	5408	CLA	O2A-CGA-CBA	3.70	122.67	111.90
24	BB	5611	CLA	C3A-C2A-C1A	3.70	106.89	101.34
31	AJ	102	LMG	C12-C11-C10	3.71	127.11	113.58
24	BC	5508	CLA	O2A-CGA-CBA	3.71	122.69	111.90
24	BC	5508	CLA	CBA-CAA-C2A	3.71	124.90	113.80
27	BD	5407	BCR	C24-C23-C22	3.71	131.79	126.21
30	BB	5625	SQD	C44-O6-C1	3.71	121.37	113.76
30	BA	5414	SQD	C31-C30-C29	3.71	133.59	114.45
24	AA	404	CLA	C4A-NA-C1A	3.72	111.07	106.45
30	BB	5625	SQD	C11-C10-C9	3.72	133.64	114.45
31	AJ	102	LMG	C9-C8-C7	3.72	120.25	111.86
31	BD	5408	LMG	C9-C8-C7	3.73	120.26	111.86
24	BC	5507	CLA	O2D-CGD-CBD	3.73	117.96	111.30
27	BB	5621	BCR	C29-C30-C25	3.73	116.31	110.48
24	AC	505	CLA	C3A-C2A-C1A	3.73	106.92	101.34
30	AA	413	SQD	C31-C30-C29	3.74	133.70	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	403	PHO	C4A-NA-C1A	3.74	111.19	108.16
30	AB	622	SQD	C11-C10-C9	3.74	133.75	114.45
24	BC	5503	CLA	O2D-CGD-CBD	3.75	118.01	111.30
24	AC	505	CLA	O2D-CGD-CBD	3.75	118.01	111.30
24	BB	5607	CLA	O2A-CGA-CBA	3.76	122.84	111.90
24	BC	5503	CLA	O2A-CGA-CBA	3.76	122.85	111.90
24	AC	503	CLA	O2D-CGD-CBD	3.76	118.03	111.30
24	BA	5405	CLA	C4A-NA-C1A	3.77	111.13	106.45
31	BD	5408	LMG	O1-C7-C8	3.77	119.96	110.99
24	AC	506	CLA	O2A-CGA-CBA	3.77	122.88	111.90
27	AA	410	BCR	C7-C8-C9	3.78	131.89	126.21
24	AC	510	CLA	O2D-CGD-CBD	3.78	118.05	111.30
31	BA	5402	LMG	O7-C8-C7	3.79	122.22	108.44
24	BC	5501	CLA	C3A-C2A-C1A	3.79	107.02	101.34
24	BC	5513	CLA	O2A-CGA-CBA	3.79	122.94	111.90
24	AC	507	CLA	O2A-CGA-CBA	3.80	122.95	111.90
27	AC	515	BCR	C23-C24-C25	3.80	137.89	127.25
24	BC	5507	CLA	O2A-CGA-CBA	3.81	122.98	111.90
24	BC	5501	CLA	O2A-CGA-CBA	3.81	122.98	111.90
24	AC	502	CLA	CBA-CAA-C2A	3.81	125.19	113.80
24	AC	503	CLA	O2A-CGA-CBA	3.81	122.98	111.90
27	BX	5101	BCR	C2-C1-C6	3.81	116.43	110.48
34	AD	403	PHO	C3A-C2A-C1A	3.81	106.17	101.68
24	BB	5606	CLA	O2A-CGA-CBA	3.81	122.99	111.90
35	BD	5406	PL9	C15-C14-C16	3.81	121.90	115.29
30	AA	416	SQD	C11-C10-C9	3.82	134.12	114.45
31	BB	5624	LMG	C34-C33-C32	3.82	134.12	114.45
30	BA	5414	SQD	C45-O47-C7	3.82	126.89	117.88
24	AC	509	CLA	O2A-CGA-CBA	3.82	123.01	111.90
31	BC	5521	LMG	O7-C8-C7	3.82	122.32	108.44
24	BB	5610	CLA	C3A-C2A-C1A	3.82	107.06	101.34
27	BC	5515	BCR	C23-C24-C25	3.82	137.95	127.25
30	BA	5401	SQD	C11-C10-C9	3.82	134.14	114.45
28	AA	411	DGD	O6E-C1E-O5D	3.82	119.10	110.02
30	AA	413	SQD	C45-O47-C7	3.83	126.92	117.88
27	AD	406	BCR	C29-C30-C25	3.83	116.46	110.48
28	BA	5412	DGD	O6E-C1E-O5D	3.83	119.11	110.02
27	BJ	5101	BCR	C23-C24-C25	3.83	137.97	127.25
24	AA	406	CLA	C4A-NA-C1A	3.83	111.21	106.45
24	AC	508	CLA	CBA-CAA-C2A	3.84	125.28	113.80
24	AC	508	CLA	O2A-CGA-CBA	3.84	123.08	111.90
24	AB	612	CLA	C4A-NA-C1A	3.84	111.22	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AB	621	LMG	C34-C33-C32	3.85	134.27	114.45
24	AB	608	CLA	C3A-C2A-C1A	3.85	107.11	101.34
24	BB	5607	CLA	C4A-NA-C1A	3.86	111.24	106.45
31	AC	521	LMG	O7-C8-C7	3.86	122.46	108.44
24	AB	605	CLA	CBA-CAA-C2A	3.86	125.35	113.80
24	AB	603	CLA	O2A-CGA-CBA	3.86	123.14	111.90
31	BD	5409	LMG	C21-C20-C19	3.87	134.40	114.45
24	BC	5506	CLA	O2A-CGA-CBA	3.88	123.18	111.90
24	AD	401	CLA	O2A-CGA-CBA	3.88	123.18	111.90
28	BE	5102	DGD	C1G-O1G-C1A	3.88	128.80	117.13
27	AJ	101	BCR	C7-C8-C9	3.88	132.05	126.21
36	BF	5101	HEM	CAD-CBD-CGD	3.88	119.30	112.66
24	AC	513	CLA	C4A-NA-C1A	3.90	111.29	106.45
24	AB	606	CLA	C3A-C2A-C1A	3.90	107.18	101.34
24	AC	504	CLA	O2D-CGD-CBD	3.90	118.27	111.30
27	AD	406	BCR	C24-C23-C22	3.91	132.08	126.21
28	AH	101	DGD	O6D-C5D-C6D	3.91	114.44	106.64
30	AB	622	SQD	C44-O6-C1	3.91	121.78	113.76
34	BD	5404	PHO	C4A-NA-C1A	3.91	111.33	108.16
30	AA	416	SQD	C31-C30-C29	3.92	134.63	114.45
31	AA	417	LMG	O7-C8-C7	3.92	122.67	108.44
24	BB	5609	CLA	CBA-CAA-C2A	3.92	125.53	113.80
28	AE	101	DGD	C1G-O1G-C1A	3.92	128.93	117.13
24	AB	603	CLA	C4A-NA-C1A	3.92	111.32	106.45
27	BT	5101	BCR	C29-C30-C25	3.92	116.61	110.48
24	BB	5612	CLA	C3A-C2A-C1A	3.92	107.22	101.34
30	BA	5401	SQD	C31-C30-C29	3.93	134.68	114.45
27	AX	101	BCR	C29-C30-C25	3.93	116.62	110.48
32	AD	409	LMT	O1B-C1B-C2B	3.93	116.97	108.11
30	BB	5625	SQD	O48-C23-C24	3.94	123.35	111.90
24	BD	5405	CLA	O2D-CGD-CBD	3.94	118.34	111.30
24	AB	602	CLA	O2A-CGA-CBA	3.94	123.37	111.90
24	AC	513	CLA	O2A-CGA-CBA	3.94	123.37	111.90
24	AC	511	CLA	O2D-CGD-CBD	3.94	118.34	111.30
24	BA	5408	CLA	O2D-CGD-CBD	3.95	118.36	111.30
32	BD	5411	LMT	O1B-C1B-C2B	3.96	117.04	108.11
28	BH	5101	DGD	O6D-C5D-C6D	3.97	114.56	106.64
27	AJ	101	BCR	C23-C24-C25	3.97	138.36	127.25
30	BF	5102	SQD	O48-C23-C24	3.97	123.45	111.90
24	AC	501	CLA	C3A-C2A-C1A	3.97	107.29	101.34
24	BB	5607	CLA	C2A-C1A-CHA	3.98	130.97	123.92
30	AB	627	SQD	O48-C23-C24	3.98	123.47	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	611	CLA	O2A-CGA-CBA	3.98	123.48	111.90
30	AF	102	SQD	O48-C23-C24	4.00	123.53	111.90
24	AA	405	CLA	C4A-NA-C1A	4.00	111.41	106.45
27	BX	5101	BCR	C29-C30-C25	4.00	116.73	110.48
24	BA	5407	CLA	O2D-CGD-CBD	4.00	118.45	111.30
36	AF	101	HEM	CAD-CBD-CGD	4.00	119.50	112.66
27	BA	5411	BCR	C7-C8-C9	4.00	132.22	126.21
24	BD	5402	CLA	O2A-CGA-CBA	4.01	123.56	111.90
30	BB	5601	SQD	O48-C23-C24	4.01	123.57	111.90
31	BL	5101	LMG	C8-O7-C10	4.01	127.36	117.88
24	BB	5615	CLA	O2A-CGA-CBA	4.01	123.58	111.90
31	AD	407	LMG	C21-C20-C19	4.01	135.14	114.45
24	BB	5616	CLA	O2D-CGD-CBD	4.02	118.48	111.30
27	BK	5102	BCR	C2-C1-C6	4.02	116.76	110.48
24	AB	603	CLA	C2A-C1A-CHA	4.02	131.05	123.92
24	AA	407	CLA	O2D-CGD-CBD	4.02	118.48	111.30
31	BL	5101	LMG	O1-C7-C8	4.02	120.56	110.99
24	BC	5513	CLA	C4A-NA-C1A	4.04	111.46	106.45
27	AT	101	BCR	C29-C30-C25	4.06	116.82	110.48
24	BC	5504	CLA	O2D-CGD-CBD	4.06	118.55	111.30
24	AC	511	CLA	CBA-CAA-C2A	4.07	125.98	113.80
24	AB	609	CLA	O2A-CGA-CBA	4.08	123.77	111.90
24	BB	5616	CLA	C4A-NA-C1A	4.08	111.52	106.45
31	BD	5408	LMG	C9-O8-C28	4.09	129.43	117.13
27	BK	5102	BCR	C7-C8-C9	4.09	132.36	126.21
24	AB	605	CLA	C4A-NA-C1A	4.09	111.53	106.45
27	BD	5407	BCR	C29-C30-C25	4.10	116.89	110.48
24	AD	404	CLA	O2D-CGD-CBD	4.11	118.64	111.30
24	BC	5511	CLA	CBA-CAA-C2A	4.11	126.10	113.80
24	BB	5609	CLA	C4A-NA-C1A	4.11	111.56	106.45
34	BD	5404	PHO	C3A-C2A-C1A	4.11	106.53	101.68
24	BB	5608	CLA	O2A-CGA-CBA	4.12	123.89	111.90
27	AC	514	BCR	C24-C23-C22	4.13	132.41	126.21
24	AB	604	CLA	O2A-CGA-CBA	4.13	123.91	111.90
27	AC	516	BCR	C2-C1-C6	4.13	116.94	110.48
24	AC	511	CLA	C4A-NA-C1A	4.14	111.59	106.45
29	BA	5415	LHG	O7-C7-C8	4.14	120.15	111.55
24	BB	5613	CLA	O2A-CGA-CBA	4.15	123.96	111.90
29	AA	415	LHG	O7-C7-C8	4.15	120.16	111.55
24	BB	5607	CLA	C3A-C2A-C1A	4.15	107.55	101.34
24	AA	406	CLA	O2D-CGD-CBD	4.15	118.72	111.30
27	BC	5516	BCR	C29-C30-C25	4.15	116.97	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5406	CLA	C4A-NA-C1A	4.16	111.61	106.45
24	BA	5407	CLA	C4A-NA-C1A	4.16	111.62	106.45
31	AB	620	LMG	O1-C7-C8	4.16	120.90	110.99
24	AB	609	CLA	C4A-NA-C1A	4.17	111.62	106.45
24	BB	5613	CLA	C4A-NA-C1A	4.17	111.62	106.45
30	AA	416	SQD	O48-C23-C24	4.17	124.04	111.90
24	BA	5406	CLA	O2D-CGD-CBD	4.17	118.76	111.30
30	BA	5401	SQD	O48-C23-C24	4.18	124.05	111.90
24	AA	405	CLA	O2D-CGD-CBD	4.18	118.77	111.30
30	AA	416	SQD	C44-O6-C1	4.19	122.34	113.76
24	AB	603	CLA	C3A-C2A-C1A	4.19	107.61	101.34
31	AB	620	LMG	C8-O7-C10	4.20	127.81	117.88
24	AB	607	CLA	C4A-NA-C1A	4.21	111.67	106.45
24	BC	5504	CLA	C4A-NA-C1A	4.21	111.68	106.45
24	BB	5618	CLA	C4A-NA-C1A	4.21	111.68	106.45
25	BA	5409	MST	C6-N5-C4	4.22	120.26	113.89
27	AK	102	BCR	C2-C1-C6	4.22	117.07	110.48
27	AK	102	BCR	C7-C8-C9	4.22	132.55	126.21
31	AD	408	LMG	C9-O8-C28	4.22	129.82	117.13
31	BD	5410	LMG	C9-O8-C28	4.23	129.84	117.13
24	AC	504	CLA	C4A-NA-C1A	4.23	111.70	106.45
24	AB	612	CLA	O2D-CGD-CBD	4.23	118.85	111.30
31	AJ	102	LMG	C9-O8-C28	4.23	129.86	117.13
24	BC	5511	CLA	C4A-NA-C1A	4.24	111.71	106.45
32	BC	5522	LMT	C1-O1'-C1'	4.25	121.17	113.87
24	AB	604	CLA	C4A-NA-C1A	4.25	111.73	106.45
30	AB	622	SQD	O48-C23-C24	4.26	124.29	111.90
35	AD	405	PL9	C35-C34-C36	4.26	122.68	115.29
24	BB	5611	CLA	C4A-NA-C1A	4.27	111.75	106.45
25	AA	408	MST	C6-N5-C4	4.27	120.34	113.89
30	BA	5401	SQD	C44-O6-C1	4.28	122.53	113.76
27	BC	5514	BCR	C24-C23-C22	4.30	132.67	126.21
24	AC	504	CLA	CBA-CAA-C2A	4.31	126.70	113.80
24	AB	614	CLA	C4A-NA-C1A	4.32	111.81	106.45
24	AA	406	CLA	O2A-CGA-CBA	4.32	124.48	111.90
27	BC	5514	BCR	C33-C5-C6	4.34	129.37	124.51
24	BB	5617	CLA	C4A-NA-C1A	4.35	111.85	106.45
24	BC	5504	CLA	CBA-CAA-C2A	4.35	126.81	113.80
24	AA	405	CLA	O2A-CGA-CBA	4.36	124.59	111.90
24	AB	613	CLA	C4A-NA-C1A	4.36	111.86	106.45
35	BD	5406	PL9	C35-C34-C36	4.36	122.86	115.29
30	BA	5414	SQD	C44-O6-C1	4.37	122.71	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	517	DGD	O5D-C1E-C2E	4.37	115.36	108.23
24	BA	5407	CLA	O2A-CGA-CBA	4.37	124.62	111.90
24	BA	5408	CLA	C4A-NA-C1A	4.37	111.88	106.45
24	BC	5507	CLA	C1C-NC-C4C	4.38	109.57	107.06
32	AI	103	LMT	C1-O1'-C1'	4.38	121.39	113.87
24	BD	5402	CLA	C4A-NA-C1A	4.39	111.89	106.45
27	BK	5102	BCR	C11-C10-C9	4.39	133.57	127.31
28	BE	5102	DGD	O2G-C1B-C2B	4.39	120.66	111.55
27	BB	5622	BCR	C33-C5-C6	4.39	129.42	124.51
24	BB	5614	CLA	C4A-NA-C1A	4.40	111.91	106.45
24	AD	401	CLA	C4A-NA-C1A	4.40	111.91	106.45
31	AD	407	LMG	C18-C17-C16	4.40	137.13	114.45
27	AC	516	BCR	C29-C30-C25	4.40	117.36	110.48
28	AE	101	DGD	O2G-C1B-C2B	4.41	120.70	111.55
24	AB	610	CLA	C4A-NA-C1A	4.41	111.93	106.45
24	AB	606	CLA	C4A-NA-C1A	4.41	111.93	106.45
24	AB	608	CLA	C4A-NA-C1A	4.43	111.95	106.45
24	AC	507	CLA	C1C-NC-C4C	4.44	109.61	107.06
24	BB	5615	CLA	C4A-NA-C1A	4.44	111.96	106.45
24	BB	5612	CLA	C4A-NA-C1A	4.45	111.97	106.45
28	BC	5517	DGD	O5D-C1E-C2E	4.45	115.49	108.23
30	AA	413	SQD	C44-O6-C1	4.45	122.89	113.76
24	AC	505	CLA	CBA-CAA-C2A	4.45	127.12	113.80
24	AB	602	CLA	C4A-NA-C1A	4.45	111.98	106.45
24	AB	611	CLA	C4A-NA-C1A	4.46	111.99	106.45
24	BB	5608	CLA	C4A-NA-C1A	4.46	111.99	106.45
24	AC	506	CLA	C4A-NA-C1A	4.46	111.99	106.45
24	BB	5610	CLA	C4A-NA-C1A	4.47	112.00	106.45
31	BD	5409	LMG	C18-C17-C16	4.48	137.54	114.45
24	AC	509	CLA	C4A-NA-C1A	4.48	112.02	106.45
24	AB	607	CLA	O2A-CGA-CBA	4.48	124.95	111.90
31	BA	5402	LMG	C9-C8-C7	4.50	122.00	111.86
31	AA	417	LMG	C9-C8-C7	4.50	122.00	111.86
31	AA	417	LMG	C9-O8-C28	4.51	130.69	117.13
24	AC	508	CLA	C4A-NA-C1A	4.52	112.07	106.45
24	BA	5406	CLA	O2A-CGA-CBA	4.53	125.08	111.90
24	AC	502	CLA	C4A-NA-C1A	4.53	112.08	106.45
24	BC	5506	CLA	C4A-NA-C1A	4.54	112.08	106.45
24	BC	5503	CLA	C4A-NA-C1A	4.54	112.09	106.45
24	BC	5509	CLA	C4A-NA-C1A	4.55	112.10	106.45
24	AC	510	CLA	C4A-NA-C1A	4.56	112.11	106.45
35	BD	5406	PL9	C20-C19-C21	4.56	123.19	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	601	CLA	C1C-NC-C4C	4.57	109.68	107.06
24	AB	606	CLA	O2A-CGA-CBA	4.57	125.20	111.90
24	BB	5611	CLA	O2A-CGA-CBA	4.57	125.20	111.90
24	AB	616	CLA	C1C-NC-C4C	4.57	109.69	107.06
24	BC	5505	CLA	CBA-CAA-C2A	4.57	127.48	113.80
24	BC	5510	CLA	C4A-NA-C1A	4.57	112.13	106.45
24	BB	5620	CLA	C1C-NC-C4C	4.58	109.69	107.06
24	BB	5606	CLA	C4A-NA-C1A	4.58	112.13	106.45
24	AD	401	CLA	C1C-NC-C4C	4.58	109.69	107.06
24	BC	5503	CLA	C1C-NC-C4C	4.58	109.69	107.06
24	AC	505	CLA	C4A-NA-C1A	4.59	112.15	106.45
31	AA	414	LMG	C8-O7-C10	4.61	128.76	117.88
24	BC	5510	CLA	C1C-NC-C4C	4.61	109.71	107.06
31	BI	5101	LMG	C9-O8-C28	4.62	131.01	117.13
31	BA	5402	LMG	C9-O8-C28	4.62	131.02	117.13
28	BC	5519	DGD	O6E-C1E-O5D	4.62	121.00	110.02
28	AC	519	DGD	O6E-C1E-O5D	4.63	121.00	110.02
27	AK	102	BCR	C11-C10-C9	4.63	133.91	127.31
24	AA	407	CLA	C4A-NA-C1A	4.64	112.21	106.45
28	AC	519	DGD	O6D-C5D-C4D	4.65	118.22	109.66
24	AB	614	CLA	CBA-CAA-C2A	4.65	127.70	113.80
31	BE	5101	LMG	C8-O7-C10	4.65	128.86	117.88
27	AC	514	BCR	C33-C5-C6	4.65	129.71	124.51
31	AI	101	LMG	C9-O8-C28	4.66	131.14	117.13
24	BC	5505	CLA	C4A-NA-C1A	4.67	112.24	106.45
24	BB	5610	CLA	O2A-CGA-CBA	4.67	125.50	111.90
24	BB	5618	CLA	CBA-CAA-C2A	4.69	127.82	113.80
24	BB	5605	CLA	C1C-NC-C4C	4.69	109.75	107.06
24	BC	5507	CLA	C4A-NA-C1A	4.69	112.27	106.45
24	AC	510	CLA	C1C-NC-C4C	4.70	109.76	107.06
31	AD	407	LMG	C20-C19-C18	4.71	138.73	114.45
35	AD	405	PL9	C20-C19-C21	4.72	123.47	115.29
24	AC	506	CLA	C1C-NC-C4C	4.73	109.77	107.06
24	BC	5506	CLA	C1C-NC-C4C	4.74	109.78	107.06
24	BD	5402	CLA	C1C-NC-C4C	4.74	109.78	107.06
24	BB	5620	CLA	C4A-NA-C1A	4.75	112.35	106.45
24	AC	507	CLA	C4A-NA-C1A	4.76	112.36	106.45
32	BC	5522	LMT	O1B-C1B-C2B	4.76	118.83	108.11
24	AD	404	CLA	C4A-NA-C1A	4.76	112.36	106.45
31	BD	5409	LMG	C20-C19-C18	4.76	139.00	114.45
24	AB	616	CLA	C4A-NA-C1A	4.76	112.37	106.45
24	AC	503	CLA	C4A-NA-C1A	4.79	112.40	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BD	5405	CLA	C4A-NA-C1A	4.82	112.44	106.45
24	AC	501	CLA	C4A-NA-C1A	4.82	112.44	106.45
24	BC	5512	CLA	C1C-NC-C4C	4.83	109.83	107.06
24	BC	5505	CLA	C1C-NC-C4C	4.85	109.84	107.06
27	AB	618	BCR	C33-C5-C6	4.85	129.94	124.51
27	BB	5623	BCR	C33-C5-C6	4.87	129.96	124.51
24	AB	615	CLA	C4A-NA-C1A	4.87	112.50	106.45
27	AD	406	BCR	C33-C5-C6	4.92	130.02	124.51
24	AA	405	CLA	C1C-NC-C4C	4.94	109.89	107.06
24	BC	5502	CLA	C4A-NA-C1A	4.95	112.59	106.45
24	BC	5508	CLA	C4A-NA-C1A	4.95	112.59	106.45
24	AB	602	CLA	C1C-NC-C4C	4.96	109.91	107.06
30	AF	102	SQD	C44-O6-C1	4.97	123.94	113.76
24	BC	5501	CLA	C4A-NA-C1A	4.99	112.65	106.45
24	BB	5614	CLA	C1C-NC-C4C	4.99	109.93	107.06
24	AC	512	CLA	C1C-NC-C4C	5.00	109.93	107.06
32	AI	103	LMT	O1B-C1B-C2B	5.00	119.38	108.11
27	AX	101	BCR	C33-C5-C6	5.02	130.13	124.51
24	BB	5611	CLA	CBA-CAA-C2A	5.03	128.83	113.80
27	BX	5101	BCR	C33-C5-C6	5.06	130.17	124.51
24	BB	5619	CLA	C4A-NA-C1A	5.06	112.74	106.45
27	BB	5623	BCR	C38-C26-C25	5.07	130.18	124.51
27	AB	619	BCR	C38-C26-C25	5.07	130.18	124.51
28	BC	5519	DGD	O6D-C5D-C4D	5.09	119.03	109.66
24	BC	5501	CLA	C1C-NC-C4C	5.09	109.98	107.06
28	BH	5101	DGD	O5D-C6D-C5D	5.10	117.47	108.94
31	AM	101	LMG	C9-O8-C28	5.10	132.46	117.13
24	BC	5512	CLA	C4A-NA-C1A	5.10	112.78	106.45
27	BD	5407	BCR	C33-C5-C6	5.10	130.22	124.51
24	AC	512	CLA	C4A-NA-C1A	5.10	112.78	106.45
31	AC	521	LMG	C9-O8-C28	5.11	132.49	117.13
30	BF	5102	SQD	C44-O6-C1	5.12	124.26	113.76
31	BM	5102	LMG	C9-O8-C28	5.12	132.54	117.13
24	AB	608	CLA	CBA-CAA-C2A	5.13	129.16	113.80
27	AB	619	BCR	C33-C5-C6	5.14	130.27	124.51
24	BB	5606	CLA	C1C-NC-C4C	5.15	110.02	107.06
31	AB	620	LMG	O7-C8-C7	5.18	127.26	108.44
24	AC	505	CLA	C1C-NC-C4C	5.19	110.04	107.06
36	BV	5201	HEM	CAD-CBD-CGD	5.19	121.54	112.66
31	BC	5521	LMG	C9-O8-C28	5.20	132.78	117.13
31	BL	5101	LMG	O7-C8-C7	5.21	127.36	108.44
36	AV	201	HEM	CAD-CBD-CGD	5.23	121.59	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5605	CLA	C4A-NA-C1A	5.23	112.94	106.45
24	AB	607	CLA	CBA-CAA-C2A	5.23	129.45	113.80
28	AH	101	DGD	O5D-C6D-C5D	5.24	117.70	108.94
25	BA	5409	MST	C8-S7-C2	5.26	106.17	102.29
24	BB	5612	CLA	CBA-CAA-C2A	5.26	129.52	113.80
25	AA	408	MST	C8-S7-C2	5.27	106.18	102.29
27	AA	410	BCR	C38-C26-C25	5.28	130.42	124.51
27	AJ	101	BCR	C33-C5-C6	5.28	130.42	124.51
27	AA	410	BCR	C33-C5-C6	5.28	130.42	124.51
27	BJ	5101	BCR	C33-C5-C6	5.29	130.43	124.51
27	AB	617	BCR	C33-C5-C6	5.29	130.44	124.51
24	AB	615	CLA	C1C-NC-C4C	5.30	110.11	107.06
24	BA	5406	CLA	C1C-NC-C4C	5.32	110.11	107.06
27	BB	5621	BCR	C33-C5-C6	5.33	130.48	124.51
27	BC	5514	BCR	C38-C26-C25	5.34	130.48	124.51
24	BB	5617	CLA	C1C-NC-C4C	5.34	110.13	107.06
24	BC	5508	CLA	C1C-NC-C4C	5.35	110.13	107.06
24	AC	501	CLA	C1C-NC-C4C	5.38	110.15	107.06
24	AB	601	CLA	C4A-NA-C1A	5.39	113.14	106.45
27	BA	5411	BCR	C38-C26-C25	5.40	130.55	124.51
24	AB	609	CLA	C1C-NC-C4C	5.41	110.17	107.06
30	BB	5625	SQD	C25-C24-C23	5.41	133.35	113.58
27	BA	5411	BCR	C33-C5-C6	5.42	130.57	124.51
27	AT	101	BCR	C38-C26-C25	5.43	130.58	124.51
30	AB	622	SQD	C25-C24-C23	5.43	133.39	113.58
24	AC	508	CLA	C1C-NC-C4C	5.46	110.19	107.06
24	AC	503	CLA	C1C-NC-C4C	5.46	110.20	107.06
24	AB	610	CLA	C1C-NC-C4C	5.49	110.21	107.06
28	AA	411	DGD	O2G-C1B-C2B	5.49	122.96	111.55
27	BC	5516	BCR	C38-C26-C25	5.51	130.68	124.51
24	AB	611	CLA	C1C-NC-C4C	5.52	110.23	107.06
28	BA	5412	DGD	O2G-C1B-C2B	5.52	123.02	111.55
27	AC	514	BCR	C38-C26-C25	5.53	130.70	124.51
24	BA	5408	CLA	C1C-NC-C4C	5.54	110.24	107.06
24	AB	604	CLA	C1C-NC-C4C	5.54	110.24	107.06
28	AB	628	DGD	C1G-O1G-C1A	5.54	133.79	117.13
28	BB	5602	DGD	C1G-O1G-C1A	5.54	133.80	117.13
31	BD	5408	LMG	O7-C8-C7	5.55	128.61	108.44
24	BB	5615	CLA	C1C-NC-C4C	5.55	110.25	107.06
24	AC	502	CLA	C1C-NC-C4C	5.57	110.26	107.06
24	BB	5613	CLA	C1C-NC-C4C	5.58	110.26	107.06
24	AB	608	CLA	C1C-NC-C4C	5.58	110.27	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AJ	102	LMG	O7-C8-C7	5.60	128.79	108.44
30	AA	416	SQD	C25-C24-C23	5.62	134.10	113.58
27	BT	5101	BCR	C38-C26-C25	5.62	130.80	124.51
27	AJ	101	BCR	C31-C1-C6	5.63	119.44	110.31
27	AK	102	BCR	C38-C26-C25	5.65	130.83	124.51
30	BA	5401	SQD	C25-C24-C23	5.65	134.22	113.58
31	BD	5409	LMG	O7-C8-C7	5.66	129.03	108.44
24	BB	5608	CLA	C1C-NC-C4C	5.67	110.32	107.06
24	BD	5405	CLA	C1C-NC-C4C	5.67	110.32	107.06
27	BK	5102	BCR	C38-C26-C25	5.69	130.87	124.51
27	AC	516	BCR	C38-C26-C25	5.71	130.90	124.51
31	AD	407	LMG	O7-C8-C7	5.73	129.26	108.44
28	AA	411	DGD	O6D-C1D-O3G	5.73	123.63	110.02
27	BJ	5101	BCR	C31-C1-C6	5.76	119.65	110.31
24	AD	404	CLA	C1C-NC-C4C	5.76	110.37	107.06
30	AB	627	SQD	C25-C24-C23	5.78	134.67	113.58
24	AB	605	CLA	C1C-NC-C4C	5.78	110.38	107.06
24	BB	5619	CLA	C1C-NC-C4C	5.79	110.38	107.06
30	BB	5601	SQD	C25-C24-C23	5.80	134.76	113.58
28	BA	5412	DGD	O6D-C1D-O3G	5.85	123.91	110.02
24	AA	407	CLA	C1C-NC-C4C	5.85	110.42	107.06
24	BB	5612	CLA	C1C-NC-C4C	5.88	110.44	107.06
30	AA	413	SQD	C25-C24-C23	5.88	135.05	113.58
30	AB	622	SQD	C10-C9-C8	5.89	134.82	113.24
24	AB	613	CLA	C1C-NC-C4C	5.89	110.44	107.06
30	BF	5102	SQD	C10-C9-C8	5.89	134.84	113.24
30	AF	102	SQD	C10-C9-C8	5.90	134.85	113.24
27	AB	617	BCR	C38-C26-C25	5.91	131.12	124.51
30	BA	5414	SQD	C25-C24-C23	5.91	135.16	113.58
27	AX	101	BCR	C38-C26-C25	5.92	131.14	124.51
27	BB	5621	BCR	C38-C26-C25	5.92	131.14	124.51
24	BB	5609	CLA	C1C-NC-C4C	5.94	110.47	107.06
27	BC	5515	BCR	C38-C26-C25	5.94	131.16	124.51
30	BB	5625	SQD	C10-C9-C8	5.95	135.04	113.24
30	AF	102	SQD	C25-C24-C23	5.96	135.35	113.58
30	AB	627	SQD	C10-C9-C8	5.97	135.12	113.24
31	BI	5101	LMG	O7-C10-C11	5.97	123.95	111.55
27	AC	515	BCR	C33-C5-C6	5.97	131.19	124.51
27	BT	5101	BCR	C33-C5-C6	5.97	131.20	124.51
30	BA	5414	SQD	O6-C1-C2	5.98	117.99	108.23
27	BJ	5101	BCR	C38-C26-C25	5.98	131.21	124.51
24	BA	5407	CLA	CBA-CAA-C2A	5.99	131.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BF	5102	SQD	C25-C24-C23	6.01	135.51	113.58
30	BA	5414	SQD	C10-C9-C8	6.02	135.31	113.24
27	AT	101	BCR	C33-C5-C6	6.03	131.25	124.51
30	AA	413	SQD	O6-C1-C2	6.03	118.06	108.23
30	AA	416	SQD	C10-C9-C8	6.04	135.38	113.24
24	BC	5502	CLA	C1C-NC-C4C	6.05	110.54	107.06
31	AI	101	LMG	O7-C10-C11	6.06	124.13	111.55
27	AC	515	BCR	C38-C26-C25	6.06	131.29	124.51
30	AA	413	SQD	C10-C9-C8	6.07	135.49	113.24
27	AJ	101	BCR	C38-C26-C25	6.08	131.31	124.51
28	AC	518	DGD	O2G-C1B-C2B	6.08	124.18	111.55
28	BC	5518	DGD	O2G-C1B-C2B	6.09	124.20	111.55
30	BA	5401	SQD	C10-C9-C8	6.10	135.57	113.24
24	BA	5405	CLA	C1C-NC-C4C	6.10	110.56	107.06
30	BB	5601	SQD	C10-C9-C8	6.11	135.62	113.24
27	BC	5515	BCR	C33-C5-C6	6.11	131.35	124.51
27	BX	5101	BCR	C38-C26-C25	6.13	131.37	124.51
28	AA	411	DGD	O1G-C1A-C2A	6.14	129.76	111.90
24	AB	606	CLA	C1C-NC-C4C	6.15	110.59	107.06
28	BA	5412	DGD	O1G-C1A-C2A	6.21	129.97	111.90
24	AA	406	CLA	CBA-CAA-C2A	6.22	132.42	113.80
29	BA	5413	LHG	C25-C24-C23	6.25	136.39	113.58
27	BC	5516	BCR	C33-C5-C6	6.25	131.50	124.51
28	BC	5517	DGD	O6D-C5D-C6D	6.25	119.12	106.64
27	BB	5622	BCR	C38-C26-C25	6.25	131.51	124.51
30	AA	416	SQD	O6-C1-C2	6.26	118.44	108.23
27	AC	516	BCR	C33-C5-C6	6.27	131.53	124.51
27	BK	5102	BCR	C33-C5-C6	6.28	131.54	124.51
29	AA	412	LHG	C25-C24-C23	6.36	136.79	113.58
24	BB	5610	CLA	C1C-NC-C4C	6.39	110.73	107.06
30	BA	5401	SQD	O6-C1-C2	6.40	118.68	108.23
27	AB	618	BCR	C38-C26-C25	6.41	131.69	124.51
24	BB	5611	CLA	C1C-NC-C4C	6.48	110.78	107.06
27	BJ	5101	BCR	C2-C1-C6	6.50	120.64	110.48
27	AK	102	BCR	C33-C5-C6	6.54	131.82	124.51
28	AC	517	DGD	O6D-C5D-C6D	6.56	119.75	106.64
27	AJ	101	BCR	C2-C1-C6	6.57	120.75	110.48
31	BC	5521	LMG	C8-O7-C10	6.57	133.41	117.88
28	AA	411	DGD	C3G-O3G-C1D	6.57	127.24	113.76
28	BA	5412	DGD	C3G-O3G-C1D	6.59	127.27	113.76
24	AB	607	CLA	C1C-NC-C4C	6.59	110.85	107.06
24	AA	406	CLA	C1C-NC-C4C	6.62	110.86	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5504	CLA	C1C-NC-C4C	6.63	110.87	107.06
31	AC	521	LMG	C8-O7-C10	6.64	133.57	117.88
28	AC	517	DGD	C1G-O1G-C1A	6.66	137.16	117.13
24	AA	405	CLA	CBA-CAA-C2A	6.69	133.82	113.80
24	BA	5406	CLA	CBA-CAA-C2A	6.77	134.05	113.80
28	BC	5517	DGD	C1G-O1G-C1A	6.77	137.50	117.13
31	AB	621	LMG	O7-C10-C11	6.82	125.72	111.55
24	AC	504	CLA	C1C-NC-C4C	6.82	110.98	107.06
27	BD	5407	BCR	C38-C26-C25	6.84	132.16	124.51
31	BB	5624	LMG	O7-C10-C11	6.85	125.77	111.55
31	AM	101	LMG	O7-C10-C11	6.88	125.83	111.55
24	AA	404	CLA	C1C-NC-C4C	6.88	111.01	107.06
31	BM	5102	LMG	O7-C10-C11	6.95	125.98	111.55
30	AF	102	SQD	O6-C1-C2	6.99	119.64	108.23
31	BD	5410	LMG	C8-O7-C10	7.02	134.47	117.88
30	BF	5102	SQD	O6-C1-C2	7.04	119.72	108.23
24	BA	5407	CLA	C1C-NC-C4C	7.04	111.11	107.06
31	AD	408	LMG	C8-O7-C10	7.06	134.55	117.88
28	BC	5517	DGD	O5D-C6D-C5D	7.08	120.78	108.94
28	AC	517	DGD	O5D-C6D-C5D	7.09	120.81	108.94
28	BH	5101	DGD	O2G-C1B-C2B	7.10	126.30	111.55
27	AD	406	BCR	C38-C26-C25	7.12	132.47	124.51
28	AH	101	DGD	O2G-C1B-C2B	7.13	126.36	111.55
30	AB	627	SQD	O6-C1-C2	7.13	119.87	108.23
30	AB	622	SQD	O6-C1-C2	7.22	120.01	108.23
30	BB	5625	SQD	O6-C1-C2	7.24	120.05	108.23
30	BB	5601	SQD	O6-C1-C2	7.27	120.09	108.23
28	BC	5518	DGD	O6D-C5D-C6D	7.43	121.48	106.64
31	BC	5520	LMG	O7-C10-C11	7.52	127.16	111.55
31	BD	5409	LMG	C8-O7-C10	7.63	135.90	117.88
28	AC	518	DGD	O6D-C5D-C6D	7.64	121.89	106.64
31	AA	417	LMG	C8-O7-C10	7.67	136.00	117.88
31	AD	407	LMG	C8-O7-C10	7.69	136.04	117.88
31	AC	520	LMG	O7-C10-C11	7.73	127.60	111.55
36	BV	5201	HEM	CMA-C3A-C4A	7.83	140.50	128.46
36	AV	201	HEM	CMA-C3A-C4A	7.85	140.52	128.46
31	BA	5402	LMG	C8-O7-C10	7.86	136.44	117.88
24	BC	5509	CLA	C1C-NC-C4C	7.98	111.65	107.06
28	AA	411	DGD	O5D-C1E-C2E	8.10	121.44	108.23
30	BB	5625	SQD	O5-C1-O6	8.10	129.25	110.02
28	BC	5519	DGD	O6D-C5D-C6D	8.10	122.82	106.64
30	AB	627	SQD	O5-C1-O6	8.13	129.33	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BB	5601	SQD	O5-C1-O6	8.17	129.41	110.02
30	AB	622	SQD	O5-C1-O6	8.22	129.55	110.02
28	BC	5519	DGD	C2G-O2G-C1B	8.27	137.41	117.88
28	BA	5412	DGD	O5D-C1E-C2E	8.27	121.73	108.23
36	AF	101	HEM	CMA-C3A-C4A	8.27	141.18	128.46
36	BF	5101	HEM	CMA-C3A-C4A	8.39	141.36	128.46
24	AC	509	CLA	C1C-NC-C4C	8.40	111.89	107.06
28	AC	519	DGD	C2G-O2G-C1B	8.50	137.95	117.88
28	AA	411	DGD	O6D-C5D-C6D	8.60	123.81	106.64
28	BA	5412	DGD	O6D-C5D-C6D	8.64	123.89	106.64
30	AF	102	SQD	O5-C1-O6	8.70	130.67	110.02
28	AC	519	DGD	O6D-C5D-C6D	8.70	124.01	106.64
28	AC	519	DGD	O5D-C1E-C2E	8.72	122.46	108.23
30	BF	5102	SQD	O5-C1-O6	8.74	130.76	110.02
24	AB	612	CLA	C1C-NC-C4C	8.83	112.14	107.06
28	BC	5519	DGD	O5D-C1E-C2E	8.87	122.70	108.23
35	BD	5406	PL9	C7-C3-C4	8.89	124.11	116.88
30	BA	5414	SQD	O5-C1-O6	8.93	131.22	110.02
30	BA	5401	SQD	O5-C1-O6	8.96	131.28	110.02
24	AB	614	CLA	C1C-NC-C4C	8.98	112.22	107.06
30	AA	416	SQD	O5-C1-O6	9.00	131.39	110.02
30	AA	413	SQD	O5-C1-O6	9.05	131.51	110.02
35	AD	405	PL9	C7-C3-C4	9.05	124.24	116.88
30	BB	5625	SQD	C5-C6-S	9.11	127.02	114.34
30	AB	622	SQD	C5-C6-S	9.14	127.07	114.34
28	BC	5518	DGD	O5D-C6D-C5D	9.15	124.25	108.94
28	AC	517	DGD	C2G-O2G-C1B	9.18	139.56	117.88
25	BA	5409	MST	C2-N3-C4	9.18	119.56	113.70
24	BB	5618	CLA	C1C-NC-C4C	9.19	112.34	107.06
28	AC	518	DGD	O5D-C6D-C5D	9.20	124.33	108.94
30	BB	5601	SQD	C5-C6-S	9.23	127.19	114.34
24	BB	5616	CLA	C1C-NC-C4C	9.34	112.43	107.06
28	BC	5517	DGD	C2G-O2G-C1B	9.41	140.10	117.88
30	BA	5401	SQD	C5-C6-S	9.42	127.45	114.34
30	AB	627	SQD	C5-C6-S	9.44	127.48	114.34
24	AB	603	CLA	C1C-NC-C4C	9.51	112.52	107.06
25	AA	408	MST	C2-N3-C4	9.51	119.78	113.70
31	BD	5408	LMG	C8-O7-C10	9.56	140.46	117.88
30	AA	416	SQD	C5-C6-S	9.56	127.66	114.34
28	AB	628	DGD	C2G-O2G-C1B	9.65	140.68	117.88
31	AJ	102	LMG	C8-O7-C10	9.78	140.99	117.88
24	BC	5513	CLA	C1C-NC-C4C	9.78	112.68	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	513	CLA	C1C-NC-C4C	9.82	112.71	107.06
28	BB	5602	DGD	C2G-O2G-C1B	9.89	141.23	117.88
24	BB	5607	CLA	C1C-NC-C4C	9.90	112.75	107.06
25	BA	5409	MST	C2-N1-C6	9.95	120.06	113.70
30	BF	5102	SQD	C5-C6-S	9.97	128.23	114.34
24	AC	511	CLA	C1C-NC-C4C	10.02	112.82	107.06
24	BC	5511	CLA	C1C-NC-C4C	10.03	112.83	107.06
25	AA	408	MST	C2-N1-C6	10.06	120.12	113.70
30	AF	102	SQD	C5-C6-S	10.06	128.34	114.34
28	AA	411	DGD	O1G-C1G-C2G	10.45	134.92	108.66
28	BA	5412	DGD	O1G-C1G-C2G	10.47	134.96	108.66
30	BB	5601	SQD	O7-S-C6	10.53	115.83	106.83
28	BC	5518	DGD	O5D-C1E-C2E	10.54	125.43	108.23
28	AC	518	DGD	O5D-C1E-C2E	10.74	125.75	108.23
30	AB	627	SQD	O7-S-C6	11.01	116.23	106.83
30	AB	622	SQD	O7-S-C6	11.33	116.51	106.83
30	BA	5401	SQD	O7-S-C6	11.41	116.58	106.83
30	AA	416	SQD	O7-S-C6	11.69	116.82	106.83
30	BA	5414	SQD	O7-S-C6	11.79	116.91	106.83
30	BB	5625	SQD	O7-S-C6	11.89	116.99	106.83
30	AA	413	SQD	C5-C6-S	11.92	130.94	114.34
30	BA	5414	SQD	C5-C6-S	11.97	131.01	114.34
28	BA	5412	DGD	O5D-C6D-C5D	12.07	129.13	108.94
28	AA	411	DGD	O5D-C6D-C5D	12.10	129.19	108.94
30	AA	413	SQD	O7-S-C6	12.14	117.20	106.83
30	AF	102	SQD	O7-S-C6	13.08	118.01	106.83
30	BF	5102	SQD	O7-S-C6	13.16	118.07	106.83
28	BC	5519	DGD	O5D-C6D-C5D	13.36	131.30	108.94
28	AC	519	DGD	O5D-C6D-C5D	13.45	131.44	108.94

All (288) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	C8
24	BC	5502	CLA	NC
24	BC	5502	CLA	ND
24	BC	5502	CLA	NA
24	BC	5511	CLA	C8
24	BC	5511	CLA	NC
24	BC	5511	CLA	ND
24	BC	5511	CLA	NA
24	AC	507	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AC	507	CLA	NC
24	AC	507	CLA	ND
24	AC	507	CLA	NA
24	BB	5617	CLA	C8
24	BB	5617	CLA	NC
24	BB	5617	CLA	ND
24	BB	5617	CLA	NA
34	BD	5403	PHO	C8
24	BB	5612	CLA	C8
24	BB	5612	CLA	NC
24	BB	5612	CLA	ND
24	BB	5612	CLA	NA
24	AC	504	CLA	C8
24	AC	504	CLA	NC
24	AC	504	CLA	ND
24	AC	504	CLA	NA
24	BC	5512	CLA	C8
24	BC	5512	CLA	NC
24	BC	5512	CLA	ND
24	BC	5512	CLA	NA
34	AD	402	PHO	C8
24	AC	506	CLA	C8
24	AC	506	CLA	NC
24	AC	506	CLA	ND
24	AC	506	CLA	NA
24	BB	5619	CLA	C8
24	BB	5619	CLA	NC
24	BB	5619	CLA	ND
24	BB	5619	CLA	NA
24	BB	5614	CLA	C8
24	BB	5614	CLA	NC
24	BB	5614	CLA	ND
24	BB	5614	CLA	NA
24	AA	405	CLA	C8
24	AA	405	CLA	NC
24	AA	405	CLA	ND
24	AA	405	CLA	NA
24	BC	5507	CLA	C8
24	BC	5507	CLA	NC
24	BC	5507	CLA	ND
24	BC	5507	CLA	NA
24	AB	612	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AB	612	CLA	NC
24	AB	612	CLA	ND
24	AB	612	CLA	NA
24	BC	5508	CLA	C8
24	BC	5508	CLA	NC
24	BC	5508	CLA	ND
24	BC	5508	CLA	NA
24	BB	5608	CLA	C8
24	BB	5608	CLA	NC
24	BB	5608	CLA	ND
24	BB	5608	CLA	NA
24	BC	5501	CLA	C8
24	BC	5501	CLA	NC
24	BC	5501	CLA	ND
24	BC	5501	CLA	NA
24	BD	5402	CLA	C8
24	BD	5402	CLA	NC
24	BD	5402	CLA	ND
24	BD	5402	CLA	NA
24	BB	5610	CLA	C8
24	BB	5610	CLA	NC
24	BB	5610	CLA	ND
24	BB	5610	CLA	NA
24	AB	606	CLA	C8
24	AB	606	CLA	NC
24	AB	606	CLA	ND
24	AB	606	CLA	NA
24	BD	5405	CLA	C8
24	BD	5405	CLA	NC
24	BD	5405	CLA	ND
24	BD	5405	CLA	NA
24	AD	401	CLA	C8
24	AD	401	CLA	NC
24	AD	401	CLA	ND
24	AD	401	CLA	NA
24	AD	404	CLA	C8
24	AD	404	CLA	NC
24	AD	404	CLA	ND
24	AD	404	CLA	NA
34	AD	403	PHO	C8
28	AC	518	DGD	C1E
24	AB	602	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AB	602	CLA	NC
24	AB	602	CLA	ND
24	AB	602	CLA	NA
24	AC	511	CLA	C8
24	AC	511	CLA	NC
24	AC	511	CLA	ND
24	AC	511	CLA	NA
24	AC	503	CLA	C8
24	AC	503	CLA	NC
24	AC	503	CLA	ND
24	AC	503	CLA	NA
24	AA	404	CLA	C8
24	AA	404	CLA	NC
24	AA	404	CLA	ND
24	AA	404	CLA	NA
24	BC	5503	CLA	C8
24	BC	5503	CLA	NC
24	BC	5503	CLA	ND
24	BC	5503	CLA	NA
24	AB	615	CLA	C8
24	AB	615	CLA	NC
24	AB	615	CLA	ND
24	AB	615	CLA	NA
24	BB	5620	CLA	C8
24	BB	5620	CLA	NC
24	BB	5620	CLA	ND
24	BB	5620	CLA	NA
24	AB	610	CLA	C8
24	AB	610	CLA	NC
24	AB	610	CLA	ND
24	AB	610	CLA	NA
24	BB	5606	CLA	C8
24	BB	5606	CLA	NC
24	BB	5606	CLA	ND
24	BB	5606	CLA	NA
24	AB	616	CLA	C8
24	AB	616	CLA	NC
24	AB	616	CLA	ND
24	AB	616	CLA	NA
24	AB	614	CLA	C8
24	AB	614	CLA	NC
24	AB	614	CLA	ND

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Mol	Chain	Res	Type	Atom
24	AB	614	CLA	NA
24	AB	611	CLA	C8
24	AB	611	CLA	NC
24	AB	611	CLA	ND
24	AB	611	CLA	NA
24	AB	613	CLA	C8
24	AB	613	CLA	NC
24	AB	613	CLA	ND
24	AB	613	CLA	NA
24	AC	509	CLA	C8
24	AC	509	CLA	NC
24	AC	509	CLA	ND
24	AC	509	CLA	NA
24	AA	407	CLA	C8
24	AA	407	CLA	NC
24	AA	407	CLA	ND
24	AA	407	CLA	NA
24	BC	5510	CLA	C8
24	BC	5510	CLA	NC
24	BC	5510	CLA	ND
24	BC	5510	CLA	NA
24	AC	501	CLA	C8
24	AC	501	CLA	NC
24	AC	501	CLA	ND
24	AC	501	CLA	NA
24	BB	5616	CLA	C8
24	BB	5616	CLA	NC
24	BB	5616	CLA	ND
24	BB	5616	CLA	NA
24	BA	5405	CLA	C8
24	BA	5405	CLA	NC
24	BA	5405	CLA	ND
24	BA	5405	CLA	NA
24	AA	406	CLA	C8
24	AA	406	CLA	NC
24	AA	406	CLA	ND
24	AA	406	CLA	NA
24	BC	5504	CLA	C8
24	BC	5504	CLA	NC
24	BC	5504	CLA	ND
24	BC	5504	CLA	NA
24	AB	609	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AB	609	CLA	NC
24	AB	609	CLA	ND
24	AB	609	CLA	NA
24	AC	502	CLA	C8
24	AC	502	CLA	NC
24	AC	502	CLA	ND
24	AC	502	CLA	NA
24	BC	5509	CLA	C8
24	BC	5509	CLA	NC
24	BC	5509	CLA	ND
24	BC	5509	CLA	NA
24	AB	607	CLA	C8
24	AB	607	CLA	NC
24	AB	607	CLA	ND
24	AB	607	CLA	NA
28	AC	519	DGD	C1E
24	BC	5506	CLA	C8
24	BC	5506	CLA	NC
24	BC	5506	CLA	ND
24	BC	5506	CLA	NA
24	AC	505	CLA	C8
24	AC	505	CLA	NC
24	AC	505	CLA	ND
24	AC	505	CLA	NA
24	AC	508	CLA	C8
24	AC	508	CLA	NC
24	AC	508	CLA	ND
24	AC	508	CLA	NA
24	AC	513	CLA	C8
24	AC	513	CLA	NC
24	AC	513	CLA	ND
24	AC	513	CLA	NA
24	BB	5609	CLA	C8
24	BB	5609	CLA	NC
24	BB	5609	CLA	ND
24	BB	5609	CLA	NA
24	BC	5505	CLA	C8
24	BC	5505	CLA	NC
24	BC	5505	CLA	ND
24	BC	5505	CLA	NA
34	BD	5404	PHO	C8
24	AB	603	CLA	C8

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Mol	Chain	Res	Type	Atom
24	AB	603	CLA	NC
24	AB	603	CLA	ND
24	AB	603	CLA	NA
24	BB	5615	CLA	C8
24	BB	5615	CLA	NC
24	BB	5615	CLA	ND
24	BB	5615	CLA	NA
24	BA	5407	CLA	C8
24	BA	5407	CLA	NC
24	BA	5407	CLA	ND
24	BA	5407	CLA	NA
24	AB	601	CLA	C8
24	AB	601	CLA	NC
24	AB	601	CLA	ND
24	AB	601	CLA	NA
24	AC	512	CLA	C8
24	AC	512	CLA	NC
24	AC	512	CLA	ND
24	AC	512	CLA	NA
24	BB	5613	CLA	C8
24	BB	5613	CLA	NC
24	BB	5613	CLA	ND
24	BB	5613	CLA	NA
24	BB	5607	CLA	C8
24	BB	5607	CLA	NC
24	BB	5607	CLA	ND
24	BB	5607	CLA	NA
24	AB	608	CLA	C8
24	AB	608	CLA	NC
24	AB	608	CLA	ND
24	AB	608	CLA	NA
24	AC	510	CLA	C8
24	AC	510	CLA	NC
24	AC	510	CLA	ND
24	AC	510	CLA	NA
28	BC	5519	DGD	C1E
24	BB	5605	CLA	C8
24	BB	5605	CLA	NC
24	BB	5605	CLA	ND
24	BB	5605	CLA	NA
24	AB	605	CLA	C8
24	AB	605	CLA	NC

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Mol	Chain	Res	Type	Atom
24	AB	605	CLA	ND
24	AB	605	CLA	NA
24	AB	604	CLA	C8
24	AB	604	CLA	NC
24	AB	604	CLA	ND
24	AB	604	CLA	NA
24	BA	5408	CLA	C8
24	BA	5408	CLA	NC
24	BA	5408	CLA	ND
24	BA	5408	CLA	NA
24	BC	5513	CLA	C8
24	BC	5513	CLA	NC
24	BC	5513	CLA	ND
24	BC	5513	CLA	NA
28	BC	5518	DGD	C1E
24	BA	5406	CLA	C8
24	BA	5406	CLA	NC
24	BA	5406	CLA	ND
24	BA	5406	CLA	NA
24	BB	5611	CLA	C8
24	BB	5611	CLA	NC
24	BB	5611	CLA	ND
24	BB	5611	CLA	NA
24	BB	5618	CLA	C8
24	BB	5618	CLA	NC
24	BB	5618	CLA	ND
24	BB	5618	CLA	NA

All (3) torsion outliers are listed below:

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

There are no ring outliers.

167 monomers are involved in 1068 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	404	CLA	12	0
24	AA	405	CLA	20	0
24	AA	406	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	407	CLA	9	0
25	AA	408	MST	9	0
27	AA	410	BCR	4	0
28	AA	411	DGD	9	0
29	AA	412	LHG	5	0
31	AA	414	LMG	11	0
29	AA	415	LHG	2	0
30	AA	416	SQD	2	0
31	AA	417	LMG	6	0
24	AB	601	CLA	5	0
24	AB	602	CLA	7	0
24	AB	603	CLA	15	0
24	AB	604	CLA	12	0
24	AB	605	CLA	10	0
24	AB	606	CLA	9	0
24	AB	607	CLA	10	0
24	AB	608	CLA	15	0
24	AB	609	CLA	7	0
24	AB	610	CLA	8	0
24	AB	611	CLA	15	0
24	AB	612	CLA	12	0
24	AB	613	CLA	9	0
24	AB	614	CLA	10	0
24	AB	615	CLA	8	0
24	AB	616	CLA	4	0
27	AB	617	BCR	3	0
27	AB	618	BCR	2	0
27	AB	619	BCR	3	0
31	AB	620	LMG	17	0
31	AB	621	LMG	4	0
30	AB	622	SQD	6	0
32	AB	624	LMT	9	0
30	AB	627	SQD	3	0
32	AB	629	LMT	4	0
32	AB	630	LMT	2	0
24	AC	501	CLA	5	0
24	AC	502	CLA	6	0
24	AC	503	CLA	6	0
24	AC	504	CLA	10	0
24	AC	505	CLA	9	0
24	AC	506	CLA	5	0
24	AC	507	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AC	508	CLA	10	0
24	AC	509	CLA	6	0
24	AC	510	CLA	6	0
24	AC	511	CLA	22	0
24	AC	512	CLA	4	0
24	AC	513	CLA	3	0
27	AC	514	BCR	6	0
27	AC	515	BCR	6	0
27	AC	516	BCR	12	0
28	AC	517	DGD	10	0
28	AC	518	DGD	12	0
28	AC	519	DGD	42	0
31	AC	520	LMG	4	0
31	AC	521	LMG	7	0
24	AD	401	CLA	9	0
34	AD	402	PHO	11	0
34	AD	403	PHO	3	0
24	AD	404	CLA	8	0
35	AD	405	PL9	15	0
27	AD	406	BCR	2	0
31	AD	407	LMG	4	0
31	AD	408	LMG	11	0
28	AE	101	DGD	1	0
36	AF	101	HEM	8	0
30	AF	102	SQD	1	0
28	AH	101	DGD	9	0
31	AI	101	LMG	3	0
32	AI	102	LMT	5	0
32	AI	103	LMT	4	0
27	AJ	101	BCR	4	0
31	AJ	102	LMG	2	0
27	AK	102	BCR	5	0
31	AM	101	LMG	6	0
32	AM	102	LMT	1	0
27	AT	101	BCR	10	0
36	AV	201	HEM	4	0
27	AX	101	BCR	8	0
30	BA	5401	SQD	3	0
31	BA	5402	LMG	3	0
24	BA	5405	CLA	11	0
24	BA	5406	CLA	22	0
24	BA	5407	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	BA	5408	CLA	11	0
25	BA	5409	MST	9	0
27	BA	5411	BCR	3	0
28	BA	5412	DGD	9	0
29	BA	5413	LHG	6	0
29	BA	5415	LHG	3	0
30	BB	5601	SQD	5	0
28	BB	5602	DGD	5	0
32	BB	5603	LMT	2	0
32	BB	5604	LMT	2	0
24	BB	5605	CLA	5	0
24	BB	5606	CLA	7	0
24	BB	5607	CLA	15	0
24	BB	5608	CLA	12	0
24	BB	5609	CLA	12	0
24	BB	5610	CLA	9	0
24	BB	5611	CLA	10	0
24	BB	5612	CLA	14	0
24	BB	5613	CLA	7	0
24	BB	5614	CLA	9	0
24	BB	5615	CLA	19	0
24	BB	5616	CLA	12	0
24	BB	5617	CLA	8	0
24	BB	5618	CLA	14	0
24	BB	5619	CLA	8	0
24	BB	5620	CLA	4	0
27	BB	5621	BCR	3	0
27	BB	5622	BCR	1	0
27	BB	5623	BCR	4	0
31	BB	5624	LMG	4	0
30	BB	5625	SQD	6	0
32	BB	5626	LMT	2	0
32	BB	5627	LMT	10	0
24	BC	5501	CLA	6	0
24	BC	5502	CLA	6	0
24	BC	5503	CLA	5	0
24	BC	5504	CLA	8	0
24	BC	5505	CLA	9	0
24	BC	5506	CLA	4	0
24	BC	5507	CLA	7	0
24	BC	5508	CLA	9	0
24	BC	5509	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	BC	5510	CLA	6	0
24	BC	5511	CLA	23	0
24	BC	5512	CLA	5	0
24	BC	5513	CLA	5	0
27	BC	5514	BCR	6	0
27	BC	5515	BCR	6	0
27	BC	5516	BCR	13	0
28	BC	5517	DGD	10	0
28	BC	5518	DGD	10	0
28	BC	5519	DGD	45	0
31	BC	5520	LMG	3	0
31	BC	5521	LMG	7	0
32	BC	5522	LMT	3	0
24	BD	5402	CLA	10	0
34	BD	5403	PHO	12	0
34	BD	5404	PHO	3	0
24	BD	5405	CLA	8	0
35	BD	5406	PL9	16	0
27	BD	5407	BCR	2	0
31	BD	5408	LMG	1	0
31	BD	5409	LMG	4	0
31	BD	5410	LMG	10	0
32	BD	5411	LMT	1	0
31	BE	5101	LMG	4	0
28	BE	5102	DGD	1	0
36	BF	5101	HEM	7	0
30	BF	5102	SQD	1	0
28	BH	5101	DGD	8	0
31	BI	5101	LMG	4	0
32	BI	5102	LMT	5	0
27	BJ	5101	BCR	3	0
27	BK	5102	BCR	5	0
31	BL	5101	LMG	18	0
32	BM	5101	LMT	2	0
31	BM	5102	LMG	4	0
27	BT	5101	BCR	6	0
36	BV	5201	HEM	6	0
27	BX	5101	BCR	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	335/344 (97%)	-0.00	6 (1%) 69 55	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.02	15 (4%) 34 21	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.02	12 (2%) 59 45	81, 103, 136, 152	0
2	BB	490/510 (96%)	0.09	21 (4%) 36 23	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.29	22 (4%) 30 18	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.24	29 (6%) 20 11	91, 124, 149, 159	0
4	AD	341/352 (96%)	0.00	6 (1%) 69 55	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.02	12 (3%) 44 29	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.45	7 (8%) 11 7	104, 126, 151, 155	0
5	BE	82/84 (97%)	1.23	23 (28%) 1 1	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.40	5 (14%) 3 2	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.27	4 (11%) 6 3	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.48	8 (12%) 5 3	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.51	6 (9%) 10 6	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.08	2 (5%) 24 14	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.70	8 (22%) 1 1	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.02	3 (7%) 13 7	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.46	7 (18%) 1 1	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.08	1 (2%) 55 40	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.13	1 (2%) 55 40	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.26	4 (10%) 6 4	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.46	6 (16%) 2 1	90, 104, 158, 160	0
12	AM	34/36 (94%)	0.24	3 (8%) 11 6	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.12	2 (5%) 23 13	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%)	0.33	16 (6%) 19 11	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.30	21 (8%) 11 6	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.35	3 (9%) 9 5	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.01	1 (3%) 49 33	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.26	4 (4%) 38 25	93, 105, 116, 125	0
15	BU	97/104 (93%)	0.16	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	0.11	2 (1%) 74 61	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.46	13 (9%) 9 5	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.62	4 (14%) 3 2	141, 154, 160, 160	0
17	By	28/46 (60%)	0.80	5 (17%) 2 1	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.42	7 (18%) 1 1	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.38	5 (13%) 3 2	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.63	11 (17%) 2 1	134, 148, 160, 160	0
20	BZ	62/62 (100%)	1.40	19 (30%) 0 1	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.20	324 (6%) 21 12	81, 113, 149, 160	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	9.3
20	BZ	5061	VAL	7.5
13	BO	5084	ASN	7.4
20	BZ	5001	MET	6.4
7	BH	5066	GLY	6.2
9	AJ	3	SER	6.0
17	By	5046	LEU	5.9
11	BL	5001	MET	5.7
20	AZ	34	ASP	5.5
1	BA	5011	ALA	5.4
7	BH	5065	LEU	5.4
2	BB	5491	VAL	5.4
18	AX	47	GLN	5.3
8	BI	5032	PRO	5.3
5	BE	5008	ARG	5.2
1	BA	5010	SER	5.0

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Mol	Chain	Res	Type	RSRZ
20	BZ	5033	TRP	4.7
8	BI	5033	LYS	4.6
11	AL	1	MET	4.4
20	AZ	62	VAL	4.4
6	AF	12	SER	4.3
20	BZ	5060	PHE	4.3
6	BF	5012	SER	4.2
9	BJ	5004	GLU	4.2
20	AZ	30	PRO	4.1
17	Ay	45	ASN	4.1
2	BB	5002	GLY	4.1
4	BD	5099	GLY	4.1
11	BL	5005	PRO	4.1
3	AC	27	ASP	4.0
20	AZ	33	TRP	4.0
11	BL	5002	GLU	4.0
8	BI	5034	ARG	4.0
6	AF	11	VAL	4.0
20	AZ	61	VAL	4.0
12	BM	5034	LYS	3.9
5	BE	5007	GLU	3.9
10	AK	46	ARG	3.9
5	AE	83	LEU	3.9
18	AX	45	LYS	3.9
3	AC	145	SER	3.9
5	BE	5021	VAL	3.9
3	AC	137	PRO	3.8
13	BO	5051	THR	3.8
3	BC	5183	GLY	3.8
17	By	5041	VAL	3.8
20	AZ	60	PHE	3.8
3	BC	5144	SER	3.7
8	BI	5002	GLU	3.7
3	BC	5204	LEU	3.7
4	AD	241	GLU	3.7
5	AE	12	ASP	3.6
4	BD	5239	GLN	3.6
4	AD	13	GLY	3.6
13	BO	5052	ALA	3.6
9	BJ	5005	GLY	3.6
11	BL	5003	PRO	3.6
18	AX	46	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
5	BE	5017	VAL	3.6
13	BO	5050	ASP	3.6
3	AC	138	GLU	3.6
13	BO	5062	GLN	3.5
14	AT	30	THR	3.5
3	BC	5203	THR	3.4
5	BE	5006	GLY	3.4
20	AZ	57	LEU	3.4
3	BC	5184	GLY	3.4
13	AO	88	GLU	3.4
2	BB	5490	GLN	3.4
2	AB	129	GLY	3.4
7	AH	26	GLY	3.4
20	BZ	5002	THR	3.4
6	BF	5011	VAL	3.4
2	BB	5128	THR	3.4
7	BH	5027	THR	3.4
6	AF	13	TYR	3.4
9	BJ	5003	SER	3.4
13	AO	51	THR	3.4
3	BC	5255	THR	3.4
5	BE	5016	SER	3.4
13	AO	114	ASN	3.3
2	AB	379	ALA	3.3
16	BV	5132	ASN	3.3
20	BZ	5004	LEU	3.3
9	AJ	4	GLU	3.3
12	AM	31	SER	3.2
7	AH	16	SER	3.2
5	AE	17	VAL	3.2
5	BE	5013	ILE	3.2
3	BC	5135	ARG	3.2
3	AC	78	GLU	3.2
7	AH	27	THR	3.2
13	BO	5060	SER	3.2
9	BJ	5008	ILE	3.2
14	AT	31	LYS	3.2
20	AZ	31	GLN	3.2
13	BO	5112	LYS	3.1
4	AD	24	ARG	3.1
13	BO	5049	ASP	3.1
7	AH	23	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
5	BE	5082	GLN	3.1
13	BO	5167	ASP	3.1
5	AE	21	VAL	3.1
5	BE	5073	LYS	3.1
2	BB	5123	PHE	3.0
17	By	5045	ASN	3.0
4	BD	5233	ARG	3.0
3	AC	141	GLU	3.0
3	BC	5057	ALA	3.0
9	BJ	5006	GLY	3.0
2	BB	5120	LEU	3.0
3	AC	198	VAL	3.0
13	BO	5063	THR	3.0
12	BM	5033	GLN	3.0
1	BA	5032	TRP	3.0
13	BO	5064	TYR	2.9
4	BD	5012	ARG	2.9
2	BB	5121	GLU	2.9
1	BA	5015	GLU	2.9
5	BE	5059	GLU	2.9
3	AC	199	ILE	2.9
17	Ay	42	ARG	2.9
6	BF	5013	TYR	2.9
11	AL	4	ASN	2.9
12	AM	33	GLN	2.9
18	BX	5043	ILE	2.8
3	BC	5207	ARG	2.8
3	BC	5030	SER	2.8
3	AC	203	THR	2.8
13	BO	5048	LEU	2.8
14	AT	32	LYS	2.8
6	BF	5015	ILE	2.8
4	AD	98	GLN	2.8
17	Ay	21	GLN	2.8
2	BB	5162	PHE	2.8
1	AA	242	GLU	2.8
13	AO	52	ALA	2.8
18	BX	5011	THR	2.8
16	BV	5111	GLU	2.8
2	BB	5161	LEU	2.8
20	BZ	5005	PHE	2.8
16	BV	5047	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
7	AH	25	TRP	2.7
13	AO	230	VAL	2.7
20	BZ	5036	SER	2.7
13	AO	84	ASN	2.7
2	BB	5219	VAL	2.7
2	AB	125	ASP	2.7
2	AB	378	LYS	2.7
3	BC	5131	TYR	2.7
3	AC	140	LEU	2.7
2	AB	118	TRP	2.7
5	BE	5018	ARG	2.7
2	AB	130	GLU	2.7
10	BK	5014	ALA	2.7
13	BO	5160	THR	2.7
4	BD	5226	GLY	2.6
1	BA	5233	ALA	2.6
3	BC	5202	PRO	2.6
5	AE	84	LYS	2.6
13	AO	232	GLY	2.6
20	BZ	5029	SER	2.6
3	BC	5256	PRO	2.6
16	BV	5043	LYS	2.6
2	BB	5352	GLU	2.6
20	AZ	32	ASP	2.6
1	BA	5268	SER	2.6
3	AC	255	THR	2.6
13	AO	120	THR	2.6
4	BD	5098	GLN	2.6
7	AH	4	ARG	2.6
8	AI	6	ILE	2.6
5	BE	5061	ARG	2.6
11	BL	5004	ASN	2.6
3	BC	5198	VAL	2.5
9	BJ	5013	VAL	2.5
17	Ay	41	VAL	2.5
16	BV	5121	LEU	2.5
1	BA	5012	ASN	2.5
2	BB	5374	ASN	2.5
3	BC	5200	THR	2.5
3	BC	5186	TYR	2.5
8	AI	2	GLU	2.5
3	BC	5143	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	5232	SER	2.5
5	BE	5083	LEU	2.5
3	AC	48	LYS	2.5
3	AC	204	LEU	2.5
11	BL	5010	VAL	2.5
13	BO	5217	SER	2.5
15	AU	69	ARG	2.5
3	AC	202	PRO	2.5
3	AC	253	LEU	2.5
1	BA	5019	ASN	2.5
16	AV	116	GLU	2.5
1	AA	11	ALA	2.5
16	BV	5031	PRO	2.5
3	AC	144	SER	2.4
2	AB	407	ASN	2.4
5	BE	5005	THR	2.4
20	AZ	35	ARG	2.4
2	BB	5294	SER	2.4
13	BO	5091	PHE	2.4
13	AO	163	THR	2.4
13	BO	5030	THR	2.4
16	AV	43	LYS	2.4
2	BB	5124	ARG	2.4
5	BE	5010	PHE	2.4
1	AA	10	SER	2.4
8	BI	5030	ARG	2.4
2	AB	120	LEU	2.4
3	BC	5230	LEU	2.4
14	BT	5030	THR	2.4
18	BX	5047	GLN	2.4
3	BC	5185	LEU	2.4
16	BV	5042	GLY	2.4
2	BB	5293	ALA	2.4
1	BA	5018	CYS	2.4
16	BV	5044	THR	2.4
2	BB	5125	ASP	2.4
3	BC	5195	ASP	2.4
2	AB	126	PRO	2.4
4	AD	227	GLU	2.4
3	BC	5249	ILE	2.3
15	AU	58	ASN	2.3
18	BX	5046	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
12	AM	34	LYS	2.3
13	AO	61	SER	2.3
18	AX	44	ASP	2.3
20	BZ	5003	ILE	2.3
11	AL	7	ARG	2.3
18	AX	42	GLN	2.3
20	BZ	5031	GLN	2.3
4	AD	234	ALA	2.3
8	BI	5024	LEU	2.3
8	BI	5031	ASN	2.3
5	BE	5015	THR	2.3
5	BE	5071	GLU	2.3
3	BC	5033	PHE	2.3
16	BV	5027	ALA	2.3
20	BZ	5034	ASP	2.3
3	BC	5137	PRO	2.3
16	BV	5133	LEU	2.3
18	BX	5045	LYS	2.3
1	BA	5309	ALA	2.3
2	AB	480	SER	2.3
20	BZ	5058	ASN	2.2
13	AO	48	LEU	2.2
20	BZ	5042	LEU	2.2
5	BE	5025	ILE	2.2
17	By	5033	PRO	2.2
3	BC	5142	GLU	2.2
2	BB	5482	ILE	2.2
15	AU	97	LEU	2.2
5	BE	5022	ILE	2.2
13	BO	5113	VAL	2.2
20	BZ	5038	GLN	2.2
5	AE	18	ARG	2.2
3	AC	277	GLY	2.2
4	BD	5059	TYR	2.2
1	AA	235	TYR	2.2
3	AC	45	LEU	2.2
9	BJ	5007	ARG	2.2
2	BB	5126	PRO	2.2
4	BD	5024	ARG	2.2
1	BA	5227	THR	2.2
5	BE	5026	THR	2.2
6	AF	42	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	AC	149	TYR	2.2
5	BE	5057	ALA	2.2
4	BD	5097	ALA	2.2
13	AO	62	GLN	2.2
13	BO	5092	VAL	2.2
5	BE	5084	LYS	2.2
20	BZ	5039	LEU	2.1
2	BB	5296	ALA	2.1
20	AZ	38	GLN	2.1
13	BO	5058	ILE	2.1
18	AX	11	THR	2.1
13	AO	87	GLN	2.1
1	AA	243	GLU	2.1
2	AB	119	ASP	2.1
8	BI	5023	PHE	2.1
13	AO	58	ILE	2.1
3	BC	5180	MET	2.1
20	BZ	5030	PRO	2.1
18	AX	12	ILE	2.1
4	BD	5025	ASP	2.1
3	BC	5209	ILE	2.1
3	BC	5100	GLY	2.1
6	AF	14	PRO	2.1
3	BC	5205	ASP	2.1
1	BA	5240	GLY	2.1
2	AB	491	VAL	2.1
7	AH	2	ALA	2.1
16	BV	5113	GLU	2.1
13	AO	162	ILE	2.1
4	BD	5013	GLY	2.1
5	AE	3	GLY	2.1
2	BB	5117	TYR	2.1
1	BA	5230	THR	2.1
7	BH	5018	TYR	2.1
7	AH	3	ARG	2.1
5	BE	5030	LEU	2.1
7	BH	5003	ARG	2.0
3	AC	143	TYR	2.0
13	BO	5225	LEU	2.0
16	BV	5045	ILE	2.0
20	BZ	5007	LEU	2.0
13	BO	5231	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
17	By	5021	GLN	2.0
1	AA	17	PHE	2.0
4	BD	5085	MET	2.0
9	AJ	7	ARG	2.0
3	AC	122	SER	2.0
16	BV	5146	LEU	2.0
2	BB	5118	TRP	2.0
3	BC	5199	ILE	2.0
7	BH	5022	ALA	2.0
11	AL	3	PRO	2.0
3	AC	61	VAL	2.0
1	BA	5013	LEU	2.0
13	AO	55	ALA	2.0
15	AU	94	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	DGD	AE	101	63/66	0.36	0.71	13.84	146,160,160,160	0
27	BCR	AJ	101	40/40	0.54	0.66	12.68	158,160,160,160	0
27	BCR	BJ	5101	40/40	0.64	0.51	7.62	160,160,160,160	0
28	DGD	BB	5602	52/66	0.50	0.53	7.62	152,160,160,160	0
31	LMG	BA	5402	42/55	0.61	0.50	7.36	144,157,160,160	0
31	LMG	AD	407	49/55	0.78	0.46	6.23	126,133,143,145	0
33	DMS	AV	202	4/4	0.83	0.64	5.99	148,148,148,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	DGD	BC	5518	62/66	0.70	0.49	5.82	147,156,160,160	0
33	DMS	BV	5203	4/4	0.93	0.67	5.72	160,160,160,160	0
32	LMT	AB	629	35/35	0.68	0.48	5.40	133,160,160,160	0
32	LMT	BB	5603	35/35	0.65	0.46	4.96	132,160,160,160	0
31	LMG	BD	5410	48/55	0.66	0.57	4.90	126,131,141,141	0
31	LMG	AA	417	42/55	0.68	0.45	4.85	145,157,160,160	0
29	LHG	BA	5415	37/49	0.48	0.62	4.83	151,160,160,160	0
28	DGD	AC	518	62/66	0.76	0.41	4.79	146,155,160,160	0
28	DGD	AB	628	52/66	0.55	0.60	4.36	154,160,160,160	0
28	DGD	BE	5102	63/66	0.44	0.70	4.36	145,160,160,160	0
27	BCR	AT	101	40/40	0.82	0.39	4.31	126,140,146,147	0
33	DMS	BB	5628	4/4	0.86	0.58	4.25	156,157,157,157	0
31	LMG	AB	621	49/55	0.69	0.44	4.13	145,150,157,160	0
27	BCR	BT	5101	40/40	0.77	0.40	4.04	124,143,147,147	0
31	LMG	BC	5520	48/55	0.57	0.55	4.02	138,159,160,160	0
33	DMS	BB	5629	4/4	0.93	0.29	3.89	125,126,127,127	0
31	LMG	BB	5624	49/55	0.76	0.40	3.88	145,150,157,160	0
31	LMG	AD	408	48/55	0.76	0.47	3.86	121,130,139,139	0
31	LMG	AB	620	51/55	0.73	0.49	3.78	125,139,150,151	0
23	CL	BA	5404[A]	1/1	0.72	0.34	3.66	29,29,29,29	1
31	LMG	BL	5101	51/55	0.79	0.46	3.46	122,138,151,152	0
31	LMG	BD	5408	46/55	0.70	0.46	3.41	139,145,160,160	0
32	LMT	BB	5604	35/35	0.71	0.52	3.37	131,160,160,160	0
33	DMS	AB	625	4/4	0.89	0.44	3.33	156,157,157,157	0
31	LMG	AC	520	48/55	0.60	0.57	3.30	136,157,160,160	0
28	DGD	BC	5519	66/66	0.80	0.36	3.29	112,121,158,159	0
32	LMT	AB	624	35/35	0.73	0.59	3.27	156,160,160,160	0
31	LMG	AA	414	44/55	0.61	0.46	3.27	140,160,160,160	0
31	LMG	AJ	102	46/55	0.74	0.43	3.27	139,144,160,160	0
32	LMT	BI	5102	35/35	0.64	0.85	3.23	151,160,160,160	0
28	DGD	AC	519	66/66	0.84	0.36	3.20	110,120,157,158	0
24	CLA	AA	406	65/65	0.87	0.34	3.15	105,112,138,139	0
27	BCR	BD	5407	40/40	0.88	0.30	3.15	112,127,132,132	0
24	CLA	AB	601	65/65	0.71	0.55	3.14	146,159,160,160	0
24	CLA	BC	5504	65/65	0.89	0.33	3.07	132,135,160,160	0
27	BCR	AK	102	40/40	0.81	0.38	2.98	133,139,151,152	0
24	CLA	AB	608	65/65	0.89	0.40	2.98	123,127,135,140	0
27	BCR	BB	5622	40/40	0.92	0.34	2.97	110,117,120,121	0
32	LMT	AM	102	35/35	0.79	0.43	2.96	126,149,154,154	0
28	DGD	AC	517	53/66	0.82	0.39	2.93	121,128,135,140	0
28	DGD	BA	5412	56/66	0.53	0.58	2.89	150,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	SQD	BB	5625	43/54	0.59	0.47	2.87	132,148,160,160	0
31	LMG	BD	5409	49/55	0.80	0.41	2.87	128,133,144,146	0
28	DGD	BH	5101	58/66	0.83	0.37	2.87	107,118,156,160	0
28	DGD	AA	411	56/66	0.56	0.54	2.85	148,158,160,160	0
24	CLA	BB	5617	65/65	0.92	0.33	2.84	98,102,138,141	0
24	CLA	AA	407	65/65	0.91	0.33	2.76	93,101,150,151	0
24	CLA	BB	5609	65/65	0.91	0.34	2.71	103,110,124,124	0
32	LMT	BB	5627	35/35	0.75	0.45	2.65	156,160,160,160	0
24	CLA	AD	404	65/65	0.87	0.35	2.63	126,130,148,149	0
30	SQD	BA	5401	54/54	0.65	0.47	2.61	136,160,160,160	0
24	CLA	BB	5612	65/65	0.91	0.39	2.56	122,127,136,139	0
24	CLA	AC	504	65/65	0.89	0.34	2.52	129,134,160,160	0
35	PL9	AD	405	55/55	0.90	0.36	2.50	99,109,113,113	0
32	LMT	AI	103	35/35	0.73	0.47	2.43	156,158,160,160	0
27	BCR	BB	5621	40/40	0.89	0.32	2.40	112,120,124,125	0
24	CLA	AC	505	65/65	0.88	0.40	2.39	121,146,150,151	0
27	BCR	AC	515	40/40	0.72	0.45	2.39	149,152,155,155	0
24	CLA	AC	503	65/65	0.88	0.48	2.38	137,144,147,152	0
24	CLA	BB	5605	65/65	0.72	0.58	2.35	146,159,160,160	0
32	LMT	AB	630	35/35	0.74	0.49	2.33	132,160,160,160	0
32	LMT	BM	5101	35/35	0.73	0.39	2.30	126,149,154,155	0
24	CLA	AB	605	65/65	0.90	0.28	2.27	105,113,122,124	0
27	BCR	AX	101	40/40	0.60	0.49	2.22	135,143,158,159	0
32	LMT	BC	5522	35/35	0.77	0.67	2.19	157,160,160,160	0
31	LMG	BE	5101	44/55	0.65	0.46	2.18	140,160,160,160	0
27	BCR	AB	617	40/40	0.87	0.32	2.15	112,121,125,125	0
24	CLA	BA	5408	65/65	0.89	0.30	2.10	95,103,150,150	0
27	BCR	BX	5101	40/40	0.62	0.49	2.10	136,143,157,158	0
24	CLA	AC	508	65/65	0.90	0.35	2.03	140,144,157,158	0
27	BCR	AC	516	40/40	0.71	0.46	1.99	135,138,143,143	0
32	LMT	AI	102	35/35	0.70	0.58	1.98	149,158,160,160	0
24	CLA	AC	502	65/65	0.91	0.36	1.94	103,109,142,143	0
30	SQD	AB	622	43/54	0.66	0.43	1.91	133,149,160,160	0
24	CLA	AC	507	65/65	0.88	0.38	1.90	137,149,152,153	0
33	DMS	AU	201	4/4	0.75	0.40	1.87	160,160,160,160	0
31	LMG	AC	521	45/55	0.40	0.63	1.86	154,160,160,160	0
24	CLA	BD	5405	65/65	0.83	0.34	1.86	125,131,148,149	0
27	BCR	BC	5514	40/40	0.80	0.43	1.84	123,126,129,129	0
24	CLA	AB	609	65/65	0.73	0.39	1.84	126,136,141,143	0
28	DGD	AH	101	58/66	0.86	0.30	1.79	108,120,155,157	0
27	BCR	AD	406	40/40	0.88	0.31	1.77	110,126,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	BC	5508	65/65	0.84	0.33	1.76	142,146,157,159	0
24	CLA	BC	5502	65/65	0.90	0.32	1.75	108,111,143,144	0
24	CLA	BB	5614	65/65	0.90	0.32	1.74	117,123,124,128	0
24	CLA	AC	501	65/65	0.88	0.37	1.73	133,136,139,143	0
23	CL	BA	5404[B]	1/1	0.72	0.34	1.72	115,115,115,115	1
34	PHO	BD	5403	64/64	0.89	0.34	1.72	102,109,118,118	0
30	SQD	BF	5102	45/54	0.68	0.57	1.71	154,160,160,160	0
24	CLA	BB	5616	65/65	0.91	0.31	1.69	108,110,120,122	0
24	CLA	AB	610	65/65	0.91	0.33	1.68	117,121,123,127	0
35	PL9	BD	5406	55/55	0.85	0.34	1.65	103,110,115,116	0
34	PHO	AD	403	64/64	0.93	0.28	1.63	119,123,128,129	0
27	BCR	BB	5623	40/40	0.82	0.37	1.63	111,116,131,131	0
24	CLA	BB	5608	65/65	0.95	0.32	1.62	96,103,124,125	0
27	BCR	BC	5515	40/40	0.71	0.43	1.58	150,152,155,156	0
33	DMS	AB	626	4/4	0.89	0.26	1.58	129,130,130,130	0
24	CLA	BA	5406	65/65	0.89	0.28	1.58	89,94,108,112	0
24	CLA	BB	5611	65/65	0.90	0.28	1.58	95,102,132,136	0
24	CLA	AB	603	65/65	0.88	0.37	1.56	107,109,119,121	0
24	CLA	AB	611	65/65	0.94	0.30	1.53	99,113,116,122	0
24	CLA	AD	401	65/65	0.93	0.27	1.52	93,100,115,119	0
24	CLA	BA	5407	65/65	0.88	0.29	1.49	110,114,138,139	0
27	BCR	BK	5102	40/40	0.80	0.37	1.47	136,140,152,152	0
34	PHO	AD	402	64/64	0.92	0.30	1.46	99,109,116,117	0
24	CLA	AB	606	65/65	0.83	0.33	1.42	120,133,140,141	0
24	CLA	AB	607	65/65	0.92	0.26	1.38	94,100,132,135	0
24	CLA	AB	602	65/65	0.86	0.33	1.37	124,127,129,132	0
31	LMG	AM	101	42/55	0.68	0.54	1.36	136,158,160,160	0
30	SQD	AF	102	45/54	0.74	0.45	1.35	154,160,160,160	0
24	CLA	AC	509	65/65	0.89	0.39	1.34	115,128,135,137	0
30	SQD	AA	416	54/54	0.76	0.34	1.33	136,160,160,160	0
24	CLA	BC	5510	65/65	0.91	0.34	1.32	113,116,130,131	0
24	CLA	AB	615	65/65	0.88	0.33	1.32	134,139,155,157	0
27	BCR	AB	618	40/40	0.87	0.27	1.32	109,117,122,122	0
24	CLA	BC	5507	65/65	0.83	0.36	1.23	136,150,153,154	0
24	CLA	AB	616	65/65	0.86	0.40	1.21	143,147,160,160	0
32	LMT	AD	409	31/35	0.71	0.43	1.21	139,154,160,160	0
23	CL	AA	403[B]	1/1	0.87	0.31	1.20	108,108,108,108	1
24	CLA	BC	5503	65/65	0.84	0.35	1.20	137,147,148,152	0
23	CL	AA	403[A]	1/1	0.87	0.31	1.19	33,33,33,33	1
29	LHG	AA	415	37/49	0.76	0.35	1.19	149,160,160,160	0
24	CLA	AC	512	65/65	0.80	0.44	1.18	154,158,160,160	0
24	CLA	BC	5513	65/65	0.72	0.50	1.17	158,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	BC	5505	65/65	0.82	0.36	1.16	123,148,152,153	0
24	CLA	BB	5615	65/65	0.92	0.26	1.16	101,113,117,120	0
24	CLA	AB	614	65/65	0.84	0.37	1.14	129,133,160,160	0
24	CLA	BB	5613	65/65	0.76	0.37	1.12	127,135,140,142	0
24	CLA	AC	506	65/65	0.75	0.37	1.12	136,143,160,160	0
32	LMT	BD	5411	31/35	0.67	0.49	1.08	140,152,160,160	0
24	CLA	AB	612	65/65	0.93	0.29	1.05	107,111,120,121	0
24	CLA	BB	5607	65/65	0.89	0.28	1.05	108,111,120,123	0
24	CLA	BA	5405	65/65	0.87	0.30	0.98	90,101,105,109	0
24	CLA	AB	604	65/65	0.93	0.30	0.95	96,104,125,127	0
27	BCR	BA	5411	40/40	0.89	0.29	0.95	94,122,132,132	0
27	BCR	AC	514	40/40	0.88	0.33	0.94	120,123,127,128	0
24	CLA	AB	613	65/65	0.93	0.26	0.94	99,102,136,140	0
27	BCR	BC	5516	40/40	0.67	0.45	0.91	136,140,145,145	0
30	SQD	AB	627	47/54	0.77	0.36	0.91	138,157,160,160	0
33	DMS	BV	5202	4/4	0.91	0.26	0.90	148,149,149,150	0
24	CLA	BC	5511	65/65	0.81	0.43	0.88	154,158,159,160	0
28	DGD	BC	5517	53/66	0.87	0.28	0.87	124,130,136,139	0
24	CLA	BB	5619	65/65	0.90	0.34	0.86	135,137,155,157	0
36	HEM	AF	101	43/43	0.94	0.38	0.85	148,152,159,160	0
24	CLA	AA	404	65/65	0.92	0.26	0.83	89,99,106,108	0
31	LMG	BM	5102	42/55	0.74	0.45	0.82	136,160,160,160	0
30	SQD	BA	5414	51/54	0.73	0.36	0.76	145,150,160,160	0
24	CLA	BC	5506	65/65	0.76	0.39	0.75	136,143,160,160	0
30	SQD	BB	5601	47/54	0.73	0.39	0.74	137,156,160,160	0
29	LHG	AA	412	39/49	0.90	0.28	0.74	110,118,128,132	0
24	CLA	BB	5606	65/65	0.85	0.30	0.73	124,127,130,131	0
24	CLA	BD	5402	65/65	0.91	0.27	0.73	97,101,117,119	0
34	PHO	BD	5404	64/64	0.90	0.28	0.72	123,125,129,130	0
24	CLA	AA	405	65/65	0.94	0.26	0.71	88,93,108,111	0
27	BCR	AB	619	40/40	0.85	0.29	0.70	111,117,131,131	0
30	SQD	AA	413	51/54	0.84	0.31	0.69	143,150,160,160	0
31	LMG	BC	5521	45/55	0.64	0.55	0.68	154,160,160,160	0
24	CLA	AC	513	65/65	0.72	0.44	0.68	158,160,160,160	0
24	CLA	AC	510	65/65	0.92	0.33	0.67	110,113,129,130	0
24	CLA	BC	5509	65/65	0.89	0.29	0.62	116,128,138,138	0
24	CLA	BC	5501	65/65	0.89	0.30	0.58	134,137,141,144	0
27	BCR	AA	410	40/40	0.91	0.27	0.55	91,122,130,130	0
24	CLA	BC	5512	65/65	0.81	0.35	0.51	157,160,160,160	0
24	CLA	BB	5618	65/65	0.87	0.32	0.50	128,133,160,160	0
24	CLA	BB	5610	65/65	0.83	0.31	0.47	121,132,140,141	0
29	LHG	BA	5413	39/49	0.88	0.27	0.42	113,122,128,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	HEM	BV	5201	43/43	0.93	0.27	0.41	97,102,106,109	0
36	HEM	AV	201	43/43	0.96	0.27	0.39	94,100,102,103	0
25	MST	AA	408	16/16	0.93	0.26	0.33	123,126,129,130	0
26	OEC	AA	409	5/9	0.95	0.28	0.31	82,83,90,110	0
36	HEM	BF	5101	43/43	0.91	0.44	0.18	148,152,160,160	0
24	CLA	AC	511	65/65	0.88	0.33	0.14	152,155,157,158	0
25	MST	BA	5409	16/16	0.92	0.23	0.06	124,129,131,132	0
24	CLA	BB	5620	65/65	0.83	0.29	0.02	143,147,160,160	0
26	OEC	BA	5410	5/9	0.73	0.22	-0.50	23,88,99,134	0
22	BCT	AA	402	4/4	0.99	0.20	-0.79	135,136,137,137	0
21	FE2	AA	401	1/1	0.98	0.17	-0.89	115,115,115,115	0
22	BCT	BA	5403	4/4	0.97	0.15	-1.25	135,136,136,137	0
21	FE2	BD	5401	1/1	0.94	0.11	-2.34	119,119,119,119	0
32	LMT	AB	623	35/35	0.53	0.72	-	135,160,160,160	0
31	LMG	AI	101	43/55	0.40	0.78	-	159,160,160,160	0
32	LMT	BB	5626	35/35	0.39	0.62	-	131,160,160,160	0
37	CA	AK	101	1/1	0.84	0.12	-	146,146,146,146	0
37	CA	BO	5301	1/1	0.65	0.34	-	160,160,160,160	0
31	LMG	BI	5101	43/55	0.58	0.71	-	160,160,160,160	0
37	CA	BF	5103	1/1	0.15	0.16	-	146,146,146,146	0
37	CA	AO	301	1/1	0.51	0.23	-	152,152,152,152	0
37	CA	AF	103	1/1	0.35	0.23	-	150,150,150,150	0
37	CA	BK	5101	1/1	0.63	0.22	-	145,145,145,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.