



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:09 pm GMT

PDB ID : 4FE1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 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

<https://www.wwpdb.org/validation/2017/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:

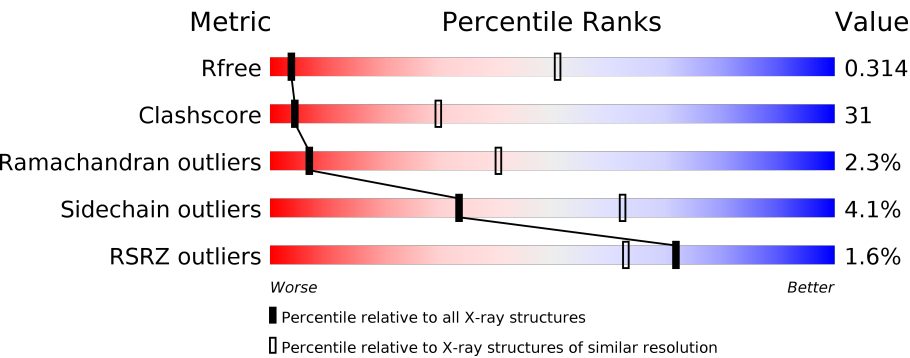
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

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 4.92 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}	111664	1012 (6.10-3.72)
Clashscore	122126	1019 (6.02-3.80)
Ramachandran outliers	120053	1008 (6.10-3.74)
Sidechain outliers	120020	1121 (6.10-3.70)
RSRZ outliers	108989	1012 (6.20-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	755	<div><div>3%</div><div><div></div><div>57%</div><div>38%</div><div></div></div><div></div></div>
2	B	740	<div><div>%</div><div><div></div><div>61%</div><div>36%</div><div></div></div><div></div></div>
3	C	80	<div><div></div><div><div></div><div>79%</div><div>19%</div><div></div></div><div></div></div>
4	D	138	<div><div></div><div><div></div><div>70%</div><div>27%</div><div></div></div><div></div></div>
5	E	75	<div><div>%</div><div><div></div><div>57%</div><div>31%</div><div></div></div><div></div></div>
6	F	164	<div><div>%</div><div><div></div><div>51%</div><div>31%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
13	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	X	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	X
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	X
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	X
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	X	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	X	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	X
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	X	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	A	845	X	-	-	-
13	CLA	A	855	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	X	-
13	CLA	B	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	X	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	I	101	X	-	-	-
13	CLA	J	1101	X	-	-	-
13	CLA	J	1102	X	-	-	-
13	CLA	J	1103	X	-	-	-
13	CLA	L	1002	X	-	-	-
13	CLA	L	1003	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1201	X	-	-	-
13	CLA	M	1202	X	-	-	X
13	CLA	X	102	X	-	-	-
15	BCR	A	847	-	-	-	X
15	BCR	A	848	-	-	-	X
15	BCR	A	849	-	-	-	X
15	BCR	B	841	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	0	0	0
			222	130	46	46			

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	CONFLICT	UNP Q8DGB4

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

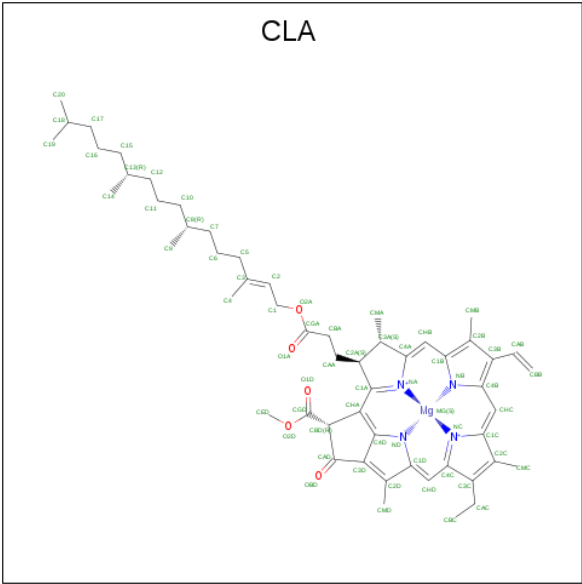
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	0	0	0
			233	164	34	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	33	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	34	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	35	ALA	-	EXPRESSION TAG	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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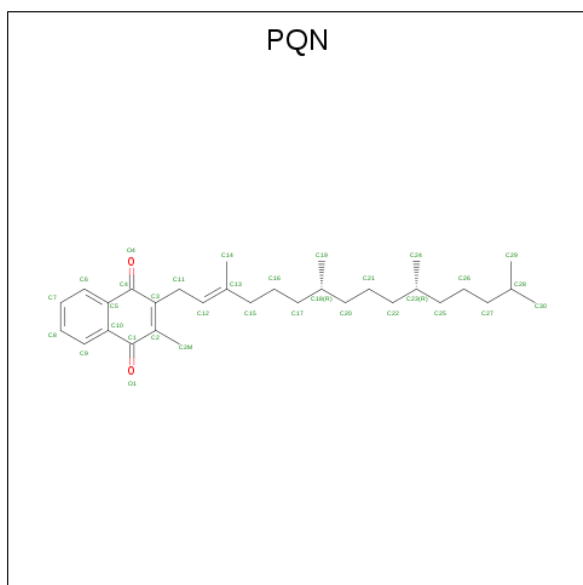
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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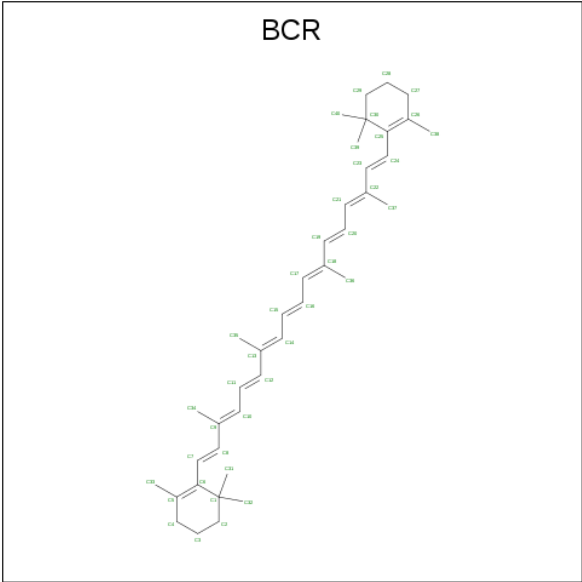
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			33	31	2		
14	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



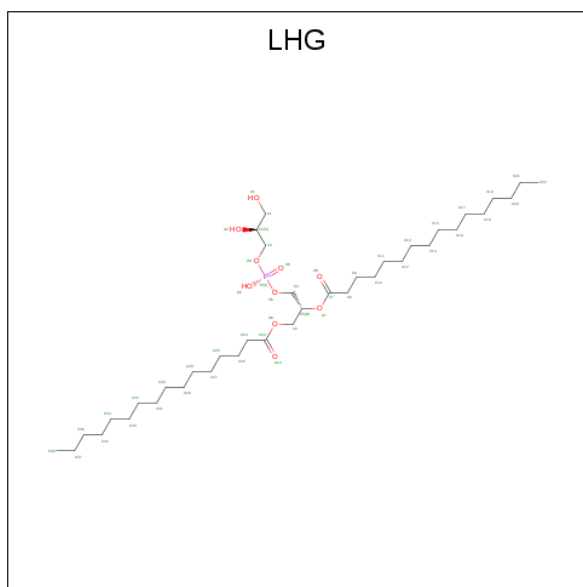
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0

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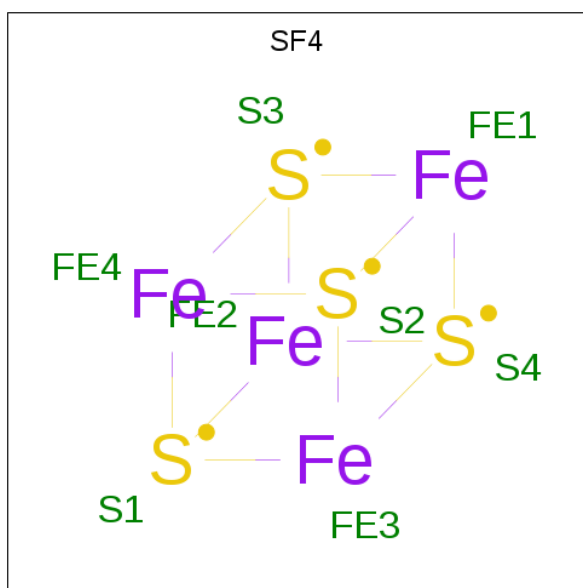
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



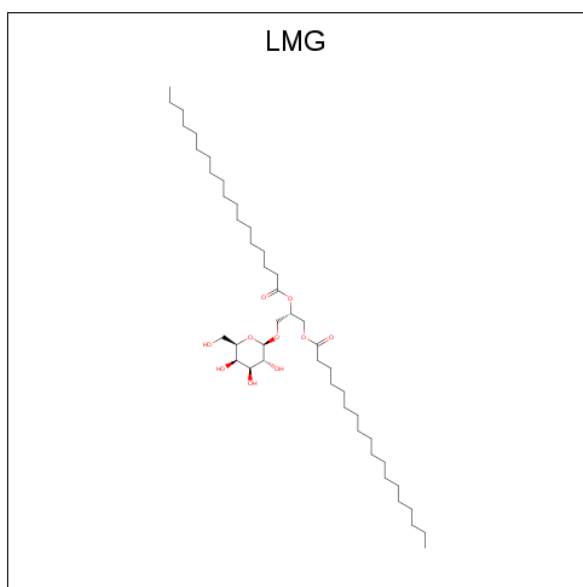
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	A	1	Total	Fe	S	0	0
			8	4	4		
17	C	1	Total	Fe	S	0	0
			8	4	4		
17	C	1	Total	Fe	S	0	0
			8	4	4		

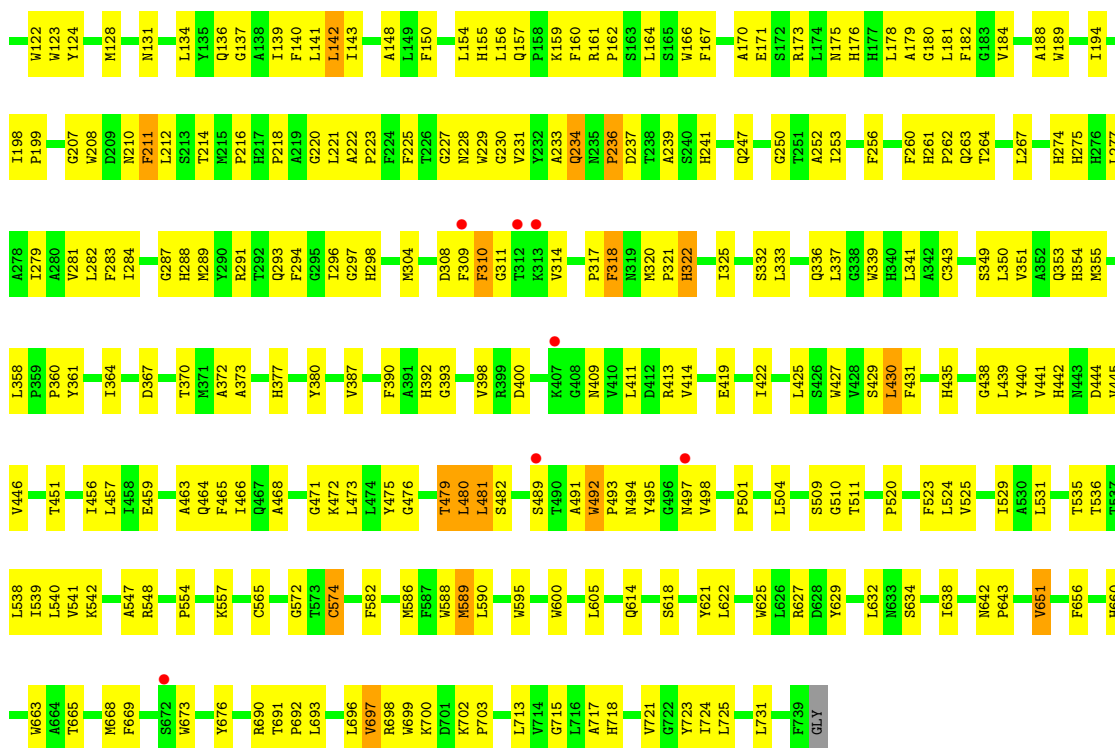
- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

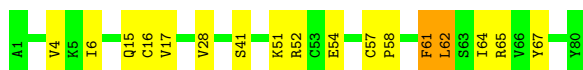
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		



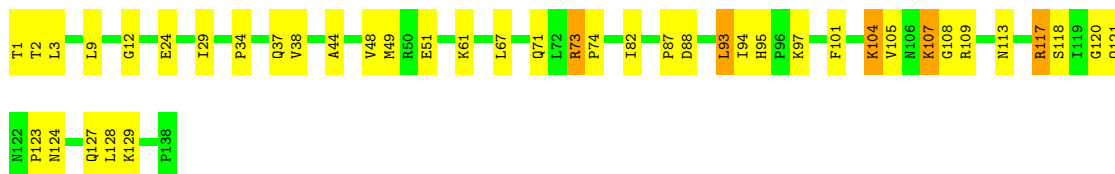
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 79% 19%



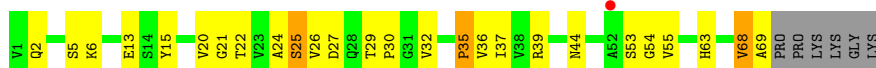
• Molecule 4: Photosystem I reaction center subunit II

Chain D: 70% 27%



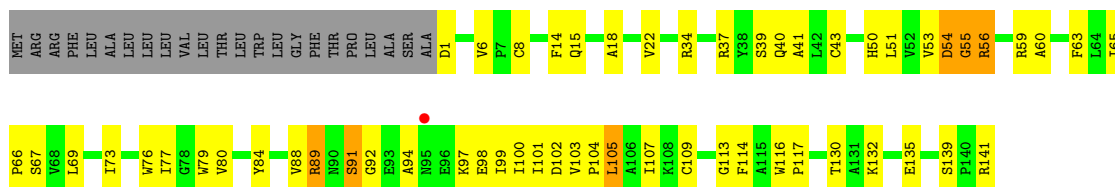
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 57% 31% 8%



• Molecule 6: Photosystem I reaction center subunit III

Chain F: 51% 31% 14%



• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 53% 42% 5%



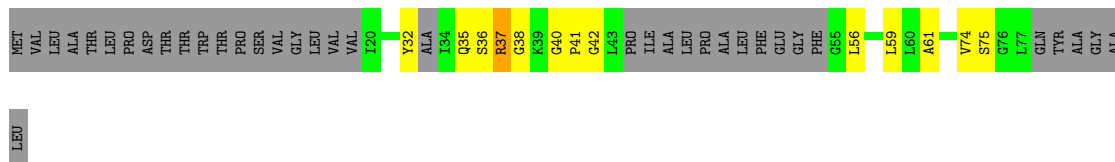
• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 56% 41% 3%



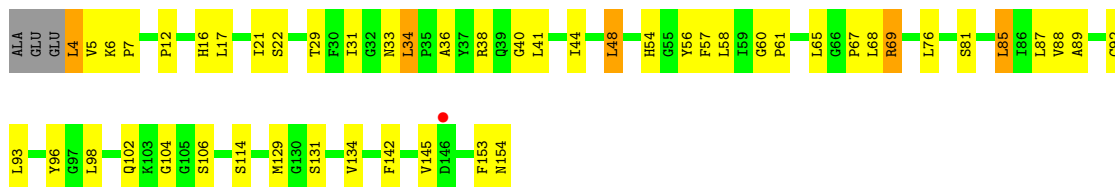
• Molecule 9: Photosystem I reaction center subunit Psak

Chain K: 40% 14% 45%



• Molecule 10: Photosystem I reaction center subunit XI

Chain L: 66% 29% 5%



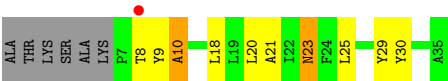
• Molecule 11: Photosystem I reaction center subunit XII

Chain M: 61% 32% 6%



• Molecule 12: Photosystem I 4.8K protein

Chain X: 3% 54% 23% 6% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.274 , 0.314	Depositor DCC
R_{free} test set	1534 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, SF4, CLA, PQN, CA, 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	A	0.38	0/5983	0.69	3/8158 (0.0%)
2	B	0.40	0/6096	0.68	2/8332 (0.0%)
3	C	0.39	0/608	0.76	0/824
4	D	0.35	0/1101	0.78	0/1492
5	E	0.42	0/551	0.85	1/750 (0.1%)
6	F	0.41	0/1087	0.76	0/1476
7	I	0.38	0/312	0.80	1/425 (0.2%)
8	J	0.40	0/350	0.80	1/477 (0.2%)
9	K	0.40	0/220	0.91	0/300
10	L	0.39	0/1148	0.79	2/1558 (0.1%)
11	M	0.47	0/244	0.91	1/332 (0.3%)
12	X	0.41	0/242	0.66	0/332
All	All	0.39	0/17942	0.72	11/24456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-8.44	110.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD1	8.11	125.60	118.30
10	L	76	LEU	CB-CG-CD2	7.19	123.22	111.00
7	I	26	VAL	CG1-CB-CG2	6.87	121.90	110.90
10	L	48	LEU	CB-CG-CD2	6.78	122.52	111.00
2	B	289	MET	CG-SD-CE	-5.94	90.70	100.20
11	M	17	LEU	CA-CB-CG	5.80	128.64	115.30
8	J	41	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	521	GLY	N-CA-C	-5.52	99.29	113.10
5	E	39	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	B	78	GLN	CA-CB-CG	5.04	124.48	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	350	0
2	B	5879	0	5632	345	0
3	C	598	0	580	15	0
4	D	1075	0	1077	30	0
5	E	539	0	528	13	0
6	F	1065	0	1077	51	0
7	I	301	0	306	23	0
8	J	338	0	347	23	0
9	K	222	0	111	9	0
10	L	1119	0	1125	50	1
11	M	241	0	264	22	0
12	X	233	0	231	11	0
13	A	2667	0	2635	478	0
13	B	2230	0	2182	427	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	F	45	0	33	5	0
13	I	65	0	72	15	0
13	J	147	0	129	17	0
13	L	195	0	216	28	0
13	M	99	0	81	18	0
13	X	45	0	33	5	0
14	A	33	0	46	7	0
14	B	33	0	46	7	0
15	A	240	0	336	39	0
15	B	345	0	481	83	0
15	F	40	0	56	13	0
15	I	40	0	56	11	0
15	J	80	0	112	11	0
15	L	80	0	112	16	0
15	M	40	0	56	13	0
16	A	76	0	98	12	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1470	1

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 31.

All (1470) 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)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:808:CLA:HMA1	13:I:101:CLA:HAB	1.31	1.06
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06
13:A:828:CLA:H51	15:A:852:BCR:H312	1.33	1.05
2:B:318:PHE:HB2	13:B:821:CLA:HMA1	1.39	1.05
15:A:852:BCR:H362	13:B:802:CLA:H42	1.37	1.05
14:A:846:PQN:H172	15:B:846:BCR:H382	1.40	1.01
2:B:425:LEU:HG	13:B:837:CLA:HBB1	1.44	0.99
1:A:487:ALA:HB2	13:A:838:CLA:HED3	1.43	0.99
13:B:807:CLA:H2	13:B:807:CLA:H13	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:153:PHE:O	10:L:154:ASN:HB2	1.65	0.96
13:B:806:CLA:H2	15:I:102:BCR:HC42	1.48	0.93
13:B:831:CLA:HED1	8:J:36:LEU:N	1.83	0.93
1:A:356:LEU:HD11	13:A:830:CLA:HBB1	1.49	0.93
8:J:31:ARG:HD3	15:J:1105:BCR:H312	1.47	0.93
15:L:1005:BCR:H23C	15:L:1005:BCR:H403	1.51	0.93
13:A:823:CLA:HMA1	13:A:845:CLA:HAC2	1.48	0.92
13:A:818:CLA:O1D	13:A:818:CLA:HAA2	1.67	0.92
1:A:318:ASN:H	13:A:820:CLA:HED1	1.33	0.92
13:A:821:CLA:H2	13:A:825:CLA:HBB1	1.49	0.92
9:K:32:TYR:HA	9:K:35:GLN:H	1.35	0.91
2:B:60:VAL:HG21	13:B:826:CLA:H43	1.53	0.91
1:A:52:HIS:HB2	16:A:853:LHG:H112	1.52	0.90
13:F:1301:CLA:O1D	13:F:1301:CLA:HAA2	1.71	0.90
10:L:61:PRO:HB3	13:L:1004:CLA:HBB1	1.54	0.89
13:A:821:CLA:HMB2	13:A:825:CLA:HMA3	1.55	0.88
2:B:492:TRP:HZ3	13:B:834:CLA:HMD3	1.38	0.88
13:B:805:CLA:H71	13:B:827:CLA:H92	1.56	0.88
13:A:803:CLA:H18	13:A:842:CLA:H52	1.54	0.88
1:A:392:SER:HB3	13:A:828:CLA:HMA1	1.53	0.87
13:B:829:CLA:HAA2	13:B:829:CLA:CGD	2.04	0.87
13:A:832:CLA:H12	2:B:692:PRO:HG2	1.58	0.86
2:B:529:ILE:HG21	13:B:835:CLA:HAB	1.59	0.85
1:A:333:LYS:H	13:A:845:CLA:HBC2	1.39	0.85
2:B:136:GLN:NE2	13:B:812:CLA:O1D	2.09	0.85
10:L:33:ASN:HB3	13:L:1002:CLA:HAC1	1.57	0.85
1:A:508:THR:HG22	1:A:510:SER:H	1.41	0.85
13:L:1003:CLA:O1D	13:L:1003:CLA:HAA2	1.76	0.84
13:A:840:CLA:H11	13:B:830:CLA:HED3	1.58	0.84
1:A:76:HIS:HB3	13:A:813:CLA:HED3	1.60	0.83
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.60	0.83
13:A:842:CLA:H72	13:J:1101:CLA:H12	1.60	0.83
13:L:1002:CLA:HAA2	13:L:1002:CLA:CGD	2.08	0.83
13:A:804:CLA:O1D	13:A:804:CLA:HAA2	1.80	0.82
13:I:101:CLA:CGD	13:I:101:CLA:HAA2	2.09	0.82
13:A:803:CLA:HED1	2:B:429:SER:HB2	1.61	0.82
8:J:12:PRO:HB2	15:J:1105:BCR:H391	1.59	0.82
1:A:118:TRP:CE3	13:A:809:CLA:H2A	2.15	0.82
13:B:804:CLA:H2	13:B:804:CLA:HED2	1.59	0.82
2:B:337:LEU:HD11	13:B:827:CLA:HBB1	1.62	0.82
13:B:806:CLA:HED3	7:I:11:PRO:HB3	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:832:CLA:HAA2	13:A:832:CLA:O1D	1.79	0.81
10:L:98:LEU:O	10:L:102:GLN:NE2	2.13	0.81
13:B:821:CLA:CGD	13:B:821:CLA:HAA2	2.10	0.81
13:B:831:CLA:H122	6:F:69:LEU:HD11	1.62	0.81
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.62	0.80
13:A:814:CLA:CGD	13:A:814:CLA:HAA2	2.10	0.80
13:B:804:CLA:HMB1	13:B:804:CLA:HBB1	1.61	0.80
1:A:308:PHE:HE2	13:A:821:CLA:HAB	1.47	0.80
13:B:807:CLA:H162	13:B:825:CLA:H203	1.64	0.80
2:B:353:GLN:HG3	13:B:823:CLA:HED3	1.64	0.80
13:A:833:CLA:HMA1	15:I:102:BCR:H292	1.62	0.79
1:A:141:SER:OG	13:A:808:CLA:HED3	1.82	0.79
2:B:373:ALA:HB1	13:B:825:CLA:HMA1	1.64	0.79
13:L:1003:CLA:CGD	13:L:1003:CLA:HAA2	2.12	0.79
13:A:826:CLA:HMA2	13:A:827:CLA:HED3	1.63	0.79
2:B:181:LEU:HD11	13:B:811:CLA:H12	1.64	0.78
13:B:803:CLA:CGD	13:B:803:CLA:HAA2	2.13	0.78
1:A:35:ASP:OD2	1:A:37:THR:OG1	2.02	0.78
1:A:444:LEU:HB2	13:A:839:CLA:HBB1	1.65	0.78
2:B:181:LEU:HG	13:B:811:CLA:H43	1.63	0.78
13:B:824:CLA:HAA2	13:B:824:CLA:CGD	2.13	0.78
13:A:805:CLA:HED3	13:A:825:CLA:H12	1.65	0.78
13:A:817:CLA:HAA2	13:A:817:CLA:CGD	2.13	0.78
13:B:814:CLA:HAA2	13:B:814:CLA:CGD	2.13	0.78
13:B:830:CLA:H152	15:F:1302:BCR:H353	1.65	0.78
13:A:806:CLA:H42	13:A:830:CLA:H52	1.65	0.78
13:A:813:CLA:HBD	13:A:825:CLA:C6	2.13	0.77
13:A:815:CLA:HAA2	13:A:815:CLA:CGD	2.14	0.77
13:A:819:CLA:H8	13:A:819:CLA:HAB	1.65	0.77
13:A:837:CLA:O2D	13:A:837:CLA:HAA2	1.85	0.77
13:B:809:CLA:CGD	13:B:809:CLA:HAA2	2.14	0.77
13:B:817:CLA:CBP	13:B:821:CLA:HED2	2.12	0.77
15:L:1006:BCR:HC8	15:L:1006:BCR:H331	1.65	0.77
1:A:118:TRP:CZ3	13:A:809:CLA:H2A	2.20	0.77
13:A:813:CLA:HBD	13:A:825:CLA:H61	1.64	0.77
13:B:801:CLA:HAA2	13:B:801:CLA:CGD	2.14	0.77
1:A:549:THR:HG21	13:A:826:CLA:HAC2	1.65	0.77
2:B:282:LEU:HD12	13:B:817:CLA:HMC1	1.67	0.77
1:A:675:LEU:HD11	13:A:828:CLA:H143	1.65	0.76
13:B:822:CLA:HBB1	13:B:822:CLA:HMB1	1.66	0.76
15:A:852:BCR:H362	13:B:802:CLA:C4	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:829:CLA:HAA2	13:A:829:CLA:CGD	2.15	0.76
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.68	0.76
13:B:805:CLA:H151	13:B:826:CLA:HBB2	1.67	0.76
13:B:830:CLA:CBB	13:B:831:CLA:HMB2	2.15	0.76
13:A:832:CLA:H72	13:L:1003:CLA:H61	1.68	0.76
13:L:1004:CLA:H62	13:L:1004:CLA:HED3	1.68	0.76
13:A:826:CLA:HAA2	13:A:826:CLA:O1D	1.86	0.76
15:A:852:BCR:H381	13:B:830:CLA:HMA1	1.66	0.76
13:F:1301:CLA:HMB3	8:J:26:LEU:HD11	1.66	0.76
13:B:823:CLA:HBA1	13:B:824:CLA:HED3	1.68	0.75
13:B:826:CLA:O2D	13:B:826:CLA:HAA2	1.87	0.75
13:A:827:CLA:CGD	13:A:827:CLA:HAA2	2.15	0.75
2:B:343:CYS:HB3	13:B:822:CLA:H42	1.68	0.75
13:B:811:CLA:H202	13:B:826:CLA:HBD	1.68	0.75
13:A:810:CLA:HMB2	13:A:812:CLA:HMD1	1.67	0.75
2:B:122:TRP:HH2	15:B:843:BCR:H391	1.51	0.75
13:A:841:CLA:CGD	13:A:841:CLA:HAA2	2.16	0.74
13:B:835:CLA:CGD	13:B:835:CLA:HAA2	2.16	0.74
13:A:813:CLA:H121	15:A:849:BCR:H353	1.68	0.74
1:A:118:TRP:CZ2	13:A:807:CLA:HED3	2.23	0.74
1:A:501:THR:O	13:A:836:CLA:ND	2.20	0.74
2:B:64:LEU:HD11	15:B:843:BCR:H271	1.67	0.74
1:A:366:LEU:HD11	13:A:819:CLA:H72	1.70	0.74
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.68	0.74
4:D:123:PRO:HB2	4:D:128:LEU:HD11	1.69	0.74
13:A:838:CLA:HBB1	13:A:839:CLA:HMD3	1.69	0.74
13:J:1101:CLA:CGD	13:J:1101:CLA:HAA2	2.16	0.74
1:A:56:HIS:CE1	13:A:806:CLA:HED1	2.23	0.74
13:B:832:CLA:HAA2	13:B:832:CLA:CGD	2.17	0.74
13:B:835:CLA:O1D	13:B:835:CLA:HAA2	1.87	0.74
13:L:1002:CLA:H2	13:L:1002:CLA:H202	1.69	0.73
2:B:221:LEU:HD22	13:B:813:CLA:HBD	1.69	0.73
2:B:439:LEU:HD11	15:B:850:BCR:H342	1.70	0.73
13:A:830:CLA:CGD	13:A:830:CLA:HAA2	2.19	0.73
2:B:49:HIS:HB3	13:B:811:CLA:HED1	1.69	0.73
2:B:227:GLY:O	13:B:814:CLA:H43	1.88	0.73
13:A:855:CLA:CGD	13:A:855:CLA:HAA2	2.18	0.73
2:B:281:VAL:HG22	15:B:841:BCR:H352	1.70	0.73
2:B:414:VAL:HG11	15:B:844:BCR:H401	1.69	0.73
13:A:824:CLA:CGD	13:A:824:CLA:HAA2	2.19	0.73
15:B:849:BCR:C21	13:L:1003:CLA:HAB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TRP:HE3	16:A:853:LHG:H111	1.53	0.72
13:A:805:CLA:CGD	13:A:805:CLA:HAA2	2.19	0.72
13:B:819:CLA:CGD	13:B:819:CLA:HAA2	2.20	0.72
13:A:842:CLA:HED1	16:A:853:LHG:H102	1.71	0.72
1:A:203:GLY:HA2	13:A:820:CLA:HBC1	1.72	0.72
13:A:810:CLA:HAA2	13:A:810:CLA:CGD	2.20	0.71
1:A:453:PHE:O	13:A:834:CLA:HBB2	1.89	0.71
13:A:816:CLA:HAA2	13:A:816:CLA:CGD	2.20	0.71
13:A:818:CLA:HBD	13:A:827:CLA:HAB	1.72	0.71
13:A:833:CLA:C2B	13:A:834:CLA:HMB2	2.19	0.71
13:B:821:CLA:O2D	13:B:821:CLA:HAA2	1.90	0.71
13:B:837:CLA:CGD	13:B:837:CLA:HAA2	2.20	0.71
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.90	0.71
13:A:831:CLA:HED2	10:L:5:VAL:HG11	1.71	0.71
13:B:823:CLA:HED2	13:B:824:CLA:CAD	2.21	0.71
13:B:839:CLA:HAA2	13:B:839:CLA:CGD	2.20	0.71
13:A:845:CLA:HAA2	13:A:845:CLA:CGD	2.21	0.71
4:D:29:ILE:HD13	4:D:67:LEU:HD23	1.72	0.71
2:B:55:ILE:HD11	15:M:1203:BCR:HC7	1.72	0.71
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.71	0.71
2:B:445:VAL:HG21	13:B:831:CLA:HAC2	1.73	0.71
13:A:832:CLA:O1D	10:L:22:SER:HB3	1.91	0.70
13:A:823:CLA:HAA2	13:A:823:CLA:CGD	2.21	0.70
2:B:294:PHE:HB2	13:B:818:CLA:HED3	1.73	0.70
13:B:830:CLA:HHC	13:B:830:CLA:HBB1	1.72	0.70
13:A:822:CLA:HED3	9:K:37:ARG:N	2.07	0.70
13:J:1102:CLA:HAA2	13:J:1102:CLA:CGD	2.21	0.70
2:B:173:ARG:HB3	13:B:822:CLA:HMD1	1.72	0.70
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.72	0.70
1:A:542:HIS:ND1	13:A:837:CLA:HAB	2.06	0.70
13:B:816:CLA:HMB2	13:B:816:CLA:H62	1.72	0.70
13:B:811:CLA:CGD	13:B:811:CLA:HAA2	2.21	0.70
13:A:818:CLA:H41	13:A:835:CLA:HED3	1.72	0.70
13:B:829:CLA:CGA	6:F:130:THR:HG21	2.22	0.70
6:F:91:SER:OG	6:F:92:GLY:N	2.24	0.70
1:A:486:PHE:HB3	13:A:837:CLA:H11	1.75	0.69
1:A:204:LEU:HD11	13:A:829:CLA:H141	1.74	0.69
13:B:812:CLA:CGD	13:B:812:CLA:HAA2	2.22	0.69
13:A:819:CLA:O2A	13:A:819:CLA:H3A	1.91	0.69
13:B:823:CLA:HMA2	13:B:824:CLA:HED3	1.74	0.69
1:A:646:ILE:HG21	13:A:802:CLA:HBA2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:817:CLA:HBD	13:B:821:CLA:CED	2.19	0.69
13:B:838:CLA:HAA2	13:B:838:CLA:CGD	2.23	0.69
1:A:216:GLN:HA	1:A:220:SER:HB3	1.75	0.68
13:B:828:CLA:HMB2	13:B:829:CLA:C2D	2.24	0.68
1:A:177:TRP:HB2	13:A:811:CLA:HMC3	1.76	0.68
1:A:432:ARG:NH2	13:A:831:CLA:HED3	2.09	0.68
13:B:817:CLA:CGD	13:B:821:CLA:HED2	2.23	0.68
2:B:318:PHE:HB2	13:B:821:CLA:CMA	2.21	0.68
2:B:665:THR:HA	13:B:803:CLA:HAB	1.75	0.68
13:A:823:CLA:HMA1	13:A:845:CLA:CAC	2.23	0.68
1:A:270:PHE:CE1	13:A:844:CLA:HMD2	2.29	0.68
13:A:822:CLA:HAA2	13:A:822:CLA:CGD	2.23	0.68
13:A:825:CLA:HED2	13:A:829:CLA:H193	1.76	0.68
13:A:802:CLA:H152	15:B:847:BCR:H12C	1.75	0.68
13:B:804:CLA:O1D	13:B:804:CLA:H101	1.94	0.68
13:A:808:CLA:HAB	13:A:828:CLA:H13	1.76	0.67
13:A:803:CLA:HED1	2:B:429:SER:CB	2.25	0.67
2:B:651:VAL:HG11	13:B:807:CLA:HAC1	1.76	0.67
13:A:840:CLA:H162	13:A:841:CLA:HED1	1.76	0.67
2:B:529:ILE:HD13	13:B:835:CLA:HAB	1.77	0.67
1:A:450:PHE:HZ	13:A:838:CLA:HMC3	1.59	0.67
13:A:838:CLA:HMB2	13:A:839:CLA:C3D	2.24	0.67
2:B:354:HIS:HB3	13:B:815:CLA:HED1	1.77	0.67
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.75	0.67
2:B:427:TRP:HD1	13:B:830:CLA:HED1	1.58	0.67
10:L:145:VAL:HG11	13:L:1004:CLA:H51	1.75	0.67
13:B:831:CLA:HBA1	8:J:36:LEU:O	1.94	0.67
13:B:836:CLA:HMB2	13:B:837:CLA:C2D	2.25	0.67
13:B:837:CLA:O1D	13:B:837:CLA:HAA2	1.95	0.67
1:A:272:TRP:CD2	13:A:817:CLA:HMB2	2.30	0.66
2:B:529:ILE:HG21	13:B:835:CLA:CAB	2.25	0.66
2:B:60:VAL:HG21	13:B:826:CLA:C4	2.25	0.66
13:B:830:CLA:CBB	15:B:846:BCR:H323	2.24	0.66
2:B:339:TRP:HE1	13:B:822:CLA:CMB	2.08	0.66
3:C:6:ILE:HG13	3:C:64:ILE:HD12	1.78	0.66
13:X:102:CLA:HAA2	13:X:102:CLA:CGD	2.26	0.66
1:A:680:HIS:HB3	13:B:802:CLA:O1D	1.95	0.66
13:A:813:CLA:CGD	13:A:813:CLA:HAA2	2.25	0.66
15:B:850:BCR:H331	15:B:850:BCR:C8	2.26	0.66
13:A:831:CLA:CGD	13:A:831:CLA:HAA2	2.25	0.66
13:B:808:CLA:CMA	13:I:101:CLA:HAB	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:826:CLA:H143	15:A:851:BCR:H391	1.78	0.66
13:A:808:CLA:HED2	13:A:828:CLA:HED2	1.78	0.66
13:A:831:CLA:HMB2	13:A:832:CLA:C2D	2.26	0.66
13:B:817:CLA:HMB2	13:B:822:CLA:H71	1.78	0.66
13:B:834:CLA:HAA2	13:B:834:CLA:CGD	2.25	0.66
13:A:835:CLA:CED	13:A:836:CLA:HMA3	2.26	0.66
15:A:852:BCR:H321	15:A:852:BCR:HC8	1.76	0.66
11:M:26:SER:HB2	13:M:1201:CLA:H2	1.77	0.66
8:J:26:LEU:HD23	15:J:1104:BCR:HC7	1.77	0.65
13:A:823:CLA:CMA	13:A:845:CLA:HAC2	2.25	0.65
13:A:803:CLA:HAA2	13:A:803:CLA:CGD	2.26	0.65
1:A:489:TRP:HZ3	13:A:837:CLA:H42	1.61	0.65
10:L:34:LEU:HD12	13:L:1003:CLA:HED3	1.79	0.65
1:A:302:LEU:HD13	13:A:815:CLA:HMC1	1.79	0.65
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.79	0.65
2:B:548:ARG:NH2	4:D:124:ASN:OD1	2.30	0.65
13:A:812:CLA:C3D	13:A:813:CLA:HMC3	2.27	0.65
13:B:804:CLA:HAA2	13:B:804:CLA:CGD	2.26	0.65
13:B:812:CLA:HMB2	15:B:843:BCR:C21	2.26	0.64
13:B:829:CLA:HAB	13:B:830:CLA:H171	1.79	0.64
13:A:806:CLA:HAA2	13:A:806:CLA:CGD	2.27	0.64
13:B:812:CLA:HAB	13:B:826:CLA:H161	1.79	0.64
1:A:449:ILE:HD13	13:B:803:CLA:HBA2	1.78	0.64
13:A:832:CLA:HBC2	13:A:839:CLA:HMC2	1.80	0.64
13:A:821:CLA:HBC3	13:A:827:CLA:H18	1.78	0.64
1:A:542:HIS:CG	13:A:837:CLA:HAB	2.31	0.64
1:A:685:PHE:HA	13:A:803:CLA:HAB	1.79	0.64
1:A:372:GLN:HG3	13:A:826:CLA:HED1	1.80	0.64
2:B:309:PHE:CE1	13:B:820:CLA:H2	2.33	0.64
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.80	0.64
13:A:825:CLA:HBA1	13:A:829:CLA:H18	1.80	0.64
13:A:826:CLA:HMA2	13:A:827:CLA:CED	2.27	0.64
1:A:118:TRP:CZ2	13:A:809:CLA:HED2	2.33	0.64
2:B:267:LEU:HD22	13:B:815:CLA:HBA1	1.80	0.64
11:M:29:LEU:HD13	13:M:1201:CLA:HMA1	1.79	0.64
1:A:83:VAL:HG11	13:A:805:CLA:H71	1.80	0.64
2:B:509:SER:O	2:B:511:THR:N	2.27	0.64
13:B:805:CLA:H51	18:B:848:LMG:H331	1.79	0.64
13:B:828:CLA:HAA2	13:B:828:CLA:CGD	2.28	0.64
13:B:831:CLA:O2D	13:B:831:CLA:HAA2	1.97	0.64
13:A:802:CLA:H143	13:I:101:CLA:HBC3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:CD1	13:A:805:CLA:HMC2	2.33	0.63
13:B:827:CLA:HAA2	13:B:827:CLA:CGD	2.28	0.63
1:A:378:PRO:HG2	1:A:384:ALA:HB2	1.79	0.63
13:A:812:CLA:HAA2	13:A:812:CLA:CGD	2.27	0.63
13:A:821:CLA:HBD	13:A:824:CLA:CED	2.28	0.63
13:B:807:CLA:H121	13:B:825:CLA:H171	1.81	0.63
1:A:120:ILE:HG12	1:A:121:VAL:HG13	1.80	0.63
13:B:808:CLA:HAA2	13:B:808:CLA:O2D	1.99	0.63
1:A:194:GLU:HG2	1:A:315:TYR:HB3	1.81	0.63
1:A:352:TRP:HB3	13:A:805:CLA:HAC1	1.81	0.63
13:A:818:CLA:H52	13:A:835:CLA:HBA1	1.81	0.63
13:B:816:CLA:CGD	13:B:816:CLA:HAA2	2.29	0.63
13:B:818:CLA:HAA2	13:B:818:CLA:CGD	2.29	0.62
1:A:345:TYR:O	1:A:349:THR:HB	1.99	0.62
13:A:837:CLA:HAA1	13:A:838:CLA:HED2	1.81	0.62
2:B:261:HIS:HD2	2:B:263:GLN:H	1.47	0.62
2:B:304:MET:HG3	2:B:322:HIS:O	2.00	0.62
8:J:16:ALA:HA	13:J:1101:CLA:H8	1.80	0.62
13:A:810:CLA:HMB2	13:A:812:CLA:CMD	2.28	0.62
2:B:466:ILE:HD13	13:B:832:CLA:HHC	1.81	0.62
13:B:806:CLA:H62	15:I:102:BCR:HC41	1.82	0.62
13:A:801:CLA:O2D	13:A:801:CLA:HAA2	2.00	0.62
13:A:821:CLA:HBD	13:A:824:CLA:HED1	1.81	0.62
2:B:308:ASP:O	13:B:820:CLA:HBA2	1.99	0.62
13:B:838:CLA:H193	15:I:102:BCR:H362	1.81	0.62
1:A:302:LEU:HD11	13:A:817:CLA:HBB1	1.82	0.62
13:A:832:CLA:HMC2	13:A:838:CLA:H203	1.82	0.62
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.00	0.62
13:A:808:CLA:HMC3	13:A:809:CLA:HMD2	1.82	0.61
2:B:122:TRP:CH2	15:B:843:BCR:H391	2.35	0.61
13:B:803:CLA:O1D	13:B:803:CLA:HAA2	2.00	0.61
2:B:358:LEU:HB2	13:B:815:CLA:HED3	1.82	0.61
13:A:825:CLA:O1D	13:A:825:CLA:HAA2	1.99	0.61
13:A:843:CLA:CGD	13:A:843:CLA:HAA2	2.30	0.61
1:A:671:ALA:HB1	13:A:808:CLA:HMC1	1.82	0.61
13:B:822:CLA:H61	13:B:824:CLA:H42	1.83	0.61
1:A:487:ALA:HA	13:A:837:CLA:HED2	1.82	0.61
2:B:188:ALA:HA	13:B:813:CLA:CBB	2.30	0.61
14:B:840:PQN:H242	15:B:847:BCR:H17C	1.81	0.61
1:A:153:THR:N	1:A:157:GLN:OE1	2.33	0.61
13:A:804:CLA:HED2	13:A:811:CLA:CGD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1201:CLA:HMB2	15:M:1203:BCR:HC42	1.83	0.61
13:A:801:CLA:CGD	13:A:801:CLA:HAA2	2.30	0.61
13:B:804:CLA:H8	13:B:822:CLA:HED2	1.81	0.61
2:B:182:PHE:CZ	13:B:811:CLA:H71	2.36	0.61
2:B:725:LEU:HD11	13:B:827:CLA:H203	1.83	0.61
1:A:300:HIS:O	1:A:304:ILE:HG12	2.01	0.61
13:A:833:CLA:C1A	15:B:849:BCR:H363	2.31	0.61
13:A:823:CLA:CBB	13:A:845:CLA:HAB	2.31	0.61
13:B:813:CLA:CGD	13:B:813:CLA:HAA2	2.30	0.61
13:B:825:CLA:H3A	13:B:825:CLA:CGA	2.30	0.61
2:B:122:TRP:CE3	13:B:826:CLA:HED1	2.36	0.61
13:A:829:CLA:H61	15:A:849:BCR:H373	1.82	0.61
13:B:808:CLA:H201	7:I:26:VAL:CG2	2.31	0.61
2:B:53:LEU:HD21	13:B:811:CLA:HBA2	1.82	0.61
13:B:831:CLA:HAA2	13:B:831:CLA:CGD	2.31	0.61
13:A:825:CLA:HBB2	15:A:850:BCR:H11C	1.83	0.60
2:B:60:VAL:HG11	15:B:843:BCR:H393	1.83	0.60
3:C:41:SER:OG	4:D:113:ASN:ND2	2.30	0.60
1:A:76:HIS:HB3	13:A:813:CLA:CED	2.31	0.60
2:B:41:LEU:O	2:B:45:ILE:HG12	2.01	0.60
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.01	0.60
13:A:821:CLA:OBD	13:A:823:CLA:HMD3	2.01	0.60
1:A:490:VAL:HB	13:A:837:CLA:HED3	1.82	0.60
13:B:801:CLA:H202	13:B:802:CLA:HMA1	1.84	0.60
2:B:188:ALA:HA	13:B:813:CLA:HBB1	1.82	0.60
9:K:36:SER:O	9:K:38:GLY:N	2.27	0.60
1:A:688:MET:HB2	13:A:803:CLA:C1C	2.31	0.60
13:A:833:CLA:CGD	13:A:833:CLA:HAA2	2.30	0.60
1:A:281:PHE:HE2	13:A:818:CLA:H43	1.66	0.60
1:A:453:PHE:C	13:A:834:CLA:HBB2	2.21	0.60
1:A:681:PHE:CD2	15:A:852:BCR:H363	2.37	0.60
2:B:339:TRP:CH2	15:B:844:BCR:H372	2.36	0.60
13:B:808:CLA:HAA2	13:B:808:CLA:CGD	2.31	0.60
13:B:823:CLA:HBA1	13:B:824:CLA:CED	2.31	0.60
1:A:143:LEU:HD12	13:A:808:CLA:HED1	1.82	0.60
13:A:809:CLA:HMC3	2:B:445:VAL:HG13	1.84	0.60
13:B:817:CLA:HMB1	13:B:822:CLA:H52	1.84	0.60
13:M:1201:CLA:CGD	13:M:1201:CLA:HAA2	2.31	0.60
11:M:29:LEU:CB	13:M:1201:CLA:HBA2	2.31	0.60
1:A:435:ARG:NH1	4:D:12:GLY:O	2.34	0.60
1:A:118:TRP:HZ3	13:A:809:CLA:HBA1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:HIS:CD2	2:B:263:GLN:H	2.20	0.60
13:B:804:CLA:H112	13:B:822:CLA:O1D	2.02	0.60
1:A:427:ASN:OD1	1:A:432:ARG:NH1	2.34	0.60
13:A:840:CLA:HED2	2:B:427:TRP:HB2	1.84	0.60
2:B:210:ASN:O	2:B:212:LEU:N	2.35	0.60
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.82	0.60
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.35	0.60
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.36	0.60
15:A:852:BCR:H393	15:J:1104:BCR:H313	1.83	0.60
15:L:1006:BCR:C8	15:L:1006:BCR:H331	2.25	0.60
1:A:379:PRO:CB	13:A:819:CLA:HBA1	2.31	0.60
2:B:380:TYR:CD1	13:B:825:CLA:HAB	2.37	0.60
1:A:660:GLN:HE22	1:A:750:ARG:HD2	1.67	0.59
13:A:802:CLA:H162	13:I:101:CLA:HMC2	1.84	0.59
1:A:272:TRP:CG	13:A:817:CLA:HMB2	2.37	0.59
13:A:825:CLA:CGD	13:A:825:CLA:HAA2	2.32	0.59
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.38	0.59
13:B:810:CLA:HBC3	13:B:811:CLA:CAB	2.32	0.59
2:B:207:GLY:HA2	13:B:812:CLA:OBD	2.02	0.59
13:B:825:CLA:O1D	13:B:825:CLA:HAA2	2.01	0.59
13:A:836:CLA:HAA2	13:A:836:CLA:CGD	2.33	0.59
13:A:842:CLA:H72	13:J:1101:CLA:C1	2.32	0.59
11:M:29:LEU:HD13	13:M:1201:CLA:CMA	2.31	0.59
1:A:250:ALA:HA	1:A:258:TRP:HD1	1.65	0.59
13:A:806:CLA:HAA2	13:A:806:CLA:O2D	2.02	0.59
2:B:713:LEU:HD11	18:B:848:LMG:H342	1.82	0.59
15:B:849:BCR:H23C	15:B:849:BCR:H392	1.83	0.59
1:A:14:VAL:HG21	13:A:810:CLA:HBA1	1.84	0.59
13:A:803:CLA:HBB1	13:B:802:CLA:C4B	2.33	0.59
13:A:821:CLA:CMB	13:A:825:CLA:HMA3	2.31	0.59
1:A:432:ARG:HH21	13:A:831:CLA:HED3	1.68	0.59
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.84	0.59
2:B:693:LEU:HD21	10:L:34:LEU:HD23	1.83	0.59
13:L:1004:CLA:CGD	13:L:1004:CLA:HAA2	2.32	0.59
13:B:817:CLA:O1A	13:B:821:CLA:HBD	2.01	0.59
13:A:804:CLA:C3C	13:J:1101:CLA:HAB	2.33	0.59
16:A:853:LHG:H172	13:J:1101:CLA:HMB2	1.85	0.59
13:A:836:CLA:HBD	13:A:855:CLA:O1D	2.02	0.59
13:B:833:CLA:O1D	13:B:834:CLA:HMA3	2.03	0.59
2:B:492:TRP:CZ3	13:B:834:CLA:HMD3	2.28	0.59
13:B:826:CLA:H203	15:B:843:BCR:H362	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:847:BCR:H383	15:A:847:BCR:H23C	1.85	0.59
2:B:663:TRP:CE3	13:B:801:CLA:HMA1	2.38	0.59
13:B:833:CLA:CGD	13:B:833:CLA:HAA2	2.33	0.58
13:B:806:CLA:H111	15:I:102:BCR:HC31	1.85	0.58
1:A:52:HIS:CG	16:A:853:LHG:H131	2.38	0.58
2:B:360:PRO:CB	13:B:816:CLA:HBA1	2.33	0.58
2:B:229:TRP:CD2	13:B:814:CLA:HMB2	2.39	0.58
8:J:15:ALA:O	8:J:19:MET:HB2	2.03	0.58
1:A:460:VAL:HG12	13:A:802:CLA:H12	1.86	0.58
13:B:801:CLA:O1A	13:B:802:CLA:HMD3	2.03	0.58
13:B:818:CLA:H3A	13:B:818:CLA:O2A	2.02	0.58
13:A:808:CLA:O1D	13:A:828:CLA:HED2	2.04	0.58
13:A:803:CLA:C9	15:A:852:BCR:H19C	2.32	0.58
1:A:90:MET:SD	13:A:808:CLA:HBA1	2.44	0.58
1:A:391:LEU:O	1:A:395:THR:HG23	2.04	0.58
1:A:503:PRO:HD2	13:A:836:CLA:C3D	2.33	0.58
1:A:379:PRO:HB2	13:A:819:CLA:HBA1	1.84	0.58
2:B:293:GLN:OE1	13:B:810:CLA:HBA2	2.04	0.58
13:B:803:CLA:H122	15:I:102:BCR:H281	1.84	0.58
1:A:446:TRP:HB2	13:A:843:CLA:HED3	1.85	0.58
13:A:803:CLA:H143	13:A:842:CLA:H111	1.86	0.58
2:B:361:TYR:CE2	13:B:816:CLA:HED3	2.38	0.58
13:X:102:CLA:HAA2	13:X:102:CLA:O2D	2.03	0.58
1:A:196:MET:HB2	13:A:813:CLA:HBC2	1.84	0.58
1:A:366:LEU:HD21	13:A:819:CLA:H72	1.84	0.58
2:B:431:PHE:CZ	15:B:850:BCR:HC41	2.38	0.58
2:B:343:CYS:SG	13:B:824:CLA:H71	2.44	0.58
13:B:829:CLA:HAA2	13:B:829:CLA:O2D	2.04	0.58
15:B:842:BCR:C8	15:B:842:BCR:H321	2.33	0.58
10:L:7:PRO:HB3	10:L:12:PRO:HA	1.86	0.58
1:A:543:ALA:HB1	13:A:838:CLA:HMB3	1.84	0.58
2:B:320:MET:SD	16:X:101:LHG:HC41	2.43	0.58
1:A:429:VAL:O	1:A:433:VAL:HG13	2.04	0.58
1:A:485:VAL:HG12	13:A:838:CLA:HMD1	1.86	0.58
6:F:139:SER:O	6:F:141:ARG:NH1	2.37	0.58
15:L:1005:BCR:HC41	13:M:1201:CLA:HMD2	1.84	0.58
2:B:419:GLU:OE1	6:F:141:ARG:NH2	2.37	0.57
13:A:803:CLA:HED2	2:B:538:LEU:CD2	2.34	0.57
4:D:61:LYS:HE2	4:D:94:ILE:HD12	1.86	0.57
6:F:97:LYS:HE2	6:F:102:ASP:HB2	1.85	0.57
6:F:54:ASP:O	6:F:56:ARG:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:835:CLA:CGD	13:A:835:CLA:HAA2	2.34	0.57
2:B:497:ASN:O	2:B:498:VAL:HB	2.04	0.57
13:B:824:CLA:H13	15:B:845:BCR:H15C	1.86	0.57
13:M:1201:CLA:CBD	13:M:1201:CLA:HAA2	2.34	0.57
1:A:95:ALA:HB2	1:A:158:LEU:HB2	1.84	0.57
13:A:804:CLA:HED2	13:A:811:CLA:O1D	2.05	0.57
2:B:427:TRP:CD1	13:B:830:CLA:HED1	2.39	0.57
1:A:300:HIS:HE2	13:A:819:CLA:C1B	2.16	0.57
13:B:803:CLA:H102	15:B:847:BCR:C36	2.34	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.57
1:A:300:HIS:HB2	13:A:818:CLA:CHB	2.34	0.57
15:A:852:BCR:H311	15:A:852:BCR:C8	2.34	0.57
2:B:139:ILE:HD12	11:M:14:ILE:HD12	1.85	0.57
13:B:816:CLA:CMB	13:B:816:CLA:H62	2.33	0.57
2:B:140:PHE:CG	13:B:812:CLA:H12	2.40	0.57
2:B:337:LEU:HB2	13:B:804:CLA:HMD3	1.87	0.57
11:M:29:LEU:HB2	13:M:1201:CLA:HBA2	1.87	0.57
1:A:156:PHE:CZ	13:A:816:CLA:HBA1	2.39	0.57
1:A:70:ARG:NE	1:A:185:PRO:O	2.31	0.57
13:A:831:CLA:HAA2	13:A:831:CLA:O1D	2.04	0.57
6:F:6:VAL:O	6:F:43:CYS:N	2.30	0.57
2:B:668:MET:HB2	13:B:803:CLA:C1C	2.33	0.57
2:B:699:TRP:HE3	13:B:838:CLA:HMD3	1.69	0.57
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.86	0.57
1:A:92:PHE:CZ	13:A:807:CLA:HMD3	2.40	0.57
2:B:354:HIS:HB3	13:B:815:CLA:CED	2.35	0.57
13:B:825:CLA:H161	18:B:848:LMG:H273	1.87	0.57
13:B:811:CLA:H203	13:B:826:CLA:H2	1.87	0.57
2:B:211:PHE:CE1	15:B:843:BCR:H352	2.40	0.57
13:A:822:CLA:HED3	9:K:37:ARG:H	1.70	0.57
13:B:802:CLA:HAA2	13:B:802:CLA:CGD	2.35	0.56
10:L:89:ALA:HB1	15:L:1005:BCR:H401	1.87	0.56
13:B:838:CLA:HED3	10:L:96:TYR:HD1	1.69	0.56
13:A:829:CLA:H61	15:A:849:BCR:C37	2.33	0.56
13:A:833:CLA:CMA	15:I:102:BCR:H292	2.33	0.56
5:E:68:VAL:HG23	5:E:69:ALA:H	1.68	0.56
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.38	0.56
2:B:236:PRO:HA	2:B:252:ALA:HB3	1.86	0.56
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.87	0.56
1:A:660:GLN:HG2	1:A:753:SER:CB	2.35	0.56
2:B:150:PHE:HD2	13:B:809:CLA:CBC	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:CYS:HB3	13:B:822:CLA:C4	2.35	0.56
1:A:660:GLN:NE2	1:A:750:ARG:HD2	2.20	0.56
13:B:815:CLA:HAA2	13:B:815:CLA:O1D	2.05	0.56
7:I:20:TRP:HZ2	13:I:101:CLA:HBB	1.71	0.56
1:A:599:LEU:HD21	13:A:830:CLA:HBC1	1.88	0.56
15:A:852:BCR:H311	15:A:852:BCR:HC8	1.87	0.56
13:B:817:CLA:HAA2	13:B:817:CLA:CGD	2.36	0.56
13:A:840:CLA:HAA2	13:A:840:CLA:O2D	2.06	0.56
13:B:805:CLA:HAA2	13:B:805:CLA:CGD	2.34	0.56
12:X:20:LEU:HD21	13:X:102:CLA:HBB1	1.88	0.56
13:A:803:CLA:H91	13:A:803:CLA:C12	2.36	0.56
13:A:822:CLA:O1D	9:K:36:SER:HA	2.06	0.56
13:A:824:CLA:HHC	13:A:831:CLA:HMD2	1.87	0.56
2:B:277:LEU:HD13	13:B:813:CLA:CMC	2.35	0.56
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.87	0.56
11:M:26:SER:HB2	15:M:1203:BCR:HC31	1.88	0.56
1:A:246:PRO:HG3	13:A:815:CLA:HED1	1.87	0.56
13:A:820:CLA:CGD	13:A:820:CLA:HAA2	2.36	0.56
1:A:433:VAL:HG12	13:A:831:CLA:HMD3	1.87	0.56
2:B:274:HIS:HE1	13:B:814:CLA:C4D	2.19	0.56
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.88	0.56
13:B:808:CLA:HMA1	13:I:101:CLA:CAB	2.21	0.56
1:A:270:PHE:CD1	13:A:844:CLA:HMD2	2.41	0.56
1:A:305:ALA:O	1:A:309:ILE:HG12	2.06	0.56
13:A:803:CLA:HAA2	13:A:803:CLA:O2D	2.05	0.56
2:B:29:ASP:CG	13:B:827:CLA:HED1	2.26	0.56
13:B:830:CLA:HBC2	13:B:830:CLA:HHD	1.87	0.56
2:B:466:ILE:HB	13:B:835:CLA:CED	2.36	0.56
2:B:184:VAL:HG11	15:B:842:BCR:C34	2.36	0.56
1:A:313:HIS:CE1	15:A:847:BCR:H363	2.41	0.55
1:A:744:TRP:CD1	15:A:852:BCR:HC22	2.40	0.55
13:A:803:CLA:H92	15:A:852:BCR:H19C	1.87	0.55
3:C:62:LEU:HB3	3:C:64:ILE:O	2.06	0.55
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.88	0.55
11:M:30:TYR:O	13:M:1201:CLA:HED2	2.06	0.55
2:B:131:ASN:HB2	11:M:1:MET:O	2.06	0.55
1:A:490:VAL:HB	13:A:837:CLA:CED	2.37	0.55
2:B:173:ARG:HE	13:B:822:CLA:HMD1	1.72	0.55
13:A:843:CLA:H92	13:L:1003:CLA:HMC1	1.89	0.55
13:A:803:CLA:HBB1	13:B:802:CLA:NB	2.21	0.55
13:I:101:CLA:O1D	13:I:101:CLA:HAA2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:CZ	13:B:809:CLA:HBB1	2.42	0.55
13:A:819:CLA:H121	13:A:821:CLA:CBB	2.36	0.55
13:A:832:CLA:CGD	13:A:832:CLA:HAA2	2.36	0.55
1:A:612:HIS:ND1	13:A:837:CLA:HMC2	2.22	0.55
2:B:229:TRP:HB2	13:B:814:CLA:O2A	2.06	0.55
13:B:810:CLA:HBD	13:B:810:CLA:HAA2	1.89	0.55
2:B:360:PRO:HB2	13:B:816:CLA:HED2	1.87	0.55
8:J:4:PHE:O	8:J:8:LEU:HG	2.06	0.55
1:A:17:ASP:HB3	1:A:20:PRO:HG3	1.88	0.55
13:A:823:CLA:O2D	13:A:823:CLA:HAA2	2.06	0.55
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.06	0.55
2:B:480:LEU:C	2:B:482:SER:H	2.11	0.55
13:B:802:CLA:HAA2	13:B:802:CLA:O2D	2.07	0.55
13:B:815:CLA:C5	13:B:832:CLA:HED2	2.36	0.55
2:B:699:TRP:CE3	13:B:838:CLA:HMD3	2.42	0.55
6:F:88:VAL:HG11	6:F:97:LYS:HB3	1.89	0.55
13:B:806:CLA:C1	7:I:18:VAL:HG21	2.23	0.55
1:A:145:GLN:NE2	1:A:382:TYR:O	2.37	0.55
13:A:826:CLA:HBA2	13:A:827:CLA:HED3	1.89	0.55
13:A:832:CLA:H2	10:L:31:ILE:HG13	1.87	0.55
2:B:39:GLU:HA	2:B:164:LEU:HD13	1.89	0.55
2:B:175:ASN:HB3	13:B:818:CLA:HMD1	1.88	0.55
13:I:101:CLA:O1D	10:L:67:PRO:HG3	2.06	0.55
1:A:339:ALA:HB1	1:A:342:LYS:HD3	1.87	0.55
1:A:374:MET:HG2	13:A:819:CLA:O1A	2.07	0.55
13:B:813:CLA:O2D	13:B:813:CLA:HAA2	2.07	0.55
13:B:822:CLA:C6	13:B:824:CLA:H42	2.36	0.55
13:B:823:CLA:HED2	13:B:824:CLA:OBD	2.06	0.55
1:A:120:ILE:HD12	15:J:1105:BCR:H311	1.89	0.55
13:A:832:CLA:HBD	10:L:21:ILE:CG2	2.37	0.55
13:A:834:CLA:H52	10:L:61:PRO:HG3	1.89	0.54
13:B:830:CLA:HAA2	13:B:830:CLA:O1D	2.07	0.54
2:B:466:ILE:HD11	13:B:835:CLA:H43	1.88	0.54
5:E:26:VAL:HG13	5:E:35:PRO:HB2	1.88	0.54
8:J:5:LEU:HD23	8:J:8:LEU:HD12	1.89	0.54
13:A:826:CLA:HAA1	13:A:839:CLA:HED2	1.89	0.54
13:A:842:CLA:CED	16:A:853:LHG:H102	2.36	0.54
2:B:372:ALA:HB1	2:B:731:LEU:HD11	1.88	0.54
13:B:824:CLA:HMB3	13:B:832:CLA:O2A	2.07	0.54
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.88	0.54
6:F:73:ILE:O	6:F:77:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:833:CLA:HMA2	15:I:102:BCR:H272	1.89	0.54
11:M:29:LEU:O	11:M:30:TYR:HB2	2.06	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.41	0.54
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.89	0.54
13:A:838:CLA:HMB2	13:A:839:CLA:CAD	2.37	0.54
12:X:23:ASN:HD21	13:X:102:CLA:CHA	2.21	0.54
2:B:373:ALA:HB1	13:B:825:CLA:CMA	2.36	0.54
13:B:827:CLA:HAA2	13:B:827:CLA:O2D	2.07	0.54
1:A:375:TYR:CZ	13:A:837:CLA:HBC3	2.42	0.54
2:B:194:ILE:HA	2:B:198:ILE:HD12	1.90	0.54
2:B:277:LEU:HD13	13:B:813:CLA:HMC1	1.88	0.54
2:B:39:GLU:O	2:B:43:GLN:HG3	2.07	0.54
13:B:831:CLA:CED	8:J:36:LEU:H	1.98	0.54
13:A:813:CLA:HBC3	13:A:813:CLA:HMC1	1.90	0.54
2:B:446:VAL:HG13	2:B:451:THR:O	2.07	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.43	0.54
15:L:1006:BCR:HC8	15:L:1006:BCR:C33	2.35	0.54
1:A:356:LEU:HB2	13:A:805:CLA:HMD3	1.90	0.54
13:A:804:CLA:O1D	13:A:811:CLA:H2	2.08	0.54
13:A:826:CLA:H162	13:A:826:CLA:H112	1.88	0.54
15:B:849:BCR:C33	15:B:849:BCR:H343	2.38	0.54
2:B:236:PRO:O	2:B:250:GLY:HA3	2.08	0.53
2:B:216:PRO:HD2	13:B:813:CLA:CAD	2.38	0.53
3:C:4:VAL:HG12	3:C:64:ILE:HD11	1.88	0.53
1:A:28:TRP:CD2	13:A:811:CLA:H12	2.43	0.53
13:A:830:CLA:O1D	13:A:830:CLA:HAA2	2.08	0.53
2:B:392:HIS:CE1	13:B:827:CLA:NA	2.76	0.53
13:B:815:CLA:HAA2	13:B:815:CLA:CGD	2.39	0.53
13:B:806:CLA:HMB2	15:I:102:BCR:HC22	1.90	0.53
8:J:31:ARG:CD	15:J:1105:BCR:H312	2.30	0.53
1:A:253:TYR:O	1:A:258:TRP:NE1	2.36	0.53
2:B:614:GLN:O	2:B:618:SER:HB2	2.09	0.53
14:B:840:PQN:H291	18:B:848:LMG:H181	1.90	0.53
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.90	0.53
1:A:67:ASP:O	1:A:71:LYS:HG3	2.07	0.53
1:A:646:ILE:HG21	13:A:802:CLA:CBA	2.39	0.53
13:B:805:CLA:H51	18:B:848:LMG:C33	2.38	0.53
2:B:24:ILE:HG21	18:B:848:LMG:H182	1.90	0.53
6:F:79:TRP:HE3	15:F:1302:BCR:HC41	1.72	0.53
13:J:1102:CLA:HMC3	15:J:1105:BCR:H352	1.90	0.53
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:815:CLA:O1D	13:A:815:CLA:HAA2	2.07	0.53
13:A:819:CLA:CGD	13:A:819:CLA:HAA2	2.38	0.53
1:A:336:PHE:CD1	16:A:854:LHG:HC42	2.44	0.53
2:B:310:PHE:HE1	13:B:820:CLA:H71	1.74	0.53
2:B:622:LEU:HD13	13:B:802:CLA:HMA2	1.90	0.53
13:A:834:CLA:H101	15:B:849:BCR:H362	1.91	0.53
6:F:76:TRP:CH2	6:F:114:PHE:HB3	2.44	0.53
15:L:1005:BCR:C8	15:L:1005:BCR:H331	2.38	0.53
1:A:356:LEU:O	1:A:360:LEU:HB2	2.08	0.53
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.90	0.53
13:A:842:CLA:H101	13:J:1101:CLA:H43	1.91	0.53
2:B:351:VAL:HA	13:B:816:CLA:H42	1.90	0.53
13:B:832:CLA:HAA2	13:B:832:CLA:O1D	2.08	0.53
4:D:9:LEU:HB2	4:D:48:VAL:HB	1.90	0.53
1:A:74:SER:OG	1:A:180:TYR:HB2	2.09	0.53
13:B:822:CLA:O2D	13:B:822:CLA:HAA2	2.09	0.53
1:A:466:ARG:HB2	1:A:474:MET:SD	2.49	0.53
1:A:722:LEU:HD11	13:A:842:CLA:HMD3	1.90	0.53
13:B:806:CLA:HED3	7:I:11:PRO:CB	2.34	0.53
13:B:810:CLA:HAA2	13:B:810:CLA:CB	2.39	0.53
13:B:803:CLA:H143	15:B:847:BCR:H362	1.90	0.53
1:A:141:SER:CB	13:A:808:CLA:HED3	2.37	0.53
1:A:323:HIS:CE1	13:A:822:CLA:NA	2.77	0.53
1:A:730:VAL:HG22	13:A:842:CLA:CAD	2.38	0.53
13:A:810:CLA:O2D	13:A:810:CLA:HAA2	2.08	0.53
2:B:466:ILE:HD13	13:B:832:CLA:CHC	2.39	0.53
1:A:203:GLY:HA3	13:A:813:CLA:CBB	2.39	0.53
13:A:840:CLA:C1	13:B:830:CLA:HED3	2.33	0.53
13:B:826:CLA:H192	15:B:843:BCR:H362	1.89	0.53
13:B:824:CLA:H101	15:B:845:BCR:H17C	1.91	0.53
1:A:80:LEU:O	1:A:83:VAL:HG12	2.09	0.52
1:A:302:LEU:HD13	13:A:815:CLA:CMC	2.39	0.52
2:B:625:TRP:O	2:B:629:TYR:HB3	2.09	0.52
13:A:828:CLA:HAA2	13:A:828:CLA:CGD	2.40	0.52
13:A:832:CLA:HBC2	13:A:839:CLA:CMC	2.39	0.52
13:B:825:CLA:CGD	13:B:825:CLA:HAA2	2.40	0.52
13:B:825:CLA:H3A	13:B:825:CLA:O2A	2.09	0.52
2:B:466:ILE:HB	13:B:835:CLA:HED1	1.90	0.52
2:B:693:LEU:HB2	15:B:849:BCR:H282	1.91	0.52
15:B:849:BCR:H333	13:I:101:CLA:H41	1.91	0.52
10:L:54:HIS:HA	10:L:57:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:OD1	1:A:156:PHE:HB3	2.10	0.52
13:A:803:CLA:CGA	13:A:803:CLA:H3A	2.40	0.52
13:A:808:CLA:H201	13:A:842:CLA:H12	1.90	0.52
2:B:29:ASP:OD2	13:B:827:CLA:HED1	2.09	0.52
2:B:277:LEU:HG	13:B:814:CLA:HBB1	1.91	0.52
2:B:122:TRP:HB2	13:B:826:CLA:HED2	1.92	0.52
13:A:831:CLA:HBB2	13:A:839:CLA:HMC2	1.91	0.52
1:A:93:HIS:CE1	13:A:807:CLA:NA	2.78	0.52
13:B:816:CLA:O2A	13:B:816:CLA:H3A	2.10	0.52
13:A:832:CLA:HED2	10:L:16:HIS:NE2	2.23	0.52
15:M:1203:BCR:HC8	15:M:1203:BCR:H321	1.92	0.52
11:M:13:VAL:O	11:M:16:LEU:HB2	2.10	0.52
1:A:534:ALA:O	1:A:538:VAL:HG22	2.10	0.52
1:A:683:TRP:CE3	13:A:801:CLA:HMA1	2.44	0.52
13:A:820:CLA:HMA2	9:K:61:ALA:CB	2.40	0.52
15:B:843:BCR:H23C	15:B:843:BCR:H383	1.91	0.52
13:B:838:CLA:H142	10:L:85:LEU:HD23	1.92	0.52
1:A:587:CYS:HB2	2:B:673:TRP:HB3	1.90	0.52
13:A:832:CLA:HMA1	2:B:691:THR:OG1	2.10	0.52
2:B:669:PHE:CZ	13:B:839:CLA:HBC3	2.45	0.52
18:B:848:LMG:H202	13:M:1201:CLA:HBC1	1.91	0.52
5:E:29:THR:HB	5:E:32:VAL:HG23	1.92	0.52
1:A:332:HIS:CE1	13:A:823:CLA:C1A	2.93	0.52
2:B:184:VAL:HG11	15:B:842:BCR:H341	1.92	0.52
13:B:803:CLA:C12	15:I:102:BCR:H281	2.40	0.52
2:B:665:THR:CA	13:B:803:CLA:HAB	2.38	0.52
5:E:24:ALA:N	5:E:37:ILE:O	2.31	0.52
13:A:834:CLA:CMC	13:B:803:CLA:H91	2.40	0.52
13:B:824:CLA:H191	13:B:837:CLA:HMB2	1.93	0.52
13:A:833:CLA:O1D	13:A:833:CLA:HAA2	2.11	0.51
2:B:7:PHE:CZ	2:B:27:ALA:HA	2.45	0.51
9:K:59:LEU:C	9:K:61:ALA:H	2.13	0.51
2:B:298:HIS:ND1	13:B:820:CLA:OBD	2.42	0.51
1:A:56:HIS:ND1	13:A:806:CLA:HED1	2.24	0.51
2:B:309:PHE:C	2:B:311:GLY:H	2.13	0.51
13:A:802:CLA:H152	15:B:847:BCR:C12	2.39	0.51
10:L:129:MET:SD	15:L:1006:BCR:H24C	2.50	0.51
10:L:60:GLY:HA2	13:L:1004:CLA:HMA3	1.92	0.51
1:A:215:HIS:CE1	13:A:814:CLA:C1A	2.92	0.51
2:B:150:PHE:HD2	13:B:809:CLA:HBC3	1.76	0.51
13:B:811:CLA:H151	13:B:826:CLA:HMD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:PRO:HB3	13:B:838:CLA:C2C	2.40	0.51
13:A:834:CLA:HED2	10:L:65:LEU:O	2.10	0.51
1:A:104:LEU:HD23	1:A:148:ARG:HH11	1.75	0.51
1:A:143:LEU:HD22	1:A:147:TRP:CH2	2.45	0.51
13:A:819:CLA:CGA	13:A:819:CLA:H3A	2.39	0.51
13:A:835:CLA:O2D	13:A:836:CLA:HMA3	2.10	0.51
2:B:156:LEU:O	2:B:161:ARG:NH1	2.37	0.51
13:B:809:CLA:HBB2	13:B:811:CLA:HMA3	1.93	0.51
5:E:27:ASP:O	5:E:35:PRO:HB3	2.11	0.51
13:A:833:CLA:C3B	13:A:834:CLA:HMB2	2.41	0.51
2:B:435:HIS:HE1	13:B:830:CLA:C4D	2.24	0.51
2:B:554:PRO:HD2	3:C:61:PHE:CE1	2.46	0.51
13:A:803:CLA:HED2	2:B:538:LEU:HD23	1.91	0.51
13:A:820:CLA:HMA2	9:K:61:ALA:HB1	1.93	0.51
1:A:454:HIS:HE1	13:A:833:CLA:C4D	2.24	0.51
2:B:180:GLY:HA3	13:B:811:CLA:CBB	2.41	0.51
7:I:17:VAL:HA	7:I:21:LEU:HB3	1.91	0.51
1:A:210:LEU:HD21	15:A:847:BCR:H342	1.93	0.51
1:A:436:HIS:CE1	13:A:831:CLA:C4D	2.93	0.51
15:A:852:BCR:C23	15:A:852:BCR:H403	2.40	0.51
2:B:157:GLN:O	2:B:161:ARG:HG3	2.11	0.51
2:B:282:LEU:HD12	13:B:817:CLA:CMC	2.40	0.51
2:B:309:PHE:HB2	2:B:314:VAL:HG11	1.92	0.51
13:B:807:CLA:C5	13:B:807:CLA:H102	2.41	0.51
10:L:56:TYR:HB2	10:L:131:SER:HB2	1.93	0.51
1:A:231:VAL:HG12	1:A:235:ASP:HB3	1.93	0.51
1:A:717:ILE:HG13	6:F:98:GLU:OE1	2.11	0.51
13:A:830:CLA:H121	13:A:842:CLA:HBA1	1.93	0.51
13:B:824:CLA:H101	15:B:845:BCR:C17	2.40	0.51
15:L:1005:BCR:C23	15:L:1005:BCR:H403	2.34	0.51
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.93	0.51
1:A:118:TRP:CZ2	13:A:807:CLA:HAA2	2.46	0.51
2:B:318:PHE:CD1	13:B:820:CLA:HAB	2.45	0.51
13:A:803:CLA:HBA2	2:B:430:LEU:HD13	1.93	0.51
13:B:808:CLA:H13	18:B:848:LMG:H221	1.93	0.51
3:C:6:ILE:HG13	3:C:64:ILE:CD1	2.40	0.51
1:A:104:LEU:HD11	1:A:153:THR:HA	1.93	0.50
1:A:548:VAL:O	1:A:552:ILE:HD13	2.11	0.50
4:D:101:PHE:HB2	4:D:104:LYS:HE3	1.94	0.50
6:F:80:VAL:HG22	6:F:109:CYS:O	2.11	0.50
1:A:660:GLN:HG2	1:A:753:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PHE:CE2	13:A:821:CLA:HAB	2.36	0.50
13:A:825:CLA:HAB	15:A:850:BCR:C34	2.41	0.50
2:B:123:TRP:HB3	2:B:128:MET:HB2	1.93	0.50
2:B:463:ALA:HB2	13:B:836:CLA:HED3	1.93	0.50
15:F:1302:BCR:C33	15:F:1302:BCR:H342	2.41	0.50
1:A:197:LEU:HG	13:A:825:CLA:HMD3	1.93	0.50
1:A:237:PRO:HB3	1:A:248:LEU:HD21	1.93	0.50
1:A:691:PHE:HB2	13:A:803:CLA:HBC2	1.93	0.50
13:A:807:CLA:HAA1	13:A:807:CLA:HBD	1.94	0.50
2:B:651:VAL:HG13	13:B:808:CLA:HAC1	1.93	0.50
4:D:120:GLY:HA3	5:E:13:GLU:CD	2.32	0.50
2:B:231:VAL:O	2:B:234:GLN:HG2	2.11	0.50
4:D:24:GLU:O	4:D:87:PRO:HD3	2.12	0.50
8:J:33:TYR:N	8:J:34:PRO:HD3	2.26	0.50
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.94	0.50
13:A:813:CLA:O1D	13:A:825:CLA:H62	2.12	0.50
2:B:713:LEU:CD1	18:B:848:LMG:H342	2.42	0.50
4:D:34:PRO:O	4:D:51:GLU:HG3	2.12	0.50
10:L:67:PRO:HG2	10:L:68:LEU:HD23	1.94	0.50
1:A:191:GLN:HG2	13:A:825:CLA:H201	1.94	0.50
1:A:472:GLN:N	1:A:472:GLN:OE1	2.38	0.50
13:A:839:CLA:CGD	13:A:839:CLA:HAA2	2.42	0.50
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.47	0.50
1:A:118:TRP:HE3	13:A:809:CLA:H2A	1.70	0.50
13:A:802:CLA:HED1	2:B:660:HIS:CD2	2.46	0.50
2:B:693:LEU:CB	15:B:849:BCR:H282	2.42	0.50
13:A:840:CLA:H43	13:B:830:CLA:O1D	2.11	0.50
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.94	0.50
1:A:737:LEU:HD22	13:A:842:CLA:HMA1	1.94	0.50
13:B:806:CLA:CGD	13:B:806:CLA:CAA	2.89	0.50
2:B:360:PRO:HG3	13:B:816:CLA:HBA1	1.94	0.50
1:A:207:LEU:HD22	15:A:848:BCR:H361	1.93	0.50
1:A:161:THR:HG22	15:A:848:BCR:HC32	1.94	0.50
2:B:468:ALA:HA	2:B:472:LYS:O	2.12	0.50
6:F:73:ILE:O	6:F:76:TRP:HB3	2.12	0.50
1:A:377:MET:HE2	13:A:827:CLA:HMC2	1.94	0.49
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.10	0.49
2:B:210:ASN:C	2:B:212:LEU:H	2.15	0.49
2:B:288:HIS:CE1	15:B:841:BCR:H363	2.47	0.49
2:B:155:HIS:HE1	13:B:809:CLA:C1A	2.25	0.49
13:B:828:CLA:O1D	13:B:828:CLA:HAA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:101:CLA:H42	10:L:81:SER:HA	1.94	0.49
13:A:826:CLA:HAA1	13:A:839:CLA:CED	2.42	0.49
2:B:339:TRP:HE1	13:B:822:CLA:C2B	2.25	0.49
2:B:718:HIS:HE1	13:B:839:CLA:C4D	2.25	0.49
13:B:838:CLA:H2	13:B:839:CLA:H142	1.94	0.49
15:B:843:BCR:H331	15:B:843:BCR:C8	2.41	0.49
13:A:813:CLA:HAA1	13:A:825:CLA:C4	2.42	0.49
2:B:194:ILE:HG12	2:B:253:ILE:HB	1.95	0.49
6:F:53:VAL:O	15:F:1302:BCR:H291	2.11	0.49
1:A:364:GLY:O	1:A:368:ILE:HD12	2.13	0.49
2:B:367:ASP:CG	2:B:370:THR:HG23	2.32	0.49
2:B:634:SER:O	2:B:638:ILE:HB	2.11	0.49
2:B:52:HIS:CE1	13:B:804:CLA:HMA2	2.48	0.49
4:D:67:LEU:HD12	4:D:71:GLN:HG3	1.93	0.49
10:L:38:ARG:HE	13:L:1002:CLA:HAC2	1.76	0.49
13:A:819:CLA:HBA2	13:A:819:CLA:HMA2	1.94	0.49
2:B:275:HIS:HB2	13:B:815:CLA:CHB	2.42	0.49
13:B:838:CLA:C19	15:I:102:BCR:H362	2.42	0.49
13:M:1201:CLA:HBD	13:M:1201:CLA:HAA2	1.94	0.49
1:A:233:ALA:O	1:A:235:ASP:N	2.43	0.49
13:A:805:CLA:O1A	13:A:813:CLA:HED2	2.12	0.49
13:A:826:CLA:HBA1	13:A:827:CLA:CGD	2.42	0.49
15:A:852:BCR:C8	15:A:852:BCR:H321	2.43	0.49
2:B:651:VAL:HG13	13:B:808:CLA:HHD	1.94	0.49
15:B:841:BCR:H383	15:B:841:BCR:H23C	1.95	0.49
13:B:807:CLA:O1D	13:B:825:CLA:HED2	2.13	0.49
1:A:215:HIS:CE1	13:A:814:CLA:NA	2.79	0.49
1:A:292:LEU:HD22	13:A:818:CLA:HBA1	1.95	0.49
1:A:215:HIS:HE1	13:A:814:CLA:C1A	2.25	0.49
13:A:820:CLA:O1D	13:A:820:CLA:HAA2	2.12	0.49
13:A:834:CLA:H3A	13:A:834:CLA:HBA2	1.56	0.49
13:A:840:CLA:H11	13:B:830:CLA:CED	2.37	0.49
2:B:291:ARG:HB2	2:B:297:GLY:O	2.12	0.49
1:A:601:TRP:CH2	13:A:802:CLA:HAB	2.48	0.49
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.48	0.49
2:B:529:ILE:CG2	13:B:835:CLA:HAB	2.38	0.49
13:I:101:CLA:H143	10:L:87:LEU:HD11	1.95	0.49
11:M:16:LEU:HD21	15:M:1203:BCR:H19C	1.95	0.49
1:A:220:SER:O	1:A:224:ASN:HB2	2.13	0.49
1:A:24:SER:O	13:A:811:CLA:HMA1	2.13	0.49
13:A:808:CLA:HED2	13:A:828:CLA:CED	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:828:CLA:HBB1	13:A:828:CLA:HMB1	1.95	0.49
13:A:842:CLA:H112	13:A:842:CLA:H91	1.62	0.49
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.48	0.49
1:A:28:TRP:CZ3	13:A:811:CLA:H43	2.47	0.48
1:A:332:HIS:CE1	13:A:823:CLA:NA	2.81	0.48
13:B:804:CLA:HED3	13:B:804:CLA:C10	2.43	0.48
13:B:838:CLA:H143	10:L:88:VAL:HG11	1.95	0.48
1:A:273:ALA:O	1:A:276:SER:OG	2.24	0.48
13:A:801:CLA:HAB	13:B:801:CLA:NA	2.28	0.48
13:A:822:CLA:HAA2	13:A:822:CLA:O2D	2.13	0.48
13:B:811:CLA:H143	13:B:811:CLA:H112	1.66	0.48
1:A:473:ASP:HA	10:L:69:ARG:HH22	1.77	0.48
1:A:370:VAL:CG1	13:A:829:CLA:HMD3	2.43	0.48
13:A:812:CLA:C4D	13:A:813:CLA:HMC3	2.44	0.48
2:B:154:LEU:O	2:B:160:PHE:HB2	2.13	0.48
13:B:806:CLA:CGD	13:B:806:CLA:HAA2	2.43	0.48
13:B:830:CLA:HBB1	13:B:831:CLA:HMB2	1.92	0.48
13:A:843:CLA:HBC1	14:B:840:PQN:H192	1.95	0.48
1:A:146:LEU:HA	1:A:380:TYR:CD2	2.47	0.48
1:A:377:MET:SD	13:A:827:CLA:HMC2	2.53	0.48
1:A:725:ILE:HG22	16:A:853:LHG:HC41	1.94	0.48
2:B:361:TYR:O	2:B:364:ILE:HG22	2.13	0.48
2:B:116:TYR:HB2	13:B:825:CLA:O1A	2.13	0.48
2:B:339:TRP:HZ3	15:B:845:BCR:H401	1.77	0.48
3:C:51:LYS:HD3	3:C:54:GLU:OE1	2.13	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.13	0.48
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.96	0.48
1:A:82:VAL:HG12	13:A:809:CLA:H193	1.96	0.48
2:B:491:ALA:HB3	2:B:495:TYR:HA	1.95	0.48
13:B:828:CLA:HBA2	13:B:828:CLA:HMA2	1.94	0.48
5:E:2:GLN:HG2	5:E:5:SER:OG	2.13	0.48
1:A:266:PRO:HB2	1:A:275:TYR:CZ	2.48	0.48
13:A:813:CLA:HBD	13:A:825:CLA:H62	1.92	0.48
1:A:395:THR:OG1	13:A:828:CLA:HBB1	2.14	0.48
2:B:339:TRP:CZ3	15:B:845:BCR:H401	2.48	0.48
2:B:498:VAL:O	2:B:501:PRO:HD2	2.13	0.48
13:B:804:CLA:HAA2	13:B:804:CLA:O1D	2.14	0.48
13:B:825:CLA:HBC3	18:B:848:LMG:H421	1.95	0.48
11:M:10:VAL:O	11:M:14:ILE:HG13	2.14	0.48
1:A:509:ALA:HA	13:A:818:CLA:H11	1.95	0.48
2:B:166:TRP:CZ3	13:B:811:CLA:HMD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:92:CYS:HB3	15:L:1005:BCR:C21	2.44	0.48
1:A:15:VAL:HG12	1:A:186:LYS:HD3	1.95	0.48
2:B:76:TRP:HZ3	2:B:124:TYR:HB2	1.78	0.48
1:A:678:GLY:HA2	13:B:802:CLA:H41	1.95	0.48
13:B:836:CLA:C9	15:F:1302:BCR:H20C	2.44	0.48
12:X:25:LEU:O	12:X:29:TYR:HD1	1.96	0.48
1:A:511:VAL:HB	1:A:526:MET:HG3	1.96	0.48
13:B:838:CLA:H151	13:B:839:CLA:H13	1.95	0.48
2:B:14:ASP:HB3	2:B:19:ARG:HB2	1.96	0.48
13:B:806:CLA:HED2	7:I:15:ILE:CD1	2.43	0.48
7:I:27:MET:HB3	15:L:1005:BCR:H352	1.96	0.48
12:X:18:LEU:O	12:X:21:ALA:HB3	2.14	0.48
1:A:714:ALA:O	6:F:89:ARG:NH2	2.42	0.47
13:A:802:CLA:H152	15:B:847:BCR:C10	2.44	0.47
13:A:813:CLA:H61	13:A:813:CLA:H102	1.68	0.47
13:A:813:CLA:HAA1	13:A:825:CLA:H41	1.96	0.47
15:A:850:BCR:C8	15:A:850:BCR:H331	2.43	0.47
2:B:68:ALA:HB2	2:B:134:LEU:HB2	1.96	0.47
2:B:317:PRO:HB2	13:B:821:CLA:HMA3	1.97	0.47
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.63	0.47
13:A:842:CLA:H161	13:J:1101:CLA:H203	1.95	0.47
1:A:120:ILE:O	1:A:123:GLN:HG2	2.14	0.47
1:A:143:LEU:CD1	13:A:808:CLA:HED1	2.44	0.47
2:B:339:TRP:HH2	13:B:821:CLA:HBC2	1.79	0.47
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.94	0.47
13:B:817:CLA:CMB	13:B:822:CLA:H71	2.44	0.47
6:F:79:TRP:CZ3	15:F:1302:BCR:H332	2.49	0.47
13:A:832:CLA:HBD	10:L:21:ILE:HG21	1.96	0.47
1:A:346:GLU:N	1:A:346:GLU:OE1	2.42	0.47
2:B:358:LEU:CB	13:B:815:CLA:HED3	2.44	0.47
13:B:807:CLA:HAB	13:B:808:CLA:HAA1	1.95	0.47
2:B:220:GLY:HA3	13:B:813:CLA:HMD1	1.97	0.47
4:D:117:ARG:HG2	4:D:118:SER:N	2.29	0.47
6:F:22:VAL:O	6:F:34:ARG:NH2	2.29	0.47
1:A:118:TRP:CH2	13:A:807:CLA:HAA2	2.50	0.47
15:A:852:BCR:HC7	15:A:852:BCR:H331	1.67	0.47
1:A:31:PRO:HB2	1:A:47:TRP:HH2	1.80	0.47
2:B:463:ALA:HA	13:B:835:CLA:HED3	1.96	0.47
2:B:717:ALA:HA	18:B:848:LMG:H371	1.95	0.47
13:B:801:CLA:H2	13:B:802:CLA:C2D	2.45	0.47
1:A:290:GLY:HA3	1:A:520:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:805:CLA:HBB1	13:A:805:CLA:HMB1	1.96	0.47
2:B:481:LEU:HD11	13:B:832:CLA:CAD	2.45	0.47
13:B:821:CLA:CED	13:B:821:CLA:HAA2	2.44	0.47
13:B:827:CLA:HBD	18:B:848:LMG:H302	1.97	0.47
13:B:836:CLA:H203	6:F:67:SER:OG	2.14	0.47
5:E:6:LYS:HA	5:E:21:GLY:O	2.14	0.47
7:I:3:GLY:HA3	7:I:5:TYR:CE2	2.49	0.47
8:J:20:THR:HG23	15:J:1105:BCR:H351	1.97	0.47
1:A:396:HIS:HE1	13:A:828:CLA:ND	2.08	0.47
13:A:826:CLA:OBD	13:A:837:CLA:HBB1	2.15	0.47
13:A:838:CLA:H3A	13:A:838:CLA:HBA2	1.56	0.47
13:A:843:CLA:CAA	13:A:843:CLA:CGD	2.93	0.47
13:B:807:CLA:CMC	15:B:847:BCR:HC32	2.44	0.47
6:F:54:ASP:C	6:F:56:ARG:H	2.18	0.47
13:A:807:CLA:CBD	13:A:807:CLA:HAA1	2.44	0.47
2:B:178:LEU:O	2:B:283:PHE:HB3	2.15	0.47
13:B:807:CLA:HMC2	15:B:847:BCR:HC32	1.97	0.47
10:L:29:THR:O	10:L:33:ASN:ND2	2.44	0.47
1:A:35:ASP:HB3	1:A:38:LEU:HD12	1.97	0.47
13:A:811:CLA:H3A	13:A:811:CLA:HBA2	1.55	0.47
1:A:94:GLY:O	1:A:98:SER:OG	2.16	0.47
2:B:702:LYS:HZ1	4:D:24:GLU:CD	2.17	0.47
13:B:817:CLA:OBD	13:B:820:CLA:HMD3	2.15	0.47
2:B:466:ILE:HG21	13:B:835:CLA:HED1	1.97	0.47
6:F:84:TYR:CZ	6:F:101:ILE:HG23	2.50	0.47
11:M:26:SER:CB	13:M:1201:CLA:H2	2.45	0.47
1:A:203:GLY:O	1:A:207:LEU:HB2	2.14	0.47
1:A:86:TRP:HA	13:A:807:CLA:HBB2	1.96	0.47
1:A:33:HIS:NE2	13:A:811:CLA:HED2	2.30	0.47
2:B:531:LEU:HD21	13:B:802:CLA:CBB	2.45	0.47
13:B:805:CLA:HMA1	13:B:827:CLA:HAB	1.96	0.47
13:A:832:CLA:H61	13:L:1003:CLA:H72	1.97	0.47
1:A:449:ILE:HD11	15:B:847:BCR:H403	1.97	0.47
13:A:802:CLA:H142	13:A:802:CLA:H111	1.57	0.47
13:A:827:CLA:H2	13:A:827:CLA:H61	1.66	0.47
15:A:852:BCR:H23C	15:A:852:BCR:H403	1.97	0.47
2:B:221:LEU:O	2:B:225:PHE:HD1	1.98	0.47
2:B:25:ALA:HB2	18:B:848:LMG:H121	1.97	0.47
2:B:466:ILE:CG2	13:B:835:CLA:HED1	2.45	0.47
2:B:595:TRP:CZ2	13:B:801:CLA:H172	2.50	0.47
13:B:804:CLA:CBB	13:B:804:CLA:HMB1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:24:GLY:HA3	13:J:1102:CLA:HBB1	1.96	0.47
11:M:14:ILE:O	11:M:18:PRO:HD2	2.15	0.47
13:A:828:CLA:HMB1	13:A:828:CLA:CBB	2.45	0.46
2:B:166:TRP:CZ2	13:B:809:CLA:HMA1	2.50	0.46
2:B:261:HIS:HD2	2:B:263:GLN:N	2.13	0.46
2:B:520:PRO:O	2:B:523:PHE:HB3	2.15	0.46
13:B:814:CLA:O2D	13:B:814:CLA:HAA2	2.15	0.46
13:B:816:CLA:H122	13:B:824:CLA:O1A	2.14	0.46
6:F:84:TYR:O	6:F:88:VAL:HG23	2.15	0.46
1:A:679:ALA:HB1	1:A:738:GLY:O	2.15	0.46
13:A:806:CLA:H42	13:A:830:CLA:C5	2.39	0.46
13:A:808:CLA:O1D	13:A:828:CLA:HAA2	2.16	0.46
13:A:832:CLA:H102	13:L:1003:CLA:H122	1.96	0.46
2:B:188:ALA:CB	13:B:826:CLA:H202	2.45	0.46
13:B:806:CLA:H3A	13:B:806:CLA:HBA2	1.74	0.46
13:B:816:CLA:CGA	13:B:816:CLA:H3A	2.45	0.46
13:B:826:CLA:CGD	13:B:826:CLA:HAA2	2.45	0.46
13:B:833:CLA:O2D	13:B:833:CLA:HAA2	2.15	0.46
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.38	0.46
13:B:830:CLA:HBC1	6:F:67:SER:OG	2.15	0.46
9:K:32:TYR:HA	9:K:35:GLN:N	2.16	0.46
13:A:832:CLA:H61	13:L:1003:CLA:H101	1.97	0.46
1:A:297:THR:O	1:A:300:HIS:HB3	2.15	0.46
1:A:603:TYR:OH	13:A:801:CLA:HED1	2.15	0.46
1:A:28:TRP:CE3	13:A:811:CLA:H43	2.50	0.46
2:B:422:ILE:HG23	2:B:538:LEU:HD11	1.97	0.46
2:B:49:HIS:HB3	13:B:811:CLA:CED	2.40	0.46
13:A:833:CLA:H171	13:B:838:CLA:HMB2	1.96	0.46
13:A:833:CLA:H51	15:B:847:BCR:C20	2.46	0.46
1:A:314:MET:HE3	13:A:823:CLA:CMD	2.46	0.46
2:B:441:VAL:O	2:B:445:VAL:HG23	2.15	0.46
2:B:724:ILE:HD13	13:B:825:CLA:HMC2	1.98	0.46
1:A:101:GLU:HG3	1:A:155:GLU:HG2	1.97	0.46
1:A:296:ASP:HB3	13:A:818:CLA:HMA1	1.98	0.46
1:A:744:TRP:HD1	13:A:828:CLA:HMB2	1.80	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.98	0.46
2:B:358:LEU:HB2	13:B:815:CLA:CED	2.45	0.46
4:D:117:ARG:HG2	4:D:118:SER:O	2.15	0.46
6:F:88:VAL:CG1	6:F:94:ALA:HA	2.43	0.46
10:L:34:LEU:HG	13:L:1003:CLA:O1D	2.16	0.46
11:M:19:ALA:HB2	15:M:1203:BCR:C13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:CYS:SG	13:A:816:CLA:HBA2	2.56	0.46
2:B:337:LEU:HD13	13:B:804:CLA:C3D	2.46	0.46
13:B:806:CLA:H121	15:M:1203:BCR:H12C	1.97	0.46
13:B:815:CLA:H72	13:B:832:CLA:O1A	2.15	0.46
2:B:435:HIS:CE1	13:B:830:CLA:C4D	2.99	0.46
1:A:231:VAL:O	1:A:232:ALA:HB3	2.16	0.46
1:A:497:ALA:O	1:A:502:ALA:HB3	2.15	0.46
1:A:660:GLN:NE2	1:A:754:VAL:HG13	2.29	0.46
13:A:803:CLA:HBD	2:B:535:THR:CG2	2.46	0.46
13:A:828:CLA:H8	15:A:852:BCR:H343	1.98	0.46
13:A:833:CLA:CBB	13:A:834:CLA:H2	2.46	0.46
2:B:304:MET:HG3	2:B:322:HIS:HB3	1.97	0.46
13:B:824:CLA:H142	13:B:824:CLA:H111	1.63	0.46
13:B:826:CLA:H51	15:B:842:BCR:H23C	1.97	0.46
13:B:828:CLA:HMB2	13:B:829:CLA:C3D	2.46	0.46
13:B:836:CLA:H93	13:B:837:CLA:HBC1	1.97	0.46
13:B:825:CLA:H111	18:B:848:LMG:H442	1.97	0.46
15:F:1302:BCR:H311	15:F:1302:BCR:C8	2.46	0.46
11:M:13:VAL:HG23	15:M:1203:BCR:H402	1.98	0.46
13:B:827:CLA:C14	18:B:848:LMG:H231	2.46	0.46
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.98	0.46
10:L:16:HIS:CD2	10:L:17:LEU:H	2.34	0.46
11:M:18:PRO:HB2	15:M:1203:BCR:H352	1.97	0.46
1:A:626:ALA:C	1:A:628:ASP:H	2.19	0.46
1:A:454:HIS:CE1	13:A:833:CLA:C4D	2.98	0.46
2:B:697:VAL:HA	10:L:96:TYR:OH	2.16	0.46
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.56	0.46
1:A:503:PRO:HG2	13:A:836:CLA:CMD	2.46	0.46
1:A:547:HIS:CE1	13:A:839:CLA:C1A	2.99	0.46
13:B:823:CLA:H3A	13:B:823:CLA:HBA2	1.66	0.46
2:B:466:ILE:CB	13:B:835:CLA:HED1	2.46	0.46
15:B:846:BCR:C8	15:B:846:BCR:H331	2.45	0.46
14:A:846:PQN:C17	15:B:846:BCR:H382	2.28	0.46
3:C:57:CYS:HB3	3:C:62:LEU:CD2	2.46	0.46
1:A:118:TRP:CE2	13:A:809:CLA:HED2	2.50	0.45
1:A:356:LEU:HD13	13:A:805:CLA:C3D	2.45	0.45
1:A:409:ALA:HA	15:A:851:BCR:HC41	1.98	0.45
1:A:444:LEU:HG	1:A:551:LEU:HB2	1.98	0.45
1:A:303:ALA:HB1	13:A:817:CLA:HBC2	1.98	0.45
1:A:207:LEU:HD21	13:A:820:CLA:HMC1	1.98	0.45
2:B:122:TRP:CZ2	15:B:843:BCR:H401	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:PHE:O	2:B:311:GLY:N	2.49	0.45
2:B:531:LEU:HD21	13:B:802:CLA:HBB1	1.98	0.45
6:F:8:CYS:HB3	6:F:14:PHE:CD2	2.51	0.45
2:B:207:GLY:H	2:B:210:ASN:ND2	2.13	0.45
2:B:229:TRP:CE3	13:B:814:CLA:HMB2	2.51	0.45
13:B:815:CLA:H112	13:B:815:CLA:H91	1.72	0.45
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.51	0.45
1:A:464:THR:HG22	1:A:468:PHE:CE1	2.52	0.45
1:A:579:ASP:OD1	3:C:52:ARG:NH2	2.48	0.45
13:A:808:CLA:H142	13:A:808:CLA:H111	1.77	0.45
13:A:820:CLA:H111	13:A:820:CLA:H142	1.53	0.45
13:A:833:CLA:HBC3	13:A:838:CLA:HMC1	1.98	0.45
2:B:111:PRO:HG2	7:I:1:MET:CE	2.46	0.45
13:A:801:CLA:NA	13:B:801:CLA:HAB	2.31	0.45
1:A:685:PHE:CA	13:A:803:CLA:HAB	2.43	0.45
13:A:830:CLA:H161	13:A:830:CLA:H121	1.86	0.45
1:A:454:HIS:HE1	13:A:833:CLA:C1A	2.30	0.45
13:A:840:CLA:H11	13:B:830:CLA:O1D	2.17	0.45
13:A:841:CLA:HAB	14:A:846:PQN:H202	1.98	0.45
2:B:284:ILE:O	2:B:288:HIS:ND1	2.42	0.45
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.97	0.45
13:A:830:CLA:HBD	16:A:853:LHG:H262	1.98	0.45
13:B:807:CLA:H102	13:B:807:CLA:H51	1.98	0.45
13:B:824:CLA:H143	15:B:844:BCR:C19	2.47	0.45
6:F:37:ARG:O	6:F:40:GLN:HG2	2.17	0.45
13:A:804:CLA:HAA1	13:A:811:CLA:H51	1.98	0.45
13:A:840:CLA:H202	13:A:841:CLA:HED1	1.98	0.45
2:B:170:ALA:O	13:B:822:CLA:HMD3	2.16	0.45
2:B:236:PRO:HB2	2:B:237:ASP:H	1.53	0.45
2:B:466:ILE:HD11	13:B:832:CLA:HMC3	1.98	0.45
2:B:702:LYS:HA	2:B:703:PRO:HD3	1.84	0.45
2:B:724:ILE:HG23	13:B:825:CLA:CBB	2.46	0.45
2:B:173:ARG:HG2	13:B:822:CLA:OBD	2.16	0.45
11:M:26:SER:CB	15:M:1203:BCR:HC41	2.47	0.45
13:A:820:CLA:H62	13:A:820:CLA:H102	1.79	0.45
14:A:846:PQN:H172	15:B:846:BCR:C38	2.30	0.45
2:B:350:LEU:HD23	13:B:816:CLA:H61	1.99	0.45
15:B:846:BCR:H383	15:B:846:BCR:H23C	1.99	0.45
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.98	0.45
1:A:436:HIS:CD2	13:A:831:CLA:NA	2.85	0.45
1:A:517:VAL:HG13	1:A:527:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TRP:CD1	13:A:812:CLA:HED3	2.52	0.45
14:A:846:PQN:H141	14:A:846:PQN:H161	1.75	0.45
2:B:143:ILE:HG23	2:B:143:ILE:HD12	1.76	0.45
2:B:176:HIS:CE1	13:B:810:CLA:NA	2.84	0.45
13:B:804:CLA:HED3	13:B:804:CLA:H102	1.99	0.45
3:C:62:LEU:H	3:C:62:LEU:HG	1.54	0.45
15:F:1302:BCR:H351	15:F:1302:BCR:H15C	1.85	0.45
6:F:8:CYS:HB2	6:F:39:SER:HA	1.99	0.45
13:A:842:CLA:H202	13:J:1101:CLA:H203	1.99	0.45
13:X:102:CLA:HMA2	13:X:102:CLA:HBA2	1.97	0.45
1:A:174:PHE:HD2	13:A:810:CLA:CBC	2.29	0.45
13:A:818:CLA:H91	13:A:836:CLA:O1A	2.17	0.45
13:A:834:CLA:H112	13:A:834:CLA:H91	1.57	0.45
2:B:207:GLY:H	2:B:210:ASN:HD21	1.65	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.32	0.45
13:B:811:CLA:CGA	13:B:811:CLA:H3A	2.47	0.45
2:B:438:GLY:HA3	13:B:831:CLA:CBB	2.47	0.45
13:A:834:CLA:H151	15:B:849:BCR:H372	1.99	0.45
6:F:54:ASP:OD1	12:X:30:TYR:CE2	2.69	0.45
1:A:278:PHE:CZ	13:A:815:CLA:HMD3	2.52	0.45
1:A:717:ILE:HD11	6:F:99:ILE:HG23	1.99	0.45
1:A:304:ILE:HD12	13:A:819:CLA:HBB1	1.99	0.45
13:A:826:CLA:HAA2	13:A:826:CLA:CGD	2.47	0.45
2:B:208:TRP:NE1	13:B:812:CLA:O1D	2.50	0.45
13:A:801:CLA:CHB	13:B:801:CLA:HMB2	2.47	0.45
13:B:808:CLA:H201	7:I:26:VAL:HG21	1.99	0.45
13:B:809:CLA:HAA2	13:B:809:CLA:O1D	2.17	0.45
13:B:834:CLA:HBA1	13:B:834:CLA:HMA2	1.98	0.45
13:B:836:CLA:H71	13:B:836:CLA:C4	2.47	0.45
13:B:838:CLA:HAB	14:B:840:PQN:H172	1.99	0.45
4:D:38:VAL:HG22	4:D:48:VAL:HG22	1.98	0.45
6:F:15:GLN:O	6:F:18:ALA:HB3	2.17	0.45
1:A:269:THR:O	1:A:270:PHE:HB2	2.16	0.44
1:A:649:TRP:O	1:A:653:PHE:HB3	2.17	0.44
13:A:801:CLA:H62	13:A:801:CLA:H102	1.79	0.44
13:A:804:CLA:H91	13:A:804:CLA:H112	1.77	0.44
13:A:809:CLA:H91	13:A:809:CLA:H111	1.63	0.44
15:A:847:BCR:HC8	15:A:848:BCR:H383	1.99	0.44
13:B:801:CLA:HAA2	13:B:801:CLA:O1D	2.15	0.44
13:B:820:CLA:CAA	13:B:820:CLA:CGD	2.95	0.44
13:A:840:CLA:H61	13:B:830:CLA:H42	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:TRP:HB2	13:B:835:CLA:HMC1	1.99	0.44
13:B:812:CLA:H8	15:B:843:BCR:H363	1.99	0.44
13:B:838:CLA:HED2	7:I:31:PHE:CZ	2.52	0.44
13:M:1201:CLA:C3B	15:M:1203:BCR:H312	2.47	0.44
1:A:219:VAL:HG13	1:A:239:PRO:HB3	1.99	0.44
1:A:487:ALA:O	1:A:491:GLN:HG3	2.17	0.44
1:A:451:LEU:HD13	1:A:544:PHE:HA	1.98	0.44
1:A:588:GLN:HA	1:A:593:ASP:CG	2.38	0.44
1:A:748:LEU:O	1:A:752:ILE:HB	2.17	0.44
2:B:481:LEU:HA	2:B:489:SER:OG	2.17	0.44
13:B:808:CLA:H151	13:B:808:CLA:H111	1.77	0.44
13:L:1003:CLA:H112	13:L:1003:CLA:H91	1.59	0.44
10:L:93:LEU:HD21	15:L:1005:BCR:H383	1.99	0.44
1:A:104:LEU:HD23	1:A:148:ARG:NH1	2.33	0.44
13:A:804:CLA:CGD	13:A:804:CLA:HAA2	2.46	0.44
1:A:118:TRP:HH2	13:A:807:CLA:CGA	2.30	0.44
13:A:826:CLA:HMB2	13:A:839:CLA:O1A	2.18	0.44
13:A:830:CLA:H143	16:A:853:LHG:H351	1.98	0.44
13:A:806:CLA:HMA1	13:A:830:CLA:HAB	1.99	0.44
1:A:168:MET:HG3	15:A:848:BCR:H322	1.99	0.44
2:B:230:GLY:HA2	13:B:814:CLA:CBA	2.48	0.44
13:B:816:CLA:H111	13:B:816:CLA:H143	1.77	0.44
6:F:76:TRP:CZ2	13:F:1301:CLA:HED3	2.53	0.44
13:L:1004:CLA:H91	13:L:1004:CLA:H112	1.73	0.44
15:M:1203:BCR:H321	15:M:1203:BCR:C8	2.47	0.44
1:A:329:LEU:HD12	1:A:345:TYR:HB2	1.98	0.44
13:A:842:CLA:H41	13:A:842:CLA:H62	1.71	0.44
15:A:852:BCR:H15C	15:A:852:BCR:H351	1.65	0.44
1:A:334:GLY:N	16:A:854:LHG:HC32	2.32	0.44
13:B:807:CLA:H51	13:B:807:CLA:C10	2.44	0.44
13:B:805:CLA:HHB	13:B:827:CLA:HAB	2.00	0.44
13:A:840:CLA:H2	13:B:830:CLA:H42	1.98	0.44
2:B:393:GLY:HA2	15:B:845:BCR:H393	1.99	0.44
13:L:1004:CLA:HMA2	13:L:1004:CLA:HBA1	1.99	0.44
13:A:839:CLA:O2D	13:A:839:CLA:HAA2	2.17	0.44
15:A:849:BCR:C8	15:A:849:BCR:H331	2.48	0.44
2:B:400:ASP:OD1	4:D:129:LYS:NZ	2.43	0.44
13:B:803:CLA:H151	13:B:803:CLA:H111	1.80	0.44
13:B:822:CLA:HBA1	13:B:822:CLA:H3A	1.66	0.44
8:J:12:PRO:HD3	13:J:1101:CLA:C3D	2.48	0.44
1:A:237:PRO:HB2	1:A:242:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:CG2	13:J:1101:CLA:HBD	2.48	0.44
1:A:552:ILE:HG13	2:B:676:TYR:OH	2.18	0.44
1:A:44:THR:HB	1:A:720:ARG:HG2	1.99	0.44
13:A:803:CLA:HBA2	2:B:430:LEU:CD1	2.48	0.44
1:A:360:LEU:HD21	13:A:830:CLA:CHC	2.48	0.44
13:A:843:CLA:H192	10:L:58:LEU:HD21	1.99	0.44
2:B:60:VAL:HB	2:B:141:LEU:HD13	1.99	0.44
2:B:718:HIS:CE1	13:B:839:CLA:C4D	3.00	0.44
13:B:803:CLA:H3A	13:B:803:CLA:CGA	2.48	0.44
2:B:136:GLN:HE21	13:B:812:CLA:CGA	2.31	0.44
2:B:439:LEU:CD1	15:B:850:BCR:H342	2.45	0.44
4:D:107:LYS:HB3	4:D:107:LYS:HE3	1.80	0.44
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.63	0.44
1:A:215:HIS:HB2	13:A:814:CLA:C1C	2.48	0.44
2:B:291:ARG:HB2	2:B:297:GLY:C	2.38	0.44
13:B:826:CLA:H192	15:B:843:BCR:C36	2.48	0.44
14:B:840:PQN:H161	14:B:840:PQN:H202	1.77	0.44
13:M:1202:CLA:HBA2	13:M:1202:CLA:H3A	1.72	0.44
1:A:205:LEU:HA	13:A:819:CLA:HMC1	1.99	0.44
1:A:449:ILE:HD13	13:B:803:CLA:CBA	2.47	0.44
13:A:811:CLA:H112	13:A:811:CLA:H91	1.67	0.44
13:A:824:CLA:HMA1	13:A:845:CLA:CBB	2.47	0.44
2:B:332:SER:O	2:B:336:GLN:HG3	2.17	0.44
2:B:390:PHE:CE1	15:B:845:BCR:H373	2.53	0.44
4:D:82:ILE:O	4:D:93:LEU:HD23	2.17	0.44
5:E:5:SER:O	5:E:22:THR:HA	2.17	0.44
6:F:41:ALA:HA	6:F:59:ARG:HH22	1.82	0.44
1:A:120:ILE:HD13	8:J:27:ILE:HG23	2.00	0.44
1:A:79:HIS:O	1:A:82:VAL:HG22	2.17	0.44
13:A:809:CLA:HMA1	8:J:27:ILE:HD13	1.99	0.44
13:A:803:CLA:C15	13:A:842:CLA:HAB	2.26	0.44
2:B:669:PHE:HB2	2:B:715:GLY:CA	2.48	0.44
13:B:805:CLA:H152	13:B:805:CLA:H112	1.58	0.44
1:A:285:LEU:HD21	1:A:378:PRO:HD2	1.99	0.43
1:A:317:THR:OG1	1:A:318:ASN:N	2.49	0.43
1:A:299:HIS:HE1	13:A:817:CLA:CHA	2.31	0.43
13:A:832:CLA:HBA2	2:B:690:ARG:O	2.18	0.43
2:B:523:PHE:HE1	13:B:836:CLA:C2D	2.31	0.43
1:A:587:CYS:HB3	2:B:673:TRP:HE3	1.83	0.43
2:B:90:ILE:HG12	13:B:808:CLA:OBD	2.17	0.43
13:B:827:CLA:H142	18:B:848:LMG:H231	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:1301:CLA:HBA1	13:F:1301:CLA:HMA2	2.00	0.43
1:A:699:GLU:HB2	2:B:542:LYS:NZ	2.34	0.43
1:A:356:LEU:HD13	13:A:805:CLA:C2D	2.48	0.43
13:A:819:CLA:H93	13:A:829:CLA:H203	2.00	0.43
13:A:834:CLA:HAA2	13:A:834:CLA:CGD	2.48	0.43
13:A:838:CLA:CBB	13:A:839:CLA:HMD3	2.45	0.43
13:A:840:CLA:HAB	13:A:840:CLA:H122	2.00	0.43
13:A:823:CLA:C1B	13:A:845:CLA:HMC2	2.48	0.43
2:B:208:TRP:CE2	13:B:812:CLA:HBD	2.54	0.43
15:L:1005:BCR:H331	15:L:1005:BCR:HC8	2.00	0.43
1:A:510:SER:HB2	13:A:827:CLA:HMC3	1.99	0.43
13:A:803:CLA:H18	13:A:842:CLA:C5	2.37	0.43
13:A:822:CLA:HMA2	13:A:822:CLA:HBA2	2.00	0.43
13:A:805:CLA:CED	13:A:825:CLA:H12	2.43	0.43
2:B:261:HIS:CD2	2:B:264:THR:H	2.36	0.43
2:B:355:MET:HE1	13:B:826:CLA:HMD1	1.99	0.43
2:B:466:ILE:CD1	13:B:832:CLA:HMC3	2.47	0.43
1:A:88:SER:HB3	1:A:165:GLY:HA3	2.00	0.43
1:A:211:ALA:HA	13:A:815:CLA:CBB	2.48	0.43
13:A:806:CLA:H152	13:A:806:CLA:H112	1.68	0.43
13:A:834:CLA:O1D	10:L:67:PRO:HD3	2.17	0.43
1:A:92:PHE:CE2	13:A:807:CLA:HMD3	2.54	0.43
2:B:337:LEU:HD13	13:B:804:CLA:C2D	2.48	0.43
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.43
3:C:57:CYS:HB3	3:C:62:LEU:HD23	1.99	0.43
13:A:827:CLA:H91	13:A:827:CLA:H112	1.77	0.43
13:A:843:CLA:H91	13:A:843:CLA:H111	1.77	0.43
2:B:308:ASP:O	13:B:820:CLA:CBA	2.66	0.43
2:B:480:LEU:HD21	12:X:29:TYR:CE2	2.53	0.43
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.48	0.43
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.47	0.43
13:B:813:CLA:HAB	15:B:841:BCR:H333	2.00	0.43
6:F:76:TRP:NE1	6:F:113:GLY:HA3	2.33	0.43
2:B:91:TRP:HA	7:I:1:MET:SD	2.59	0.43
13:L:1002:CLA:HAA2	13:L:1002:CLA:O1D	2.18	0.43
13:B:806:CLA:H121	15:M:1203:BCR:C12	2.49	0.43
1:A:587:CYS:HB2	2:B:673:TRP:CB	2.49	0.43
1:A:75:ALA:HB1	13:A:805:CLA:HBB1	2.00	0.43
13:A:840:CLA:C16	13:A:841:CLA:HED1	2.47	0.43
2:B:337:LEU:O	2:B:341:LEU:HG	2.19	0.43
2:B:390:PHE:HB3	2:B:540:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:693:LEU:O	2:B:696:LEU:HB2	2.17	0.43
2:B:52:HIS:CD2	13:B:804:CLA:HMA1	2.54	0.43
6:F:76:TRP:HZ2	13:F:1301:CLA:HED3	1.84	0.43
10:L:92:CYS:HB3	15:L:1005:BCR:C19	2.49	0.43
1:A:177:TRP:HB2	13:A:811:CLA:CMC	2.45	0.43
1:A:689:PHE:HA	14:A:846:PQN:H9	2.00	0.43
4:D:95:HIS:HA	4:D:97:LYS:N	2.34	0.43
1:A:510:SER:HB2	13:A:827:CLA:CMC	2.48	0.43
1:A:536:PHE:HE1	13:A:838:CLA:C2D	2.31	0.43
1:A:547:HIS:CE1	13:A:839:CLA:NA	2.87	0.43
1:A:461:HIS:HE1	13:A:834:CLA:CHA	2.31	0.43
13:A:826:CLA:H71	13:A:835:CLA:HAB	2.01	0.43
2:B:260:PHE:CZ	2:B:358:LEU:HD23	2.53	0.43
13:B:808:CLA:H201	7:I:26:VAL:HG23	1.99	0.43
10:L:41:LEU:HA	10:L:41:LEU:HD23	1.69	0.43
1:A:395:THR:HB	1:A:610:ILE:HG21	2.01	0.43
13:B:815:CLA:H42	13:B:824:CLA:CBB	2.49	0.43
10:L:89:ALA:O	10:L:92:CYS:HB2	2.18	0.43
1:A:152:ILE:HG23	1:A:157:GLN:HB2	2.00	0.43
13:A:810:CLA:HBB2	13:A:813:CLA:HMA3	2.01	0.43
1:A:202:ALA:HB1	13:A:820:CLA:HBC3	2.01	0.43
13:A:834:CLA:HAA2	13:A:834:CLA:O1D	2.19	0.43
13:A:840:CLA:HBA2	13:A:840:CLA:H3A	1.58	0.43
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.54	0.43
2:B:588:TRP:HH2	13:B:802:CLA:CBB	2.32	0.43
6:F:99:ILE:HG13	6:F:100:ILE:N	2.33	0.43
6:F:34:ARG:HD3	8:J:35:ASP:CG	2.40	0.43
1:A:14:VAL:HG22	13:A:812:CLA:O1D	2.19	0.42
2:B:279:ILE:HA	2:B:279:ILE:HD13	1.89	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.19	0.42
13:B:822:CLA:CBB	13:B:822:CLA:HMB1	2.44	0.42
13:A:803:CLA:HMD2	2:B:539:ILE:HD13	2.01	0.42
1:A:28:TRP:CZ2	13:A:804:CLA:H11	2.54	0.42
1:A:547:HIS:HE1	13:A:839:CLA:CHA	2.33	0.42
13:A:803:CLA:H162	13:A:842:CLA:H102	2.01	0.42
2:B:536:THR:HG21	13:B:823:CLA:HBC3	2.01	0.42
13:B:803:CLA:H201	13:B:839:CLA:H71	2.00	0.42
13:B:811:CLA:O1D	13:B:811:CLA:HAA2	2.18	0.42
13:B:815:CLA:H51	13:B:832:CLA:HED2	2.01	0.42
15:B:845:BCR:H331	15:B:845:BCR:C8	2.48	0.42
1:A:242:PHE:HB3	1:A:249:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HB2	1:A:345:TYR:HE1	1.84	0.42
1:A:443:HIS:CE1	13:A:832:CLA:NA	2.86	0.42
13:A:808:CLA:H91	13:A:808:CLA:H112	1.82	0.42
1:A:86:TRP:O	1:A:90:MET:HG2	2.19	0.42
2:B:233:ALA:O	2:B:234:GLN:O	2.37	0.42
2:B:360:PRO:CG	13:B:816:CLA:HBA1	2.49	0.42
2:B:493:PRO:HG2	2:B:494:ASN:H	1.84	0.42
13:B:820:CLA:CGD	13:B:820:CLA:HAA1	2.49	0.42
13:B:805:CLA:H191	18:B:848:LMG:H272	2.02	0.42
2:B:3:LYS:HG3	7:I:38:ALA:OXT	2.19	0.42
7:I:7:ALA:CB	7:I:10:LEU:HD22	2.50	0.42
13:L:1003:CLA:C4C	15:L:1005:BCR:H281	2.49	0.42
1:A:33:HIS:CE1	13:A:804:CLA:HED3	2.54	0.42
1:A:461:HIS:HE1	13:A:834:CLA:C1A	2.32	0.42
13:A:840:CLA:H101	13:B:830:CLA:H11	2.02	0.42
14:B:840:PQN:H301	18:B:848:LMG:H201	2.01	0.42
15:B:849:BCR:H15C	15:B:849:BCR:H351	1.68	0.42
6:F:102:ASP:OD2	6:F:105:LEU:HB2	2.20	0.42
10:L:34:LEU:HG	13:L:1003:CLA:CGD	2.49	0.42
1:A:268:PHE:HA	13:A:844:CLA:HAC1	2.02	0.42
1:A:429:VAL:HG23	13:A:824:CLA:HBC3	2.01	0.42
1:A:380:TYR:OH	13:A:829:CLA:O1D	2.34	0.42
13:A:836:CLA:HMB1	15:A:851:BCR:H292	2.01	0.42
13:A:842:CLA:CAA	13:A:842:CLA:CGD	2.98	0.42
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.49	0.42
13:A:830:CLA:H61	13:A:830:CLA:H41	1.63	0.42
13:A:823:CLA:HBB1	13:A:845:CLA:HAB	1.99	0.42
1:A:210:LEU:HD21	15:A:847:BCR:C34	2.50	0.42
2:B:481:LEU:HD11	13:B:832:CLA:OBD	2.20	0.42
2:B:360:PRO:HB3	13:B:816:CLA:HBA1	2.01	0.42
13:B:834:CLA:O1A	13:B:834:CLA:HED2	2.19	0.42
15:F:1302:BCR:H11C	15:F:1302:BCR:H341	1.87	0.42
1:A:146:LEU:HA	1:A:380:TYR:HD2	1.84	0.42
1:A:674:LEU:HD13	13:A:809:CLA:HMC1	2.01	0.42
13:A:809:CLA:HMC3	2:B:445:VAL:CG1	2.47	0.42
13:A:825:CLA:C7	13:A:825:CLA:H2	2.50	0.42
13:A:833:CLA:H51	15:B:847:BCR:C21	2.50	0.42
13:A:835:CLA:H3A	13:A:835:CLA:HBA2	1.75	0.42
13:A:843:CLA:HBB1	13:A:843:CLA:H72	2.00	0.42
2:B:325:ILE:CG2	13:B:821:CLA:HMD3	2.50	0.42
2:B:333:LEU:HB3	13:B:804:CLA:HAC1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:TRP:CD1	13:B:801:CLA:HBC1	2.55	0.42
15:B:844:BCR:H351	15:B:844:BCR:H15C	1.74	0.42
6:F:55:GLY:H	15:F:1302:BCR:H282	1.84	0.42
7:I:18:VAL:O	7:I:23:PRO:HD3	2.19	0.42
1:A:624:THR:OG1	1:A:625:VAL:N	2.52	0.42
13:A:807:CLA:HBA2	13:A:807:CLA:H3A	1.80	0.42
1:A:215:HIS:HB2	13:A:814:CLA:NC	2.34	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.82	0.42
2:B:668:MET:HB2	13:B:803:CLA:CHC	2.50	0.42
2:B:699:TRP:CZ3	13:B:838:CLA:HBC3	2.54	0.42
2:B:703:PRO:HG2	13:B:838:CLA:CBC	2.49	0.42
13:B:820:CLA:H93	13:B:820:CLA:HBB1	2.00	0.42
13:B:812:CLA:HMB1	13:B:826:CLA:H122	2.01	0.42
13:B:831:CLA:H41	13:B:831:CLA:H61	1.47	0.42
13:B:836:CLA:H91	15:F:1302:BCR:H20C	2.02	0.42
1:A:429:VAL:HG23	13:A:824:CLA:CBC	2.50	0.42
1:A:502:ALA:N	1:A:503:PRO:HD3	2.35	0.42
13:A:809:CLA:H111	13:A:809:CLA:H142	1.85	0.42
1:A:513:PHE:CE2	13:A:827:CLA:HBC2	2.55	0.42
13:A:806:CLA:CHC	13:A:829:CLA:HAB	2.49	0.42
2:B:182:PHE:HB3	2:B:283:PHE:CD2	2.54	0.42
2:B:309:PHE:CD1	13:B:820:CLA:HMB2	2.55	0.42
2:B:724:ILE:HG23	13:B:825:CLA:CAB	2.50	0.42
2:B:64:LEU:HD21	15:B:843:BCR:H271	2.01	0.42
3:C:16:CYS:SG	3:C:17:VAL:N	2.93	0.42
15:J:1104:BCR:H383	15:J:1104:BCR:H23C	2.02	0.42
13:A:832:CLA:C4	13:L:1003:CLA:H93	2.50	0.42
1:A:118:TRP:HZ3	13:A:809:CLA:CBA	2.33	0.42
1:A:348:LEU:HD12	13:A:825:CLA:HMC2	2.01	0.42
1:A:713:VAL:O	13:A:841:CLA:HMD3	2.20	0.42
13:A:805:CLA:CBB	13:A:805:CLA:HMB1	2.50	0.42
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.55	0.42
13:B:807:CLA:CGD	13:B:807:CLA:HAA2	2.50	0.42
13:B:812:CLA:CAC	15:B:843:BCR:H353	2.50	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.93	0.41
1:A:626:ALA:C	1:A:628:ASP:N	2.73	0.41
13:B:811:CLA:H111	13:B:811:CLA:H91	1.78	0.41
13:B:826:CLA:H42	15:B:843:BCR:C39	2.49	0.41
13:B:830:CLA:H102	13:B:830:CLA:H62	1.76	0.41
13:B:836:CLA:H3A	13:B:837:CLA:OBD	2.20	0.41
13:B:838:CLA:O1D	13:B:838:CLA:HAA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.41
13:I:101:CLA:O2A	13:I:101:CLA:HMA2	2.20	0.41
7:I:17:VAL:HG22	7:I:21:LEU:HD23	2.02	0.41
15:B:849:BCR:H21C	13:L:1003:CLA:HAB	2.01	0.41
1:A:403:PHE:O	13:A:830:CLA:HMC1	2.20	0.41
1:A:53:ALA:HB2	16:A:853:LHG:HC82	2.02	0.41
1:A:118:TRP:HZ2	13:A:807:CLA:HED3	1.78	0.41
2:B:189:TRP:CD2	13:B:816:CLA:HMD3	2.54	0.41
11:M:29:LEU:HB3	13:M:1201:CLA:HBA2	2.01	0.41
1:A:225:LYS:HD3	1:A:252:LEU:HB3	2.02	0.41
1:A:511:VAL:HB	1:A:526:MET:CG	2.49	0.41
1:A:377:MET:CE	13:A:827:CLA:HMC2	2.50	0.41
13:A:835:CLA:HMC3	13:A:837:CLA:H43	2.01	0.41
2:B:11:LEU:HA	2:B:11:LEU:HD23	1.90	0.41
2:B:239:ALA:HA	2:B:262:PRO:HG3	2.01	0.41
2:B:140:PHE:CE1	13:B:812:CLA:H61	2.56	0.41
11:M:26:SER:O	13:M:1201:CLA:CGA	2.68	0.41
1:A:16:VAL:HG11	1:A:183:ARG:HB3	2.03	0.41
1:A:660:GLN:HE21	1:A:754:VAL:HG13	1.85	0.41
13:A:817:CLA:CAA	13:A:817:CLA:CGD	2.94	0.41
13:A:838:CLA:CGD	13:A:838:CLA:CAA	2.98	0.41
2:B:241:HIS:HD2	2:B:247:GLN:O	2.03	0.41
2:B:274:HIS:HE1	13:B:814:CLA:CHA	2.33	0.41
2:B:309:PHE:CE1	13:B:820:CLA:H72	2.55	0.41
13:B:822:CLA:HAA2	13:B:822:CLA:CGD	2.50	0.41
1:A:157:GLN:HG2	13:A:814:CLA:CED	2.50	0.41
1:A:86:TRP:HA	13:A:807:CLA:CBB	2.50	0.41
5:E:6:LYS:HB3	5:E:20:VAL:CG1	2.50	0.41
1:A:118:TRP:CZ3	13:A:809:CLA:HBA1	2.51	0.41
13:A:826:CLA:HBB1	13:A:839:CLA:HMA1	2.02	0.41
2:B:377:HIS:HB2	13:B:825:CLA:CHB	2.51	0.41
15:B:850:BCR:H21C	8:J:36:LEU:HD22	2.03	0.41
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.01	0.41
10:L:4:LEU:HD22	10:L:5:VAL:N	2.36	0.41
2:B:479:THR:HG21	12:X:29:TYR:O	2.21	0.41
1:A:178:PHE:O	1:A:182:LYS:HB2	2.21	0.41
1:A:356:LEU:HD23	1:A:411:HIS:CG	2.56	0.41
1:A:396:HIS:O	1:A:400:ILE:HG12	2.20	0.41
13:A:832:CLA:H91	13:A:832:CLA:H112	1.68	0.41
13:A:842:CLA:H202	13:J:1101:CLA:H171	2.03	0.41
1:A:161:THR:CG2	15:A:848:BCR:HC32	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ASN:O	2:B:231:VAL:HG23	2.20	0.41
2:B:457:LEU:O	6:F:51:LEU:N	2.53	0.41
2:B:64:LEU:HD21	15:B:843:BCR:H281	2.01	0.41
2:B:723:TYR:CE1	13:B:801:CLA:CGA	3.04	0.41
13:B:836:CLA:H62	13:B:836:CLA:H102	1.88	0.41
15:B:849:BCR:H321	15:B:849:BCR:C8	2.50	0.41
15:B:850:BCR:H351	15:B:850:BCR:H15C	1.85	0.41
13:J:1101:CLA:H61	13:J:1101:CLA:H41	1.94	0.41
1:A:120:ILE:HD12	15:J:1105:BCR:C31	2.51	0.41
1:A:221:LEU:HD11	1:A:295:SER:HB3	2.02	0.41
1:A:343:GLY:O	1:A:347:VAL:HG23	2.21	0.41
1:A:299:HIS:HE1	13:A:817:CLA:C4D	2.34	0.41
13:A:843:CLA:H191	13:L:1003:CLA:CBB	2.51	0.41
14:A:846:PQN:H212	14:A:846:PQN:H191	1.77	0.41
2:B:444:ASP:OD1	2:B:621:TYR:HB2	2.21	0.41
13:B:829:CLA:HMB2	15:F:1302:BCR:H10C	2.02	0.41
15:B:849:BCR:H11C	15:B:849:BCR:H341	1.77	0.41
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.36	0.41
12:X:23:ASN:HD22	12:X:23:ASN:C	2.23	0.41
1:A:292:LEU:CD2	13:A:818:CLA:HBA1	2.51	0.41
1:A:605:CYS:O	1:A:609:VAL:HG23	2.20	0.41
13:A:826:CLA:H51	13:A:837:CLA:C2	2.51	0.41
13:B:822:CLA:H61	13:B:822:CLA:H41	1.55	0.41
15:B:849:BCR:C23	15:B:849:BCR:H392	2.50	0.41
4:D:37:GLN:O	4:D:49:MET:HG2	2.21	0.41
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.41
1:A:411:HIS:HA	1:A:414:ILE:HD12	2.03	0.41
1:A:484:PRO:HD2	1:A:488:GLN:NE2	2.35	0.41
1:A:718:GLN:HA	1:A:719:PRO:HD3	1.97	0.41
13:A:821:CLA:H3A	13:A:821:CLA:HBA2	1.31	0.41
13:A:821:CLA:H143	13:A:824:CLA:H93	2.02	0.41
13:A:833:CLA:HAA1	15:B:849:BCR:H363	2.03	0.41
2:B:413:ARG:HD3	13:B:828:CLA:OBD	2.20	0.41
13:A:840:CLA:O1D	2:B:427:TRP:HB2	2.21	0.41
13:A:802:CLA:C15	15:B:847:BCR:H12C	2.47	0.41
2:B:24:ILE:HA	13:M:1201:CLA:HMD3	2.02	0.41
1:A:252:LEU:HG	1:A:252:LEU:H	1.50	0.41
1:A:695:GLY:O	1:A:699:GLU:HG3	2.21	0.41
13:A:817:CLA:OBD	13:A:836:CLA:HED3	2.21	0.41
13:A:808:CLA:H62	13:A:828:CLA:H92	2.03	0.41
2:B:6:LYS:NZ	11:M:30:TYR:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:804:CLA:H142	13:B:804:CLA:H111	1.83	0.41
2:B:425:LEU:CG	13:B:837:CLA:HBB1	2.31	0.41
4:D:12:GLY:HA2	10:L:12:PRO:O	2.21	0.41
13:I:101:CLA:H91	13:I:101:CLA:H111	1.74	0.41
1:A:143:LEU:O	1:A:146:LEU:HB3	2.21	0.40
1:A:204:LEU:HB2	13:A:813:CLA:HMB2	2.03	0.40
1:A:257:ASP:O	1:A:258:TRP:HB2	2.20	0.40
1:A:28:TRP:CG	13:A:811:CLA:H12	2.55	0.40
1:A:332:HIS:HE1	13:A:823:CLA:CHA	2.33	0.40
13:A:833:CLA:C1B	13:A:834:CLA:HMB2	2.50	0.40
2:B:140:PHE:CZ	13:B:812:CLA:H61	2.55	0.40
2:B:387:VAL:HG11	2:B:586:MET:SD	2.61	0.40
2:B:465:PHE:HB2	12:X:30:TYR:CE1	2.55	0.40
2:B:473:LEU:O	2:B:476:GLY:N	2.46	0.40
15:A:852:BCR:C36	13:B:802:CLA:H42	2.27	0.40
13:B:834:CLA:HHC	13:B:834:CLA:HBB1	2.03	0.40
4:D:124:ASN:HB2	4:D:127:GLN:CD	2.41	0.40
6:F:99:ILE:HG13	6:F:100:ILE:HG13	2.04	0.40
2:B:260:PHE:HZ	2:B:358:LEU:HD23	1.86	0.40
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.57	0.40
2:B:703:PRO:HG2	13:B:838:CLA:HBC3	2.04	0.40
14:B:840:PQN:H2M1	14:B:840:PQN:H111	1.69	0.40
8:J:24:GLY:C	13:J:1102:CLA:HBB1	2.42	0.40
1:A:480:ILE:HD11	10:L:69:ARG:NH1	2.37	0.40
1:A:622:TRP:O	1:A:633:HIS:HD2	2.05	0.40
13:A:833:CLA:CED	13:A:843:CLA:H11	2.51	0.40
13:A:845:CLA:HAA2	13:A:845:CLA:CBF	2.50	0.40
1:A:333:LYS:O	13:A:845:CLA:HBC3	2.21	0.40
13:A:825:CLA:HAB	15:A:850:BCR:H341	2.03	0.40
2:B:279:ILE:CD1	13:B:815:CLA:HBC2	2.51	0.40
13:B:806:CLA:H12	7:I:18:VAL:CG2	2.27	0.40
2:B:122:TRP:HZ2	15:B:843:BCR:H401	1.86	0.40
13:B:824:CLA:H122	15:B:845:BCR:H17C	2.02	0.40
15:B:849:BCR:H23C	15:B:849:BCR:C39	2.49	0.40
15:F:1302:BCR:H331	15:F:1302:BCR:H342	2.04	0.40
10:L:92:CYS:HB3	15:L:1005:BCR:C20	2.51	0.40
12:X:20:LEU:O	12:X:23:ASN:HB3	2.22	0.40
1:A:137:ILE:HG21	13:A:808:CLA:CHD	2.52	0.40
1:A:182:LYS:HA	1:A:182:LYS:HD3	1.87	0.40
1:A:688:MET:HB2	13:A:803:CLA:CHC	2.51	0.40
2:B:137:GLY:HA2	13:B:812:CLA:O1A	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HD12	2:B:142:LEU:HA	1.89	0.40
2:B:466:ILE:HD12	13:B:835:CLA:CED	2.51	0.40
2:B:642:ASN:HB2	2:B:643:PRO:HD2	2.03	0.40
2:B:721:VAL:CG2	13:B:827:CLA:H152	2.52	0.40
13:B:824:CLA:H121	15:B:844:BCR:C20	2.52	0.40
6:F:63:PHE:C	6:F:66:PRO:HD2	2.41	0.40
2:B:700:LYS:NZ	7:I:35:GLU:O	2.47	0.40
1:A:171:LEU:HD12	13:A:810:CLA:HBC1	2.02	0.40
1:A:325:LEU:HB2	1:A:345:TYR:CE1	2.57	0.40
1:A:741:ALA:O	1:A:744:TRP:HB3	2.22	0.40
13:A:814:CLA:CGD	13:A:814:CLA:CAA	2.93	0.40
13:A:819:CLA:H8	13:A:819:CLA:CAB	2.46	0.40
13:A:836:CLA:HMA2	13:A:836:CLA:HBA2	2.03	0.40
2:B:43:GLN:NE2	2:B:161:ARG:HB3	2.36	0.40
2:B:541:VAL:HG22	15:B:844:BCR:H281	2.04	0.40
13:B:801:CLA:H2	13:B:802:CLA:C3D	2.51	0.40
13:B:835:CLA:H91	13:B:835:CLA:H112	1.71	0.40
2:B:288:HIS:NE2	15:B:841:BCR:H363	2.37	0.40
13:B:830:CLA:HBB2	15:B:846:BCR:HC41	2.04	0.40
5:E:15:TYR:CE2	5:E:44:ASN:HA	2.57	0.40
7:I:19:CYS:HB3	13:I:101:CLA:CBB	2.51	0.40
8:J:30:ASN:ND2	15:J:1104:BCR:H332	2.36	0.40
12:X:9:TYR:O	12:X:10:ALA:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	685 (93%)	39 (5%)	12 (2%)	11	49
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	14	54
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	13	53
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	4	31
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0	7
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	5	36
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	4
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	13	53
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	4	33
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	4	31
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	7	40

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU
2	B	492	TRP
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	55	GLY
6	F	91	SER
9	K	37	ARG
9	K	41	PRO
9	K	42	GLY
12	X	10	ALA
1	A	578	CYS
2	B	236	PRO
2	B	565	CYS
4	D	3	LEU
5	E	36	VAL
5	E	55	VAL
6	F	60	ALA

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Mol	Chain	Res	Type
9	K	74	VAL
10	L	104	GLY
10	L	106	SER
1	A	115	GLN
1	A	234	LYS
1	A	499	GLY
2	B	310	PHE
4	D	44	ALA
5	E	53	SER
6	F	89	ARG
9	K	75	SER
1	A	232	ALA
1	A	250	ALA
1	A	625	VAL
4	D	107	LYS
5	E	25	SER
5	E	35	PRO
5	E	68	VAL
1	A	42	PRO
1	A	182	LYS
1	A	498	PRO
2	B	481	LEU
4	D	108	GLY
11	M	30	TYR
5	E	30	PRO
9	K	40	GLY
9	K	56	LEU
5	E	54	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	567 (96%)	22 (4%)	37	65
2	B	595/597 (100%)	572 (96%)	23 (4%)	35	63
3	C	67/67 (100%)	65 (97%)	2 (3%)	44	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	115/115 (100%)	109 (95%)	6 (5%)	25	57
5	E	59/64 (92%)	58 (98%)	1 (2%)	63	83
6	F	109/128 (85%)	105 (96%)	4 (4%)	37	65
7	I	32/32 (100%)	31 (97%)	1 (3%)	43	69
8	J	36/36 (100%)	35 (97%)	1 (3%)	47	71
10	L	117/119 (98%)	109 (93%)	8 (7%)	17	49
11	M	26/26 (100%)	24 (92%)	2 (8%)	14	45
12	X	20/24 (83%)	18 (90%)	2 (10%)	8	32
All	All	1765/1811 (98%)	1693 (96%)	72 (4%)	33	62

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU
1	A	260	PHE
1	A	276	SER
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	395	THR
1	A	433	VAL
1	A	466	ARG
1	A	538	VAL
1	A	587	CYS
1	A	632	SER
1	A	675	LEU
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU

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Mol	Chain	Res	Type
2	B	214	THR
2	B	218	PRO
2	B	256	PHE
2	B	296	ILE
2	B	318	PHE
2	B	322	HIS
2	B	349	SER
2	B	411	LEU
2	B	430	LEU
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	605	LEU
2	B	632	LEU
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	15	GLN
3	C	61	PHE
4	D	1	THR
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
5	E	63	HIS
6	F	1	ASP
6	F	54	ASP
6	F	56	ARG
6	F	105	LEU
7	I	10	LEU
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
10	L	142	PHE

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Mol	Chain	Res	Type
11	M	3	LEU
11	M	17	LEU
12	X	8	THR
12	X	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	542	HIS
1	A	633	HIS
2	B	136	GLN
2	B	261	HIS
6	F	40	GLN
6	F	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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
13	CLA	A	801	-	58,73,73	1.48	10 (17%)	66,113,113	1.91	12 (18%)
13	CLA	A	802	-	58,73,73	1.47	10 (17%)	66,113,113	1.51	8 (12%)
13	CLA	A	803	-	58,73,73	1.44	9 (15%)	66,113,113	1.58	10 (15%)
13	CLA	A	804	13	52,67,73	1.55	9 (17%)	58,105,113	1.62	9 (15%)
13	CLA	A	805	-	58,73,73	1.46	10 (17%)	66,113,113	1.55	8 (12%)
13	CLA	A	806	-	58,73,73	1.42	9 (15%)	66,113,113	1.51	10 (15%)
13	CLA	A	807	-	44,59,73	1.63	8 (18%)	49,96,113	1.78	10 (20%)
13	CLA	A	808	1	58,73,73	1.46	9 (15%)	66,113,113	1.92	12 (18%)
13	CLA	A	809	1	58,73,73	1.45	9 (15%)	66,113,113	1.78	16 (24%)
13	CLA	A	810	-	35,53,73	1.57	6 (17%)	38,89,113	2.11	6 (15%)
13	CLA	A	811	13	58,73,73	1.45	9 (15%)	66,113,113	1.73	9 (13%)
13	CLA	A	812	-	47,62,73	1.55	10 (21%)	52,99,113	1.96	10 (19%)
13	CLA	A	813	-	53,68,73	1.50	9 (16%)	60,107,113	1.82	11 (18%)
13	CLA	A	814	-	35,53,73	1.58	5 (14%)	38,89,113	1.97	6 (15%)
13	CLA	A	815	-	35,53,73	1.56	6 (17%)	38,89,113	2.07	8 (21%)
13	CLA	A	816	-	42,57,73	1.57	8 (19%)	47,93,113	1.69	8 (17%)
13	CLA	A	817	-	47,62,73	1.61	9 (19%)	52,99,113	1.62	9 (17%)
13	CLA	A	818	-	47,62,73	1.57	9 (19%)	52,99,113	1.89	9 (17%)
13	CLA	A	819	-	58,73,73	1.41	10 (17%)	66,113,113	1.86	15 (22%)
13	CLA	A	820	-	54,69,73	1.52	10 (18%)	61,108,113	1.56	12 (19%)
13	CLA	A	821	-	58,73,73	1.44	10 (17%)	66,113,113	1.72	11 (16%)
13	CLA	A	822	-	42,57,73	1.61	7 (16%)	47,93,113	2.24	7 (14%)
13	CLA	A	823	-	44,59,73	1.63	9 (20%)	49,96,113	1.56	9 (18%)
13	CLA	A	824	-	52,67,73	1.53	10 (19%)	58,105,113	2.21	13 (22%)
13	CLA	A	825	-	58,73,73	1.45	9 (15%)	66,113,113	1.64	9 (13%)
13	CLA	A	826	-	58,73,73	1.48	10 (17%)	66,113,113	1.63	12 (18%)
13	CLA	A	827	-	58,73,73	1.43	9 (15%)	66,113,113	1.69	12 (18%)
13	CLA	A	828	-	58,73,73	1.45	9 (15%)	66,113,113	1.69	9 (13%)
13	CLA	A	829	-	58,73,73	1.44	10 (17%)	66,113,113	1.82	10 (15%)
13	CLA	A	830	-	58,73,73	1.44	9 (15%)	66,113,113	1.73	10 (15%)
13	CLA	A	831	-	43,58,73	1.67	10 (23%)	48,95,113	1.68	8 (16%)
13	CLA	A	832	-	58,73,73	1.45	11 (18%)	66,113,113	1.81	9 (13%)
13	CLA	A	833	-	58,73,73	1.45	10 (17%)	66,113,113	1.45	7 (10%)
13	CLA	A	834	-	58,73,73	1.47	11 (18%)	66,113,113	1.49	7 (10%)
13	CLA	A	835	-	47,62,73	1.61	10 (21%)	52,99,113	1.63	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	836	1	35,53,73	1.56	7 (20%)	38,89,113	1.73	7 (18%)
13	CLA	A	837	-	44,59,73	1.66	7 (15%)	49,96,113	2.10	11 (22%)
13	CLA	A	838	-	58,73,73	1.45	10 (17%)	66,113,113	1.73	11 (16%)
13	CLA	A	839	-	40,55,73	1.58	7 (17%)	45,91,113	1.81	9 (20%)
13	CLA	A	840	-	58,73,73	1.45	10 (17%)	66,113,113	1.74	10 (15%)
13	CLA	A	841	-	44,59,73	1.62	8 (18%)	49,96,113	1.69	8 (16%)
13	CLA	A	842	-	58,73,73	1.48	10 (17%)	66,113,113	1.39	8 (12%)
13	CLA	A	843	-	58,73,73	1.41	9 (15%)	66,113,113	1.74	12 (18%)
13	CLA	A	844	-	32,49,73	1.69	6 (18%)	34,83,113	1.40	6 (17%)
13	CLA	A	845	16	45,60,73	1.60	9 (20%)	50,97,113	2.02	13 (26%)
14	PQN	A	846	-	34,34,34	0.93	1 (2%)	42,45,45	1.13	3 (7%)
15	BCR	A	847	-	41,41,41	2.21	23 (56%)	56,56,56	2.05	23 (41%)
15	BCR	A	848	-	41,41,41	2.22	23 (56%)	56,56,56	2.14	21 (37%)
15	BCR	A	849	-	41,41,41	2.08	21 (51%)	56,56,56	2.23	24 (42%)
15	BCR	A	850	-	41,41,41	2.26	22 (53%)	56,56,56	2.19	22 (39%)
15	BCR	A	851	-	41,41,41	2.18	22 (53%)	56,56,56	2.17	18 (32%)
15	BCR	A	852	-	41,41,41	2.24	22 (53%)	56,56,56	2.27	20 (35%)
16	LHG	A	853	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	2 (3%)
16	LHG	A	854	13	26,26,48	1.23	2 (7%)	29,32,54	1.20	2 (6%)
13	CLA	A	855	-	35,53,73	1.57	6 (17%)	38,89,113	1.95	6 (15%)
17	SF4	A	856	1,2	0,12,12	0.00	-	0,24,24	0.00	-
13	CLA	B	801	-	58,73,73	1.48	10 (17%)	66,113,113	1.81	10 (15%)
13	CLA	B	802	-	58,73,73	1.45	9 (15%)	66,113,113	2.01	9 (13%)
13	CLA	B	803	-	58,73,73	1.46	11 (18%)	66,113,113	1.73	10 (15%)
13	CLA	B	804	-	58,73,73	1.45	9 (15%)	66,113,113	1.61	10 (15%)
13	CLA	B	805	-	58,73,73	1.43	10 (17%)	66,113,113	1.50	8 (12%)
13	CLA	B	806	-	58,73,73	1.44	11 (18%)	66,113,113	1.65	9 (13%)
13	CLA	B	807	-	58,73,73	1.46	11 (18%)	66,113,113	1.67	11 (16%)
13	CLA	B	808	2	58,73,73	1.43	9 (15%)	66,113,113	1.78	10 (15%)
13	CLA	B	809	-	35,53,73	1.58	6 (17%)	38,89,113	2.04	6 (15%)
13	CLA	B	810	-	35,53,73	1.59	7 (20%)	38,89,113	1.64	7 (18%)
13	CLA	B	811	-	58,73,73	1.48	10 (17%)	66,113,113	1.80	9 (13%)
13	CLA	B	812	-	58,73,73	1.43	10 (17%)	66,113,113	1.78	9 (13%)
13	CLA	B	813	-	35,53,73	1.54	6 (17%)	38,89,113	2.07	8 (21%)
13	CLA	B	814	-	48,63,73	1.54	9 (18%)	54,101,113	1.85	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	815	-	52,67,73	1.53	9 (17%)	58,105,113	1.48	8 (13%)
13	CLA	B	816	-	53,68,73	1.51	10 (18%)	60,107,113	1.70	11 (18%)
13	CLA	B	817	-	58,73,73	1.43	10 (17%)	66,113,113	1.66	9 (13%)
13	CLA	B	818	-	40,55,73	1.61	7 (17%)	45,91,113	1.68	6 (13%)
13	CLA	B	819	-	35,53,73	1.58	6 (17%)	38,89,113	2.07	6 (15%)
13	CLA	B	820	-	48,63,73	1.56	10 (20%)	54,101,113	1.55	10 (18%)
13	CLA	B	821	-	35,53,73	1.63	7 (20%)	38,89,113	1.79	7 (18%)
13	CLA	B	822	-	47,62,73	1.59	9 (19%)	52,99,113	1.86	10 (19%)
13	CLA	B	823	-	39,54,73	1.61	7 (17%)	44,90,113	1.78	8 (18%)
13	CLA	B	824	-	58,73,73	1.44	9 (15%)	66,113,113	1.83	10 (15%)
13	CLA	B	825	-	58,73,73	1.48	9 (15%)	66,113,113	1.51	7 (10%)
13	CLA	B	826	-	58,73,73	1.46	9 (15%)	66,113,113	1.39	6 (9%)
13	CLA	B	827	-	58,73,73	1.45	9 (15%)	66,113,113	1.87	12 (18%)
13	CLA	B	828	-	35,53,73	1.58	8 (22%)	38,89,113	1.96	6 (15%)
13	CLA	B	829	-	42,57,73	1.58	7 (16%)	47,93,113	1.60	7 (14%)
13	CLA	B	830	-	58,73,73	1.45	9 (15%)	66,113,113	1.64	10 (15%)
13	CLA	B	831	-	51,66,73	1.53	9 (17%)	57,104,113	2.19	10 (17%)
13	CLA	B	832	-	35,53,73	1.59	6 (17%)	38,89,113	1.95	6 (15%)
13	CLA	B	833	-	35,53,73	1.54	6 (17%)	38,89,113	1.99	6 (15%)
13	CLA	B	834	-	35,53,73	1.55	6 (17%)	38,89,113	1.99	6 (15%)
13	CLA	B	835	-	53,68,73	1.52	9 (16%)	60,107,113	1.92	13 (21%)
13	CLA	B	836	-	58,73,73	1.44	10 (17%)	66,113,113	1.62	9 (13%)
13	CLA	B	837	-	40,55,73	1.59	8 (20%)	45,91,113	1.85	7 (15%)
13	CLA	B	838	-	58,73,73	1.44	9 (15%)	66,113,113	1.76	12 (18%)
13	CLA	B	839	-	58,73,73	1.45	9 (15%)	66,113,113	1.59	10 (15%)
14	PQN	B	840	-	34,34,34	0.86	1 (2%)	42,45,45	1.30	4 (9%)
15	BCR	B	841	-	41,41,41	2.18	23 (56%)	56,56,56	2.11	22 (39%)
15	BCR	B	842	-	41,41,41	2.24	24 (58%)	56,56,56	2.27	21 (37%)
15	BCR	B	843	-	41,41,41	2.15	21 (51%)	56,56,56	2.39	26 (46%)
15	BCR	B	844	-	25,25,41	2.29	15 (60%)	33,33,56	2.14	13 (39%)
15	BCR	B	845	-	41,41,41	2.16	22 (53%)	56,56,56	2.35	23 (41%)
15	BCR	B	846	-	41,41,41	2.20	23 (56%)	56,56,56	2.08	21 (37%)
15	BCR	B	847	-	41,41,41	2.19	22 (53%)	56,56,56	2.28	22 (39%)
18	LMG	B	848	-	55,55,55	1.05	8 (14%)	63,63,63	1.22	3 (4%)
15	BCR	B	849	-	41,41,41	2.10	21 (51%)	56,56,56	2.34	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	B	850	-	41,41,41	2.19	22 (53%)	56,56,56	2.36	24 (42%)
17	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
13	CLA	F	1301	-	35,53,73	1.59	6 (17%)	38,89,113	1.98	9 (23%)
15	BCR	F	1302	-	41,41,41	2.16	22 (53%)	56,56,56	2.20	21 (37%)
13	CLA	I	101	-	58,73,73	1.45	10 (17%)	66,113,113	1.76	11 (16%)
15	BCR	I	102	-	41,41,41	2.08	19 (46%)	56,56,56	2.33	23 (41%)
13	CLA	J	1101	-	58,73,73	1.42	9 (15%)	66,113,113	1.72	12 (18%)
13	CLA	J	1102	8	35,53,73	1.55	6 (17%)	38,89,113	2.12	7 (18%)
13	CLA	J	1103	-	31,45,73	1.89	7 (22%)	34,78,113	1.31	2 (5%)
15	BCR	J	1104	-	41,41,41	2.21	23 (56%)	56,56,56	2.24	25 (44%)
15	BCR	J	1105	-	41,41,41	2.21	23 (56%)	56,56,56	2.15	23 (41%)
13	CLA	L	1002	10	58,73,73	1.44	10 (17%)	66,113,113	1.77	11 (16%)
13	CLA	L	1003	-	58,73,73	1.45	10 (17%)	66,113,113	1.94	13 (19%)
13	CLA	L	1004	-	58,73,73	1.43	9 (15%)	66,113,113	1.69	10 (15%)
15	BCR	L	1005	-	41,41,41	2.16	23 (56%)	56,56,56	2.26	23 (41%)
15	BCR	L	1006	-	41,41,41	2.20	22 (53%)	56,56,56	2.03	19 (33%)
13	CLA	M	1201	-	47,62,73	1.62	10 (21%)	52,99,113	1.91	11 (21%)
13	CLA	M	1202	-	35,53,73	1.55	6 (17%)	38,89,113	1.97	6 (15%)
15	BCR	M	1203	-	41,41,41	2.15	22 (53%)	56,56,56	2.28	21 (37%)
16	LHG	X	101	-	22,22,48	1.31	2 (9%)	25,28,54	1.01	1 (4%)
13	CLA	X	102	12	35,53,73	1.56	6 (17%)	38,89,113	2.47	6 (15%)

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
13	CLA	A	801	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	802	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	803	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	804	13	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	805	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	A	806	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	807	-	3/3/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	808	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	809	1	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	A	810	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	811	13	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	812	-	2/2/17/25	0/24/122/135	0/0/9/9
13	CLA	A	813	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	A	814	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	815	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	A	816	-	2/2/16/25	0/18/116/135	0/0/9/9
13	CLA	A	817	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	818	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	819	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	820	-	3/3/19/25	0/33/131/135	0/0/9/9
13	CLA	A	821	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	822	-	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	A	823	-	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	824	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	825	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	826	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	827	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	828	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	829	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	830	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	831	-	3/3/17/25	0/19/117/135	0/0/9/9
13	CLA	A	832	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	833	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	834	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	835	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	836	1	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	A	837	-	1/1/17/25	0/21/119/135	0/0/9/9
13	CLA	A	838	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	839	-	3/3/16/25	0/16/114/135	0/0/9/9
13	CLA	A	840	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	841	-	3/3/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	842	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	843	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	844	-	1/1/14/25	0/5/101/135	0/0/9/9
13	CLA	A	845	16	3/3/17/25	0/22/120/135	0/0/9/9
14	PQN	A	846	-	-	0/23/43/43	0/2/2/2
15	BCR	A	847	-	-	0/29/63/63	0/2/2/2
15	BCR	A	848	-	-	0/29/63/63	0/2/2/2
15	BCR	A	849	-	-	0/29/63/63	0/2/2/2
15	BCR	A	850	-	-	0/29/63/63	0/2/2/2
15	BCR	A	851	-	-	0/29/63/63	0/2/2/2
15	BCR	A	852	-	-	0/29/63/63	0/2/2/2
16	LHG	A	853	-	-	0/53/53/53	0/0/0/0
16	LHG	A	854	13	-	0/31/31/53	0/0/0/0
13	CLA	A	855	-	2/2/16/25	0/11/111/135	0/0/9/9
17	SF4	A	856	1,2	-	0/0/48/48	0/6/5/5
13	CLA	B	801	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	802	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	803	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	804	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	805	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	806	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	807	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	808	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	809	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	810	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	811	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	812	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	813	-	1/1/16/25	0/11/111/135	0/0/9/9
13	CLA	B	814	-	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	815	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	B	816	-	2/2/19/25	0/31/129/135	0/0/9/9
13	CLA	B	817	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	818	-	2/2/16/25	0/16/114/135	0/0/9/9
13	CLA	B	819	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	820	-	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	821	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	822	-	2/2/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	823	-	2/2/16/25	0/15/113/135	0/0/9/9
13	CLA	B	824	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	825	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	826	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	827	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	828	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	829	-	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	B	830	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	831	-	3/3/18/25	0/29/127/135	0/0/9/9
13	CLA	B	832	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	833	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	834	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	835	-	2/2/19/25	0/31/129/135	0/0/9/9
13	CLA	B	836	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	837	-	3/3/16/25	0/16/114/135	0/0/9/9
13	CLA	B	838	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	839	-	3/3/20/25	0/37/135/135	0/0/9/9
14	PQN	B	840	-	-	0/23/43/43	0/2/2/2
15	BCR	B	841	-	-	0/29/63/63	0/2/2/2
15	BCR	B	842	-	-	0/29/63/63	0/2/2/2
15	BCR	B	843	-	-	0/29/63/63	0/2/2/2
15	BCR	B	844	-	-	0/18/35/63	0/1/1/2
15	BCR	B	845	-	-	0/29/63/63	0/2/2/2
15	BCR	B	846	-	-	0/29/63/63	0/2/2/2
15	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	LMG	B	848	-	-	0/50/70/70	0/1/1/1
15	BCR	B	849	-	-	0/29/63/63	0/2/2/2
15	BCR	B	850	-	-	0/29/63/63	0/2/2/2
17	SF4	C	101	3	-	0/0/48/48	0/6/5/5
17	SF4	C	102	3	-	0/0/48/48	0/6/5/5
13	CLA	F	1301	-	1/1/16/25	0/11/111/135	0/0/9/9
15	BCR	F	1302	-	-	0/29/63/63	0/2/2/2
13	CLA	I	101	-	2/2/20/25	0/37/135/135	0/0/9/9
15	BCR	I	102	-	-	0/29/63/63	0/2/2/2
13	CLA	J	1101	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	J	1102	8	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	J	1103	-	2/2/13/25	0/2/96/135	0/0/9/9
15	BCR	J	1104	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	J	1105	-	-	0/29/63/63	0/2/2/2
13	CLA	L	1002	10	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1003	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1004	-	3/3/20/25	0/37/135/135	0/0/9/9
15	BCR	L	1005	-	-	0/29/63/63	0/2/2/2
15	BCR	L	1006	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1201	-	2/2/17/25	0/24/122/135	0/0/9/9
13	CLA	M	1202	-	2/2/16/25	0/11/111/135	0/0/9/9
15	BCR	M	1203	-	-	0/29/63/63	0/2/2/2
16	LHG	X	101	-	-	0/26/26/53	0/0/0/0
13	CLA	X	102	12	2/2/16/25	0/11/111/135	0/0/9/9

All (1327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3A-C2A	-4.17	1.50	1.54
13	A	824	CLA	C1B-CHB	-3.87	1.29	1.40
13	A	834	CLA	C1B-CHB	-3.83	1.30	1.40
13	B	816	CLA	C1B-CHB	-3.80	1.30	1.40
13	L	1002	CLA	C1B-CHB	-3.78	1.30	1.40
13	A	801	CLA	C1B-CHB	-3.76	1.30	1.40
13	B	801	CLA	C1B-CHB	-3.75	1.30	1.40
13	A	822	CLA	C1B-CHB	-3.74	1.30	1.40
13	A	802	CLA	C1B-CHB	-3.74	1.30	1.40
13	B	803	CLA	C1B-CHB	-3.73	1.30	1.40
13	B	828	CLA	C1B-CHB	-3.73	1.30	1.40
13	A	835	CLA	C1B-CHB	-3.73	1.30	1.40
13	B	804	CLA	C1B-CHB	-3.70	1.30	1.40
13	L	1003	CLA	C1B-CHB	-3.70	1.30	1.40
13	B	818	CLA	C1B-CHB	-3.69	1.30	1.40
13	B	821	CLA	C1B-CHB	-3.69	1.30	1.40
13	A	831	CLA	C1B-CHB	-3.69	1.30	1.40
13	B	825	CLA	C1B-CHB	-3.69	1.30	1.40
13	B	826	CLA	C1B-CHB	-3.68	1.30	1.40
13	B	819	CLA	C1B-CHB	-3.68	1.30	1.40
13	A	804	CLA	C1B-CHB	-3.67	1.30	1.40
13	B	809	CLA	C1B-CHB	-3.67	1.30	1.40
13	J	1103	CLA	C1B-CHB	-3.67	1.30	1.40
13	F	1301	CLA	C1B-CHB	-3.67	1.30	1.40
13	A	803	CLA	C1B-CHB	-3.66	1.30	1.40
13	A	828	CLA	C1B-CHB	-3.66	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	809	CLA	C1B-CHB	-3.66	1.30	1.40
13	A	820	CLA	C1B-CHB	-3.66	1.30	1.40
13	A	818	CLA	C1B-CHB	-3.65	1.30	1.40
13	A	815	CLA	C1B-CHB	-3.65	1.30	1.40
13	A	826	CLA	C1B-CHB	-3.64	1.30	1.40
13	A	810	CLA	C1B-CHB	-3.64	1.30	1.40
13	B	810	CLA	C1B-CHB	-3.64	1.30	1.40
13	B	829	CLA	C1B-CHB	-3.63	1.30	1.40
13	A	837	CLA	C1B-CHB	-3.63	1.30	1.40
13	X	102	CLA	C1B-CHB	-3.62	1.30	1.40
13	A	836	CLA	C1B-CHB	-3.62	1.30	1.40
13	A	811	CLA	C1B-CHB	-3.61	1.30	1.40
13	B	802	CLA	C1B-CHB	-3.61	1.30	1.40
13	B	837	CLA	C1B-CHB	-3.60	1.30	1.40
13	A	820	CLA	C4A-NA	-3.60	1.32	1.38
13	B	813	CLA	C1B-CHB	-3.60	1.30	1.40
13	A	817	CLA	C1B-CHB	-3.60	1.30	1.40
13	B	830	CLA	C1B-CHB	-3.59	1.30	1.40
13	A	814	CLA	C1B-CHB	-3.59	1.30	1.40
13	A	838	CLA	C1B-CHB	-3.59	1.30	1.40
13	B	807	CLA	C1B-CHB	-3.59	1.30	1.40
13	B	832	CLA	C1B-CHB	-3.58	1.30	1.40
13	B	839	CLA	C1B-CHB	-3.58	1.30	1.40
13	A	839	CLA	C1B-CHB	-3.58	1.30	1.40
13	A	805	CLA	C1B-CHB	-3.57	1.30	1.40
13	B	827	CLA	C1B-CHB	-3.57	1.30	1.40
13	A	833	CLA	C1B-CHB	-3.57	1.30	1.40
13	B	823	CLA	C1B-CHB	-3.56	1.30	1.40
13	B	822	CLA	C1B-CHB	-3.56	1.30	1.40
13	A	845	CLA	C1B-CHB	-3.56	1.30	1.40
13	A	813	CLA	C1B-CHB	-3.56	1.30	1.40
13	I	101	CLA	C1B-CHB	-3.55	1.30	1.40
13	A	819	CLA	C1B-CHB	-3.55	1.30	1.40
13	A	808	CLA	C1B-CHB	-3.55	1.30	1.40
13	B	806	CLA	C1B-CHB	-3.55	1.30	1.40
13	A	802	CLA	C4A-NA	-3.54	1.32	1.38
13	A	816	CLA	C1B-CHB	-3.54	1.30	1.40
13	A	855	CLA	C1B-CHB	-3.54	1.30	1.40
13	B	833	CLA	C1B-CHB	-3.53	1.30	1.40
13	A	842	CLA	C1B-CHB	-3.53	1.30	1.40
13	B	811	CLA	C1B-CHB	-3.53	1.30	1.40
13	B	801	CLA	C4A-NA	-3.53	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	825	CLA	C1B-CHB	-3.52	1.30	1.40
13	J	1102	CLA	C1B-CHB	-3.52	1.30	1.40
13	B	817	CLA	C1B-CHB	-3.52	1.30	1.40
13	A	844	CLA	C1B-CHB	-3.52	1.30	1.40
13	M	1201	CLA	C1B-CHB	-3.52	1.30	1.40
13	B	815	CLA	C1B-CHB	-3.52	1.30	1.40
13	B	834	CLA	C1B-CHB	-3.52	1.30	1.40
13	A	844	CLA	C4A-NA	-3.51	1.32	1.38
13	B	816	CLA	C4A-NA	-3.51	1.32	1.38
13	B	824	CLA	C1B-CHB	-3.51	1.30	1.40
13	B	831	CLA	C1B-CHB	-3.51	1.30	1.40
13	L	1003	CLA	C4A-NA	-3.51	1.32	1.38
13	L	1004	CLA	C1B-CHB	-3.50	1.30	1.40
13	B	808	CLA	C1B-CHB	-3.50	1.30	1.40
13	A	829	CLA	C1B-CHB	-3.50	1.30	1.40
13	M	1202	CLA	C1B-CHB	-3.50	1.30	1.40
13	B	838	CLA	C1B-CHB	-3.49	1.30	1.40
13	B	836	CLA	C1B-CHB	-3.49	1.30	1.40
13	A	807	CLA	C1B-CHB	-3.49	1.30	1.40
13	A	806	CLA	C1B-CHB	-3.49	1.30	1.40
13	B	814	CLA	C1B-CHB	-3.49	1.30	1.40
13	A	823	CLA	C1B-CHB	-3.48	1.30	1.40
13	A	841	CLA	C1B-CHB	-3.47	1.30	1.40
13	J	1101	CLA	C1B-CHB	-3.47	1.31	1.40
13	B	812	CLA	C1B-CHB	-3.47	1.31	1.40
13	B	820	CLA	C1B-CHB	-3.47	1.31	1.40
13	M	1201	CLA	C4A-NA	-3.47	1.32	1.38
13	A	821	CLA	C1B-CHB	-3.47	1.31	1.40
13	A	819	CLA	C4A-NA	-3.46	1.32	1.38
13	A	843	CLA	C1B-CHB	-3.46	1.31	1.40
13	B	837	CLA	C4A-NA	-3.46	1.32	1.38
13	B	835	CLA	O2D-CED	-3.45	1.37	1.45
13	A	830	CLA	C1B-CHB	-3.45	1.31	1.40
13	A	827	CLA	C1B-CHB	-3.45	1.31	1.40
13	B	805	CLA	C1B-CHB	-3.45	1.31	1.40
13	A	835	CLA	C4A-NA	-3.45	1.32	1.38
13	B	826	CLA	C4A-NA	-3.45	1.32	1.38
13	B	821	CLA	C4A-NA	-3.44	1.32	1.38
13	B	835	CLA	C1B-CHB	-3.43	1.31	1.40
13	B	810	CLA	C4A-NA	-3.43	1.32	1.38
13	B	807	CLA	C4A-NA	-3.42	1.32	1.38
13	A	801	CLA	C4A-NA	-3.42	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	855	CLA	C4A-NA	-3.42	1.32	1.38
16	A	854	LHG	O7-C5	-3.42	1.37	1.46
16	X	101	LHG	O7-C5	-3.42	1.37	1.46
13	A	812	CLA	C1B-CHB	-3.41	1.31	1.40
13	A	840	CLA	C1B-CHB	-3.40	1.31	1.40
13	B	803	CLA	C4A-NA	-3.39	1.32	1.38
13	A	813	CLA	C4A-NA	-3.37	1.33	1.38
13	A	829	CLA	C4A-NA	-3.37	1.33	1.38
13	A	821	CLA	C4A-NA	-3.37	1.33	1.38
13	A	832	CLA	C1B-CHB	-3.36	1.31	1.40
13	A	823	CLA	C4A-NA	-3.36	1.33	1.38
13	B	839	CLA	C4A-NA	-3.36	1.33	1.38
13	J	1103	CLA	C4A-NA	-3.35	1.33	1.38
13	B	825	CLA	C4A-NA	-3.35	1.33	1.38
13	A	845	CLA	C4A-NA	-3.35	1.33	1.38
13	B	836	CLA	C4A-NA	-3.35	1.33	1.38
13	B	830	CLA	C4A-NA	-3.35	1.33	1.38
13	J	1101	CLA	C4A-NA	-3.34	1.33	1.38
13	A	822	CLA	C4A-NA	-3.33	1.33	1.38
13	A	826	CLA	C4A-NA	-3.33	1.33	1.38
13	A	816	CLA	C4A-NA	-3.33	1.33	1.38
13	A	824	CLA	C4A-NA	-3.32	1.33	1.38
13	B	804	CLA	C4A-NA	-3.32	1.33	1.38
13	B	818	CLA	C4A-NA	-3.32	1.33	1.38
13	B	822	CLA	C4A-NA	-3.32	1.33	1.38
13	B	824	CLA	C4A-NA	-3.31	1.33	1.38
13	A	837	CLA	O2D-CED	-3.31	1.37	1.45
13	B	812	CLA	C4A-NA	-3.30	1.33	1.38
13	A	838	CLA	C4A-NA	-3.30	1.33	1.38
13	A	804	CLA	C4A-NA	-3.30	1.33	1.38
13	L	1002	CLA	C4A-NA	-3.30	1.33	1.38
13	B	832	CLA	C4A-NA	-3.30	1.33	1.38
13	B	827	CLA	C4A-NA	-3.30	1.33	1.38
13	A	831	CLA	C4A-NA	-3.30	1.33	1.38
13	A	828	CLA	C4A-NA	-3.29	1.33	1.38
13	A	803	CLA	C4A-NA	-3.29	1.33	1.38
13	A	841	CLA	C4A-NA	-3.29	1.33	1.38
13	X	102	CLA	C4A-NA	-3.28	1.33	1.38
13	B	806	CLA	C4A-NA	-3.28	1.33	1.38
13	B	815	CLA	C4A-NA	-3.28	1.33	1.38
13	A	843	CLA	C4A-NA	-3.27	1.33	1.38
13	A	832	CLA	C4A-NA	-3.27	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	817	CLA	C4A-NA	-3.27	1.33	1.38
13	A	842	CLA	C4A-NA	-3.27	1.33	1.38
16	A	854	LHG	O8-C6	-3.27	1.37	1.45
13	B	808	CLA	C4A-NA	-3.27	1.33	1.38
13	B	805	CLA	C4A-NA	-3.27	1.33	1.38
13	A	827	CLA	C4A-NA	-3.26	1.33	1.38
13	B	809	CLA	C4A-NA	-3.26	1.33	1.38
13	L	1004	CLA	C4A-NA	-3.26	1.33	1.38
13	A	825	CLA	C4A-NA	-3.26	1.33	1.38
13	B	811	CLA	C4A-NA	-3.25	1.33	1.38
13	A	814	CLA	O2D-CED	-3.25	1.37	1.45
13	A	818	CLA	C4A-NA	-3.25	1.33	1.38
13	I	101	CLA	C4A-NA	-3.24	1.33	1.38
13	B	838	CLA	C4A-NA	-3.23	1.33	1.38
13	A	817	CLA	C4A-NA	-3.23	1.33	1.38
13	B	833	CLA	C4A-NA	-3.23	1.33	1.38
13	J	1102	CLA	C4A-NA	-3.22	1.33	1.38
13	B	802	CLA	C4A-NA	-3.22	1.33	1.38
13	A	840	CLA	C4A-NA	-3.22	1.33	1.38
13	A	808	CLA	C4A-NA	-3.22	1.33	1.38
13	A	839	CLA	C4A-NA	-3.22	1.33	1.38
13	A	815	CLA	C4A-NA	-3.22	1.33	1.38
13	A	812	CLA	C4A-NA	-3.22	1.33	1.38
13	B	828	CLA	C4A-NA	-3.21	1.33	1.38
13	A	830	CLA	C4A-NA	-3.21	1.33	1.38
13	B	829	CLA	C4A-NA	-3.21	1.33	1.38
16	X	101	LHG	O8-C6	-3.21	1.38	1.45
13	A	833	CLA	C4A-NA	-3.21	1.33	1.38
13	A	811	CLA	C4A-NA	-3.20	1.33	1.38
16	A	853	LHG	O7-C5	-3.20	1.38	1.46
13	B	826	CLA	O2D-CED	-3.20	1.37	1.45
13	B	814	CLA	C4A-NA	-3.20	1.33	1.38
13	A	806	CLA	C4A-NA	-3.20	1.33	1.38
13	B	813	CLA	C4A-NA	-3.20	1.33	1.38
13	A	834	CLA	C4A-NA	-3.18	1.33	1.38
13	A	810	CLA	C4A-NA	-3.18	1.33	1.38
13	A	814	CLA	C4A-NA	-3.16	1.33	1.38
13	B	823	CLA	C4A-NA	-3.16	1.33	1.38
13	F	1301	CLA	C4A-NA	-3.16	1.33	1.38
13	A	805	CLA	C4A-NA	-3.15	1.33	1.38
13	B	819	CLA	C4A-NA	-3.15	1.33	1.38
13	B	831	CLA	C4A-NA	-3.14	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	836	CLA	C4A-NA	-3.14	1.33	1.38
13	B	820	CLA	C4A-NA	-3.14	1.33	1.38
13	B	835	CLA	C4A-NA	-3.13	1.33	1.38
13	A	837	CLA	C4A-NA	-3.13	1.33	1.38
13	A	809	CLA	C4A-NA	-3.11	1.33	1.38
13	B	834	CLA	C4A-NA	-3.11	1.33	1.38
16	A	853	LHG	O8-C6	-3.08	1.38	1.45
13	M	1202	CLA	C4A-NA	-3.08	1.33	1.38
13	A	831	CLA	O2D-CED	-3.06	1.38	1.45
13	A	808	CLA	O2D-CED	-2.98	1.38	1.45
13	B	818	CLA	O2D-CED	-2.97	1.38	1.45
13	B	831	CLA	O2D-CED	-2.96	1.38	1.45
13	B	815	CLA	O2D-CED	-2.96	1.38	1.45
13	B	821	CLA	O2D-CED	-2.92	1.38	1.45
13	A	803	CLA	O2D-CED	-2.91	1.38	1.45
13	A	807	CLA	C4A-NA	-2.89	1.33	1.38
13	A	804	CLA	O2D-CED	-2.88	1.38	1.45
13	A	826	CLA	O2D-CED	-2.83	1.38	1.45
13	A	806	CLA	O2D-CED	-2.82	1.38	1.45
13	B	823	CLA	O2D-CED	-2.81	1.38	1.45
13	B	827	CLA	O2D-CED	-2.80	1.38	1.45
13	B	806	CLA	O2D-CED	-2.78	1.38	1.45
13	B	825	CLA	O2D-CED	-2.77	1.38	1.45
13	A	842	CLA	O2D-CED	-2.77	1.38	1.45
13	B	805	CLA	O2D-CED	-2.76	1.38	1.45
13	B	838	CLA	O2D-CED	-2.76	1.38	1.45
13	B	832	CLA	O2D-CED	-2.75	1.38	1.45
13	A	834	CLA	O2D-CED	-2.75	1.38	1.45
13	A	816	CLA	O2D-CED	-2.73	1.38	1.45
13	A	827	CLA	O2D-CED	-2.73	1.38	1.45
13	A	823	CLA	O2D-CED	-2.73	1.38	1.45
13	A	822	CLA	O2D-CED	-2.73	1.38	1.45
13	B	829	CLA	O2D-CED	-2.72	1.38	1.45
13	B	820	CLA	O2D-CED	-2.72	1.38	1.45
13	B	810	CLA	O2D-CED	-2.71	1.38	1.45
13	L	1004	CLA	O2D-CED	-2.71	1.38	1.45
13	A	833	CLA	O2D-CED	-2.70	1.38	1.45
15	B	845	BCR	C40-C30	-2.70	1.48	1.53
13	B	816	CLA	O2D-CED	-2.70	1.38	1.45
13	L	1002	CLA	O2D-CED	-2.70	1.38	1.45
13	I	101	CLA	O2D-CED	-2.70	1.38	1.45
13	B	836	CLA	O2D-CED	-2.69	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	838	CLA	O2D-CED	-2.69	1.38	1.45
13	A	836	CLA	O2D-CED	-2.69	1.38	1.45
13	A	817	CLA	O2D-CED	-2.69	1.38	1.45
13	A	835	CLA	O2D-CED	-2.69	1.38	1.45
13	A	841	CLA	O2D-CED	-2.69	1.38	1.45
13	A	843	CLA	O2D-CED	-2.69	1.38	1.45
13	B	802	CLA	O2D-CED	-2.69	1.38	1.45
13	A	830	CLA	O2D-CED	-2.69	1.38	1.45
13	L	1003	CLA	O2D-CED	-2.68	1.38	1.45
15	I	102	BCR	C32-C1	-2.68	1.48	1.53
13	A	809	CLA	O2D-CED	-2.68	1.38	1.45
13	B	830	CLA	O2D-CED	-2.68	1.38	1.45
15	B	843	BCR	C32-C1	-2.68	1.48	1.53
13	A	825	CLA	O2D-CED	-2.67	1.38	1.45
13	B	803	CLA	O2D-CED	-2.67	1.39	1.45
15	B	846	BCR	C32-C1	-2.67	1.48	1.53
13	B	804	CLA	O2D-CED	-2.67	1.39	1.45
13	A	801	CLA	O2D-CED	-2.66	1.39	1.45
13	F	1301	CLA	O2D-CED	-2.66	1.39	1.45
13	J	1101	CLA	O2D-CED	-2.66	1.39	1.45
13	A	845	CLA	O2D-CED	-2.66	1.39	1.45
13	A	815	CLA	O2D-CED	-2.66	1.39	1.45
13	A	829	CLA	O2D-CED	-2.66	1.39	1.45
13	A	805	CLA	O2D-CED	-2.65	1.39	1.45
13	A	855	CLA	O2D-CED	-2.65	1.39	1.45
13	A	802	CLA	O2D-CED	-2.65	1.39	1.45
13	B	811	CLA	O2D-CED	-2.65	1.39	1.45
13	A	820	CLA	O2D-CED	-2.65	1.39	1.45
13	B	837	CLA	O2D-CED	-2.65	1.39	1.45
15	L	1005	BCR	C32-C1	-2.65	1.48	1.53
15	J	1105	BCR	C32-C1	-2.65	1.48	1.53
13	A	824	CLA	O2D-CED	-2.65	1.39	1.45
15	B	847	BCR	C32-C1	-2.64	1.48	1.53
13	A	811	CLA	O2D-CED	-2.64	1.39	1.45
13	A	821	CLA	O2D-CED	-2.64	1.39	1.45
13	B	822	CLA	O2D-CED	-2.64	1.39	1.45
13	A	813	CLA	O2D-CED	-2.64	1.39	1.45
13	B	814	CLA	O2D-CED	-2.64	1.39	1.45
13	B	839	CLA	O2D-CED	-2.63	1.39	1.45
13	M	1201	CLA	O2D-CED	-2.63	1.39	1.45
13	A	810	CLA	O2D-CED	-2.63	1.39	1.45
13	A	840	CLA	O2D-CED	-2.63	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	850	BCR	C32-C1	-2.63	1.48	1.53
15	A	849	BCR	C32-C1	-2.63	1.48	1.53
13	B	808	CLA	O2D-CED	-2.62	1.39	1.45
13	A	832	CLA	O2D-CED	-2.62	1.39	1.45
13	B	834	CLA	O2D-CED	-2.62	1.39	1.45
13	B	801	CLA	O2D-CED	-2.62	1.39	1.45
13	B	812	CLA	O2D-CED	-2.61	1.39	1.45
13	B	819	CLA	O2D-CED	-2.61	1.39	1.45
13	X	102	CLA	O2D-CED	-2.61	1.39	1.45
15	A	851	BCR	C32-C1	-2.61	1.48	1.53
13	A	839	CLA	O2D-CED	-2.61	1.39	1.45
15	B	842	BCR	C32-C1	-2.61	1.48	1.53
13	B	807	CLA	O2D-CED	-2.61	1.39	1.45
13	B	828	CLA	O2D-CED	-2.60	1.39	1.45
13	A	818	CLA	O2D-CED	-2.60	1.39	1.45
13	B	809	CLA	O2D-CED	-2.60	1.39	1.45
13	A	812	CLA	O2D-CED	-2.60	1.39	1.45
13	B	833	CLA	O2D-CED	-2.60	1.39	1.45
15	B	849	BCR	C32-C1	-2.59	1.48	1.53
13	B	824	CLA	O2D-CED	-2.59	1.39	1.45
15	J	1104	BCR	C32-C1	-2.59	1.48	1.53
13	A	828	CLA	O2D-CED	-2.58	1.39	1.45
13	A	819	CLA	O2D-CED	-2.58	1.39	1.45
15	A	850	BCR	C32-C1	-2.58	1.48	1.53
15	M	1203	BCR	C32-C1	-2.57	1.48	1.53
15	L	1006	BCR	C32-C1	-2.57	1.48	1.53
13	M	1202	CLA	O2D-CED	-2.57	1.39	1.45
15	A	848	BCR	C32-C1	-2.57	1.48	1.53
15	A	852	BCR	C32-C1	-2.56	1.48	1.53
15	A	847	BCR	C32-C1	-2.56	1.48	1.53
13	J	1102	CLA	O2D-CED	-2.55	1.39	1.45
15	B	847	BCR	C40-C30	-2.55	1.48	1.53
15	B	845	BCR	C32-C1	-2.54	1.48	1.53
13	B	813	CLA	O2D-CED	-2.54	1.39	1.45
13	A	807	CLA	O2D-CED	-2.54	1.39	1.45
15	B	841	BCR	C32-C1	-2.53	1.48	1.53
15	F	1302	BCR	C32-C1	-2.52	1.48	1.53
13	B	817	CLA	O2D-CED	-2.52	1.39	1.45
15	B	842	BCR	C40-C30	-2.49	1.48	1.53
15	M	1203	BCR	C40-C30	-2.48	1.48	1.53
15	B	843	BCR	C40-C30	-2.47	1.48	1.53
15	B	844	BCR	C40-C30	-2.46	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	102	BCR	C40-C30	-2.45	1.48	1.53
15	J	1105	BCR	C40-C30	-2.44	1.48	1.53
15	L	1005	BCR	C40-C30	-2.43	1.48	1.53
15	J	1104	BCR	C40-C30	-2.41	1.48	1.53
15	A	848	BCR	C40-C30	-2.40	1.48	1.53
15	A	851	BCR	C40-C30	-2.40	1.48	1.53
15	A	850	BCR	C40-C30	-2.40	1.48	1.53
15	B	846	BCR	C40-C30	-2.39	1.48	1.53
15	B	850	BCR	C40-C30	-2.39	1.48	1.53
15	B	849	BCR	C40-C30	-2.38	1.48	1.53
15	A	849	BCR	C40-C30	-2.36	1.48	1.53
15	A	847	BCR	C40-C30	-2.36	1.48	1.53
15	B	841	BCR	C40-C30	-2.35	1.48	1.53
15	L	1006	BCR	C40-C30	-2.34	1.48	1.53
15	F	1302	BCR	C40-C30	-2.33	1.48	1.53
13	A	844	CLA	C1A-CHA	-2.33	1.33	1.43
15	A	852	BCR	C40-C30	-2.32	1.49	1.53
15	B	846	BCR	C39-C30	-2.29	1.49	1.53
15	J	1105	BCR	C39-C30	-2.27	1.49	1.53
18	B	848	LMG	O7-C8	-2.26	1.40	1.46
13	B	820	CLA	O2A-C1	-2.26	1.39	1.46
13	J	1103	CLA	C1A-CHA	-2.26	1.33	1.43
15	B	844	BCR	C39-C30	-2.25	1.49	1.53
15	A	851	BCR	C39-C30	-2.25	1.49	1.53
15	B	847	BCR	C39-C30	-2.23	1.49	1.53
15	L	1005	BCR	C39-C30	-2.23	1.49	1.53
15	M	1203	BCR	C39-C30	-2.23	1.49	1.53
15	B	841	BCR	C39-C30	-2.21	1.49	1.53
15	A	847	BCR	C39-C30	-2.20	1.49	1.53
18	B	848	LMG	O1-C7	-2.20	1.39	1.43
15	F	1302	BCR	C39-C30	-2.19	1.49	1.53
15	A	848	BCR	C39-C30	-2.19	1.49	1.53
13	B	828	CLA	C3B-C2B	-2.18	1.37	1.40
15	A	849	BCR	C39-C30	-2.17	1.49	1.53
15	B	842	BCR	C39-C30	-2.17	1.49	1.53
15	A	852	BCR	C39-C30	-2.16	1.49	1.53
13	A	834	CLA	C3B-C2B	-2.16	1.37	1.40
15	L	1006	BCR	C39-C30	-2.16	1.49	1.53
15	B	845	BCR	C39-C30	-2.16	1.49	1.53
15	I	102	BCR	C39-C30	-2.16	1.49	1.53
15	B	850	BCR	C39-C30	-2.15	1.49	1.53
15	J	1105	BCR	C31-C1	-2.15	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	836	CLA	C1A-CHA	-2.14	1.34	1.43
15	B	843	BCR	C39-C30	-2.14	1.49	1.53
13	A	819	CLA	C1A-CHA	-2.13	1.34	1.43
15	J	1104	BCR	C39-C30	-2.12	1.49	1.53
13	A	842	CLA	C1A-CHA	-2.12	1.34	1.43
15	B	844	BCR	C29-C28	-2.12	1.47	1.52
15	B	849	BCR	C39-C30	-2.12	1.49	1.53
13	A	802	CLA	C1A-CHA	-2.10	1.34	1.43
13	B	817	CLA	C1A-CHA	-2.10	1.34	1.43
15	A	850	BCR	C39-C30	-2.10	1.49	1.53
13	B	806	CLA	O2A-C1	-2.09	1.40	1.46
13	A	820	CLA	C1A-CHA	-2.08	1.34	1.43
15	B	845	BCR	C31-C1	-2.08	1.49	1.53
13	M	1201	CLA	C1A-CHA	-2.08	1.34	1.43
13	B	837	CLA	C1A-CHA	-2.07	1.34	1.43
15	L	1005	BCR	C31-C1	-2.07	1.49	1.53
15	B	842	BCR	C29-C28	-2.07	1.47	1.52
15	B	846	BCR	C29-C28	-2.07	1.47	1.52
15	M	1203	BCR	C29-C28	-2.07	1.47	1.52
13	B	801	CLA	C1A-CHA	-2.07	1.34	1.43
13	B	810	CLA	C1A-CHA	-2.07	1.34	1.43
15	B	846	BCR	C31-C1	-2.07	1.49	1.53
13	A	821	CLA	C1A-CHA	-2.06	1.34	1.43
15	B	841	BCR	C29-C28	-2.06	1.47	1.52
13	B	807	CLA	C1A-CHA	-2.06	1.34	1.43
13	A	833	CLA	C4B-CHC	-2.06	1.34	1.40
15	B	847	BCR	C29-C28	-2.06	1.47	1.52
15	A	848	BCR	C31-C1	-2.05	1.49	1.53
13	B	816	CLA	C1A-CHA	-2.05	1.34	1.43
13	B	807	CLA	C1D-C2D	-2.05	1.37	1.42
13	A	840	CLA	C1A-CHA	-2.04	1.34	1.43
15	J	1104	BCR	C31-C1	-2.04	1.49	1.53
15	B	841	BCR	C31-C1	-2.04	1.49	1.53
15	A	851	BCR	C29-C28	-2.04	1.47	1.52
13	L	1002	CLA	C1A-CHA	-2.04	1.34	1.43
13	B	812	CLA	C1A-CHA	-2.04	1.34	1.43
13	L	1003	CLA	C1A-CHA	-2.04	1.34	1.43
15	A	847	BCR	C29-C28	-2.04	1.47	1.52
15	B	849	BCR	C29-C28	-2.04	1.47	1.52
15	L	1006	BCR	C31-C1	-2.04	1.49	1.53
13	A	816	CLA	C1A-CHA	-2.03	1.34	1.43
15	F	1302	BCR	C31-C1	-2.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	838	CLA	C1A-CHA	-2.03	1.34	1.43
13	I	101	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	834	CLA	C1A-CHA	-2.03	1.34	1.43
13	B	805	CLA	C1A-CHA	-2.03	1.34	1.43
13	A	831	CLA	C3B-C2B	-2.03	1.37	1.40
13	A	832	CLA	C1A-CHA	-2.03	1.34	1.43
15	L	1005	BCR	C29-C28	-2.02	1.47	1.52
15	A	849	BCR	C29-C28	-2.02	1.47	1.52
15	A	847	BCR	C31-C1	-2.02	1.49	1.53
13	B	806	CLA	C1A-CHA	-2.02	1.34	1.43
13	B	803	CLA	C3B-C2B	-2.02	1.37	1.40
13	A	824	CLA	C1A-CHA	-2.02	1.34	1.43
13	A	835	CLA	C1A-CHA	-2.01	1.34	1.43
15	J	1105	BCR	C29-C28	-2.01	1.47	1.52
13	B	803	CLA	C1A-CHA	-2.01	1.34	1.43
13	A	836	CLA	C1A-CHA	-2.01	1.34	1.43
15	A	848	BCR	C29-C28	-2.01	1.47	1.52
13	B	828	CLA	C4B-CHC	-2.01	1.34	1.40
15	A	852	BCR	C29-C28	-2.01	1.47	1.52
15	M	1203	BCR	C31-C1	-2.01	1.49	1.53
13	A	823	CLA	C1A-CHA	-2.01	1.34	1.43
13	B	831	CLA	C4B-CHC	-2.01	1.34	1.40
13	A	812	CLA	C1A-CHA	-2.00	1.34	1.43
15	A	850	BCR	C29-C28	-2.00	1.47	1.52
13	B	821	CLA	C1A-CHA	-2.00	1.34	1.43
13	A	801	CLA	C1-C2	2.00	1.55	1.49
15	F	1302	BCR	C8-C7	2.00	1.39	1.33
15	B	850	BCR	C7-C6	2.00	1.52	1.45
15	I	102	BCR	C10-C9	2.00	1.38	1.35
15	M	1203	BCR	C24-C25	2.01	1.52	1.45
13	A	826	CLA	C1-C2	2.01	1.55	1.49
15	J	1104	BCR	C8-C7	2.01	1.39	1.33
15	I	102	BCR	C5-C6	2.01	1.37	1.34
15	A	851	BCR	C24-C25	2.01	1.52	1.45
13	A	808	CLA	C1-C2	2.02	1.55	1.49
13	A	829	CLA	C1-C2	2.02	1.55	1.49
15	A	849	BCR	C24-C25	2.03	1.52	1.45
15	A	848	BCR	C24-C25	2.04	1.52	1.45
15	B	843	BCR	C8-C7	2.04	1.39	1.33
15	B	844	BCR	C24-C25	2.05	1.52	1.45
15	B	849	BCR	C11-C12	2.05	1.39	1.34
15	B	842	BCR	C7-C6	2.06	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	848	LMG	O7-C10	2.07	1.40	1.34
15	B	845	BCR	C11-C12	2.07	1.39	1.34
15	L	1006	BCR	C24-C25	2.08	1.53	1.45
15	A	849	BCR	C20-C19	2.08	1.39	1.34
15	B	849	BCR	C10-C9	2.08	1.38	1.35
15	B	847	BCR	C24-C25	2.08	1.53	1.45
13	B	826	CLA	O2D-CGD	2.09	1.38	1.33
13	A	831	CLA	C5-C3	2.09	1.56	1.50
13	B	835	CLA	C1-C2	2.09	1.55	1.49
15	B	850	BCR	C8-C7	2.09	1.39	1.33
15	B	846	BCR	C24-C25	2.10	1.53	1.45
15	B	844	BCR	C14-C13	2.10	1.39	1.34
13	B	826	CLA	C5-C3	2.10	1.55	1.51
13	B	827	CLA	O2D-CGD	2.10	1.38	1.33
15	M	1203	BCR	C11-C12	2.10	1.39	1.34
15	B	843	BCR	C24-C23	2.10	1.39	1.33
15	J	1105	BCR	C24-C25	2.10	1.53	1.45
15	I	102	BCR	C20-C19	2.11	1.39	1.34
15	B	842	BCR	C8-C7	2.11	1.39	1.33
15	A	849	BCR	C10-C9	2.11	1.38	1.35
15	B	845	BCR	C24-C25	2.12	1.53	1.45
15	I	102	BCR	C24-C23	2.12	1.39	1.33
15	F	1302	BCR	C11-C12	2.13	1.39	1.34
15	L	1005	BCR	C11-C12	2.13	1.39	1.34
15	L	1005	BCR	C24-C25	2.14	1.53	1.45
15	A	851	BCR	C11-C12	2.14	1.39	1.34
15	F	1302	BCR	C24-C23	2.14	1.39	1.33
13	B	816	CLA	C5-C3	2.14	1.55	1.51
13	A	805	CLA	C1-C2	2.14	1.55	1.49
15	A	852	BCR	C24-C25	2.15	1.53	1.45
15	L	1006	BCR	C11-C12	2.15	1.40	1.34
15	M	1203	BCR	C10-C9	2.16	1.38	1.35
15	B	841	BCR	C24-C25	2.16	1.53	1.45
15	B	843	BCR	C11-C12	2.16	1.40	1.34
15	J	1104	BCR	C11-C12	2.16	1.40	1.34
13	A	843	CLA	C5-C3	2.16	1.56	1.51
15	B	842	BCR	C24-C25	2.17	1.53	1.45
15	B	850	BCR	C11-C12	2.17	1.40	1.34
15	A	848	BCR	C11-C12	2.17	1.40	1.34
15	B	846	BCR	C11-C12	2.17	1.40	1.34
15	J	1105	BCR	C11-C12	2.17	1.40	1.34
15	B	847	BCR	C11-C12	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	1104	BCR	C24-C25	2.17	1.53	1.45
15	B	849	BCR	C24-C23	2.17	1.39	1.33
13	B	801	CLA	C5-C3	2.18	1.56	1.51
15	A	847	BCR	C24-C25	2.18	1.53	1.45
15	B	841	BCR	C11-C12	2.18	1.40	1.34
15	A	849	BCR	C24-C23	2.19	1.39	1.33
15	B	847	BCR	C5-C6	2.19	1.38	1.34
13	B	814	CLA	C5-C3	2.19	1.56	1.51
15	M	1203	BCR	C24-C23	2.19	1.39	1.33
13	L	1002	CLA	C5-C3	2.19	1.56	1.51
15	A	851	BCR	C24-C23	2.20	1.39	1.33
15	F	1302	BCR	C20-C19	2.20	1.40	1.34
13	A	832	CLA	C1-C2	2.20	1.55	1.49
15	B	842	BCR	C11-C12	2.20	1.40	1.34
13	B	811	CLA	C1-C2	2.20	1.55	1.49
15	A	850	BCR	C24-C25	2.20	1.53	1.45
15	A	847	BCR	C11-C12	2.20	1.40	1.34
15	A	852	BCR	C11-C12	2.20	1.40	1.34
15	B	843	BCR	C10-C9	2.21	1.38	1.35
13	B	812	CLA	C5-C3	2.21	1.56	1.51
15	B	850	BCR	C24-C23	2.21	1.39	1.33
13	A	806	CLA	C5-C3	2.22	1.56	1.51
13	A	817	CLA	C5-C3	2.22	1.56	1.51
15	L	1005	BCR	C24-C23	2.22	1.39	1.33
13	A	824	CLA	O2D-CGD	2.22	1.38	1.33
15	A	848	BCR	C24-C23	2.22	1.39	1.33
15	B	845	BCR	C26-C25	2.23	1.38	1.34
15	B	841	BCR	C20-C19	2.23	1.40	1.34
13	A	845	CLA	C5-C3	2.23	1.56	1.51
15	B	846	BCR	C20-C19	2.23	1.40	1.34
13	A	813	CLA	C5-C3	2.23	1.56	1.51
13	L	1003	CLA	C5-C3	2.23	1.56	1.51
15	B	845	BCR	C10-C9	2.23	1.38	1.35
15	L	1006	BCR	C24-C23	2.23	1.39	1.33
15	B	841	BCR	C24-C23	2.23	1.39	1.33
13	B	808	CLA	C5-C3	2.24	1.56	1.51
13	B	805	CLA	C5-C3	2.24	1.56	1.51
13	A	803	CLA	C5-C3	2.24	1.56	1.51
13	A	802	CLA	C5-C3	2.24	1.56	1.51
15	J	1105	BCR	C24-C23	2.25	1.40	1.33
15	B	843	BCR	C5-C6	2.25	1.38	1.34
15	A	847	BCR	C20-C19	2.25	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	812	CLA	C5-C3	2.26	1.56	1.51
15	B	846	BCR	C24-C23	2.26	1.40	1.33
13	A	820	CLA	C5-C3	2.26	1.56	1.51
13	A	831	CLA	O2D-CGD	2.26	1.38	1.33
15	B	847	BCR	C20-C19	2.26	1.40	1.34
15	B	849	BCR	C20-C19	2.27	1.40	1.34
13	A	811	CLA	O2D-CGD	2.27	1.38	1.33
13	B	804	CLA	C5-C3	2.27	1.56	1.51
15	B	844	BCR	C24-C23	2.27	1.40	1.33
13	A	840	CLA	C5-C3	2.28	1.56	1.51
13	B	802	CLA	C5-C3	2.28	1.56	1.51
13	A	801	CLA	O2D-CGD	2.28	1.38	1.33
15	A	847	BCR	C24-C23	2.28	1.40	1.33
15	L	1005	BCR	C5-C6	2.28	1.38	1.34
15	B	842	BCR	C20-C19	2.28	1.40	1.34
15	B	847	BCR	C24-C23	2.28	1.40	1.33
15	B	845	BCR	C20-C19	2.29	1.40	1.34
15	L	1005	BCR	C20-C19	2.29	1.40	1.34
15	A	850	BCR	C11-C12	2.29	1.40	1.34
15	A	851	BCR	C10-C9	2.29	1.38	1.35
15	A	852	BCR	C5-C6	2.29	1.38	1.34
13	A	818	CLA	C5-C3	2.29	1.56	1.51
13	B	803	CLA	O2D-CGD	2.30	1.38	1.33
13	B	808	CLA	O2D-CGD	2.30	1.39	1.33
15	M	1203	BCR	C20-C19	2.30	1.40	1.34
13	A	819	CLA	C5-C3	2.30	1.56	1.51
13	B	838	CLA	O2D-CGD	2.30	1.39	1.33
13	A	833	CLA	C5-C3	2.30	1.56	1.51
13	A	828	CLA	C5-C3	2.31	1.56	1.51
13	L	1003	CLA	O2D-CGD	2.31	1.39	1.33
13	B	807	CLA	C5-C3	2.31	1.56	1.51
15	F	1302	BCR	C10-C9	2.31	1.38	1.35
15	J	1104	BCR	C24-C23	2.31	1.40	1.33
13	J	1101	CLA	C5-C3	2.31	1.56	1.51
13	B	822	CLA	O2D-CGD	2.32	1.39	1.33
13	L	1002	CLA	O2D-CGD	2.32	1.39	1.33
15	B	841	BCR	C5-C6	2.32	1.38	1.34
13	B	814	CLA	O2D-CGD	2.32	1.39	1.33
15	L	1005	BCR	C10-C9	2.32	1.38	1.35
13	B	831	CLA	C5-C3	2.32	1.56	1.51
15	J	1104	BCR	C20-C19	2.32	1.40	1.34
13	B	833	CLA	O2D-CGD	2.32	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	851	BCR	C20-C19	2.32	1.40	1.34
13	L	1004	CLA	C5-C3	2.33	1.56	1.51
15	A	848	BCR	C20-C19	2.33	1.40	1.34
13	A	830	CLA	O2D-CGD	2.33	1.39	1.33
13	B	820	CLA	C5-C3	2.33	1.56	1.51
13	B	836	CLA	C5-C3	2.33	1.56	1.51
15	J	1105	BCR	C5-C6	2.33	1.38	1.34
13	L	1004	CLA	O2D-CGD	2.33	1.39	1.33
13	A	821	CLA	O2D-CGD	2.33	1.39	1.33
15	A	850	BCR	C5-C6	2.34	1.38	1.34
15	B	842	BCR	C5-C6	2.34	1.38	1.34
13	B	806	CLA	C5-C3	2.34	1.56	1.51
15	B	843	BCR	C20-C19	2.34	1.40	1.34
15	B	850	BCR	C20-C19	2.34	1.40	1.34
13	X	102	CLA	O2D-CGD	2.34	1.39	1.33
13	B	836	CLA	O2D-CGD	2.34	1.39	1.33
13	B	815	CLA	C5-C3	2.34	1.56	1.51
13	A	803	CLA	O2D-CGD	2.34	1.39	1.33
15	A	852	BCR	C10-C9	2.34	1.38	1.35
13	A	813	CLA	O2D-CGD	2.35	1.39	1.33
13	A	827	CLA	O2D-CGD	2.35	1.39	1.33
15	B	847	BCR	C10-C9	2.35	1.38	1.35
13	B	811	CLA	O2D-CGD	2.35	1.39	1.33
13	I	101	CLA	C5-C3	2.35	1.56	1.51
13	A	824	CLA	C5-C3	2.35	1.56	1.51
13	A	822	CLA	O2D-CGD	2.35	1.39	1.33
13	B	807	CLA	O2D-CGD	2.35	1.39	1.33
13	A	829	CLA	O2D-CGD	2.35	1.39	1.33
13	B	817	CLA	O2D-CGD	2.36	1.39	1.33
15	B	845	BCR	C24-C23	2.36	1.40	1.33
15	L	1006	BCR	C20-C19	2.36	1.40	1.34
13	J	1101	CLA	O2D-CGD	2.36	1.39	1.33
13	B	817	CLA	C5-C3	2.36	1.56	1.51
13	A	827	CLA	C5-C3	2.36	1.56	1.51
13	B	839	CLA	C5-C3	2.36	1.56	1.51
13	B	809	CLA	O2D-CGD	2.36	1.39	1.33
13	B	824	CLA	C5-C3	2.37	1.56	1.51
15	A	852	BCR	C24-C23	2.37	1.40	1.33
15	A	849	BCR	C14-C13	2.37	1.38	1.35
13	A	839	CLA	O2D-CGD	2.37	1.39	1.33
13	A	805	CLA	O2D-CGD	2.37	1.39	1.33
15	B	846	BCR	C10-C9	2.38	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	850	BCR	C24-C23	2.38	1.40	1.33
13	B	834	CLA	O2D-CGD	2.38	1.39	1.33
15	F	1302	BCR	C5-C6	2.38	1.38	1.34
13	A	835	CLA	C5-C3	2.38	1.56	1.51
13	M	1201	CLA	O2D-CGD	2.38	1.39	1.33
13	B	824	CLA	O2D-CGD	2.38	1.39	1.33
13	A	812	CLA	O2D-CGD	2.38	1.39	1.33
13	B	802	CLA	O2D-CGD	2.38	1.39	1.33
13	A	826	CLA	C5-C3	2.38	1.56	1.51
13	A	810	CLA	O2D-CGD	2.38	1.39	1.33
18	B	848	LMG	C3-C2	2.38	1.58	1.52
15	A	851	BCR	C5-C6	2.38	1.38	1.34
18	B	848	LMG	C4-C3	2.38	1.58	1.52
13	B	825	CLA	C5-C3	2.38	1.56	1.51
13	A	804	CLA	O2D-CGD	2.39	1.39	1.33
13	B	822	CLA	C5-C3	2.39	1.56	1.51
13	B	818	CLA	O2D-CGD	2.39	1.39	1.33
15	B	850	BCR	C5-C6	2.40	1.38	1.34
15	J	1105	BCR	C20-C19	2.40	1.40	1.34
13	A	832	CLA	O2D-CGD	2.40	1.39	1.33
13	A	801	CLA	C5-C3	2.40	1.56	1.51
13	A	825	CLA	O2D-CGD	2.40	1.39	1.33
15	B	850	BCR	C10-C9	2.40	1.39	1.35
13	B	832	CLA	O2D-CGD	2.40	1.39	1.33
13	A	845	CLA	O2D-CGD	2.40	1.39	1.33
13	B	806	CLA	O2D-CGD	2.40	1.39	1.33
13	A	826	CLA	O2D-CGD	2.40	1.39	1.33
15	A	850	BCR	C20-C19	2.40	1.40	1.34
13	B	803	CLA	C5-C3	2.41	1.56	1.51
13	B	838	CLA	C5-C3	2.41	1.56	1.51
13	B	804	CLA	O2D-CGD	2.41	1.39	1.33
13	A	843	CLA	O2D-CGD	2.41	1.39	1.33
13	A	804	CLA	C5-C3	2.41	1.56	1.51
15	B	842	BCR	C24-C23	2.41	1.40	1.33
15	J	1105	BCR	C10-C9	2.41	1.39	1.35
15	A	848	BCR	C5-C6	2.41	1.38	1.34
13	B	839	CLA	O2D-CGD	2.41	1.39	1.33
13	A	855	CLA	O2D-CGD	2.42	1.39	1.33
18	B	848	LMG	O6-C1	2.42	1.48	1.41
13	A	838	CLA	O2D-CGD	2.42	1.39	1.33
13	B	837	CLA	O2D-CGD	2.42	1.39	1.33
13	B	827	CLA	C5-C3	2.42	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	808	CLA	C5-C3	2.42	1.56	1.51
13	M	1201	CLA	C5-C3	2.42	1.56	1.51
13	B	823	CLA	O2D-CGD	2.42	1.39	1.33
13	A	836	CLA	O2D-CGD	2.43	1.39	1.33
13	A	811	CLA	C5-C3	2.43	1.56	1.51
13	A	809	CLA	C5-C3	2.43	1.56	1.51
15	B	845	BCR	C5-C6	2.43	1.38	1.34
13	A	819	CLA	O2D-CGD	2.43	1.39	1.33
13	B	815	CLA	O2D-CGD	2.43	1.39	1.33
15	B	844	BCR	C20-C19	2.43	1.40	1.34
13	A	834	CLA	O2D-CGD	2.43	1.39	1.33
13	B	827	CLA	C4C-C3C	2.43	1.49	1.45
13	A	802	CLA	O2D-CGD	2.44	1.39	1.33
13	B	819	CLA	O2D-CGD	2.44	1.39	1.33
13	A	805	CLA	C5-C3	2.45	1.56	1.51
13	A	821	CLA	C5-C3	2.45	1.56	1.51
13	A	815	CLA	O2D-CGD	2.45	1.39	1.33
13	B	835	CLA	C5-C3	2.45	1.56	1.51
13	A	806	CLA	O2D-CGD	2.45	1.39	1.33
13	A	840	CLA	O2D-CGD	2.45	1.39	1.33
13	B	812	CLA	O2D-CGD	2.45	1.39	1.33
13	B	830	CLA	C5-C3	2.46	1.56	1.51
13	B	805	CLA	O2D-CGD	2.46	1.39	1.33
13	B	801	CLA	O2D-CGD	2.46	1.39	1.33
13	B	816	CLA	O2D-CGD	2.46	1.39	1.33
13	J	1102	CLA	O2D-CGD	2.46	1.39	1.33
13	A	818	CLA	O2D-CGD	2.47	1.39	1.33
13	B	825	CLA	O2D-CGD	2.47	1.39	1.33
15	B	841	BCR	C10-C9	2.47	1.39	1.35
13	B	813	CLA	O2D-CGD	2.47	1.39	1.33
13	A	830	CLA	C5-C3	2.47	1.56	1.51
13	F	1301	CLA	O2D-CGD	2.47	1.39	1.33
13	A	838	CLA	C5-C3	2.47	1.56	1.51
15	A	847	BCR	C10-C9	2.48	1.39	1.35
15	A	847	BCR	C5-C6	2.48	1.38	1.34
15	A	848	BCR	C10-C9	2.48	1.39	1.35
13	B	828	CLA	O2D-CGD	2.48	1.39	1.33
13	A	829	CLA	C5-C3	2.49	1.56	1.51
15	B	846	BCR	C5-C6	2.49	1.38	1.34
13	B	820	CLA	O2A-CGA	2.49	1.40	1.33
13	A	842	CLA	C5-C3	2.50	1.56	1.51
15	J	1104	BCR	C5-C6	2.50	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	827	CLA	C4C-C3C	2.50	1.49	1.45
13	M	1202	CLA	O2D-CGD	2.51	1.39	1.33
15	B	849	BCR	C5-C6	2.51	1.38	1.34
15	B	849	BCR	C14-C13	2.51	1.39	1.35
15	B	850	BCR	C14-C13	2.52	1.39	1.35
15	J	1104	BCR	C10-C9	2.52	1.39	1.35
13	A	820	CLA	O2D-CGD	2.53	1.39	1.33
15	B	845	BCR	C14-C13	2.53	1.39	1.35
13	A	834	CLA	C5-C3	2.54	1.56	1.51
15	J	1105	BCR	C26-C25	2.54	1.38	1.34
15	B	842	BCR	C10-C9	2.54	1.39	1.35
13	A	835	CLA	O2D-CGD	2.54	1.39	1.33
15	I	102	BCR	C12-C13	2.54	1.51	1.45
15	J	1104	BCR	C26-C25	2.54	1.38	1.34
13	A	825	CLA	C5-C3	2.55	1.56	1.51
13	A	809	CLA	O2D-CGD	2.55	1.39	1.33
13	B	811	CLA	C5-C3	2.55	1.56	1.51
15	B	843	BCR	C26-C25	2.55	1.38	1.34
13	A	823	CLA	O2D-CGD	2.55	1.39	1.33
13	B	830	CLA	O2D-CGD	2.55	1.39	1.33
15	A	849	BCR	C5-C6	2.55	1.38	1.34
15	I	102	BCR	C21-C22	2.56	1.39	1.35
15	B	850	BCR	C26-C25	2.56	1.38	1.34
15	L	1005	BCR	C14-C13	2.56	1.39	1.35
13	B	820	CLA	O2D-CGD	2.57	1.39	1.33
13	A	832	CLA	C5-C3	2.57	1.56	1.51
13	A	842	CLA	O2D-CGD	2.57	1.39	1.33
13	A	828	CLA	O2D-CGD	2.58	1.39	1.33
15	I	102	BCR	C26-C25	2.58	1.38	1.34
15	A	851	BCR	C26-C25	2.58	1.38	1.34
13	I	101	CLA	O2D-CGD	2.58	1.39	1.33
13	A	816	CLA	O2D-CGD	2.59	1.39	1.33
15	A	852	BCR	C20-C19	2.59	1.41	1.34
15	L	1006	BCR	C10-C9	2.59	1.39	1.35
13	A	841	CLA	O2D-CGD	2.59	1.39	1.33
15	A	849	BCR	C21-C22	2.59	1.39	1.35
15	B	844	BCR	C26-C25	2.60	1.38	1.34
13	B	829	CLA	O2D-CGD	2.60	1.39	1.33
15	A	852	BCR	C26-C25	2.62	1.38	1.34
15	A	849	BCR	C12-C13	2.62	1.51	1.45
15	L	1006	BCR	C26-C25	2.62	1.38	1.34
15	A	850	BCR	C10-C9	2.63	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	1203	BCR	C26-C25	2.63	1.39	1.34
15	A	849	BCR	C26-C25	2.64	1.39	1.34
13	A	833	CLA	O2D-CGD	2.64	1.39	1.33
15	A	848	BCR	C26-C25	2.64	1.39	1.34
15	I	102	BCR	C14-C13	2.64	1.39	1.35
13	B	810	CLA	O2D-CGD	2.65	1.39	1.33
15	L	1005	BCR	C26-C25	2.65	1.39	1.34
15	B	849	BCR	C12-C13	2.66	1.51	1.45
18	B	848	LMG	C4-C5	2.66	1.58	1.53
13	B	821	CLA	O2D-CGD	2.66	1.39	1.33
13	A	818	CLA	O2A-CGA	2.68	1.41	1.33
15	A	851	BCR	C14-C13	2.68	1.39	1.35
13	B	823	CLA	O2A-CGA	2.68	1.41	1.32
15	B	847	BCR	C26-C25	2.68	1.39	1.34
13	A	817	CLA	O2D-CGD	2.69	1.39	1.33
13	A	807	CLA	C4C-C3C	2.69	1.49	1.45
15	B	845	BCR	C12-C13	2.70	1.51	1.45
13	A	843	CLA	O2A-CGA	2.71	1.41	1.33
15	B	843	BCR	C21-C22	2.72	1.39	1.35
13	A	808	CLA	C4C-C3C	2.73	1.49	1.45
13	A	807	CLA	C2-C3	2.73	1.39	1.33
13	I	101	CLA	C4C-C3C	2.73	1.49	1.45
15	J	1105	BCR	C14-C13	2.73	1.39	1.35
13	A	807	CLA	O2A-CGA	2.74	1.41	1.33
13	A	823	CLA	C4C-C3C	2.74	1.49	1.45
13	B	815	CLA	O2A-CGA	2.74	1.41	1.33
15	F	1302	BCR	C21-C22	2.75	1.39	1.35
13	B	814	CLA	O2A-CGA	2.75	1.41	1.33
13	A	819	CLA	C4C-C3C	2.75	1.49	1.45
13	A	809	CLA	C4C-C3C	2.75	1.49	1.45
13	A	822	CLA	C4C-C3C	2.75	1.49	1.45
15	L	1006	BCR	C12-C13	2.75	1.51	1.45
13	A	819	CLA	O2A-CGA	2.76	1.41	1.33
13	A	838	CLA	O2A-CGA	2.76	1.41	1.33
15	L	1005	BCR	C21-C22	2.76	1.39	1.35
13	B	807	CLA	O2A-CGA	2.76	1.41	1.33
13	A	834	CLA	C4C-C3C	2.76	1.49	1.45
13	B	814	CLA	C4C-C3C	2.76	1.49	1.45
15	F	1302	BCR	C26-C25	2.76	1.39	1.34
15	B	849	BCR	C26-C25	2.77	1.39	1.34
15	A	849	BCR	C19-C18	2.77	1.51	1.45
15	I	102	BCR	C19-C18	2.77	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	806	CLA	O2A-CGA	2.77	1.41	1.33
15	B	841	BCR	C14-C13	2.78	1.39	1.35
15	J	1104	BCR	C14-C13	2.78	1.39	1.35
15	B	841	BCR	C21-C22	2.78	1.39	1.35
13	A	831	CLA	O2A-CGA	2.78	1.41	1.33
13	B	816	CLA	O2A-CGA	2.78	1.41	1.33
13	B	806	CLA	C4C-C3C	2.78	1.49	1.45
15	B	842	BCR	C26-C25	2.78	1.39	1.34
15	A	852	BCR	C12-C13	2.79	1.52	1.45
13	B	802	CLA	C4C-C3C	2.79	1.49	1.45
13	B	821	CLA	C4C-C3C	2.79	1.49	1.45
15	B	846	BCR	C26-C25	2.79	1.39	1.34
15	M	1203	BCR	C8-C9	2.80	1.52	1.45
13	B	804	CLA	C4C-C3C	2.80	1.49	1.45
13	B	817	CLA	O2A-CGA	2.80	1.41	1.33
15	M	1203	BCR	C12-C13	2.80	1.52	1.45
13	A	823	CLA	O2A-CGA	2.80	1.41	1.33
13	B	816	CLA	C4C-C3C	2.80	1.49	1.45
15	A	850	BCR	C26-C25	2.81	1.39	1.34
15	M	1203	BCR	C14-C13	2.81	1.39	1.35
13	A	818	CLA	C1C-C2C	2.81	1.50	1.44
13	A	831	CLA	C2-C3	2.82	1.40	1.32
15	B	847	BCR	C21-C22	2.82	1.39	1.35
13	X	102	CLA	C4C-C3C	2.82	1.49	1.45
13	B	807	CLA	C4C-C3C	2.82	1.49	1.45
13	B	805	CLA	O2A-CGA	2.82	1.41	1.33
13	A	845	CLA	O2A-CGA	2.82	1.41	1.33
15	A	851	BCR	C12-C13	2.82	1.52	1.45
13	A	830	CLA	C4C-C3C	2.82	1.49	1.45
15	F	1302	BCR	C14-C13	2.83	1.39	1.35
13	A	843	CLA	C4C-C3C	2.83	1.49	1.45
13	B	830	CLA	C4C-C3C	2.83	1.49	1.45
13	A	838	CLA	C4C-C3C	2.83	1.49	1.45
15	B	847	BCR	C14-C13	2.83	1.39	1.35
13	B	825	CLA	O2A-CGA	2.83	1.41	1.33
13	B	832	CLA	C4C-C3C	2.83	1.49	1.45
15	B	843	BCR	C14-C13	2.84	1.39	1.35
13	A	806	CLA	O2A-CGA	2.84	1.41	1.33
13	A	819	CLA	C1C-C2C	2.84	1.50	1.44
13	B	817	CLA	C1C-C2C	2.85	1.50	1.44
15	L	1006	BCR	C5-C6	2.85	1.39	1.34
13	A	840	CLA	O2A-CGA	2.85	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	811	CLA	C4C-C3C	2.85	1.50	1.45
13	B	826	CLA	C1C-C2C	2.85	1.50	1.44
13	B	829	CLA	C4C-C3C	2.85	1.50	1.45
13	B	812	CLA	O2A-CGA	2.86	1.41	1.33
15	A	847	BCR	C26-C25	2.86	1.39	1.34
15	B	847	BCR	C12-C13	2.86	1.52	1.45
13	B	833	CLA	C4C-C3C	2.86	1.50	1.45
15	J	1104	BCR	C12-C13	2.86	1.52	1.45
13	A	845	CLA	C1C-C2C	2.86	1.50	1.44
15	L	1006	BCR	C14-C13	2.86	1.39	1.35
13	B	836	CLA	C4C-C3C	2.86	1.50	1.45
13	B	835	CLA	C1C-C2C	2.87	1.50	1.44
15	B	849	BCR	C19-C18	2.87	1.52	1.45
13	B	828	CLA	C4C-C3C	2.87	1.50	1.45
15	B	849	BCR	C11-C10	2.87	1.52	1.43
13	L	1002	CLA	O2A-CGA	2.87	1.41	1.33
13	A	825	CLA	C4C-C3C	2.87	1.50	1.45
13	A	810	CLA	C4C-C3C	2.87	1.50	1.45
13	A	828	CLA	O2A-CGA	2.87	1.41	1.33
13	A	828	CLA	C4C-C3C	2.87	1.50	1.45
13	F	1301	CLA	C4C-C3C	2.88	1.50	1.45
13	B	835	CLA	C4C-C3C	2.88	1.50	1.45
13	A	843	CLA	C2-C3	2.88	1.40	1.33
15	A	847	BCR	C21-C22	2.88	1.39	1.35
15	I	102	BCR	C11-C10	2.88	1.52	1.43
13	B	820	CLA	C2-C3	2.88	1.40	1.33
15	A	849	BCR	C16-C17	2.88	1.52	1.43
15	B	846	BCR	C12-C13	2.89	1.52	1.45
13	M	1201	CLA	C4C-C3C	2.89	1.50	1.45
13	A	812	CLA	O2A-CGA	2.89	1.41	1.33
13	A	837	CLA	C4C-C3C	2.89	1.50	1.45
13	A	827	CLA	C1C-C2C	2.89	1.50	1.44
13	B	803	CLA	C4C-C3C	2.89	1.50	1.45
15	L	1005	BCR	C16-C17	2.89	1.52	1.43
15	F	1302	BCR	C12-C13	2.89	1.52	1.45
13	A	831	CLA	C4C-C3C	2.89	1.50	1.45
13	B	829	CLA	O2A-CGA	2.89	1.41	1.33
13	A	801	CLA	C4C-C3C	2.90	1.50	1.45
13	A	804	CLA	C4C-C3C	2.90	1.50	1.45
13	A	834	CLA	C1C-C2C	2.90	1.50	1.44
13	A	815	CLA	C1C-C2C	2.90	1.50	1.44
15	A	849	BCR	C17-C18	2.90	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	820	CLA	C1C-C2C	2.90	1.50	1.44
13	J	1101	CLA	C4C-C3C	2.90	1.50	1.45
13	B	838	CLA	C4C-C3C	2.90	1.50	1.45
13	A	812	CLA	C4C-C3C	2.90	1.50	1.45
15	A	850	BCR	C14-C13	2.90	1.39	1.35
15	A	849	BCR	C8-C9	2.91	1.52	1.45
13	A	835	CLA	O2A-CGA	2.91	1.41	1.33
13	A	809	CLA	O2A-CGA	2.91	1.41	1.33
13	B	836	CLA	O2A-CGA	2.91	1.41	1.33
13	A	818	CLA	C2-C3	2.91	1.40	1.33
15	B	842	BCR	C12-C13	2.91	1.52	1.45
13	L	1003	CLA	C4C-C3C	2.91	1.50	1.45
15	B	841	BCR	C26-C25	2.91	1.39	1.34
15	A	847	BCR	C19-C18	2.91	1.52	1.45
13	B	837	CLA	O2A-CGA	2.91	1.41	1.33
13	B	838	CLA	O2A-CGA	2.91	1.41	1.33
13	B	830	CLA	O2A-CGA	2.91	1.41	1.33
13	A	842	CLA	O2A-CGA	2.91	1.41	1.33
15	B	849	BCR	C8-C9	2.91	1.52	1.45
13	A	833	CLA	O2A-CGA	2.91	1.41	1.33
13	B	803	CLA	O2A-CGA	2.91	1.41	1.33
13	B	825	CLA	C4C-C3C	2.91	1.50	1.45
13	A	814	CLA	C4C-C3C	2.91	1.50	1.45
13	A	826	CLA	C4C-C3C	2.91	1.50	1.45
18	B	848	LMG	O8-C28	2.91	1.41	1.33
13	I	101	CLA	O2A-CGA	2.91	1.41	1.33
13	A	842	CLA	C4C-C3C	2.92	1.50	1.45
15	A	852	BCR	C8-C9	2.92	1.52	1.45
13	A	813	CLA	O2A-CGA	2.92	1.41	1.33
13	B	831	CLA	C4C-C3C	2.92	1.50	1.45
13	B	826	CLA	O2A-CGA	2.92	1.41	1.33
15	I	102	BCR	C8-C9	2.92	1.52	1.45
13	B	831	CLA	C1C-C2C	2.92	1.50	1.44
13	B	810	CLA	C4C-C3C	2.92	1.50	1.45
15	B	841	BCR	C19-C18	2.93	1.52	1.45
13	A	806	CLA	C2-C3	2.93	1.40	1.33
13	B	810	CLA	C1C-C2C	2.93	1.50	1.44
13	B	819	CLA	C1C-C2C	2.93	1.50	1.44
13	A	818	CLA	C4C-C3C	2.93	1.50	1.45
15	L	1006	BCR	C8-C9	2.93	1.52	1.45
15	F	1302	BCR	C19-C18	2.93	1.52	1.45
13	A	833	CLA	C1C-C2C	2.93	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	841	BCR	C12-C13	2.93	1.52	1.45
15	L	1005	BCR	C8-C9	2.93	1.52	1.45
13	A	840	CLA	C4C-C3C	2.93	1.50	1.45
13	J	1102	CLA	C4C-C3C	2.93	1.50	1.45
13	A	824	CLA	O2A-CGA	2.93	1.41	1.33
13	B	828	CLA	C1C-C2C	2.93	1.50	1.44
15	L	1006	BCR	C21-C22	2.93	1.39	1.35
15	J	1105	BCR	C12-C13	2.93	1.52	1.45
15	A	849	BCR	C11-C10	2.93	1.52	1.43
15	A	852	BCR	C14-C13	2.93	1.39	1.35
13	B	804	CLA	C2-C3	2.93	1.40	1.33
13	A	817	CLA	C4C-C3C	2.94	1.50	1.45
15	B	847	BCR	C19-C18	2.94	1.52	1.45
13	B	827	CLA	O2A-CGA	2.94	1.41	1.33
13	B	826	CLA	C4C-C3C	2.94	1.50	1.45
13	L	1003	CLA	C1C-C2C	2.94	1.50	1.44
13	B	820	CLA	C4C-C3C	2.94	1.50	1.45
15	A	847	BCR	C12-C13	2.94	1.52	1.45
15	B	845	BCR	C11-C10	2.94	1.52	1.43
13	A	803	CLA	O2A-CGA	2.94	1.41	1.33
15	A	848	BCR	C12-C13	2.94	1.52	1.45
13	B	813	CLA	C1C-C2C	2.94	1.50	1.44
13	A	810	CLA	C1C-C2C	2.94	1.50	1.44
13	B	813	CLA	C4C-C3C	2.94	1.50	1.45
13	A	836	CLA	C4C-C3C	2.95	1.50	1.45
13	A	839	CLA	O2A-CGA	2.95	1.41	1.33
13	A	820	CLA	O2A-CGA	2.95	1.41	1.33
13	B	814	CLA	C1C-C2C	2.95	1.50	1.44
13	B	809	CLA	C4C-C3C	2.95	1.50	1.45
13	A	817	CLA	O2A-CGA	2.95	1.41	1.33
13	L	1002	CLA	C4C-C3C	2.95	1.50	1.45
13	A	820	CLA	C4C-C3C	2.95	1.50	1.45
13	A	805	CLA	O2A-CGA	2.95	1.41	1.33
13	B	839	CLA	O2A-CGA	2.95	1.41	1.33
13	A	803	CLA	C4C-C3C	2.95	1.50	1.45
15	B	846	BCR	C14-C13	2.95	1.39	1.35
13	A	821	CLA	C4C-C3C	2.96	1.50	1.45
13	A	819	CLA	C2-C3	2.96	1.40	1.33
15	A	849	BCR	C15-C14	2.96	1.52	1.43
15	I	102	BCR	C16-C17	2.96	1.52	1.43
13	A	805	CLA	C4C-C3C	2.96	1.50	1.45
13	B	821	CLA	C1C-C2C	2.96	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	822	CLA	C1C-C2C	2.96	1.50	1.44
13	B	806	CLA	C2-C3	2.96	1.40	1.33
13	A	816	CLA	O2A-CGA	2.96	1.41	1.33
13	A	832	CLA	C4C-C3C	2.96	1.50	1.45
15	J	1104	BCR	C21-C22	2.97	1.39	1.35
13	B	812	CLA	C2-C3	2.97	1.40	1.33
13	B	807	CLA	C2-C3	2.97	1.40	1.33
13	L	1004	CLA	O2A-CGA	2.97	1.41	1.33
13	A	821	CLA	O2A-CGA	2.97	1.41	1.33
13	X	102	CLA	C1C-C2C	2.97	1.50	1.44
15	M	1203	BCR	C11-C10	2.97	1.52	1.43
13	B	818	CLA	O2A-CGA	2.97	1.41	1.33
13	B	837	CLA	C4C-C3C	2.97	1.50	1.45
13	A	816	CLA	C4C-C3C	2.97	1.50	1.45
13	B	803	CLA	C1C-C2C	2.97	1.50	1.44
13	A	834	CLA	O2A-CGA	2.97	1.41	1.33
13	B	817	CLA	C4C-C3C	2.98	1.50	1.45
13	A	833	CLA	C4C-C3C	2.98	1.50	1.45
13	A	803	CLA	C2-C3	2.98	1.40	1.33
15	B	842	BCR	C14-C13	2.98	1.39	1.35
13	A	829	CLA	O2A-CGA	2.98	1.41	1.33
13	J	1101	CLA	O2A-CGA	2.98	1.42	1.33
13	B	808	CLA	C4C-C3C	2.98	1.50	1.45
13	B	818	CLA	C4C-C3C	2.98	1.50	1.45
15	A	852	BCR	C11-C10	2.98	1.52	1.43
13	B	805	CLA	C1C-C2C	2.98	1.50	1.44
15	L	1005	BCR	C12-C13	2.98	1.52	1.45
13	A	841	CLA	C1C-C2C	2.98	1.50	1.44
13	B	816	CLA	C2-C3	2.99	1.40	1.33
15	B	845	BCR	C19-C18	2.99	1.52	1.45
13	B	822	CLA	C4C-C3C	2.99	1.50	1.45
13	A	839	CLA	C4C-C3C	2.99	1.50	1.45
15	A	848	BCR	C14-C13	2.99	1.39	1.35
13	A	822	CLA	C1C-C2C	2.99	1.50	1.44
13	B	802	CLA	C2-C3	2.99	1.40	1.33
13	A	835	CLA	C4C-C3C	2.99	1.50	1.45
13	A	804	CLA	O2A-CGA	2.99	1.42	1.33
13	B	812	CLA	C4C-C3C	2.99	1.50	1.45
15	B	843	BCR	C8-C9	3.00	1.52	1.45
13	L	1004	CLA	C2-C3	3.00	1.40	1.33
15	A	851	BCR	C16-C17	3.00	1.52	1.43
13	B	804	CLA	C1C-C2C	3.00	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	845	BCR	C16-C17	3.00	1.52	1.43
15	B	846	BCR	C16-C17	3.00	1.52	1.43
13	A	855	CLA	C4C-C3C	3.00	1.50	1.45
15	A	851	BCR	C19-C18	3.00	1.52	1.45
13	B	815	CLA	C1C-C2C	3.00	1.50	1.44
15	M	1203	BCR	C21-C22	3.00	1.39	1.35
13	A	801	CLA	O2A-CGA	3.00	1.42	1.33
15	B	846	BCR	C19-C18	3.00	1.52	1.45
13	B	834	CLA	C4C-C3C	3.00	1.50	1.45
15	L	1005	BCR	C19-C18	3.00	1.52	1.45
13	B	839	CLA	C1C-C2C	3.00	1.50	1.44
15	F	1302	BCR	C11-C10	3.00	1.52	1.43
13	L	1004	CLA	C1C-C2C	3.00	1.50	1.44
13	A	828	CLA	C2-C3	3.00	1.40	1.33
13	A	811	CLA	O2A-CGA	3.00	1.42	1.33
15	B	843	BCR	C16-C17	3.00	1.52	1.43
15	B	843	BCR	C12-C13	3.01	1.52	1.45
15	B	850	BCR	C12-C13	3.01	1.52	1.45
13	A	830	CLA	O2A-CGA	3.01	1.42	1.33
15	A	847	BCR	C14-C13	3.01	1.39	1.35
15	B	846	BCR	C11-C10	3.01	1.52	1.43
15	L	1006	BCR	C19-C18	3.01	1.52	1.45
13	A	855	CLA	C1C-C2C	3.01	1.50	1.44
15	B	843	BCR	C23-C22	3.01	1.52	1.45
13	B	808	CLA	O2A-CGA	3.01	1.42	1.33
15	J	1105	BCR	C8-C9	3.01	1.52	1.45
15	B	849	BCR	C17-C18	3.01	1.39	1.35
13	B	801	CLA	C4C-C3C	3.01	1.50	1.45
15	B	845	BCR	C15-C14	3.01	1.52	1.43
13	B	822	CLA	O2A-CGA	3.01	1.42	1.33
15	B	847	BCR	C8-C9	3.01	1.52	1.45
13	A	824	CLA	C1C-C2C	3.01	1.50	1.44
13	B	829	CLA	C1C-C2C	3.01	1.50	1.44
15	J	1105	BCR	C19-C18	3.01	1.52	1.45
13	B	801	CLA	C2-C3	3.02	1.40	1.33
13	A	812	CLA	C1C-C2C	3.02	1.50	1.44
15	B	842	BCR	C21-C22	3.02	1.39	1.35
13	A	815	CLA	C4C-C3C	3.02	1.50	1.45
15	A	851	BCR	C11-C10	3.02	1.52	1.43
13	B	831	CLA	O2A-CGA	3.02	1.42	1.33
15	B	850	BCR	C19-C18	3.02	1.52	1.45
13	B	809	CLA	C1C-C2C	3.02	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	1203	BCR	C16-C17	3.02	1.52	1.43
15	B	850	BCR	C16-C17	3.02	1.52	1.43
15	I	102	BCR	C15-C14	3.03	1.52	1.43
15	B	849	BCR	C16-C17	3.03	1.52	1.43
13	A	822	CLA	O2A-CGA	3.03	1.42	1.33
15	J	1105	BCR	C11-C10	3.03	1.52	1.43
13	M	1202	CLA	C4C-C3C	3.03	1.50	1.45
15	B	846	BCR	C21-C22	3.03	1.39	1.35
13	B	824	CLA	C4C-C3C	3.03	1.50	1.45
15	L	1006	BCR	C16-C17	3.03	1.52	1.43
15	B	847	BCR	C11-C10	3.03	1.52	1.43
13	A	835	CLA	C1C-C2C	3.03	1.50	1.44
15	M	1203	BCR	C19-C18	3.03	1.52	1.45
15	B	841	BCR	C16-C17	3.03	1.52	1.43
15	F	1302	BCR	C8-C9	3.03	1.52	1.45
13	B	812	CLA	C1C-C2C	3.03	1.50	1.44
13	A	841	CLA	O2A-CGA	3.03	1.42	1.33
13	B	817	CLA	C2-C3	3.04	1.40	1.33
13	A	823	CLA	C2-C3	3.04	1.40	1.33
15	B	843	BCR	C19-C18	3.04	1.52	1.45
15	J	1105	BCR	C16-C17	3.04	1.52	1.43
15	A	850	BCR	C8-C9	3.04	1.52	1.45
15	B	845	BCR	C8-C9	3.04	1.52	1.45
13	B	823	CLA	C4C-C3C	3.04	1.50	1.45
13	A	813	CLA	C2-C3	3.05	1.40	1.33
13	B	816	CLA	C1C-C2C	3.05	1.50	1.44
13	B	815	CLA	C4C-C3C	3.05	1.50	1.45
13	I	101	CLA	C2-C3	3.05	1.40	1.33
13	B	819	CLA	C4C-C3C	3.05	1.50	1.45
13	A	820	CLA	C2-C3	3.05	1.40	1.33
13	B	823	CLA	C1C-C2C	3.05	1.50	1.44
15	L	1005	BCR	C15-C14	3.05	1.52	1.43
15	I	102	BCR	C23-C22	3.05	1.52	1.45
13	A	841	CLA	C2-C3	3.05	1.40	1.33
13	B	802	CLA	O2A-CGA	3.05	1.42	1.33
15	A	848	BCR	C16-C17	3.05	1.52	1.43
15	B	846	BCR	C17-C18	3.05	1.39	1.35
15	B	849	BCR	C21-C22	3.05	1.39	1.35
13	A	812	CLA	C2-C3	3.05	1.40	1.33
13	B	808	CLA	C2-C3	3.05	1.40	1.33
13	B	820	CLA	C1C-C2C	3.05	1.50	1.44
13	A	829	CLA	C1C-C2C	3.05	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	842	CLA	C1C-C2C	3.06	1.50	1.44
15	B	846	BCR	C8-C9	3.06	1.52	1.45
13	A	816	CLA	C1C-C2C	3.06	1.50	1.44
13	A	801	CLA	C1C-C2C	3.06	1.50	1.44
13	A	827	CLA	O2A-CGA	3.06	1.42	1.33
13	B	804	CLA	O2A-CGA	3.06	1.42	1.33
15	B	850	BCR	C21-C22	3.06	1.39	1.35
13	A	802	CLA	C1C-C2C	3.06	1.50	1.44
13	B	834	CLA	C1C-C2C	3.06	1.50	1.44
13	A	824	CLA	C4C-C3C	3.06	1.50	1.45
15	A	848	BCR	C8-C9	3.07	1.52	1.45
15	B	847	BCR	C16-C17	3.07	1.53	1.43
13	A	805	CLA	C1C-C2C	3.07	1.50	1.44
13	L	1002	CLA	C2-C3	3.07	1.40	1.33
15	B	850	BCR	C15-C14	3.07	1.53	1.43
13	B	830	CLA	C1C-C2C	3.07	1.50	1.44
15	J	1105	BCR	C21-C22	3.07	1.39	1.35
13	A	802	CLA	C4C-C3C	3.07	1.50	1.45
15	M	1203	BCR	C15-C14	3.07	1.53	1.43
13	A	841	CLA	C4C-C3C	3.07	1.50	1.45
15	A	847	BCR	C11-C10	3.07	1.53	1.43
15	J	1104	BCR	C19-C18	3.07	1.52	1.45
13	A	813	CLA	C4C-C3C	3.07	1.50	1.45
15	B	841	BCR	C11-C10	3.07	1.53	1.43
13	A	803	CLA	C1C-C2C	3.07	1.50	1.44
13	J	1102	CLA	C1C-C2C	3.08	1.50	1.44
13	B	803	CLA	C2-C3	3.08	1.40	1.33
15	B	842	BCR	C11-C10	3.08	1.53	1.43
15	B	845	BCR	C17-C18	3.08	1.39	1.35
15	A	847	BCR	C16-C17	3.08	1.53	1.43
15	A	851	BCR	C15-C14	3.08	1.53	1.43
13	B	801	CLA	O2A-CGA	3.08	1.42	1.33
13	A	825	CLA	O2A-CGA	3.08	1.42	1.33
15	A	852	BCR	C15-C14	3.08	1.53	1.43
15	A	848	BCR	C19-C18	3.08	1.52	1.45
13	B	825	CLA	C2-C3	3.08	1.40	1.33
13	L	1003	CLA	C2-C3	3.08	1.40	1.33
15	B	843	BCR	C11-C10	3.08	1.53	1.43
13	A	837	CLA	C1C-C2C	3.08	1.50	1.44
13	B	811	CLA	C4C-C3C	3.08	1.50	1.45
13	J	1103	CLA	C1C-C2C	3.08	1.50	1.44
13	B	805	CLA	C2-C3	3.08	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	836	CLA	C1C-C2C	3.08	1.50	1.44
13	J	1101	CLA	C2-C3	3.08	1.40	1.33
13	L	1004	CLA	C4C-C3C	3.08	1.50	1.45
13	A	829	CLA	C2-C3	3.09	1.40	1.33
13	B	833	CLA	C1C-C2C	3.09	1.50	1.44
13	A	802	CLA	C2-C3	3.09	1.40	1.33
15	A	848	BCR	C21-C22	3.09	1.39	1.35
13	A	838	CLA	C2-C3	3.09	1.40	1.33
13	B	824	CLA	O2A-CGA	3.09	1.42	1.33
15	L	1006	BCR	C11-C10	3.09	1.53	1.43
13	A	802	CLA	O2A-CGA	3.09	1.42	1.33
15	J	1104	BCR	C16-C17	3.09	1.53	1.43
15	B	842	BCR	C19-C18	3.09	1.52	1.45
13	A	825	CLA	C1C-C2C	3.09	1.50	1.44
13	A	845	CLA	C2-C3	3.09	1.40	1.33
13	A	831	CLA	C1C-C2C	3.09	1.50	1.44
15	A	848	BCR	C11-C10	3.09	1.53	1.43
15	A	851	BCR	C17-C18	3.10	1.39	1.35
15	B	841	BCR	C15-C14	3.10	1.53	1.43
15	L	1006	BCR	C17-C18	3.10	1.39	1.35
13	A	827	CLA	C2-C3	3.10	1.40	1.33
15	B	849	BCR	C15-C14	3.10	1.53	1.43
15	B	844	BCR	C19-C18	3.10	1.52	1.45
15	A	851	BCR	C8-C9	3.10	1.52	1.45
13	J	1103	CLA	C4C-C3C	3.10	1.50	1.45
13	A	824	CLA	C2-C3	3.10	1.40	1.33
13	B	801	CLA	C1C-C2C	3.10	1.50	1.44
13	A	806	CLA	C1C-C2C	3.10	1.50	1.44
13	A	821	CLA	C1C-C2C	3.10	1.50	1.44
15	F	1302	BCR	C16-C17	3.10	1.53	1.43
15	L	1005	BCR	C11-C10	3.10	1.53	1.43
13	A	806	CLA	C4C-C3C	3.10	1.50	1.45
13	L	1003	CLA	O2A-CGA	3.11	1.42	1.33
13	J	1101	CLA	C1C-C2C	3.11	1.50	1.44
13	A	811	CLA	C1C-C2C	3.11	1.50	1.44
13	A	830	CLA	C1C-C2C	3.11	1.50	1.44
13	I	101	CLA	C1C-C2C	3.11	1.50	1.44
13	A	833	CLA	C2-C3	3.11	1.40	1.33
15	B	843	BCR	C15-C14	3.12	1.53	1.43
13	B	839	CLA	C4C-C3C	3.12	1.50	1.45
13	M	1201	CLA	C1C-C2C	3.12	1.50	1.44
13	A	840	CLA	C2-C3	3.12	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	850	BCR	C16-C17	3.12	1.53	1.43
13	A	829	CLA	C4C-C3C	3.12	1.50	1.45
13	B	806	CLA	C1C-C2C	3.12	1.50	1.44
13	B	838	CLA	C2-C3	3.13	1.40	1.33
15	B	850	BCR	C8-C9	3.13	1.52	1.45
13	A	808	CLA	O2A-CGA	3.13	1.42	1.33
13	A	821	CLA	C2-C3	3.13	1.40	1.33
13	B	814	CLA	C2-C3	3.13	1.40	1.33
13	B	839	CLA	C2-C3	3.13	1.40	1.33
13	A	817	CLA	C2-C3	3.13	1.40	1.33
15	B	841	BCR	C8-C9	3.13	1.52	1.45
13	M	1201	CLA	O2A-CGA	3.13	1.42	1.33
15	A	850	BCR	C19-C18	3.13	1.52	1.45
15	B	846	BCR	C15-C14	3.13	1.53	1.43
13	A	817	CLA	C1C-C2C	3.13	1.50	1.44
15	A	850	BCR	C12-C13	3.14	1.52	1.45
13	B	836	CLA	C2-C3	3.14	1.40	1.33
13	B	836	CLA	C1C-C2C	3.14	1.50	1.44
15	J	1105	BCR	C15-C14	3.14	1.53	1.43
15	F	1302	BCR	C23-C22	3.14	1.52	1.45
13	B	837	CLA	C1C-C2C	3.14	1.50	1.44
13	A	832	CLA	C1C-C2C	3.14	1.50	1.44
15	B	844	BCR	C16-C17	3.14	1.53	1.43
15	J	1104	BCR	C15-C14	3.14	1.53	1.43
13	A	845	CLA	C4C-C3C	3.15	1.50	1.45
15	J	1104	BCR	C11-C10	3.15	1.53	1.43
13	A	843	CLA	C1C-C2C	3.15	1.50	1.44
15	B	841	BCR	C17-C18	3.15	1.40	1.35
13	A	838	CLA	C1C-C2C	3.15	1.50	1.44
13	B	824	CLA	C2-C3	3.15	1.40	1.33
13	B	831	CLA	C2-C3	3.15	1.40	1.33
13	A	830	CLA	C2-C3	3.15	1.40	1.33
13	B	822	CLA	C2-C3	3.16	1.40	1.33
13	A	844	CLA	C4C-C3C	3.16	1.50	1.45
13	A	834	CLA	C2-C3	3.16	1.40	1.33
13	B	815	CLA	C2-C3	3.16	1.40	1.33
15	L	1005	BCR	C17-C18	3.16	1.40	1.35
15	A	847	BCR	C8-C9	3.16	1.52	1.45
13	A	804	CLA	C2-C3	3.16	1.40	1.33
15	B	842	BCR	C16-C17	3.16	1.53	1.43
15	B	850	BCR	C11-C10	3.16	1.53	1.43
15	A	849	BCR	C23-C22	3.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	823	CLA	C1C-C2C	3.16	1.50	1.44
15	I	102	BCR	C17-C18	3.16	1.40	1.35
13	A	826	CLA	O2A-CGA	3.16	1.42	1.33
13	B	824	CLA	C1C-C2C	3.16	1.50	1.44
15	A	850	BCR	C15-C14	3.17	1.53	1.43
15	A	850	BCR	C21-C22	3.17	1.40	1.35
15	A	848	BCR	C15-C14	3.17	1.53	1.43
13	B	818	CLA	C1C-C2C	3.17	1.50	1.44
13	B	830	CLA	C2-C3	3.17	1.40	1.33
15	B	847	BCR	C15-C14	3.18	1.53	1.43
15	F	1302	BCR	C15-C14	3.18	1.53	1.43
13	M	1202	CLA	C1C-C2C	3.18	1.50	1.44
13	A	801	CLA	C2-C3	3.18	1.40	1.33
13	M	1201	CLA	C2-C3	3.18	1.40	1.33
15	B	843	BCR	C17-C18	3.18	1.40	1.35
13	F	1301	CLA	C1C-C2C	3.18	1.50	1.44
15	A	847	BCR	C17-C18	3.18	1.40	1.35
13	A	828	CLA	C1C-C2C	3.18	1.50	1.44
13	A	804	CLA	C1C-C2C	3.18	1.50	1.44
15	A	847	BCR	C15-C14	3.19	1.53	1.43
13	A	813	CLA	C1C-C2C	3.19	1.50	1.44
13	A	826	CLA	C1C-C2C	3.19	1.50	1.44
13	B	825	CLA	C1C-C2C	3.19	1.50	1.44
15	B	845	BCR	C21-C22	3.19	1.40	1.35
13	A	811	CLA	C2-C3	3.19	1.40	1.33
13	A	835	CLA	C2-C3	3.19	1.40	1.33
15	A	852	BCR	C16-C17	3.19	1.53	1.43
13	A	844	CLA	C1C-C2C	3.19	1.50	1.44
13	A	809	CLA	C2-C3	3.19	1.40	1.33
15	L	1006	BCR	C15-C14	3.20	1.53	1.43
13	A	839	CLA	C1C-C2C	3.20	1.50	1.44
13	A	809	CLA	C1C-C2C	3.20	1.50	1.44
13	A	837	CLA	C2-C3	3.20	1.40	1.33
13	B	811	CLA	C1C-C2C	3.20	1.50	1.44
15	J	1104	BCR	C8-C9	3.20	1.52	1.45
15	B	849	BCR	C23-C22	3.20	1.52	1.45
13	L	1002	CLA	C1C-C2C	3.20	1.50	1.44
15	F	1302	BCR	C17-C18	3.20	1.40	1.35
13	B	835	CLA	O2A-CGA	3.20	1.42	1.33
15	B	842	BCR	C8-C9	3.21	1.52	1.45
15	A	851	BCR	C21-C22	3.21	1.40	1.35
13	A	807	CLA	O2D-CGD	3.21	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	808	CLA	C1C-C2C	3.21	1.50	1.44
13	B	808	CLA	C1C-C2C	3.21	1.50	1.44
15	B	842	BCR	C15-C14	3.21	1.53	1.43
15	B	844	BCR	C15-C14	3.21	1.53	1.43
13	B	835	CLA	C2-C3	3.21	1.40	1.33
13	B	811	CLA	O2A-CGA	3.22	1.42	1.33
15	L	1005	BCR	C23-C22	3.22	1.52	1.45
13	B	802	CLA	C1C-C2C	3.22	1.50	1.44
15	B	844	BCR	C21-C22	3.22	1.40	1.35
15	A	850	BCR	C11-C10	3.23	1.53	1.43
13	A	837	CLA	O2A-CGA	3.23	1.42	1.33
13	A	832	CLA	O2A-CGA	3.23	1.42	1.33
13	B	807	CLA	C1C-C2C	3.23	1.50	1.44
15	B	850	BCR	C17-C18	3.23	1.40	1.35
13	B	827	CLA	C2-C3	3.23	1.41	1.33
15	M	1203	BCR	C17-C18	3.24	1.40	1.35
13	A	808	CLA	C2-C3	3.24	1.41	1.33
15	A	849	BCR	C20-C21	3.24	1.53	1.43
13	B	832	CLA	C1C-C2C	3.24	1.50	1.44
13	B	826	CLA	C2-C3	3.24	1.41	1.33
13	A	842	CLA	C2-C3	3.24	1.41	1.33
15	I	102	BCR	C20-C21	3.25	1.53	1.43
13	A	832	CLA	C2-C3	3.25	1.41	1.33
15	B	850	BCR	C23-C22	3.25	1.53	1.45
15	A	852	BCR	C19-C18	3.26	1.53	1.45
13	A	807	CLA	C1C-C2C	3.26	1.50	1.44
13	A	814	CLA	C1C-C2C	3.27	1.50	1.44
13	B	805	CLA	C4C-C3C	3.27	1.50	1.45
15	B	841	BCR	C23-C22	3.27	1.53	1.45
15	B	842	BCR	C17-C18	3.28	1.40	1.35
13	B	838	CLA	C1C-C2C	3.28	1.50	1.44
15	A	851	BCR	C23-C22	3.28	1.53	1.45
13	A	826	CLA	C2-C3	3.29	1.41	1.33
13	A	805	CLA	C2-C3	3.29	1.41	1.33
15	A	848	BCR	C17-C18	3.30	1.40	1.35
13	A	825	CLA	C2-C3	3.30	1.41	1.33
15	J	1105	BCR	C17-C18	3.31	1.40	1.35
15	L	1006	BCR	C23-C22	3.31	1.53	1.45
15	A	847	BCR	C23-C22	3.32	1.53	1.45
15	B	844	BCR	C23-C22	3.32	1.53	1.45
13	B	827	CLA	C1C-C2C	3.32	1.51	1.44
15	M	1203	BCR	C23-C22	3.32	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	847	BCR	C17-C18	3.33	1.40	1.35
15	B	841	BCR	C20-C21	3.33	1.53	1.43
15	B	843	BCR	C20-C21	3.33	1.53	1.43
13	A	840	CLA	C1C-C2C	3.34	1.51	1.44
15	J	1104	BCR	C17-C18	3.35	1.40	1.35
15	F	1302	BCR	C20-C21	3.35	1.53	1.43
15	B	846	BCR	C23-C22	3.36	1.53	1.45
15	A	852	BCR	C17-C18	3.36	1.40	1.35
15	B	849	BCR	C20-C21	3.39	1.54	1.43
15	B	847	BCR	C23-C22	3.39	1.53	1.45
15	A	848	BCR	C23-C22	3.41	1.53	1.45
15	A	847	BCR	C20-C21	3.41	1.54	1.43
15	J	1104	BCR	C23-C22	3.41	1.53	1.45
15	B	845	BCR	C23-C22	3.42	1.53	1.45
15	B	846	BCR	C20-C21	3.42	1.54	1.43
15	B	847	BCR	C20-C21	3.43	1.54	1.43
14	B	840	PQN	C12-C13	3.44	1.41	1.33
15	M	1203	BCR	C20-C21	3.45	1.54	1.43
15	J	1105	BCR	C23-C22	3.45	1.53	1.45
15	J	1104	BCR	C20-C21	3.46	1.54	1.43
15	B	842	BCR	C23-C22	3.47	1.53	1.45
13	B	811	CLA	C2-C3	3.48	1.41	1.33
15	L	1006	BCR	C20-C21	3.49	1.54	1.43
15	A	852	BCR	C23-C22	3.49	1.53	1.45
15	B	845	BCR	C20-C21	3.50	1.54	1.43
15	B	850	BCR	C20-C21	3.50	1.54	1.43
15	B	844	BCR	C17-C18	3.51	1.40	1.35
15	L	1005	BCR	C20-C21	3.51	1.54	1.43
15	J	1105	BCR	C20-C21	3.53	1.54	1.43
15	A	850	BCR	C23-C22	3.53	1.53	1.45
15	A	850	BCR	C17-C18	3.53	1.40	1.35
15	A	851	BCR	C20-C21	3.53	1.54	1.43
15	A	848	BCR	C20-C21	3.54	1.54	1.43
15	B	844	BCR	C20-C21	3.55	1.54	1.43
15	B	842	BCR	C20-C21	3.56	1.54	1.43
15	A	850	BCR	C20-C21	3.56	1.54	1.43
15	A	852	BCR	C21-C22	3.56	1.40	1.35
14	A	846	PQN	C12-C13	3.63	1.41	1.33
15	A	852	BCR	C20-C21	3.64	1.54	1.43
13	A	844	CLA	CBD-CHA	3.90	1.55	1.50
13	J	1103	CLA	CBD-CHA	3.92	1.55	1.50

All (1371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C3D-CAD-CBD	-9.31	95.07	107.61
13	B	831	CLA	C3D-CAD-CBD	-8.69	95.90	107.61
13	B	835	CLA	C3D-CAD-CBD	-8.14	96.65	107.61
13	A	801	CLA	C3D-CAD-CBD	-8.00	96.83	107.61
13	X	102	CLA	C3D-CAD-CBD	-7.77	97.14	107.61
13	A	837	CLA	C3D-CAD-CBD	-7.71	97.22	107.61
15	A	852	BCR	C15-C14-C13	-7.52	116.57	127.31
13	L	1003	CLA	C3D-CAD-CBD	-7.34	97.72	107.61
13	B	827	CLA	C3D-CAD-CBD	-7.27	97.82	107.61
15	B	849	BCR	C15-C14-C13	-7.17	117.08	127.31
13	A	814	CLA	C3D-CAD-CBD	-7.10	98.05	107.61
13	A	822	CLA	C3D-CAD-CBD	-6.81	98.44	107.61
13	J	1102	CLA	C3D-CAD-CBD	-6.80	98.45	107.61
13	B	824	CLA	C3D-CAD-CBD	-6.78	98.48	107.61
13	B	819	CLA	C3D-CAD-CBD	-6.70	98.59	107.61
13	A	830	CLA	C3D-CAD-CBD	-6.58	98.76	107.61
13	B	811	CLA	C3D-CAD-CBD	-6.51	98.84	107.61
13	A	810	CLA	C3D-CAD-CBD	-6.49	98.87	107.61
13	L	1002	CLA	C3D-CAD-CBD	-6.43	98.95	107.61
13	B	802	CLA	O1D-CGD-CBD	-6.37	112.77	124.58
13	A	822	CLA	O1D-CGD-CBD	-6.34	112.82	124.58
13	B	821	CLA	C3D-CAD-CBD	-6.33	99.08	107.61
13	B	809	CLA	C3D-CAD-CBD	-6.31	99.11	107.61
13	B	801	CLA	C3D-CAD-CBD	-6.17	99.30	107.61
13	B	828	CLA	C3D-CAD-CBD	-6.15	99.33	107.61
13	B	832	CLA	C3D-CAD-CBD	-6.13	99.35	107.61
13	B	803	CLA	C3D-CAD-CBD	-6.07	99.43	107.61
13	B	812	CLA	C3D-CAD-CBD	-5.97	99.57	107.61
15	A	850	BCR	C7-C8-C9	-5.92	117.31	126.21
13	B	814	CLA	C3D-CAD-CBD	-5.85	99.74	107.61
13	X	102	CLA	O1D-CGD-CBD	-5.81	113.81	124.58
15	B	849	BCR	C11-C10-C9	-5.80	119.03	127.31
15	B	844	BCR	C15-C14-C13	-5.78	119.01	127.30
13	A	816	CLA	C3D-CAD-CBD	-5.71	99.92	107.61
13	A	813	CLA	C3D-CAD-CBD	-5.61	100.06	107.61
15	F	1302	BCR	C15-C14-C13	-5.56	119.38	127.31
13	A	815	CLA	C3D-CAD-CBD	-5.52	100.17	107.61
13	A	832	CLA	C3D-CAD-CBD	-5.51	100.19	107.61
13	A	808	CLA	C3D-CAD-CBD	-5.50	100.20	107.61
13	I	101	CLA	O1D-CGD-CBD	-5.48	114.42	124.58
13	A	843	CLA	C3D-CAD-CBD	-5.48	100.24	107.61
13	B	802	CLA	C3D-CAD-CBD	-5.39	100.35	107.61
15	B	845	BCR	C15-C14-C13	-5.36	119.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	834	CLA	C3D-CAD-CBD	-5.34	100.42	107.61
13	A	827	CLA	C3D-CAD-CBD	-5.33	100.43	107.61
13	B	837	CLA	C3D-CAD-CBD	-5.30	100.47	107.61
13	A	803	CLA	C3D-CAD-CBD	-5.28	100.50	107.61
15	M	1203	BCR	C33-C5-C6	-5.27	118.61	124.51
15	B	845	BCR	C38-C26-C25	-5.27	118.61	124.51
13	M	1202	CLA	C3D-CAD-CBD	-5.26	100.53	107.61
13	A	855	CLA	C3D-CAD-CBD	-5.20	100.61	107.61
13	B	818	CLA	C3D-CAD-CBD	-5.10	100.74	107.61
15	B	847	BCR	C33-C5-C6	-5.08	118.82	124.51
13	I	101	CLA	C3D-CAD-CBD	-5.08	100.78	107.61
13	B	808	CLA	C3D-CAD-CBD	-5.05	100.81	107.61
13	B	813	CLA	C3D-CAD-CBD	-5.04	100.83	107.61
13	A	828	CLA	C3D-CAD-CBD	-5.03	100.83	107.61
15	L	1005	BCR	C16-C17-C18	-5.01	120.16	127.31
13	A	829	CLA	C3D-CAD-CBD	-4.99	100.89	107.61
15	B	850	BCR	C7-C8-C9	-4.98	118.73	126.21
15	B	842	BCR	C15-C14-C13	-4.97	120.22	127.31
13	A	840	CLA	O1D-CGD-CBD	-4.97	115.37	124.58
15	A	852	BCR	C15-C16-C17	-4.93	112.94	123.46
15	A	852	BCR	C33-C5-C6	-4.91	119.02	124.51
13	A	817	CLA	C3D-CAD-CBD	-4.89	101.02	107.61
15	B	842	BCR	C33-C5-C6	-4.86	119.06	124.51
13	A	838	CLA	C3D-CAD-CBD	-4.86	101.06	107.61
13	A	832	CLA	O1D-CGD-CBD	-4.83	115.62	124.58
13	M	1201	CLA	C3D-CAD-CBD	-4.79	101.15	107.61
13	A	845	CLA	C3D-CAD-CBD	-4.77	101.18	107.61
15	B	850	BCR	C38-C26-C25	-4.73	119.21	124.51
13	A	831	CLA	C3D-CAD-CBD	-4.71	101.27	107.61
13	A	811	CLA	C3D-CAD-CBD	-4.70	101.28	107.61
13	A	826	CLA	C3D-CAD-CBD	-4.69	101.29	107.61
13	A	840	CLA	C3D-CAD-CBD	-4.67	101.32	107.61
13	A	841	CLA	C3D-CAD-CBD	-4.60	101.42	107.61
13	A	812	CLA	C3D-CAD-CBD	-4.58	101.44	107.61
13	A	825	CLA	C3D-CAD-CBD	-4.57	101.45	107.61
13	B	838	CLA	C3D-CAD-CBD	-4.57	101.46	107.61
15	I	102	BCR	C33-C5-C6	-4.55	119.42	124.51
15	A	851	BCR	C15-C14-C13	-4.55	120.82	127.31
13	B	829	CLA	C3D-CAD-CBD	-4.54	101.49	107.61
15	L	1006	BCR	C16-C17-C18	-4.53	120.84	127.31
13	B	806	CLA	C3D-CAD-CBD	-4.53	101.51	107.61
15	I	102	BCR	C38-C26-C25	-4.49	119.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	843	BCR	C16-C17-C18	-4.48	120.92	127.31
15	L	1005	BCR	C38-C26-C25	-4.48	119.50	124.51
15	A	849	BCR	C16-C17-C18	-4.46	120.94	127.31
13	A	809	CLA	C3D-CAD-CBD	-4.45	101.61	107.61
15	B	843	BCR	C33-C5-C6	-4.44	119.54	124.51
15	B	850	BCR	C15-C14-C13	-4.44	120.98	127.31
15	B	847	BCR	C16-C17-C18	-4.43	120.99	127.31
15	F	1302	BCR	C33-C5-C6	-4.43	119.55	124.51
13	B	831	CLA	O1D-CGD-CBD	-4.41	116.39	124.58
15	A	852	BCR	C38-C26-C25	-4.41	119.58	124.51
13	B	812	CLA	O1D-CGD-CBD	-4.40	116.42	124.58
13	B	816	CLA	C3D-CAD-CBD	-4.39	101.70	107.61
15	A	851	BCR	C38-C26-C25	-4.38	119.61	124.51
15	J	1105	BCR	C38-C26-C25	-4.36	119.63	124.51
15	L	1006	BCR	C38-C26-C25	-4.29	119.70	124.51
15	F	1302	BCR	C11-C10-C9	-4.29	121.19	127.31
15	B	850	BCR	C16-C17-C18	-4.29	121.19	127.31
13	A	829	CLA	CAA-CBA-CGA	-4.28	100.57	113.35
13	A	819	CLA	O1D-CGD-CBD	-4.26	116.67	124.58
15	A	851	BCR	C33-C5-C6	-4.26	119.74	124.51
15	L	1006	BCR	C24-C23-C22	-4.25	119.82	126.21
13	A	842	CLA	C3D-CAD-CBD	-4.25	101.89	107.61
15	A	850	BCR	C24-C23-C22	-4.24	119.84	126.21
15	A	851	BCR	C24-C23-C22	-4.24	119.85	126.21
15	B	849	BCR	C38-C26-C25	-4.23	119.78	124.51
13	A	812	CLA	O1D-CGD-CBD	-4.22	116.75	124.58
14	B	840	PQN	C11-C12-C13	-4.21	119.66	126.79
13	B	806	CLA	C1-C2-C3	-4.21	118.20	125.96
15	B	843	BCR	C23-C24-C25	-4.19	115.52	127.25
15	L	1005	BCR	C33-C5-C6	-4.18	119.83	124.51
13	B	838	CLA	CAA-CBA-CGA	-4.16	100.92	113.35
13	B	833	CLA	C3D-CAD-CBD	-4.16	102.00	107.61
15	A	848	BCR	C38-C26-C25	-4.14	119.87	124.51
15	B	842	BCR	C24-C23-C22	-4.13	120.00	126.21
15	B	847	BCR	C38-C26-C25	-4.13	119.89	124.51
13	B	802	CLA	C1-C2-C3	-4.13	118.35	125.96
15	B	841	BCR	C16-C17-C18	-4.13	121.42	127.31
15	J	1105	BCR	C33-C5-C6	-4.12	119.89	124.51
15	B	850	BCR	C11-C10-C9	-4.12	121.43	127.31
15	A	849	BCR	C20-C21-C22	-4.12	121.43	127.31
15	A	848	BCR	C33-C5-C6	-4.11	119.91	124.51
13	B	810	CLA	C3D-CAD-CBD	-4.10	102.09	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	1301	CLA	C3D-CAD-CBD	-4.10	102.09	107.61
13	B	807	CLA	O1D-CGD-CBD	-4.09	116.99	124.58
15	J	1104	BCR	C38-C26-C25	-4.09	119.93	124.51
15	A	850	BCR	C38-C26-C25	-4.08	119.94	124.51
15	B	846	BCR	C16-C17-C18	-4.08	121.48	127.31
15	B	841	BCR	C33-C5-C6	-4.08	119.94	124.51
15	J	1104	BCR	C33-C5-C6	-4.07	119.95	124.51
15	L	1005	BCR	C7-C8-C9	-4.07	120.10	126.21
13	A	815	CLA	O1D-CGD-CBD	-4.06	117.05	124.58
13	A	804	CLA	C3D-CAD-CBD	-4.05	102.16	107.61
15	A	848	BCR	C24-C23-C22	-4.04	120.14	126.21
15	M	1203	BCR	C8-C7-C6	-4.03	115.97	127.25
13	A	845	CLA	CAA-CBA-CGA	-4.02	101.36	113.35
15	B	842	BCR	C11-C10-C9	-4.01	121.58	127.31
13	A	806	CLA	C1-C2-C3	-4.01	118.57	125.96
15	A	848	BCR	C16-C17-C18	-4.00	121.60	127.31
13	A	808	CLA	O2D-CGD-O1D	-3.99	115.89	123.82
13	J	1101	CLA	C3D-CAD-CBD	-3.98	102.25	107.61
15	B	844	BCR	C38-C26-C25	-3.98	120.06	124.51
15	B	843	BCR	C38-C26-C25	-3.97	120.06	124.51
15	B	845	BCR	C24-C23-C22	-3.96	120.26	126.21
15	A	851	BCR	C16-C17-C18	-3.95	121.67	127.31
15	A	849	BCR	C33-C5-C6	-3.95	120.09	124.51
13	A	843	CLA	O1D-CGD-CBD	-3.95	117.26	124.58
15	A	848	BCR	C7-C8-C9	-3.95	120.28	126.21
15	A	847	BCR	C16-C17-C18	-3.94	121.69	127.31
13	L	1003	CLA	O1D-CGD-CBD	-3.91	117.33	124.58
15	J	1104	BCR	C7-C8-C9	-3.90	120.36	126.21
13	M	1201	CLA	O1D-CGD-CBD	-3.90	117.35	124.58
15	B	846	BCR	C20-C21-C22	-3.88	121.78	127.31
13	A	825	CLA	O1D-CGD-CBD	-3.86	117.41	124.58
15	A	849	BCR	C7-C8-C9	-3.86	120.42	126.21
15	A	847	BCR	C33-C5-C6	-3.84	120.21	124.51
15	B	842	BCR	C20-C21-C22	-3.83	121.84	127.31
15	I	102	BCR	C7-C8-C9	-3.82	120.47	126.21
15	B	850	BCR	C24-C23-C22	-3.82	120.47	126.21
15	A	849	BCR	C38-C26-C25	-3.81	120.24	124.51
15	B	842	BCR	C38-C26-C25	-3.81	120.24	124.51
15	B	846	BCR	C33-C5-C6	-3.80	120.25	124.51
15	J	1104	BCR	C15-C14-C13	-3.79	121.90	127.31
15	A	849	BCR	C15-C14-C13	-3.78	121.91	127.31
13	B	829	CLA	CAA-CBA-CGA	-3.78	102.06	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1005	BCR	C24-C23-C22	-3.78	120.54	126.21
13	B	839	CLA	C3D-CAD-CBD	-3.77	102.53	107.61
15	B	849	BCR	C33-C5-C6	-3.77	120.29	124.51
15	L	1006	BCR	C20-C21-C22	-3.76	121.94	127.31
15	I	102	BCR	C23-C24-C25	-3.76	116.73	127.25
13	A	824	CLA	O1D-CGD-CBD	-3.76	117.61	124.58
13	B	805	CLA	C1-C2-C3	-3.74	119.06	125.96
13	L	1004	CLA	C3D-CAD-CBD	-3.73	102.58	107.61
13	B	837	CLA	O1D-CGD-CBD	-3.72	117.68	124.58
13	A	819	CLA	C3D-CAD-CBD	-3.72	102.60	107.61
15	B	849	BCR	C7-C8-C9	-3.72	120.63	126.21
13	A	835	CLA	C3D-CAD-CBD	-3.71	102.61	107.61
15	M	1203	BCR	C38-C26-C25	-3.70	120.36	124.51
15	L	1005	BCR	C16-C15-C14	-3.70	115.56	123.46
15	B	847	BCR	C20-C21-C22	-3.70	122.03	127.31
15	B	849	BCR	C16-C17-C18	-3.70	122.04	127.31
15	B	845	BCR	C33-C5-C6	-3.68	120.39	124.51
13	A	818	CLA	O2D-CGD-O1D	-3.68	116.52	123.82
15	J	1105	BCR	C24-C23-C22	-3.66	120.71	126.21
15	A	850	BCR	C20-C21-C22	-3.66	122.08	127.31
13	A	811	CLA	O1D-CGD-CBD	-3.66	117.79	124.58
13	B	822	CLA	C3D-CAD-CBD	-3.65	102.69	107.61
15	A	850	BCR	C16-C17-C18	-3.65	122.10	127.31
13	A	831	CLA	C1-C2-C3	-3.64	120.86	126.77
15	J	1105	BCR	C16-C17-C18	-3.63	122.13	127.31
15	F	1302	BCR	C38-C26-C25	-3.63	120.45	124.51
15	B	846	BCR	C10-C11-C12	-3.63	112.22	123.26
13	A	839	CLA	O2D-CGD-O1D	-3.63	116.62	123.82
15	M	1203	BCR	C10-C11-C12	-3.62	112.23	123.26
13	B	836	CLA	C3D-CAD-CBD	-3.61	102.75	107.61
13	B	801	CLA	O1D-CGD-CBD	-3.60	117.90	124.58
13	B	813	CLA	O1D-CGD-CBD	-3.59	117.92	124.58
15	A	850	BCR	C11-C10-C9	-3.59	122.19	127.31
13	B	830	CLA	O2D-CGD-O1D	-3.58	116.71	123.82
15	A	847	BCR	C20-C21-C22	-3.56	122.23	127.31
15	B	845	BCR	C20-C21-C22	-3.56	122.24	127.31
15	M	1203	BCR	C24-C23-C22	-3.55	120.87	126.21
13	B	817	CLA	O1D-CGD-CBD	-3.55	118.00	124.58
13	B	825	CLA	C3D-CAD-CBD	-3.55	102.83	107.61
13	A	829	CLA	O1D-CGD-CBD	-3.54	118.02	124.58
15	J	1105	BCR	C15-C14-C13	-3.54	122.26	127.31
13	B	817	CLA	O2D-CGD-O1D	-3.54	116.80	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	1005	BCR	C11-C10-C9	-3.53	122.27	127.31
15	I	102	BCR	C16-C17-C18	-3.52	122.28	127.31
13	B	823	CLA	C3D-CAD-CBD	-3.52	102.88	107.61
15	B	850	BCR	C20-C21-C22	-3.50	122.31	127.31
13	A	821	CLA	O2D-CGD-O1D	-3.50	116.87	123.82
13	A	810	CLA	O1D-CGD-CBD	-3.50	118.08	124.58
13	A	833	CLA	C3D-CAD-CBD	-3.50	102.90	107.61
13	B	808	CLA	O1D-CGD-CBD	-3.49	118.11	124.58
15	B	843	BCR	C10-C11-C12	-3.49	112.64	123.26
15	A	850	BCR	C33-C5-C6	-3.48	120.61	124.51
15	B	845	BCR	C15-C16-C17	-3.48	116.03	123.46
13	B	811	CLA	O1D-CGD-CBD	-3.47	118.15	124.58
15	B	850	BCR	C33-C5-C6	-3.47	120.63	124.51
15	B	841	BCR	C20-C21-C22	-3.46	122.38	127.31
13	B	822	CLA	O1D-CGD-CBD	-3.45	118.17	124.58
15	B	849	BCR	C15-C16-C17	-3.45	116.09	123.46
15	F	1302	BCR	C15-C16-C17	-3.45	116.10	123.46
15	F	1302	BCR	C20-C21-C22	-3.45	122.39	127.31
13	B	824	CLA	O1D-CGD-CBD	-3.44	118.20	124.58
13	A	823	CLA	C3D-CAD-CBD	-3.43	102.99	107.61
15	B	849	BCR	C23-C24-C25	-3.43	117.66	127.25
13	B	836	CLA	O1D-CGD-CBD	-3.42	118.24	124.58
13	A	828	CLA	O1D-CGD-CBD	-3.42	118.24	124.58
15	M	1203	BCR	C16-C17-C18	-3.42	122.43	127.31
15	B	841	BCR	C10-C11-C12	-3.41	112.87	123.26
13	B	833	CLA	O1D-CGD-CBD	-3.40	118.27	124.58
13	A	801	CLA	O1D-CGD-CBD	-3.39	118.29	124.58
13	A	805	CLA	C3D-CAD-CBD	-3.39	103.05	107.61
15	A	849	BCR	C10-C11-C12	-3.39	112.95	123.26
15	I	102	BCR	C10-C11-C12	-3.38	112.95	123.26
13	A	823	CLA	C1-C2-C3	-3.38	119.72	125.96
13	B	804	CLA	C1-C2-C3	-3.38	119.73	125.96
15	B	850	BCR	C23-C24-C25	-3.38	117.80	127.25
13	A	855	CLA	O1D-CGD-CBD	-3.37	118.32	124.58
13	J	1102	CLA	O1D-CGD-CBD	-3.37	118.33	124.58
15	B	843	BCR	C23-C22-C21	-3.37	113.77	118.94
13	B	834	CLA	O1D-CGD-CBD	-3.37	118.33	124.58
13	A	807	CLA	C3D-CAD-CBD	-3.37	103.08	107.61
13	B	804	CLA	C3D-CAD-CBD	-3.36	103.08	107.61
13	B	819	CLA	O1D-CGD-CBD	-3.36	118.34	124.58
13	M	1202	CLA	O1D-CGD-CBD	-3.36	118.35	124.58
15	B	846	BCR	C24-C23-C22	-3.36	121.17	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	832	CLA	O1D-CGD-CBD	-3.36	118.35	124.58
15	I	102	BCR	C15-C14-C13	-3.35	122.53	127.31
15	F	1302	BCR	C7-C8-C9	-3.35	121.18	126.21
13	A	821	CLA	C1-C2-C3	-3.34	119.81	125.96
14	A	846	PQN	C11-C12-C13	-3.34	121.14	126.79
13	A	819	CLA	CBA-CAA-C2A	-3.33	103.95	113.82
13	L	1002	CLA	O1D-CGD-CBD	-3.33	118.41	124.58
13	F	1301	CLA	O2D-CGD-O1D	-3.32	117.22	123.82
13	A	809	CLA	CAA-CBA-CGA	-3.32	103.43	113.35
15	J	1104	BCR	C16-C17-C18	-3.32	122.57	127.31
13	A	813	CLA	O1D-CGD-CBD	-3.32	118.43	124.58
15	A	847	BCR	C10-C11-C12	-3.32	113.16	123.26
15	A	847	BCR	C24-C23-C22	-3.31	121.24	126.21
13	B	826	CLA	C3D-CAD-CBD	-3.31	103.16	107.61
15	B	845	BCR	C10-C11-C12	-3.30	113.20	123.26
13	A	817	CLA	CAA-CBA-CGA	-3.30	103.50	113.35
13	B	807	CLA	C3D-CAD-CBD	-3.30	103.17	107.61
15	A	848	BCR	C20-C21-C22	-3.30	122.61	127.31
13	A	818	CLA	C3D-CAD-CBD	-3.29	103.18	107.61
15	A	851	BCR	C20-C21-C22	-3.29	122.61	127.31
13	B	814	CLA	O1D-CGD-CBD	-3.29	118.48	124.58
15	F	1302	BCR	C24-C23-C22	-3.28	121.29	126.21
13	A	837	CLA	O1D-CGD-CBD	-3.27	118.51	124.58
15	B	847	BCR	C12-C13-C14	-3.27	113.92	118.94
13	A	838	CLA	O1D-CGD-CBD	-3.27	118.52	124.58
15	B	841	BCR	C24-C23-C22	-3.26	121.31	126.21
15	B	847	BCR	C8-C7-C6	-3.26	118.11	127.25
15	I	102	BCR	C8-C7-C6	-3.26	118.13	127.25
13	B	827	CLA	O1D-CGD-CBD	-3.25	118.54	124.58
13	A	806	CLA	C3D-CAD-CBD	-3.25	103.24	107.61
13	B	831	CLA	O2D-CGD-O1D	-3.23	117.41	123.82
15	B	841	BCR	C15-C14-C13	-3.23	122.70	127.31
13	A	820	CLA	C3D-CAD-CBD	-3.23	103.27	107.61
13	A	845	CLA	C6-C5-C3	-3.21	109.14	114.63
15	B	846	BCR	C8-C7-C6	-3.20	118.28	127.25
15	M	1203	BCR	C15-C14-C13	-3.20	122.75	127.31
15	B	847	BCR	C24-C23-C22	-3.19	121.41	126.21
15	J	1105	BCR	C8-C7-C6	-3.19	118.31	127.25
15	A	849	BCR	C23-C24-C25	-3.19	118.32	127.25
13	B	833	CLA	O2D-CGD-O1D	-3.18	117.51	123.82
13	A	821	CLA	O1D-CGD-CBD	-3.17	118.70	124.58
13	A	834	CLA	O1D-CGD-CBD	-3.17	118.70	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	845	CLA	O1D-CGD-CBD	-3.17	118.70	124.58
15	M	1203	BCR	C20-C21-C22	-3.16	122.80	127.31
13	B	803	CLA	O1D-CGD-CBD	-3.15	118.73	124.58
15	J	1105	BCR	C20-C21-C22	-3.15	122.81	127.31
13	B	809	CLA	O1D-CGD-CBD	-3.15	118.74	124.58
13	A	808	CLA	CGD-CBD-CAD	-3.15	100.54	110.73
13	A	802	CLA	C1-C2-C3	-3.14	120.17	125.96
15	B	843	BCR	C7-C8-C9	-3.14	121.50	126.21
15	I	102	BCR	C21-C20-C19	-3.13	113.73	123.26
13	B	804	CLA	O1D-CGD-CBD	-3.13	118.78	124.58
13	A	828	CLA	C1-C2-C3	-3.12	120.20	125.96
15	I	102	BCR	C24-C23-C22	-3.12	121.52	126.21
13	A	805	CLA	O1D-CGD-CBD	-3.12	118.80	124.58
15	B	842	BCR	C15-C16-C17	-3.11	116.82	123.46
13	B	839	CLA	O1D-CGD-CBD	-3.11	118.81	124.58
13	B	828	CLA	O1D-CGD-CBD	-3.11	118.82	124.58
15	F	1302	BCR	C23-C24-C25	-3.10	118.56	127.25
13	B	827	CLA	O2D-CGD-O1D	-3.10	117.67	123.82
13	A	812	CLA	C1-C2-C3	-3.09	120.26	125.96
15	A	851	BCR	C7-C8-C9	-3.08	121.58	126.21
13	L	1003	CLA	CAA-CBA-CGA	-3.08	104.15	113.35
15	B	846	BCR	C38-C26-C25	-3.08	121.06	124.51
15	L	1006	BCR	C8-C7-C6	-3.07	118.65	127.25
13	J	1101	CLA	O1D-CGD-CBD	-3.07	118.89	124.58
15	A	850	BCR	C15-C14-C13	-3.06	122.94	127.31
15	A	852	BCR	C7-C8-C9	-3.05	121.62	126.21
15	B	846	BCR	C12-C13-C14	-3.04	114.27	118.94
13	A	824	CLA	O2D-CGD-O1D	-3.04	117.78	123.82
13	B	801	CLA	C1-C2-C3	-3.04	120.36	125.96
13	B	809	CLA	O2D-CGD-O1D	-3.03	117.80	123.82
13	A	808	CLA	O1D-CGD-CBD	-3.03	118.96	124.58
15	J	1105	BCR	C7-C8-C9	-3.03	121.66	126.21
15	B	847	BCR	C10-C11-C12	-3.03	114.04	123.26
13	L	1003	CLA	C1-C2-C3	-3.03	120.38	125.96
13	A	838	CLA	OBD-CAD-C3D	-3.02	122.59	128.09
15	I	102	BCR	C12-C13-C14	-3.02	114.30	118.94
15	B	844	BCR	C24-C23-C22	-3.02	121.67	126.21
15	B	844	BCR	C15-C16-C17	-3.02	117.02	123.46
15	B	845	BCR	C8-C7-C6	-3.02	118.80	127.25
13	L	1004	CLA	O1D-CGD-CBD	-3.02	118.98	124.58
15	B	843	BCR	C15-C14-C13	-3.02	123.01	127.31
15	L	1005	BCR	C20-C21-C22	-3.01	123.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	830	CLA	O1D-CGD-CBD	-3.00	119.01	124.58
13	B	816	CLA	O1D-CGD-CBD	-3.00	119.02	124.58
13	B	807	CLA	C1-C2-C3	-3.00	120.44	125.96
13	A	803	CLA	C1-C2-C3	-2.99	120.44	125.96
15	L	1006	BCR	C10-C11-C12	-2.99	114.15	123.26
13	A	820	CLA	C1-C2-C3	-2.97	120.48	125.96
15	J	1104	BCR	C20-C21-C22	-2.97	123.08	127.31
13	B	808	CLA	O2D-CGD-O1D	-2.96	117.94	123.82
13	A	801	CLA	O2D-CGD-O1D	-2.96	117.94	123.82
13	A	811	CLA	O2D-CGD-O1D	-2.96	117.95	123.82
13	B	823	CLA	O1D-CGD-CBD	-2.95	119.10	124.58
13	B	813	CLA	O2D-CGD-O1D	-2.95	117.97	123.82
15	B	847	BCR	C7-C8-C9	-2.95	121.79	126.21
15	B	849	BCR	C11-C12-C13	-2.94	118.15	126.42
13	B	806	CLA	CAA-CBA-CGA	-2.94	104.57	113.35
15	A	849	BCR	C8-C7-C6	-2.94	119.02	127.25
13	B	822	CLA	O2D-CGD-O1D	-2.94	117.99	123.82
15	B	844	BCR	C23-C24-C25	-2.94	119.03	127.25
13	I	101	CLA	C1-C2-C3	-2.94	120.55	125.96
15	A	847	BCR	C7-C8-C9	-2.92	121.82	126.21
15	J	1104	BCR	C10-C11-C12	-2.92	114.36	123.26
13	B	814	CLA	O2D-CGD-O1D	-2.92	118.03	123.82
13	B	838	CLA	C1-C2-C3	-2.91	120.60	125.96
13	A	836	CLA	O1D-CGD-CBD	-2.91	119.19	124.58
13	B	815	CLA	C3D-CAD-CBD	-2.90	103.70	107.61
15	B	841	BCR	C7-C8-C9	-2.90	121.86	126.21
13	L	1004	CLA	O2D-CGD-O1D	-2.89	118.09	123.82
13	A	807	CLA	CGD-CBD-CAD	-2.88	101.39	110.73
13	B	820	CLA	C1-C2-C3	-2.88	120.66	125.96
15	B	841	BCR	C38-C26-C25	-2.88	121.29	124.51
15	A	847	BCR	C38-C26-C25	-2.87	121.29	124.51
15	A	851	BCR	C8-C7-C6	-2.87	119.21	127.25
15	I	102	BCR	C20-C21-C22	-2.87	123.21	127.31
13	B	812	CLA	CAA-CBA-CGA	-2.87	104.79	113.35
15	J	1105	BCR	C11-C10-C9	-2.87	123.22	127.31
13	A	817	CLA	C1-C2-C3	-2.86	120.68	125.96
13	A	827	CLA	O1D-CGD-CBD	-2.86	119.27	124.58
13	A	810	CLA	O2D-CGD-O1D	-2.86	118.14	123.82
15	B	841	BCR	C8-C7-C6	-2.86	119.25	127.25
13	B	838	CLA	O1D-CGD-CBD	-2.85	119.29	124.58
15	L	1006	BCR	C36-C18-C17	-2.85	118.93	122.92
15	L	1005	BCR	C21-C20-C19	-2.85	114.58	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	847	BCR	C16-C15-C14	-2.85	117.38	123.46
15	B	843	BCR	C8-C7-C6	-2.84	119.29	127.25
15	L	1005	BCR	C8-C7-C6	-2.84	119.29	127.25
13	B	806	CLA	O1D-CGD-CBD	-2.84	119.31	124.58
13	F	1301	CLA	OBD-CAD-C3D	-2.84	122.93	128.09
15	B	842	BCR	C7-C8-C9	-2.84	121.95	126.21
13	A	819	CLA	C5-C3-C2	-2.82	115.35	121.10
15	I	102	BCR	C11-C10-C9	-2.82	123.28	127.31
13	A	845	CLA	O2D-CGD-O1D	-2.82	118.23	123.82
15	J	1105	BCR	C10-C11-C12	-2.80	114.73	123.26
13	B	820	CLA	C3D-CAD-CBD	-2.80	103.84	107.61
13	A	821	CLA	C3D-CAD-CBD	-2.79	103.85	107.61
15	F	1302	BCR	C34-C9-C10	-2.78	119.03	122.92
15	A	851	BCR	C10-C11-C12	-2.78	114.80	123.26
15	A	851	BCR	C15-C16-C17	-2.78	117.54	123.46
13	A	809	CLA	C1-C2-C3	-2.76	120.86	125.96
13	A	814	CLA	O1D-CGD-CBD	-2.76	119.45	124.58
15	B	843	BCR	C34-C9-C10	-2.76	119.05	122.92
13	B	831	CLA	C1-C2-C3	-2.75	120.88	125.96
15	B	849	BCR	C8-C7-C6	-2.75	119.55	127.25
13	A	812	CLA	O2D-CGD-O1D	-2.74	118.37	123.82
15	A	848	BCR	C10-C11-C12	-2.74	114.91	123.26
13	J	1101	CLA	O2D-CGD-O1D	-2.74	118.39	123.82
15	L	1006	BCR	C15-C14-C13	-2.73	123.41	127.31
15	M	1203	BCR	C12-C13-C14	-2.73	114.75	118.94
13	B	835	CLA	O1D-CGD-CBD	-2.73	119.52	124.58
15	A	851	BCR	C11-C10-C9	-2.73	123.42	127.31
15	B	845	BCR	C7-C8-C9	-2.72	122.13	126.21
15	A	847	BCR	C8-C7-C6	-2.71	119.66	127.25
13	M	1201	CLA	O2D-CGD-O1D	-2.71	118.44	123.82
13	J	1102	CLA	O2D-CGD-O1D	-2.71	118.45	123.82
13	A	824	CLA	C1-C2-C3	-2.70	120.98	125.96
13	L	1002	CLA	C1-C2-C3	-2.70	120.98	125.96
15	A	849	BCR	C15-C16-C17	-2.70	117.70	123.46
15	A	849	BCR	C24-C23-C22	-2.70	122.15	126.21
13	A	845	CLA	C1-C2-C3	-2.69	121.00	125.96
15	M	1203	BCR	C23-C24-C25	-2.69	119.71	127.25
15	L	1006	BCR	C37-C22-C21	-2.69	119.15	122.92
15	L	1005	BCR	C10-C11-C12	-2.69	115.07	123.26
13	A	818	CLA	CAA-CBA-CGA	-2.68	105.34	113.35
15	A	848	BCR	C8-C7-C6	-2.68	119.75	127.25
15	J	1104	BCR	C11-C10-C9	-2.68	123.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	845	BCR	C16-C17-C18	-2.68	123.49	127.31
13	A	807	CLA	C1-C2-C3	-2.67	121.03	125.96
15	B	847	BCR	C23-C24-C25	-2.66	119.80	127.25
15	I	102	BCR	C15-C16-C17	-2.66	117.78	123.46
13	L	1003	CLA	CAA-C2A-C3A	-2.66	105.52	112.81
13	B	824	CLA	O2D-CGD-O1D	-2.66	118.54	123.82
13	A	813	CLA	O2D-CGD-O1D	-2.66	118.55	123.82
13	A	805	CLA	O2D-CGD-O1D	-2.65	118.55	123.82
13	A	802	CLA	O2D-CGD-O1D	-2.65	118.55	123.82
15	B	849	BCR	C34-C9-C10	-2.65	119.21	122.92
13	A	808	CLA	C1-C2-C3	-2.65	121.08	125.96
15	J	1104	BCR	C23-C24-C25	-2.64	119.86	127.25
15	M	1203	BCR	C15-C16-C17	-2.64	117.83	123.46
13	B	819	CLA	O2D-CGD-O1D	-2.62	118.61	123.82
15	A	852	BCR	C23-C24-C25	-2.62	119.91	127.25
15	A	849	BCR	C11-C10-C9	-2.62	123.57	127.31
15	B	845	BCR	C23-C24-C25	-2.62	119.92	127.25
15	B	846	BCR	C16-C15-C14	-2.62	117.88	123.46
15	A	852	BCR	C11-C10-C9	-2.62	123.58	127.31
15	A	848	BCR	C15-C14-C13	-2.62	123.58	127.31
15	A	852	BCR	C10-C11-C12	-2.61	115.30	123.26
15	A	849	BCR	C12-C13-C14	-2.61	114.93	118.94
15	A	851	BCR	C23-C24-C25	-2.61	119.94	127.25
15	A	848	BCR	C23-C24-C25	-2.61	119.94	127.25
13	A	804	CLA	OBD-CAD-C3D	-2.61	123.34	128.09
13	B	811	CLA	O2D-CGD-O1D	-2.61	118.65	123.82
13	A	809	CLA	O2D-CGD-O1D	-2.61	118.65	123.82
13	B	822	CLA	C1-C2-C3	-2.61	121.16	125.96
13	A	804	CLA	O2D-CGD-O1D	-2.60	118.65	123.82
15	B	843	BCR	C39-C30-C25	-2.60	106.09	110.31
13	A	839	CLA	O1D-CGD-CBD	-2.59	119.78	124.58
15	A	849	BCR	C16-C15-C14	-2.59	117.94	123.46
15	B	843	BCR	C36-C18-C17	-2.58	119.31	122.92
13	B	827	CLA	C2C-C1C-NC	-2.58	107.42	110.09
13	B	811	CLA	C1-C2-C3	-2.58	121.20	125.96
13	B	822	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
13	B	828	CLA	O2D-CGD-O1D	-2.57	118.72	123.82
15	A	851	BCR	C36-C18-C17	-2.57	119.32	122.92
15	B	841	BCR	C12-C13-C14	-2.57	115.00	118.94
13	B	805	CLA	C3D-CAD-CBD	-2.57	104.16	107.61
13	A	801	CLA	C1-C2-C3	-2.56	121.23	125.96
15	B	841	BCR	C27-C26-C25	-2.55	119.00	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	829	CLA	O2D-CGD-O1D	-2.54	118.77	123.82
13	A	809	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
15	J	1104	BCR	C15-C16-C17	-2.54	118.04	123.46
15	B	843	BCR	C21-C20-C19	-2.54	115.53	123.26
13	J	1101	CLA	C1-C2-C3	-2.54	121.28	125.96
15	A	848	BCR	C12-C13-C14	-2.53	115.05	118.94
13	B	814	CLA	C7-C6-C5	-2.53	106.28	113.17
15	A	848	BCR	C11-C10-C9	-2.53	123.70	127.31
15	J	1105	BCR	C23-C24-C25	-2.53	120.17	127.25
15	B	850	BCR	C10-C11-C12	-2.52	115.57	123.26
15	B	849	BCR	C24-C23-C22	-2.52	122.43	126.21
13	B	830	CLA	CAA-CBA-CGA	-2.52	105.84	113.35
15	B	847	BCR	C31-C1-C6	-2.51	106.23	110.31
15	B	844	BCR	C16-C17-C18	-2.51	123.72	127.31
13	B	816	CLA	C7-C6-C5	-2.51	106.34	113.17
13	A	837	CLA	CAA-C2A-C3A	-2.51	105.93	112.81
13	A	836	CLA	C3D-CAD-CBD	-2.51	104.23	107.61
13	B	834	CLA	O2D-CGD-O1D	-2.50	118.85	123.82
13	A	838	CLA	C11-C10-C8	-2.50	107.52	115.73
13	F	1301	CLA	O1D-CGD-CBD	-2.50	119.95	124.58
15	A	852	BCR	C24-C23-C22	-2.50	122.46	126.21
13	B	807	CLA	O2D-CGD-O1D	-2.49	118.87	123.82
15	A	847	BCR	C27-C26-C25	-2.49	119.09	122.74
15	J	1104	BCR	C24-C23-C22	-2.49	122.47	126.21
13	A	831	CLA	O1D-CGD-CBD	-2.49	119.97	124.58
13	A	838	CLA	O2D-CGD-O1D	-2.48	118.90	123.82
13	A	836	CLA	O2D-CGD-O1D	-2.47	118.91	123.82
15	A	848	BCR	C36-C18-C17	-2.46	119.48	122.92
13	A	840	CLA	CAA-CBA-CGA	-2.45	106.02	113.35
13	A	834	CLA	C3D-CAD-CBD	-2.45	104.31	107.61
15	M	1203	BCR	C27-C26-C25	-2.44	119.15	122.74
15	A	847	BCR	C15-C14-C13	-2.44	123.82	127.31
13	A	843	CLA	CAA-CBA-CGA	-2.43	106.09	113.35
13	A	855	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
15	A	850	BCR	C37-C22-C21	-2.43	119.52	122.92
15	B	846	BCR	C27-C26-C25	-2.43	119.18	122.74
15	B	843	BCR	C12-C13-C14	-2.42	115.22	118.94
13	B	801	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
13	B	814	CLA	CAA-CBA-CGA	-2.42	106.14	113.35
15	A	849	BCR	C37-C22-C21	-2.41	119.54	122.92
15	M	1203	BCR	C7-C8-C9	-2.41	122.59	126.21
15	A	850	BCR	C4-C5-C6	-2.41	119.20	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	820	CLA	O2D-CGD-O1D	-2.41	119.04	123.82
13	L	1002	CLA	O2D-CGD-O1D	-2.41	119.05	123.82
13	B	839	CLA	CAA-CBA-CGA	-2.40	106.18	113.35
15	A	850	BCR	C16-C15-C14	-2.40	118.33	123.46
13	B	830	CLA	C1-C2-C3	-2.40	121.53	125.96
13	B	836	CLA	O2D-CGD-O1D	-2.40	119.06	123.82
15	B	847	BCR	C37-C22-C21	-2.40	119.57	122.92
15	B	844	BCR	C21-C20-C19	-2.39	115.97	123.26
13	A	808	CLA	OBD-CAD-CBD	-2.39	122.40	125.91
13	M	1202	CLA	O2D-CGD-O1D	-2.39	119.08	123.82
15	B	846	BCR	C23-C24-C25	-2.38	120.58	127.25
15	B	845	BCR	C40-C30-C25	-2.38	106.44	110.31
13	B	835	CLA	O2D-CGD-O1D	-2.38	119.10	123.82
15	L	1006	BCR	C16-C15-C14	-2.38	118.39	123.46
13	A	844	CLA	CAD-CBD-CHA	-2.37	102.11	105.09
15	A	848	BCR	C16-C15-C14	-2.37	118.40	123.46
13	A	838	CLA	CAA-CBA-CGA	-2.37	106.28	113.35
13	A	839	CLA	CAA-CBA-CGA	-2.37	106.28	113.35
13	B	838	CLA	O2D-CGD-O1D	-2.36	119.14	123.82
13	A	819	CLA	O2D-CGD-O1D	-2.35	119.16	123.82
13	A	826	CLA	O2D-CGD-O1D	-2.35	119.16	123.82
13	M	1201	CLA	CAA-CBA-CGA	-2.35	106.35	113.35
13	B	803	CLA	C1-C2-C3	-2.34	121.64	125.96
13	B	820	CLA	CAA-CBA-CGA	-2.33	106.39	113.35
15	J	1104	BCR	C37-C22-C21	-2.33	119.66	122.92
13	L	1004	CLA	C1-C2-C3	-2.33	121.67	125.96
13	A	827	CLA	C1-C2-C3	-2.32	121.67	125.96
15	B	850	BCR	C34-C9-C10	-2.32	119.67	122.92
15	B	842	BCR	C34-C9-C10	-2.32	119.67	122.92
15	B	843	BCR	C16-C15-C14	-2.32	118.51	123.46
13	A	827	CLA	C2C-C1C-NC	-2.32	107.69	110.09
15	B	842	BCR	C37-C22-C21	-2.32	119.68	122.92
15	B	849	BCR	C21-C20-C19	-2.32	116.20	123.26
15	B	850	BCR	C36-C18-C17	-2.32	119.68	122.92
15	B	841	BCR	C16-C15-C14	-2.32	118.52	123.46
15	A	847	BCR	C12-C13-C14	-2.32	115.39	118.94
15	B	841	BCR	C23-C24-C25	-2.31	120.78	127.25
15	B	846	BCR	C8-C9-C10	-2.31	115.40	118.94
15	I	102	BCR	C16-C15-C14	-2.31	118.54	123.46
13	A	823	CLA	CAA-CBA-CGA	-2.30	106.47	113.35
15	A	849	BCR	C21-C20-C19	-2.30	116.25	123.26
15	L	1005	BCR	C15-C14-C13	-2.30	124.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	847	BCR	C34-C9-C10	-2.30	119.70	122.92
15	B	850	BCR	C15-C16-C17	-2.30	118.56	123.46
13	A	803	CLA	C11-C12-C13	-2.28	108.23	115.73
15	B	842	BCR	C16-C17-C18	-2.28	124.05	127.31
15	A	852	BCR	C8-C7-C6	-2.28	120.86	127.25
15	B	846	BCR	C37-C22-C21	-2.28	119.72	122.92
13	B	837	CLA	O2D-CGD-O1D	-2.28	119.29	123.82
15	L	1006	BCR	C12-C13-C14	-2.28	115.44	118.94
15	B	849	BCR	C4-C5-C6	-2.28	119.39	122.74
13	A	845	CLA	C3C-C4C-NC	-2.28	107.62	110.43
13	M	1201	CLA	C1-C2-C3	-2.27	121.77	125.96
15	B	846	BCR	C39-C30-C25	-2.27	106.62	110.31
15	F	1302	BCR	C21-C20-C19	-2.27	116.34	123.26
13	B	807	CLA	C11-C10-C8	-2.27	108.28	115.73
13	B	824	CLA	OBD-CAD-C3D	-2.27	123.97	128.09
15	J	1105	BCR	C15-C16-C17	-2.27	118.62	123.46
13	A	835	CLA	O2D-CGD-O1D	-2.27	119.32	123.82
15	J	1104	BCR	C39-C30-C25	-2.26	106.64	110.31
15	B	846	BCR	C36-C18-C17	-2.26	119.75	122.92
15	B	847	BCR	C21-C20-C19	-2.26	116.37	123.26
15	B	847	BCR	C36-C18-C17	-2.26	119.76	122.92
15	B	849	BCR	C36-C18-C17	-2.26	119.76	122.92
13	B	803	CLA	O2D-CGD-O1D	-2.26	119.34	123.82
15	A	848	BCR	C27-C26-C25	-2.26	119.43	122.74
15	B	843	BCR	C11-C10-C9	-2.25	124.11	127.31
13	A	830	CLA	O2D-CGD-O1D	-2.24	119.37	123.82
15	A	847	BCR	C36-C18-C17	-2.24	119.78	122.92
13	B	827	CLA	C7-C6-C5	-2.24	107.08	113.17
15	A	852	BCR	C27-C26-C25	-2.24	119.45	122.74
13	B	839	CLA	O2D-CGD-O1D	-2.24	119.38	123.82
13	B	804	CLA	O2D-CGD-O1D	-2.24	119.38	123.82
15	J	1105	BCR	C37-C22-C21	-2.23	119.79	122.92
15	B	850	BCR	C32-C1-C6	-2.23	106.69	110.31
13	A	814	CLA	OBD-CAD-C3D	-2.23	124.03	128.09
15	A	849	BCR	C27-C26-C25	-2.23	119.47	122.74
13	A	819	CLA	C7-C6-C5	-2.23	107.11	113.17
13	A	818	CLA	CAA-C2A-C3A	-2.23	106.71	112.81
15	B	841	BCR	C37-C22-C21	-2.22	119.82	122.92
13	A	809	CLA	CGD-CBD-CAD	-2.21	103.56	110.73
13	L	1003	CLA	O2D-CGD-O1D	-2.21	119.43	123.82
13	A	825	CLA	CAA-CBA-CGA	-2.21	106.74	113.35
15	A	850	BCR	C10-C11-C12	-2.21	116.52	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	1105	BCR	C27-C26-C25	-2.21	119.49	122.74
13	B	838	CLA	O2A-CGA-O1A	-2.21	118.18	123.58
15	B	842	BCR	C31-C1-C6	-2.21	106.72	110.31
15	A	847	BCR	C37-C22-C21	-2.21	119.83	122.92
15	B	841	BCR	C15-C16-C17	-2.21	118.75	123.46
15	B	841	BCR	C21-C20-C19	-2.20	116.56	123.26
13	A	841	CLA	C1-C2-C3	-2.20	121.91	125.96
15	B	849	BCR	C32-C1-C6	-2.19	106.75	110.31
15	B	841	BCR	C4-C5-C6	-2.19	119.52	122.74
15	B	846	BCR	C15-C16-C17	-2.19	118.78	123.46
13	B	821	CLA	CAA-C2A-C3A	-2.19	106.80	112.81
13	A	826	CLA	O1D-CGD-CBD	-2.19	120.51	124.58
15	B	845	BCR	C4-C5-C6	-2.19	119.53	122.74
15	A	848	BCR	C4-C5-C6	-2.19	119.53	122.74
13	B	825	CLA	O1D-CGD-CBD	-2.19	120.53	124.58
13	B	808	CLA	C7-C6-C5	-2.18	107.23	113.17
15	J	1104	BCR	C12-C13-C14	-2.18	115.59	118.94
15	B	841	BCR	C36-C18-C17	-2.18	119.87	122.92
15	B	844	BCR	C36-C18-C17	-2.18	119.87	122.92
15	A	850	BCR	C36-C18-C17	-2.18	119.87	122.92
15	J	1104	BCR	C4-C5-C6	-2.18	119.54	122.74
15	F	1302	BCR	C27-C26-C25	-2.18	119.54	122.74
15	M	1203	BCR	C21-C20-C19	-2.17	116.64	123.26
15	B	842	BCR	C36-C18-C17	-2.17	119.88	122.92
13	A	813	CLA	C11-C10-C8	-2.17	108.61	115.73
15	F	1302	BCR	C8-C7-C6	-2.17	121.19	127.25
15	J	1105	BCR	C36-C18-C17	-2.16	119.89	122.92
15	B	843	BCR	C15-C16-C17	-2.16	118.84	123.46
13	B	823	CLA	CBA-CAA-C2A	-2.16	107.40	113.82
13	A	812	CLA	CAA-CBA-CGA	-2.16	106.90	113.35
13	A	826	CLA	C1-C2-C3	-2.16	121.98	125.96
15	A	852	BCR	C20-C21-C22	-2.15	124.23	127.31
13	F	1301	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
15	F	1302	BCR	C37-C22-C21	-2.15	119.91	122.92
13	A	844	CLA	C3C-C4C-NC	-2.15	107.78	110.43
15	L	1006	BCR	C4-C5-C6	-2.15	119.59	122.74
13	A	815	CLA	C2C-C1C-NC	-2.15	107.87	110.09
13	A	844	CLA	CBD-CAD-C3D	-2.14	106.24	107.71
15	A	850	BCR	C27-C26-C25	-2.14	119.59	122.74
15	B	844	BCR	C27-C26-C25	-2.14	119.60	122.74
13	B	831	CLA	CED-O2D-CGD	-2.14	111.03	115.97
15	A	847	BCR	C16-C15-C14	-2.14	118.89	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	850	BCR	C16-C15-C14	-2.14	118.89	123.46
15	A	847	BCR	C30-C25-C26	-2.14	119.58	122.59
13	A	806	CLA	C11-C10-C8	-2.14	108.71	115.73
13	A	832	CLA	O2D-CGD-O1D	-2.14	119.58	123.82
13	A	843	CLA	C6-C7-C8	-2.14	108.72	115.73
13	A	824	CLA	C3C-C4C-NC	-2.14	107.79	110.43
15	J	1105	BCR	C4-C5-C6	-2.14	119.60	122.74
13	A	826	CLA	C11-C10-C8	-2.14	108.72	115.73
13	A	829	CLA	C7-C6-C5	-2.13	107.36	113.17
13	A	809	CLA	O2A-CGA-O1A	-2.13	118.37	123.58
15	A	850	BCR	C34-C9-C10	-2.13	119.94	122.92
13	A	824	CLA	C11-C10-C8	-2.13	108.74	115.73
15	A	847	BCR	C4-C5-C6	-2.13	119.61	122.74
15	F	1302	BCR	C16-C17-C18	-2.13	124.27	127.31
13	A	821	CLA	C16-C15-C13	-2.13	108.75	115.73
15	L	1006	BCR	C33-C5-C6	-2.13	122.13	124.51
15	B	847	BCR	C15-C14-C13	-2.13	124.28	127.31
13	B	802	CLA	CGD-CBD-CAD	-2.13	103.85	110.73
13	A	842	CLA	C1-C2-C3	-2.12	122.04	125.96
13	L	1003	CLA	C3C-C4C-NC	-2.12	107.81	110.43
13	B	812	CLA	O2D-CGD-O1D	-2.12	119.62	123.82
13	B	815	CLA	O2D-CGD-O1D	-2.12	119.62	123.82
15	A	849	BCR	C34-C9-C10	-2.12	119.96	122.92
15	L	1006	BCR	C23-C24-C25	-2.11	121.34	127.25
14	B	840	PQN	C2M-C2-C3	-2.11	120.00	124.21
15	L	1005	BCR	C27-C26-C25	-2.11	119.65	122.74
13	A	807	CLA	O1D-CGD-CBD	-2.10	120.69	124.58
15	A	850	BCR	C31-C1-C6	-2.10	106.90	110.31
13	A	840	CLA	C1-C2-C3	-2.10	122.09	125.96
13	A	835	CLA	OBD-CAD-C3D	-2.10	124.28	128.09
13	A	827	CLA	O2D-CGD-O1D	-2.10	119.66	123.82
15	J	1104	BCR	C21-C20-C19	-2.09	116.89	123.26
15	L	1005	BCR	C12-C13-C14	-2.09	115.73	118.94
13	J	1101	CLA	C11-C10-C8	-2.09	108.86	115.73
13	A	801	CLA	C11-C10-C8	-2.09	108.87	115.73
13	A	843	CLA	C11-C10-C8	-2.09	108.88	115.73
13	I	101	CLA	C11-C10-C8	-2.09	108.88	115.73
15	F	1302	BCR	C10-C11-C12	-2.08	116.91	123.26
15	I	102	BCR	C31-C1-C6	-2.08	106.93	110.31
15	M	1203	BCR	C16-C15-C14	-2.08	119.02	123.46
15	A	849	BCR	C20-C19-C18	-2.08	120.58	126.42
15	B	842	BCR	C21-C20-C19	-2.07	116.94	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	102	BCR	C19-C18-C17	-2.07	115.76	118.94
13	B	816	CLA	CAA-C2A-C3A	-2.07	107.12	112.81
15	A	848	BCR	C21-C20-C19	-2.07	116.95	123.26
15	B	845	BCR	C11-C10-C9	-2.07	124.35	127.31
15	J	1105	BCR	C39-C30-C25	-2.07	106.95	110.31
13	B	815	CLA	C11-C10-C8	-2.07	108.94	115.73
13	A	809	CLA	C11-C10-C8	-2.07	108.94	115.73
13	A	819	CLA	C16-C15-C13	-2.07	108.94	115.73
15	B	845	BCR	C19-C18-C17	-2.06	115.77	118.94
15	A	847	BCR	C1-C6-C5	-2.06	119.69	122.59
15	J	1104	BCR	C1-C6-C5	-2.06	119.69	122.59
13	B	832	CLA	O2D-CGD-O1D	-2.06	119.73	123.82
15	J	1105	BCR	C21-C20-C19	-2.06	116.98	123.26
13	A	819	CLA	C2C-C1C-NC	-2.06	107.95	110.09
15	J	1104	BCR	C36-C18-C17	-2.06	120.04	122.92
15	B	844	BCR	C20-C21-C22	-2.06	124.37	127.31
13	B	821	CLA	O1D-CGD-CBD	-2.06	120.77	124.58
13	B	817	CLA	C3D-CAD-CBD	-2.06	104.84	107.61
15	B	842	BCR	C30-C25-C26	-2.05	119.71	122.59
13	A	815	CLA	C3C-C4C-NC	-2.05	107.90	110.43
15	J	1105	BCR	C12-C13-C14	-2.05	115.80	118.94
15	F	1302	BCR	C1-C6-C5	-2.05	119.71	122.59
13	A	839	CLA	C3D-CAD-CBD	-2.05	104.86	107.61
15	B	850	BCR	C40-C30-C25	-2.05	106.99	110.31
15	B	847	BCR	C35-C13-C14	-2.04	120.06	122.92
15	B	846	BCR	C4-C5-C6	-2.04	119.74	122.74
13	B	804	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
15	A	850	BCR	C30-C25-C26	-2.04	119.72	122.59
13	B	830	CLA	O1D-CGD-CBD	-2.04	120.79	124.58
13	B	835	CLA	C1-C2-C3	-2.04	122.20	125.96
13	B	805	CLA	C11-C10-C8	-2.04	109.03	115.73
15	A	847	BCR	C21-C20-C19	-2.04	117.05	123.26
13	A	809	CLA	C2C-C1C-NC	-2.04	107.98	110.09
13	B	801	CLA	C11-C10-C8	-2.04	109.04	115.73
13	B	836	CLA	C11-C10-C8	-2.04	109.05	115.73
15	A	852	BCR	C34-C9-C10	-2.04	120.07	122.92
13	B	810	CLA	C3C-C4C-NC	-2.03	107.92	110.43
13	A	803	CLA	C7-C6-C5	-2.03	107.65	113.17
13	B	830	CLA	C3D-CAD-CBD	-2.03	104.88	107.61
13	B	817	CLA	C1-C2-C3	-2.03	122.22	125.96
13	A	840	CLA	O2D-CGD-O1D	-2.03	119.80	123.82
15	B	845	BCR	C21-C20-C19	-2.03	117.09	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	845	BCR	C37-C22-C21	-2.02	120.09	122.92
13	A	806	CLA	C11-C12-C13	-2.02	109.09	115.73
15	J	1104	BCR	C8-C7-C6	-2.02	121.59	127.25
13	A	816	CLA	C3C-C4C-NC	-2.02	107.93	110.43
15	L	1005	BCR	C4-C5-C6	-2.02	119.78	122.74
13	A	843	CLA	C11-C12-C13	-2.02	109.11	115.73
13	A	828	CLA	C11-C10-C8	-2.01	109.12	115.73
13	A	811	CLA	C1-C2-C3	-2.01	122.25	125.96
13	A	807	CLA	O2A-CGA-O1A	-2.01	118.67	123.58
13	A	801	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
15	B	850	BCR	C1-C6-C5	-2.01	119.77	122.59
13	B	835	CLA	CED-O2D-CGD	-2.01	111.33	115.97
15	L	1005	BCR	C34-C9-C10	-2.01	120.11	122.92
13	X	102	CLA	O2D-CGD-O1D	-2.01	119.84	123.82
15	B	849	BCR	C35-C13-C14	-2.00	120.11	122.92
15	L	1006	BCR	C1-C6-C5	-2.00	119.77	122.59
13	B	813	CLA	C2C-C1C-NC	-2.00	108.01	110.09
13	I	101	CLA	C11-C12-C13	-2.00	109.15	115.73
15	B	850	BCR	C35-C13-C14	-2.00	120.12	122.92
15	A	851	BCR	C21-C20-C19	-2.00	117.16	123.26
13	A	820	CLA	C3C-C4C-NC	-2.00	107.95	110.43
13	L	1002	CLA	C2C-C1C-NC	-2.00	108.02	110.09
15	A	852	BCR	C30-C25-C26	-2.00	119.78	122.59
15	B	849	BCR	C23-C22-C21	-2.00	115.87	118.94
15	A	852	BCR	C36-C18-C17	-2.00	120.12	122.92
13	A	808	CLA	CED-O2D-CGD	-2.00	111.35	115.97
14	A	846	PQN	C2M-C2-C1	2.01	119.61	116.27
13	B	811	CLA	C2A-C1A-CHA	2.01	127.45	123.92
13	A	826	CLA	C2A-C1A-CHA	2.01	127.45	123.92
13	A	822	CLA	C2A-C1A-CHA	2.01	127.46	123.92
13	A	813	CLA	O2A-CGA-CBA	2.02	117.75	111.92
13	A	836	CLA	CMD-C2D-C3D	2.02	128.57	124.88
13	A	839	CLA	OBD-CAD-CBD	2.03	128.89	125.91
13	A	841	CLA	CED-O2D-CGD	2.03	120.64	115.97
13	A	802	CLA	C1C-NC-C4C	2.03	108.19	107.05
13	A	820	CLA	C2A-C3A-C4A	2.04	105.16	101.87
13	B	807	CLA	C1D-CHD-C4C	2.04	125.28	122.48
13	B	807	CLA	O2A-CGA-CBA	2.05	117.84	111.92
13	A	813	CLA	C1C-NC-C4C	2.05	108.20	107.05
13	A	821	CLA	C1C-NC-C4C	2.05	108.20	107.05
13	B	814	CLA	O2A-CGA-CBA	2.06	117.86	111.92
13	A	801	CLA	C1-O2A-CGA	2.06	121.51	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	832	CLA	C1C-NC-C4C	2.06	108.21	107.05
13	B	835	CLA	CAA-C2A-C1A	2.06	118.74	111.97
13	A	803	CLA	C1C-NC-C4C	2.06	108.21	107.05
13	L	1004	CLA	C1C-NC-C4C	2.08	108.22	107.05
13	A	823	CLA	CED-O2D-CGD	2.08	120.76	115.97
13	A	806	CLA	C1-O2A-CGA	2.09	121.58	116.77
13	A	827	CLA	C1C-NC-C4C	2.09	108.22	107.05
13	A	805	CLA	C4-C3-C5	2.10	118.91	115.29
13	A	820	CLA	C1C-NC-C4C	2.10	108.23	107.05
13	B	829	CLA	O2A-CGA-CBA	2.10	118.00	111.92
13	A	843	CLA	CMD-C2D-C3D	2.10	128.71	124.88
13	B	826	CLA	O2A-CGA-CBA	2.11	118.01	111.92
13	B	820	CLA	CED-O2D-CGD	2.13	120.87	115.97
13	A	820	CLA	O2A-CGA-CBA	2.13	118.08	111.92
13	A	837	CLA	C1-O2A-CGA	2.14	121.71	116.77
13	B	814	CLA	C4-C3-C5	2.15	118.99	115.29
15	A	850	BCR	C35-C13-C12	2.16	121.53	118.10
15	B	843	BCR	C29-C28-C27	2.16	116.31	111.36
13	A	809	CLA	CMD-C2D-C3D	2.16	128.82	124.88
13	B	810	CLA	C1C-NC-C4C	2.17	108.27	107.05
13	B	829	CLA	C1-O2A-CGA	2.17	121.77	116.77
15	A	849	BCR	C35-C13-C12	2.17	121.56	118.10
14	A	846	PQN	C14-C13-C15	2.17	119.04	115.29
13	A	826	CLA	C1-O2A-CGA	2.18	121.80	116.77
13	A	807	CLA	C1D-CHD-C4C	2.18	125.47	122.48
13	A	823	CLA	O2A-CGA-CBA	2.18	118.23	111.92
13	A	827	CLA	C1D-CHD-C4C	2.20	125.49	122.48
15	L	1005	BCR	C36-C18-C19	2.20	121.61	118.10
13	B	835	CLA	C1-O2A-CGA	2.21	121.85	116.77
13	B	827	CLA	C1D-CHD-C4C	2.21	125.51	122.48
15	B	843	BCR	C35-C13-C12	2.22	121.64	118.10
13	A	835	CLA	C1-O2A-CGA	2.22	121.89	116.77
13	J	1102	CLA	C1C-NC-C4C	2.22	108.30	107.05
13	A	830	CLA	C1C-NC-C4C	2.22	108.30	107.05
13	B	827	CLA	O2A-CGA-CBA	2.22	118.35	111.92
13	A	833	CLA	CED-O2D-CGD	2.23	121.10	115.97
15	L	1005	BCR	C30-C25-C24	2.23	121.98	115.73
13	B	802	CLA	C1D-CHD-C4C	2.23	125.53	122.48
13	L	1002	CLA	O2A-CGA-CBA	2.23	118.37	111.92
13	A	830	CLA	O2A-CGA-CBA	2.23	118.37	111.92
13	I	101	CLA	O2A-CGA-CBA	2.24	118.39	111.92
13	B	816	CLA	C1C-NC-C4C	2.24	108.31	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	828	CLA	C1D-CHD-C4C	2.24	125.55	122.48
13	A	816	CLA	CED-O2D-CGD	2.25	121.15	115.97
13	B	824	CLA	C1-O2A-CGA	2.25	121.96	116.77
13	B	816	CLA	C1-O2A-CGA	2.25	121.96	116.77
13	A	840	CLA	C1D-CHD-C4C	2.28	125.59	122.48
13	A	816	CLA	C1C-NC-C4C	2.28	108.33	107.05
13	J	1101	CLA	CAA-CBA-CGA	2.29	120.19	113.35
13	B	838	CLA	CBA-CAA-C2A	2.30	120.63	113.82
13	A	820	CLA	C1-O2A-CGA	2.30	122.06	116.77
13	M	1201	CLA	C1-O2A-CGA	2.30	122.07	116.77
13	B	823	CLA	O2A-CGA-CBA	2.31	121.59	112.32
13	A	823	CLA	C1D-CHD-C4C	2.31	125.64	122.48
13	A	801	CLA	C1D-CHD-C4C	2.31	125.65	122.48
13	A	840	CLA	C4-C3-C5	2.32	119.29	115.29
13	A	842	CLA	CED-O2D-CGD	2.32	121.32	115.97
13	B	813	CLA	C1C-NC-C4C	2.32	108.36	107.05
13	A	834	CLA	C1D-CHD-C4C	2.33	125.67	122.48
13	A	824	CLA	CGD-CBD-CAD	2.33	118.28	110.73
13	A	817	CLA	CED-O2D-CGD	2.33	121.34	115.97
13	A	814	CLA	C1D-CHD-C4C	2.33	125.67	122.48
13	B	810	CLA	CED-O2D-CGD	2.33	121.35	115.97
13	A	806	CLA	O2A-CGA-CBA	2.34	118.67	111.92
13	I	101	CLA	C1D-CHD-C4C	2.34	125.68	122.48
13	B	831	CLA	C1D-CHD-C4C	2.35	125.69	122.48
13	A	804	CLA	O2A-CGA-CBA	2.35	118.70	111.92
15	I	102	BCR	C2-C3-C4	2.35	116.75	111.36
15	B	844	BCR	C35-C13-C12	2.36	119.92	114.59
14	B	840	PQN	C14-C13-C15	2.37	119.38	115.29
13	B	835	CLA	C2A-C1A-CHA	2.37	128.09	123.92
13	B	803	CLA	OBD-CAD-CBD	2.38	129.40	125.91
15	B	842	BCR	C2-C3-C4	2.38	116.81	111.36
15	A	852	BCR	C1-C6-C7	2.38	122.41	115.73
13	A	822	CLA	C1D-CHD-C4C	2.38	125.74	122.48
13	A	830	CLA	C1D-CHD-C4C	2.38	125.74	122.48
13	A	824	CLA	O2A-CGA-CBA	2.40	118.84	111.92
13	A	827	CLA	CMD-C2D-C3D	2.40	129.25	124.88
13	A	842	CLA	C1D-CHD-C4C	2.40	125.77	122.48
13	B	839	CLA	O2A-CGA-CBA	2.41	118.89	111.92
13	A	821	CLA	C4-C3-C5	2.42	119.46	115.29
13	B	818	CLA	C1C-NC-C4C	2.42	108.41	107.05
13	B	826	CLA	C1D-CHD-C4C	2.42	125.80	122.48
15	B	849	BCR	C29-C30-C25	2.42	114.27	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1003	CLA	C1-O2A-CGA	2.43	122.37	116.77
13	A	810	CLA	C1D-CHD-C4C	2.43	125.81	122.48
13	A	808	CLA	C4-C3-C5	2.44	119.49	115.29
13	A	817	CLA	C1D-CHD-C4C	2.44	125.82	122.48
13	B	839	CLA	C1-O2A-CGA	2.44	122.39	116.77
18	B	848	LMG	C7-O1-C1	2.44	118.69	113.80
13	A	831	CLA	C1D-CHD-C4C	2.44	125.82	122.48
13	B	801	CLA	C1D-CHD-C4C	2.44	125.82	122.48
13	B	808	CLA	CMD-C2D-C3D	2.45	129.34	124.88
13	L	1002	CLA	C1C-NC-C4C	2.46	108.43	107.05
13	J	1101	CLA	CBA-CAA-C2A	2.46	121.11	113.82
13	A	805	CLA	C1D-CHD-C4C	2.46	125.85	122.48
13	A	825	CLA	C4-C3-C5	2.46	119.53	115.29
13	A	819	CLA	C1C-NC-C4C	2.47	108.44	107.05
13	A	831	CLA	C5-C3-C4	2.47	120.17	114.59
13	A	811	CLA	C1D-CHD-C4C	2.47	125.87	122.48
13	B	835	CLA	C1D-CHD-C4C	2.48	125.87	122.48
13	A	837	CLA	CAA-C2A-C1A	2.49	120.14	111.97
15	B	850	BCR	C35-C13-C12	2.49	122.07	118.10
15	L	1006	BCR	C33-C5-C4	2.50	118.28	113.56
13	B	807	CLA	CMD-C2D-C3D	2.50	129.43	124.88
14	B	840	PQN	C2M-C2-C1	2.50	120.44	116.27
13	B	823	CLA	CAA-C2A-C1A	2.50	120.17	111.97
13	B	814	CLA	C1D-CHD-C4C	2.51	125.91	122.48
13	A	825	CLA	O2A-CGA-CBA	2.51	119.18	111.92
13	A	801	CLA	O2A-CGA-CBA	2.52	119.19	111.92
13	B	812	CLA	C1D-CHD-C4C	2.52	125.93	122.48
15	J	1104	BCR	C29-C28-C27	2.52	117.14	111.36
13	B	829	CLA	C1D-CHD-C4C	2.52	125.94	122.48
13	B	804	CLA	C1D-CHD-C4C	2.53	125.95	122.48
15	B	843	BCR	C2-C3-C4	2.54	117.17	111.36
13	A	809	CLA	C3A-C2A-C1A	2.54	105.14	101.34
15	M	1203	BCR	C2-C3-C4	2.54	117.17	111.36
13	B	831	CLA	C4-C3-C5	2.54	119.67	115.29
13	B	803	CLA	C1D-CHD-C4C	2.54	125.96	122.48
13	A	808	CLA	C1D-CHD-C4C	2.54	125.96	122.48
13	F	1301	CLA	C2A-C1A-CHA	2.54	128.39	123.92
13	B	821	CLA	C1D-CHD-C4C	2.54	125.96	122.48
13	B	806	CLA	C1D-CHD-C4C	2.54	125.96	122.48
13	B	835	CLA	C4-C3-C5	2.55	119.69	115.29
13	B	816	CLA	O2A-CGA-CBA	2.55	119.30	111.92
13	A	804	CLA	C1D-CHD-C4C	2.55	125.98	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C1D-CHD-C4C	2.55	125.98	122.48
13	B	809	CLA	C1D-CHD-C4C	2.56	125.99	122.48
13	A	835	CLA	O2A-CGA-CBA	2.57	119.34	111.92
15	B	850	BCR	C33-C5-C4	2.57	118.42	113.56
13	A	835	CLA	C1C-NC-C4C	2.57	108.50	107.05
13	F	1301	CLA	C1D-CHD-C4C	2.58	126.01	122.48
13	L	1003	CLA	C1C-NC-C4C	2.59	108.50	107.05
13	A	812	CLA	C1-O2A-CGA	2.59	122.74	116.77
13	B	805	CLA	O2A-CGA-CBA	2.60	119.42	111.92
13	B	825	CLA	C1D-CHD-C4C	2.60	126.05	122.48
13	B	837	CLA	O2A-CGA-CBA	2.61	119.45	111.92
13	A	826	CLA	C4-C3-C5	2.61	119.78	115.29
13	A	819	CLA	O2A-CGA-CBA	2.61	119.46	111.92
13	B	822	CLA	O2A-CGA-CBA	2.61	119.47	111.92
13	A	838	CLA	C1D-CHD-C4C	2.62	126.06	122.48
13	B	817	CLA	O2A-CGA-CBA	2.63	119.52	111.92
13	A	824	CLA	C1C-NC-C4C	2.64	108.53	107.05
13	X	102	CLA	C1D-CHD-C4C	2.64	126.10	122.48
15	B	845	BCR	C29-C28-C27	2.65	117.43	111.36
13	B	832	CLA	C1D-CHD-C4C	2.65	126.11	122.48
13	A	819	CLA	C1D-CHD-C4C	2.66	126.11	122.48
13	A	825	CLA	C1D-CHD-C4C	2.66	126.11	122.48
13	A	825	CLA	C1-O2A-CGA	2.66	122.89	116.77
13	B	817	CLA	C1D-CHD-C4C	2.66	126.12	122.48
13	L	1003	CLA	C1D-CHD-C4C	2.66	126.12	122.48
13	A	842	CLA	C1-O2A-CGA	2.66	122.89	116.77
13	B	838	CLA	C1D-CHD-C4C	2.66	126.12	122.48
13	M	1201	CLA	O2A-CGA-CBA	2.66	119.62	111.92
13	B	837	CLA	C1D-CHD-C4C	2.66	126.13	122.48
13	B	816	CLA	C1D-CHD-C4C	2.67	126.13	122.48
13	A	837	CLA	C1D-CHD-C4C	2.67	126.14	122.48
15	J	1104	BCR	C38-C26-C27	2.67	118.62	113.56
13	A	844	CLA	C1C-NC-C4C	2.68	108.55	107.05
13	B	821	CLA	O2D-CGD-CBD	2.68	116.03	111.28
13	B	836	CLA	C4-C3-C5	2.68	119.91	115.29
13	B	820	CLA	CAA-C2A-C3A	2.68	120.16	112.81
15	B	843	BCR	C38-C26-C27	2.68	118.64	113.56
13	B	824	CLA	C1D-CHD-C4C	2.69	126.16	122.48
13	B	828	CLA	C1D-CHD-C4C	2.69	126.16	122.48
13	A	804	CLA	C1-O2A-CGA	2.70	122.98	116.77
13	B	820	CLA	C1D-CHD-C4C	2.70	126.17	122.48
13	B	819	CLA	C1D-CHD-C4C	2.70	126.18	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	803	CLA	O2A-CGA-CBA	2.71	119.74	111.92
13	A	817	CLA	C4-C3-C5	2.71	119.95	115.29
15	I	102	BCR	C29-C30-C25	2.71	114.71	110.48
13	A	820	CLA	C4-C3-C5	2.71	119.96	115.29
13	A	839	CLA	C1D-CHD-C4C	2.71	126.19	122.48
13	A	818	CLA	C1D-CHD-C4C	2.71	126.19	122.48
13	A	843	CLA	C1D-CHD-C4C	2.72	126.20	122.48
13	B	836	CLA	C1D-CHD-C4C	2.72	126.20	122.48
13	L	1003	CLA	C4-C3-C5	2.72	119.98	115.29
13	B	827	CLA	C1-O2A-CGA	2.73	123.06	116.77
13	A	845	CLA	C4-C3-C5	2.74	120.01	115.29
13	J	1101	CLA	C4-C3-C5	2.74	120.02	115.29
13	B	815	CLA	C1D-CHD-C4C	2.75	126.24	122.48
13	M	1201	CLA	C4-C3-C5	2.75	120.02	115.29
13	A	833	CLA	C1D-CHD-C4C	2.75	126.24	122.48
13	B	833	CLA	C1D-CHD-C4C	2.75	126.24	122.48
13	A	815	CLA	C1C-NC-C4C	2.75	108.60	107.05
13	A	831	CLA	O2A-CGA-CBA	2.75	119.88	111.92
13	A	835	CLA	C1D-CHD-C4C	2.76	126.25	122.48
13	L	1002	CLA	C1D-CHD-C4C	2.76	126.26	122.48
13	J	1103	CLA	C1D-CHD-C4C	2.76	126.26	122.48
13	A	833	CLA	C4-C3-C5	2.76	120.06	115.29
13	B	827	CLA	C1C-NC-C4C	2.77	108.61	107.05
13	B	805	CLA	C4-C3-C5	2.77	120.07	115.29
13	B	811	CLA	C1D-CHD-C4C	2.77	126.27	122.48
13	B	820	CLA	C1-O2A-CGA	2.77	123.16	116.77
13	A	833	CLA	O2A-CGA-CBA	2.77	119.94	111.92
13	A	802	CLA	C4-C3-C5	2.78	120.08	115.29
13	B	810	CLA	C1D-CHD-C4C	2.78	126.28	122.48
13	A	845	CLA	C1C-NC-C4C	2.78	108.61	107.05
13	B	808	CLA	C1D-CHD-C4C	2.78	126.28	122.48
13	A	801	CLA	C4-C3-C5	2.78	120.09	115.29
13	A	822	CLA	O2A-CGA-CBA	2.78	119.97	111.92
13	J	1102	CLA	C1D-CHD-C4C	2.79	126.31	122.48
13	M	1201	CLA	C1D-CHD-C4C	2.80	126.31	122.48
15	L	1005	BCR	C35-C13-C12	2.80	122.56	118.10
13	L	1002	CLA	C4-C3-C5	2.80	120.12	115.29
13	B	822	CLA	C4-C3-C5	2.80	120.12	115.29
13	B	801	CLA	C4-C3-C5	2.81	120.13	115.29
13	B	815	CLA	C4-C3-C5	2.82	120.15	115.29
13	B	802	CLA	C4-C3-C5	2.82	120.15	115.29
13	B	807	CLA	C4-C3-C5	2.82	120.15	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	818	CLA	C1D-CHD-C4C	2.82	126.34	122.48
13	B	831	CLA	O2A-CGA-CBA	2.82	120.08	111.92
13	A	812	CLA	C1D-CHD-C4C	2.82	126.35	122.48
15	B	850	BCR	C29-C30-C25	2.83	114.90	110.48
13	A	826	CLA	O2A-CGA-CBA	2.83	120.10	111.92
13	A	836	CLA	C1D-CHD-C4C	2.83	126.35	122.48
13	A	817	CLA	C1-O2A-CGA	2.83	123.30	116.77
13	B	830	CLA	C4-C3-C5	2.84	120.18	115.29
13	A	802	CLA	O2A-CGA-CBA	2.84	120.14	111.92
13	A	813	CLA	C4-C3-C5	2.85	120.19	115.29
13	A	826	CLA	C1D-CHD-C4C	2.85	126.38	122.48
13	A	806	CLA	C4-C3-C5	2.85	120.20	115.29
13	A	811	CLA	O2A-CGA-CBA	2.85	120.16	111.92
13	A	815	CLA	C1D-CHD-C4C	2.86	126.39	122.48
13	B	822	CLA	C1D-CHD-C4C	2.86	126.39	122.48
13	B	813	CLA	C1D-CHD-C4C	2.86	126.40	122.48
13	B	801	CLA	O2A-CGA-CBA	2.87	120.21	111.92
13	A	813	CLA	C1D-CHD-C4C	2.87	126.41	122.48
13	A	828	CLA	C1-O2A-CGA	2.87	123.39	116.77
13	M	1202	CLA	C1D-CHD-C4C	2.88	126.42	122.48
13	A	806	CLA	C1D-CHD-C4C	2.88	126.42	122.48
13	A	838	CLA	C4-C3-C5	2.88	120.25	115.29
13	B	806	CLA	C4-C3-C5	2.88	120.26	115.29
13	A	821	CLA	C1D-CHD-C4C	2.88	126.42	122.48
15	A	851	BCR	C29-C30-C25	2.88	114.99	110.48
13	A	835	CLA	C4-C3-C5	2.89	120.27	115.29
13	B	812	CLA	C1-O2A-CGA	2.89	123.42	116.77
13	J	1101	CLA	C1D-CHD-C4C	2.89	126.44	122.48
13	A	820	CLA	C1D-CHD-C4C	2.89	126.44	122.48
13	A	816	CLA	C1D-CHD-C4C	2.90	126.44	122.48
13	A	829	CLA	C4-C3-C5	2.90	120.28	115.29
13	A	803	CLA	C1D-CHD-C4C	2.90	126.45	122.48
13	A	827	CLA	C4-C3-C5	2.90	120.29	115.29
13	B	803	CLA	O2A-CGA-CBA	2.91	120.34	111.92
13	A	829	CLA	C1D-CHD-C4C	2.92	126.48	122.48
13	A	824	CLA	C4-C3-C5	2.93	120.34	115.29
13	L	1004	CLA	C4-C3-C5	2.93	120.34	115.29
13	A	840	CLA	C1-O2A-CGA	2.93	123.52	116.77
13	A	811	CLA	C4-C3-C5	2.94	120.36	115.29
13	B	827	CLA	C4-C3-C5	2.94	120.36	115.29
15	B	843	BCR	C33-C5-C4	2.94	119.13	113.56
13	B	839	CLA	C1D-CHD-C4C	2.95	126.51	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C4-C3-C5	2.95	120.37	115.29
13	B	839	CLA	C4-C3-C5	2.95	120.37	115.29
13	A	803	CLA	C4-C3-C5	2.95	120.37	115.29
16	A	853	LHG	O8-C23-C24	2.95	120.46	111.92
13	A	834	CLA	O2A-CGA-CBA	2.96	120.49	111.92
13	A	837	CLA	C2A-C1A-CHA	2.97	129.14	123.92
13	A	832	CLA	C4-C3-C5	2.97	120.41	115.29
13	B	834	CLA	C1D-CHD-C4C	2.98	126.56	122.48
13	A	855	CLA	C1D-CHD-C4C	2.98	126.56	122.48
13	A	821	CLA	O2A-CGA-CBA	2.98	120.54	111.92
13	A	845	CLA	C1D-CHD-C4C	2.98	126.56	122.48
13	A	839	CLA	O2A-CGA-CBA	2.98	120.55	111.92
13	I	101	CLA	C4-C3-C5	2.99	120.44	115.29
13	B	824	CLA	O2A-CGA-CBA	2.99	120.57	111.92
13	A	830	CLA	C1-O2A-CGA	2.99	123.67	116.77
15	B	842	BCR	C33-C5-C4	3.00	119.23	113.56
13	A	834	CLA	C4-C3-C5	3.00	120.46	115.29
13	A	802	CLA	C1D-CHD-C4C	3.00	126.59	122.48
13	I	101	CLA	C1-O2A-CGA	3.00	123.69	116.77
13	A	819	CLA	C1-O2A-CGA	3.01	123.70	116.77
13	B	823	CLA	C1D-CHD-C4C	3.01	126.60	122.48
13	B	817	CLA	C4-C3-C5	3.01	120.48	115.29
13	B	824	CLA	C4-C3-C5	3.01	120.49	115.29
13	B	812	CLA	C4-C3-C5	3.02	120.49	115.29
13	B	803	CLA	C4-C3-C5	3.02	120.49	115.29
13	A	841	CLA	O2A-CGA-CBA	3.02	120.66	111.92
13	B	808	CLA	C4-C3-C5	3.02	120.50	115.29
13	B	830	CLA	C1D-CHD-C4C	3.02	126.62	122.48
13	A	841	CLA	C1D-CHD-C4C	3.03	126.62	122.48
13	A	805	CLA	O2A-CGA-CBA	3.03	120.67	111.92
13	A	804	CLA	C4-C3-C5	3.03	120.51	115.29
15	B	847	BCR	C29-C30-C25	3.03	115.22	110.48
13	A	812	CLA	C4-C3-C5	3.03	120.52	115.29
13	A	842	CLA	O2D-CGD-CBD	3.05	116.69	111.28
13	A	832	CLA	C1D-CHD-C4C	3.05	126.66	122.48
13	A	828	CLA	C4-C3-C5	3.05	120.55	115.29
13	L	1004	CLA	C1D-CHD-C4C	3.06	126.66	122.48
13	A	845	CLA	C1-O2A-CGA	3.06	123.81	116.77
13	A	837	CLA	O2A-CGA-CBA	3.06	120.77	111.92
13	B	808	CLA	O2A-CGA-CBA	3.06	120.77	111.92
13	B	825	CLA	C4-C3-C5	3.08	120.59	115.29
15	B	842	BCR	C29-C30-C25	3.08	115.29	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C1D-CHD-C4C	3.08	126.69	122.48
15	F	1302	BCR	C29-C30-C25	3.08	115.30	110.48
13	A	838	CLA	C1-O2A-CGA	3.10	123.92	116.77
13	A	844	CLA	C1D-CHD-C4C	3.10	126.73	122.48
13	B	818	CLA	O2A-CGA-CBA	3.13	120.96	111.92
13	A	827	CLA	O2A-CGA-CBA	3.15	121.02	111.92
18	B	848	LMG	O8-C28-C29	3.17	121.10	111.92
13	A	843	CLA	C4-C3-C5	3.18	120.77	115.29
13	B	820	CLA	C4-C3-C5	3.19	120.79	115.29
13	B	821	CLA	CED-O2D-CGD	3.20	123.34	115.97
15	L	1005	BCR	C29-C30-C25	3.20	115.48	110.48
15	A	847	BCR	C38-C26-C27	3.20	119.62	113.56
13	J	1101	CLA	O2A-CGA-CBA	3.21	121.19	111.92
13	B	804	CLA	C4-C3-C5	3.21	120.82	115.29
13	B	802	CLA	O2A-CGA-CBA	3.21	121.21	111.92
13	A	818	CLA	C4-C3-C5	3.21	120.83	115.29
13	A	837	CLA	C4-C3-C5	3.22	119.78	115.96
15	B	842	BCR	C38-C26-C27	3.23	119.67	113.56
15	B	849	BCR	C2-C1-C6	3.23	115.53	110.48
13	B	835	CLA	O2A-CGA-CBA	3.24	121.29	111.92
13	B	826	CLA	C1-O2A-CGA	3.24	124.24	116.77
15	L	1006	BCR	C29-C30-C25	3.25	115.56	110.48
15	A	852	BCR	C2-C1-C6	3.25	115.56	110.48
15	B	841	BCR	C38-C26-C27	3.25	119.71	113.56
13	A	816	CLA	O2A-CGA-CBA	3.25	121.33	111.92
13	B	815	CLA	C1-O2A-CGA	3.26	124.27	116.77
13	A	844	CLA	C4A-NA-C1A	3.26	110.53	106.32
13	L	1004	CLA	O2A-CGA-CBA	3.26	121.36	111.92
15	B	843	BCR	C28-C27-C26	3.26	119.72	113.99
13	B	805	CLA	C1D-CHD-C4C	3.27	126.96	122.48
15	B	846	BCR	C38-C26-C27	3.28	119.76	113.56
15	A	849	BCR	C29-C30-C25	3.28	115.60	110.48
13	B	804	CLA	O2A-CGA-CBA	3.29	121.42	111.92
15	M	1203	BCR	C29-C30-C25	3.29	115.63	110.48
15	I	102	BCR	C33-C5-C4	3.30	119.80	113.56
15	A	848	BCR	C29-C30-C25	3.30	115.63	110.48
13	B	801	CLA	C4A-NA-C1A	3.30	110.58	106.32
15	B	844	BCR	C29-C30-C25	3.30	115.64	110.48
13	A	830	CLA	C4-C3-C5	3.30	120.98	115.29
15	A	850	BCR	C29-C30-C25	3.30	115.64	110.48
13	A	807	CLA	O2A-CGA-CBA	3.31	121.48	111.92
13	A	823	CLA	C4-C3-C5	3.31	119.88	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	845	BCR	C38-C26-C27	3.31	119.82	113.56
16	A	854	LHG	O8-C23-C24	3.32	120.08	111.38
13	B	838	CLA	C4-C3-C5	3.32	121.02	115.29
15	A	849	BCR	C33-C5-C4	3.33	119.86	113.56
13	A	801	CLA	C4A-NA-C1A	3.33	110.62	106.32
13	B	830	CLA	O2A-CGA-CBA	3.34	121.58	111.92
13	B	816	CLA	C4-C3-C5	3.34	121.05	115.29
13	A	843	CLA	C1-O2A-CGA	3.34	124.47	116.77
13	B	836	CLA	C1-O2A-CGA	3.36	124.51	116.77
13	B	814	CLA	C1-O2A-CGA	3.37	124.53	116.77
13	B	815	CLA	O2D-CGD-CBD	3.37	117.25	111.28
13	J	1103	CLA	C4A-NA-C1A	3.38	110.68	106.32
15	M	1203	BCR	C33-C5-C4	3.39	119.98	113.56
15	A	849	BCR	C2-C1-C6	3.40	115.79	110.48
15	B	846	BCR	C29-C30-C25	3.41	115.81	110.48
13	A	802	CLA	C4A-NA-C1A	3.41	110.72	106.32
15	F	1302	BCR	C38-C26-C27	3.41	120.01	113.56
15	B	846	BCR	C33-C5-C4	3.41	120.01	113.56
15	B	847	BCR	C33-C5-C4	3.41	120.02	113.56
13	A	832	CLA	O2A-CGA-CBA	3.42	121.80	111.92
13	B	818	CLA	O2D-CGD-CBD	3.42	117.34	111.28
15	A	851	BCR	C2-C1-C6	3.42	115.83	110.48
15	A	852	BCR	C29-C30-C25	3.43	115.84	110.48
13	B	803	CLA	C4A-NA-C1A	3.43	110.75	106.32
13	A	813	CLA	C1-O2A-CGA	3.43	124.68	116.77
13	B	802	CLA	C4A-NA-C1A	3.44	110.76	106.32
15	B	845	BCR	C33-C5-C4	3.45	120.08	113.56
13	A	817	CLA	O2D-CGD-CBD	3.46	117.42	111.28
15	J	1105	BCR	C29-C30-C25	3.47	115.90	110.48
13	B	813	CLA	C4A-NA-C1A	3.47	110.80	106.32
13	A	824	CLA	C4A-NA-C1A	3.48	110.81	106.32
13	A	842	CLA	C4-C3-C5	3.48	121.29	115.29
15	A	851	BCR	C33-C5-C4	3.48	120.15	113.56
13	A	816	CLA	O2D-CGD-CBD	3.48	117.46	111.28
15	B	841	BCR	C29-C30-C25	3.49	115.93	110.48
15	A	847	BCR	C33-C5-C4	3.49	120.17	113.56
13	B	820	CLA	O2D-CGD-CBD	3.50	117.48	111.28
15	A	850	BCR	C33-C5-C4	3.50	120.19	113.56
16	X	101	LHG	O7-C7-C8	3.52	118.97	111.55
15	B	849	BCR	C38-C26-C27	3.53	120.23	113.56
15	F	1302	BCR	C2-C1-C6	3.54	116.01	110.48
15	A	849	BCR	C38-C26-C27	3.56	120.30	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	847	BCR	C38-C26-C27	3.56	120.30	113.56
15	B	849	BCR	C33-C5-C4	3.57	120.32	113.56
15	B	844	BCR	C38-C26-C27	3.59	120.34	113.56
13	A	841	CLA	C4-C3-C5	3.60	120.23	115.96
13	B	810	CLA	O2D-CGD-CBD	3.61	117.68	111.28
15	L	1005	BCR	C33-C5-C4	3.61	120.39	113.56
13	A	834	CLA	C4A-NA-C1A	3.61	110.98	106.32
15	F	1302	BCR	C33-C5-C4	3.62	120.41	113.56
15	L	1006	BCR	C38-C26-C27	3.62	120.41	113.56
13	B	828	CLA	C4A-NA-C1A	3.63	111.01	106.32
15	A	847	BCR	C29-C30-C25	3.65	116.18	110.48
15	A	850	BCR	C38-C26-C27	3.65	120.47	113.56
13	B	806	CLA	C1-O2A-CGA	3.65	125.18	116.77
13	A	808	CLA	O2A-CGA-CBA	3.66	122.50	111.92
15	M	1203	BCR	C38-C26-C27	3.66	120.49	113.56
15	J	1105	BCR	C2-C1-C6	3.67	116.21	110.48
15	L	1006	BCR	C2-C1-C6	3.67	116.21	110.48
15	J	1105	BCR	C33-C5-C4	3.67	120.50	113.56
15	J	1104	BCR	C33-C5-C4	3.67	120.51	113.56
13	B	825	CLA	C1-O2A-CGA	3.67	125.23	116.77
13	B	811	CLA	O2A-CGA-CBA	3.68	122.55	111.92
15	A	851	BCR	C38-C26-C27	3.68	120.52	113.56
13	X	102	CLA	C4A-NA-C1A	3.68	111.07	106.32
15	B	841	BCR	C33-C5-C4	3.69	120.54	113.56
13	A	823	CLA	O2D-CGD-CBD	3.69	117.82	111.28
13	A	833	CLA	O2D-CGD-CBD	3.69	117.83	111.28
15	A	848	BCR	C33-C5-C4	3.70	120.56	113.56
13	B	824	CLA	C4A-NA-C1A	3.70	111.10	106.32
15	B	847	BCR	C3-C4-C5	3.70	120.49	113.99
15	A	852	BCR	C33-C5-C4	3.71	120.57	113.56
13	A	814	CLA	C4A-NA-C1A	3.71	111.11	106.32
13	B	829	CLA	C4A-NA-C1A	3.71	111.11	106.32
13	B	812	CLA	C4A-NA-C1A	3.72	111.11	106.32
15	B	846	BCR	C2-C1-C6	3.72	116.30	110.48
13	B	816	CLA	C4A-NA-C1A	3.74	111.14	106.32
15	I	102	BCR	C3-C4-C5	3.74	120.55	113.99
15	I	102	BCR	C38-C26-C27	3.75	120.66	113.56
15	B	845	BCR	C2-C1-C6	3.75	116.35	110.48
13	B	808	CLA	C4A-NA-C1A	3.75	111.16	106.32
13	B	811	CLA	C4A-NA-C1A	3.76	111.17	106.32
13	A	822	CLA	C4A-NA-C1A	3.76	111.17	106.32
13	A	842	CLA	C4A-NA-C1A	3.76	111.17	106.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	850	BCR	C3-C4-C5	3.76	120.59	113.99
13	A	815	CLA	C4A-NA-C1A	3.77	111.18	106.32
13	B	825	CLA	C4A-NA-C1A	3.77	111.18	106.32
13	B	821	CLA	C4A-NA-C1A	3.77	111.18	106.32
13	B	823	CLA	C4A-NA-C1A	3.77	111.18	106.32
13	B	836	CLA	C4A-NA-C1A	3.77	111.18	106.32
15	A	848	BCR	C38-C26-C27	3.77	120.70	113.56
13	A	840	CLA	C4A-NA-C1A	3.78	111.20	106.32
15	A	848	BCR	C2-C1-C6	3.78	116.39	110.48
13	B	818	CLA	C4A-NA-C1A	3.78	111.20	106.32
13	A	828	CLA	C4A-NA-C1A	3.79	111.21	106.32
13	B	835	CLA	C4A-NA-C1A	3.80	111.22	106.32
13	J	1101	CLA	C4A-NA-C1A	3.80	111.22	106.32
13	A	835	CLA	C4A-NA-C1A	3.80	111.22	106.32
13	A	841	CLA	C4A-NA-C1A	3.80	111.22	106.32
13	A	817	CLA	C4A-NA-C1A	3.80	111.22	106.32
13	A	829	CLA	C4A-NA-C1A	3.80	111.23	106.32
13	B	815	CLA	C4A-NA-C1A	3.80	111.23	106.32
15	A	850	BCR	C2-C1-C6	3.81	116.43	110.48
13	A	803	CLA	C4A-NA-C1A	3.81	111.24	106.32
13	B	809	CLA	C4A-NA-C1A	3.82	111.25	106.32
13	B	819	CLA	C4A-NA-C1A	3.82	111.25	106.32
13	L	1002	CLA	C4A-NA-C1A	3.82	111.25	106.32
13	A	823	CLA	C4A-NA-C1A	3.82	111.25	106.32
15	B	850	BCR	C38-C26-C27	3.82	120.79	113.56
13	J	1102	CLA	C4A-NA-C1A	3.83	111.26	106.32
13	B	839	CLA	C4A-NA-C1A	3.83	111.26	106.32
13	B	804	CLA	C4A-NA-C1A	3.83	111.26	106.32
13	A	805	CLA	C4A-NA-C1A	3.84	111.27	106.32
13	B	837	CLA	C4A-NA-C1A	3.84	111.27	106.32
13	B	826	CLA	C4A-NA-C1A	3.84	111.27	106.32
13	A	806	CLA	C4A-NA-C1A	3.85	111.29	106.32
15	L	1005	BCR	C38-C26-C27	3.86	120.86	113.56
15	L	1005	BCR	C2-C1-C6	3.86	116.51	110.48
13	A	804	CLA	C4A-NA-C1A	3.86	111.30	106.32
13	A	813	CLA	C4A-NA-C1A	3.86	111.30	106.32
13	A	836	CLA	C4A-NA-C1A	3.86	111.30	106.32
13	A	855	CLA	C4A-NA-C1A	3.86	111.31	106.32
13	L	1003	CLA	C4A-NA-C1A	3.87	111.31	106.32
13	B	838	CLA	O2A-CGA-CBA	3.87	123.10	111.92
13	B	820	CLA	C4A-NA-C1A	3.87	111.31	106.32
15	J	1105	BCR	C38-C26-C27	3.87	120.88	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	841	CLA	O2D-CGD-CBD	3.87	118.14	111.28
13	L	1004	CLA	C4A-NA-C1A	3.87	111.32	106.32
13	B	834	CLA	C4A-NA-C1A	3.88	111.32	106.32
13	B	805	CLA	C4A-NA-C1A	3.88	111.33	106.32
13	A	833	CLA	C4A-NA-C1A	3.88	111.33	106.32
13	B	829	CLA	O2D-CGD-CBD	3.90	118.19	111.28
13	B	832	CLA	C4A-NA-C1A	3.90	111.35	106.32
13	B	838	CLA	C4A-NA-C1A	3.90	111.35	106.32
15	J	1104	BCR	C2-C1-C6	3.91	116.58	110.48
13	A	837	CLA	C4A-NA-C1A	3.91	111.36	106.32
13	I	101	CLA	C4A-NA-C1A	3.91	111.36	106.32
15	A	852	BCR	C38-C26-C27	3.92	120.97	113.56
16	A	853	LHG	O7-C7-C8	3.93	119.83	111.55
13	B	831	CLA	C4A-NA-C1A	3.93	111.39	106.32
13	A	820	CLA	C4A-NA-C1A	3.93	111.39	106.32
13	A	811	CLA	C4A-NA-C1A	3.94	111.40	106.32
13	A	821	CLA	C4A-NA-C1A	3.94	111.40	106.32
15	B	845	BCR	C28-C27-C26	3.94	120.91	113.99
13	A	818	CLA	C4A-NA-C1A	3.95	111.41	106.32
16	A	854	LHG	O7-C7-C8	3.95	119.88	111.55
15	B	841	BCR	C2-C1-C6	3.95	116.66	110.48
13	A	832	CLA	C4A-NA-C1A	3.95	111.42	106.32
13	B	817	CLA	C4A-NA-C1A	3.96	111.43	106.32
13	B	807	CLA	C4A-NA-C1A	3.96	111.43	106.32
15	M	1203	BCR	C3-C4-C5	3.96	120.95	113.99
13	A	827	CLA	C4A-NA-C1A	3.96	111.43	106.32
15	A	847	BCR	C2-C1-C6	3.97	116.68	110.48
13	A	831	CLA	C4A-NA-C1A	3.98	111.45	106.32
13	B	810	CLA	C4A-NA-C1A	3.98	111.46	106.32
13	A	838	CLA	C4A-NA-C1A	3.98	111.46	106.32
13	A	843	CLA	C4A-NA-C1A	3.99	111.46	106.32
13	A	816	CLA	C4A-NA-C1A	3.99	111.46	106.32
13	A	812	CLA	C4A-NA-C1A	3.99	111.47	106.32
13	A	810	CLA	C4A-NA-C1A	4.00	111.48	106.32
13	M	1201	CLA	C4A-NA-C1A	4.01	111.50	106.32
13	B	822	CLA	C4A-NA-C1A	4.02	111.50	106.32
13	B	833	CLA	C4A-NA-C1A	4.03	111.52	106.32
13	B	806	CLA	C4A-NA-C1A	4.03	111.52	106.32
13	B	830	CLA	C4A-NA-C1A	4.05	111.54	106.32
13	A	809	CLA	O2A-CGA-CBA	4.05	123.64	111.92
13	A	845	CLA	C4A-NA-C1A	4.06	111.55	106.32
15	B	842	BCR	C3-C4-C5	4.08	121.16	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	805	CLA	O2D-CGD-CBD	4.08	118.52	111.28
13	F	1301	CLA	C4A-NA-C1A	4.08	111.59	106.32
13	A	826	CLA	C4A-NA-C1A	4.09	111.59	106.32
13	B	826	CLA	O2D-CGD-CBD	4.09	118.54	111.28
13	B	814	CLA	C4A-NA-C1A	4.11	111.63	106.32
13	A	825	CLA	C4A-NA-C1A	4.13	111.65	106.32
13	A	807	CLA	C4A-NA-C1A	4.15	111.67	106.32
15	J	1104	BCR	C28-C27-C26	4.16	121.29	113.99
13	A	819	CLA	C4A-NA-C1A	4.19	111.73	106.32
13	A	839	CLA	C4A-NA-C1A	4.19	111.73	106.32
13	B	827	CLA	C4A-NA-C1A	4.20	111.74	106.32
13	M	1202	CLA	C4A-NA-C1A	4.21	111.75	106.32
13	A	806	CLA	O2D-CGD-CBD	4.22	118.76	111.28
13	A	830	CLA	C4A-NA-C1A	4.24	111.79	106.32
13	A	819	CLA	C4-C3-C5	4.25	122.62	115.29
13	A	803	CLA	O2D-CGD-CBD	4.26	118.84	111.28
13	A	808	CLA	C4A-NA-C1A	4.27	111.83	106.32
13	A	809	CLA	C4A-NA-C1A	4.31	111.88	106.32
13	A	820	CLA	O2D-CGD-CBD	4.35	118.99	111.28
15	B	843	BCR	C3-C4-C5	4.37	121.65	113.99
15	B	843	BCR	C29-C30-C25	4.39	117.34	110.48
13	A	831	CLA	O2D-CGD-CBD	4.44	119.16	111.28
13	B	825	CLA	O2D-CGD-CBD	4.57	119.39	111.28
13	A	835	CLA	O2D-CGD-CBD	4.60	119.44	111.28
15	I	102	BCR	C2-C1-C6	4.74	117.89	110.48
15	M	1203	BCR	C2-C1-C6	4.74	117.90	110.48
15	B	847	BCR	C2-C1-C6	4.95	118.21	110.48
13	A	807	CLA	C4-C3-C5	4.95	121.82	115.96
13	A	804	CLA	O2D-CGD-CBD	4.98	120.10	111.28
15	B	842	BCR	C2-C1-C6	4.99	118.28	110.48
15	B	850	BCR	C2-C1-C6	5.02	118.33	110.48
13	A	829	CLA	C1-O2A-CGA	5.03	128.35	116.77
15	B	845	BCR	C29-C30-C25	5.04	118.36	110.48
13	A	826	CLA	O2D-CGD-CBD	5.06	120.24	111.28
15	J	1104	BCR	C29-C30-C25	5.11	118.47	110.48
13	A	807	CLA	CED-O2D-CGD	5.13	127.80	115.97
15	B	843	BCR	C2-C1-C6	5.14	118.51	110.48
13	A	802	CLA	O2D-CGD-CBD	5.18	120.47	111.28
13	B	806	CLA	O2D-CGD-CBD	5.18	120.47	111.28
13	A	814	CLA	O2D-CGD-CBD	5.29	120.66	111.28
13	A	818	CLA	C1-O2A-CGA	5.33	129.04	116.77
13	A	834	CLA	O2D-CGD-CBD	5.38	120.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	837	CLA	O2D-CGD-CBD	5.42	120.89	111.28
13	B	823	CLA	O2D-CGD-CBD	5.43	120.90	111.28
13	A	827	CLA	O2D-CGD-CBD	5.52	121.07	111.28
13	B	816	CLA	O2D-CGD-CBD	5.54	121.10	111.28
13	A	809	CLA	O2D-CGD-CBD	5.65	121.30	111.28
13	B	835	CLA	O2D-CGD-CBD	5.70	121.38	111.28
13	B	838	CLA	O2D-CGD-CBD	5.78	121.53	111.28
13	A	830	CLA	O2D-CGD-CBD	5.81	121.58	111.28
13	A	828	CLA	O2D-CGD-CBD	5.83	121.61	111.28
13	B	839	CLA	O2D-CGD-CBD	5.94	121.81	111.28
13	B	804	CLA	O2D-CGD-CBD	5.95	121.83	111.28
13	A	836	CLA	O2D-CGD-CBD	5.99	121.90	111.28
13	B	832	CLA	O2D-CGD-CBD	5.99	121.91	111.28
13	B	803	CLA	O2D-CGD-CBD	6.00	121.91	111.28
18	B	848	LMG	C30-C29-C28	6.01	135.30	113.60
13	A	843	CLA	O2D-CGD-CBD	6.11	122.11	111.28
13	A	818	CLA	O2D-CGD-CBD	6.15	122.18	111.28
13	I	101	CLA	O2D-CGD-CBD	6.26	122.38	111.28
13	B	828	CLA	O2D-CGD-CBD	6.27	122.39	111.28
13	M	1202	CLA	O2D-CGD-CBD	6.29	122.44	111.28
13	B	830	CLA	O2D-CGD-CBD	6.32	122.48	111.28
13	L	1002	CLA	O2D-CGD-CBD	6.35	122.54	111.28
13	A	825	CLA	O2D-CGD-CBD	6.37	122.57	111.28
13	A	838	CLA	O2D-CGD-CBD	6.37	122.58	111.28
13	A	805	CLA	O2D-CGD-CBD	6.41	122.64	111.28
13	A	855	CLA	O2D-CGD-CBD	6.43	122.68	111.28
13	B	836	CLA	O2D-CGD-CBD	6.44	122.69	111.28
13	J	1101	CLA	O2D-CGD-CBD	6.45	122.71	111.28
13	F	1301	CLA	O2D-CGD-CBD	6.47	122.75	111.28
13	B	834	CLA	O2D-CGD-CBD	6.50	122.81	111.28
13	L	1004	CLA	O2D-CGD-CBD	6.56	122.90	111.28
13	B	819	CLA	O2D-CGD-CBD	6.61	123.00	111.28
13	B	837	CLA	O2D-CGD-CBD	6.61	123.00	111.28
13	A	813	CLA	O2D-CGD-CBD	6.62	123.02	111.28
13	A	815	CLA	O2D-CGD-CBD	6.63	123.04	111.28
13	A	845	CLA	O2D-CGD-CBD	6.64	123.06	111.28
13	B	801	CLA	O2D-CGD-CBD	6.65	123.07	111.28
13	J	1102	CLA	O2D-CGD-CBD	6.72	123.19	111.28
13	B	811	CLA	O2D-CGD-CBD	6.72	123.19	111.28
13	A	829	CLA	O2D-CGD-CBD	6.73	123.21	111.28
13	L	1003	CLA	O2D-CGD-CBD	6.75	123.24	111.28
13	B	824	CLA	O2D-CGD-CBD	6.75	123.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	809	CLA	O2D-CGD-CBD	6.85	123.43	111.28
13	B	814	CLA	O2D-CGD-CBD	6.88	123.48	111.28
13	A	839	CLA	O2D-CGD-CBD	6.94	123.59	111.28
13	A	801	CLA	O2D-CGD-CBD	7.04	123.76	111.28
13	A	810	CLA	O2D-CGD-CBD	7.05	123.77	111.28
13	B	827	CLA	O2D-CGD-CBD	7.05	123.78	111.28
13	B	822	CLA	O2D-CGD-CBD	7.08	123.83	111.28
13	B	812	CLA	O2D-CGD-CBD	7.11	123.89	111.28
13	B	808	CLA	O2D-CGD-CBD	7.15	123.95	111.28
13	B	813	CLA	O2D-CGD-CBD	7.23	124.10	111.28
13	B	807	CLA	O2D-CGD-CBD	7.24	124.12	111.28
13	A	819	CLA	O2D-CGD-CBD	7.26	124.16	111.28
13	M	1201	CLA	O2D-CGD-CBD	7.29	124.21	111.28
13	B	833	CLA	O2D-CGD-CBD	7.30	124.22	111.28
13	A	811	CLA	O2D-CGD-CBD	7.32	124.26	111.28
13	A	821	CLA	O2D-CGD-CBD	7.42	124.43	111.28
13	A	824	CLA	O2D-CGD-CBD	7.52	124.61	111.28
13	A	832	CLA	O2D-CGD-CBD	7.61	124.77	111.28
13	A	840	CLA	O2D-CGD-CBD	7.65	124.83	111.28
13	A	812	CLA	O2D-CGD-CBD	7.67	124.87	111.28
13	A	808	CLA	O2D-CGD-CBD	7.68	124.90	111.28
13	B	817	CLA	O2D-CGD-CBD	7.85	125.19	111.28
13	B	831	CLA	O2D-CGD-CBD	8.41	126.18	111.28
13	A	822	CLA	O2D-CGD-CBD	8.43	126.23	111.28
13	B	802	CLA	O2D-CGD-CBD	8.46	126.28	111.28
13	X	102	CLA	O2D-CGD-CBD	8.50	126.35	111.28

All (229) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	832	CLA	NC
13	B	832	CLA	ND
13	B	832	CLA	NA
13	A	806	CLA	ND
13	A	806	CLA	NA
13	B	837	CLA	NC
13	B	837	CLA	ND
13	B	837	CLA	NA
13	B	825	CLA	NC
13	B	825	CLA	ND
13	B	825	CLA	NA
13	M	1201	CLA	ND

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Mol	Chain	Res	Type	Atom
13	M	1201	CLA	NA
13	A	822	CLA	NC
13	A	822	CLA	ND
13	A	822	CLA	NA
13	A	805	CLA	ND
13	A	845	CLA	NC
13	A	845	CLA	ND
13	A	845	CLA	NA
13	B	817	CLA	ND
13	B	817	CLA	NA
13	B	812	CLA	NC
13	B	812	CLA	ND
13	B	812	CLA	NA
13	B	831	CLA	NC
13	B	831	CLA	ND
13	B	831	CLA	NA
13	A	828	CLA	NC
13	A	828	CLA	ND
13	A	802	CLA	ND
13	A	802	CLA	NA
13	A	815	CLA	ND
13	A	815	CLA	NA
13	A	810	CLA	NC
13	A	810	CLA	ND
13	A	810	CLA	NA
13	B	814	CLA	NC
13	B	814	CLA	ND
13	B	814	CLA	NA
13	A	801	CLA	NC
13	A	801	CLA	ND
13	B	816	CLA	NC
13	B	816	CLA	ND
13	B	835	CLA	NC
13	B	835	CLA	ND
13	B	813	CLA	NC
13	B	808	CLA	ND
13	B	811	CLA	NC
13	B	811	CLA	ND
13	B	827	CLA	NC
13	B	827	CLA	ND
13	B	827	CLA	NA
13	J	1102	CLA	NC

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Mol	Chain	Res	Type	Atom
13	J	1102	CLA	ND
13	A	811	CLA	NC
13	A	811	CLA	ND
13	A	811	CLA	NA
13	A	834	CLA	ND
13	A	834	CLA	NA
13	A	818	CLA	NC
13	A	818	CLA	ND
13	A	818	CLA	NA
13	A	820	CLA	NC
13	A	820	CLA	ND
13	A	820	CLA	NA
13	B	803	CLA	ND
13	A	842	CLA	NC
13	A	842	CLA	ND
13	A	842	CLA	NA
13	B	821	CLA	NC
13	B	821	CLA	ND
13	B	821	CLA	NA
13	A	813	CLA	NC
13	A	813	CLA	ND
13	A	813	CLA	NA
13	J	1101	CLA	NC
13	J	1101	CLA	ND
13	J	1101	CLA	NA
13	A	823	CLA	NC
13	A	823	CLA	ND
13	A	823	CLA	NA
13	B	823	CLA	ND
13	B	823	CLA	NA
13	L	1003	CLA	NC
13	L	1003	CLA	ND
13	L	1003	CLA	NA
13	A	838	CLA	ND
13	A	838	CLA	NA
13	A	808	CLA	NC
13	A	808	CLA	ND
13	A	808	CLA	NA
13	B	824	CLA	ND
13	A	807	CLA	NC
13	A	807	CLA	ND
13	A	807	CLA	NA

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Mol	Chain	Res	Type	Atom
13	A	840	CLA	NC
13	A	840	CLA	ND
13	A	840	CLA	NA
13	A	824	CLA	NC
13	A	824	CLA	ND
13	A	824	CLA	NA
13	A	827	CLA	NC
13	A	827	CLA	ND
13	A	827	CLA	NA
13	A	843	CLA	NC
13	A	843	CLA	ND
13	A	843	CLA	NA
13	I	101	CLA	ND
13	I	101	CLA	NA
13	A	814	CLA	NC
13	A	814	CLA	ND
13	A	814	CLA	NA
13	X	102	CLA	ND
13	X	102	CLA	NA
13	B	839	CLA	NC
13	B	839	CLA	ND
13	B	839	CLA	NA
13	L	1004	CLA	NC
13	L	1004	CLA	ND
13	L	1004	CLA	NA
13	B	829	CLA	NC
13	B	829	CLA	ND
13	B	829	CLA	NA
13	B	801	CLA	NC
13	B	801	CLA	ND
13	B	833	CLA	ND
13	B	833	CLA	NA
13	A	829	CLA	ND
13	A	829	CLA	NA
13	B	838	CLA	NC
13	B	838	CLA	ND
13	B	838	CLA	NA
13	A	803	CLA	NC
13	A	803	CLA	ND
13	A	803	CLA	NA
13	B	807	CLA	NC
13	B	807	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	807	CLA	NA
13	B	820	CLA	NC
13	B	820	CLA	ND
13	B	820	CLA	NA
13	B	805	CLA	NC
13	B	805	CLA	ND
13	B	805	CLA	NA
13	B	809	CLA	NC
13	B	809	CLA	ND
13	B	809	CLA	NA
13	A	839	CLA	NC
13	A	839	CLA	ND
13	A	839	CLA	NA
13	A	833	CLA	NC
13	A	833	CLA	ND
13	B	802	CLA	ND
13	A	821	CLA	ND
13	A	821	CLA	NA
13	A	831	CLA	NC
13	A	831	CLA	ND
13	A	831	CLA	NA
13	A	837	CLA	NC
13	A	819	CLA	NC
13	A	819	CLA	ND
13	A	819	CLA	NA
13	A	816	CLA	NC
13	A	816	CLA	NA
13	B	822	CLA	ND
13	B	822	CLA	NA
13	B	830	CLA	ND
13	B	830	CLA	NA
13	B	828	CLA	NC
13	B	828	CLA	ND
13	A	844	CLA	NC
13	A	835	CLA	NC
13	A	835	CLA	ND
13	A	835	CLA	NA
13	J	1103	CLA	NC
13	J	1103	CLA	ND
13	F	1301	CLA	NA
13	B	836	CLA	NC
13	B	836	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	836	CLA	NA
13	A	825	CLA	ND
13	A	825	CLA	NA
13	B	806	CLA	ND
13	B	806	CLA	NA
13	A	832	CLA	ND
13	A	832	CLA	NA
13	A	812	CLA	ND
13	A	812	CLA	NA
13	A	804	CLA	NC
13	A	804	CLA	ND
13	A	804	CLA	NA
13	A	836	CLA	ND
13	A	836	CLA	NA
13	B	826	CLA	ND
13	B	826	CLA	NA
13	A	855	CLA	ND
13	A	855	CLA	NA
13	M	1202	CLA	NC
13	M	1202	CLA	NA
13	A	841	CLA	NC
13	A	841	CLA	ND
13	A	841	CLA	NA
13	B	810	CLA	ND
13	B	810	CLA	NA
13	A	809	CLA	NA
13	B	815	CLA	NC
13	B	815	CLA	ND
13	B	815	CLA	NA
13	A	826	CLA	NC
13	A	826	CLA	NA
13	A	817	CLA	NC
13	A	817	CLA	ND
13	A	817	CLA	NA
13	A	830	CLA	NC
13	A	830	CLA	ND
13	A	830	CLA	NA
13	B	804	CLA	ND
13	B	804	CLA	NA
13	L	1002	CLA	NC
13	L	1002	CLA	ND
13	L	1002	CLA	NA

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Mol	Chain	Res	Type	Atom
13	B	818	CLA	NC
13	B	818	CLA	ND
13	B	834	CLA	NC
13	B	834	CLA	ND
13	B	819	CLA	NC
13	B	819	CLA	ND
13	B	819	CLA	NA

There are no torsion outliers.

There are no ring outliers.

123 monomers are involved in 1092 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	801	CLA	8	0
13	A	802	CLA	12	0
13	A	803	CLA	27	0
13	A	804	CLA	10	0
13	A	805	CLA	13	0
13	A	806	CLA	9	0
13	A	807	CLA	13	0
13	A	808	CLA	17	0
13	A	809	CLA	16	0
13	A	810	CLA	8	0
13	A	811	CLA	14	0
13	A	812	CLA	7	0
13	A	813	CLA	19	0
13	A	814	CLA	8	0
13	A	815	CLA	7	0
13	A	816	CLA	3	0
13	A	817	CLA	9	0
13	A	818	CLA	11	0
13	A	819	CLA	16	0
13	A	820	CLA	10	0
13	A	821	CLA	12	0
13	A	822	CLA	7	0
13	A	823	CLA	13	0
13	A	824	CLA	8	0
13	A	825	CLA	22	0
13	A	826	CLA	17	0
13	A	827	CLA	15	0
13	A	828	CLA	16	0
13	A	829	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	830	CLA	14	0
13	A	831	CLA	11	0
13	A	832	CLA	21	0
13	A	833	CLA	19	0
13	A	834	CLA	18	0
13	A	835	CLA	8	0
13	A	836	CLA	11	0
13	A	837	CLA	14	0
13	A	838	CLA	14	0
13	A	839	CLA	17	0
13	A	840	CLA	16	0
13	A	841	CLA	6	0
13	A	842	CLA	22	0
13	A	843	CLA	10	0
13	A	844	CLA	3	0
13	A	845	CLA	11	0
14	A	846	PQN	7	0
15	A	847	BCR	5	0
15	A	848	BCR	5	0
15	A	849	BCR	4	0
15	A	850	BCR	4	0
15	A	851	BCR	3	0
15	A	852	BCR	19	0
16	A	853	LHG	10	0
16	A	854	LHG	2	0
13	A	855	CLA	2	0
13	B	801	CLA	13	0
13	B	802	CLA	18	0
13	B	803	CLA	16	0
13	B	804	CLA	17	0
13	B	805	CLA	9	0
13	B	806	CLA	15	0
13	B	807	CLA	12	0
13	B	808	CLA	14	0
13	B	809	CLA	8	0
13	B	810	CLA	5	0
13	B	811	CLA	18	0
13	B	812	CLA	15	0
13	B	813	CLA	10	0
13	B	814	CLA	10	0
13	B	815	CLA	15	0
13	B	816	CLA	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	817	CLA	12	0
13	B	818	CLA	4	0
13	B	819	CLA	1	0
13	B	820	CLA	12	0
13	B	821	CLA	13	0
13	B	822	CLA	21	0
13	B	823	CLA	8	0
13	B	824	CLA	20	0
13	B	825	CLA	18	0
13	B	826	CLA	19	0
13	B	827	CLA	14	0
13	B	828	CLA	6	0
13	B	829	CLA	7	0
13	B	830	CLA	24	0
13	B	831	CLA	12	0
13	B	832	CLA	12	0
13	B	833	CLA	3	0
13	B	834	CLA	7	0
13	B	835	CLA	16	0
13	B	836	CLA	10	0
13	B	837	CLA	8	0
13	B	838	CLA	18	0
13	B	839	CLA	7	0
14	B	840	PQN	7	0
15	B	841	BCR	5	0
15	B	842	BCR	4	0
15	B	843	BCR	18	0
15	B	844	BCR	6	0
15	B	845	BCR	9	0
15	B	846	BCR	7	0
15	B	847	BCR	12	0
18	B	848	LMG	18	0
15	B	849	BCR	16	0
15	B	850	BCR	6	0
13	F	1301	CLA	5	0
15	F	1302	BCR	13	0
13	I	101	CLA	15	0
15	I	102	BCR	11	0
13	J	1101	CLA	13	0
13	J	1102	CLA	4	0
15	J	1104	BCR	4	0
15	J	1105	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	1002	CLA	5	0
13	L	1003	CLA	16	0
13	L	1004	CLA	7	0
15	L	1005	BCR	12	0
15	L	1006	BCR	4	0
13	M	1201	CLA	17	0
13	M	1202	CLA	1	0
15	M	1203	BCR	13	0
16	X	101	LHG	1	0
13	X	102	CLA	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	0.11	22 (2%) 50 39	42, 99, 157, 202	0
2	B	739/740 (99%)	0.01	10 (1%) 75 66	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.41	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	0.00	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	0.39	1 (1%) 75 66	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.23	1 (0%) 87 82	54, 83, 136, 158	0
7	I	38/38 (100%)	0.14	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.62	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.41	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.18	1 (0%) 87 82	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.03	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.27	1 (3%) 45 36	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.01	36 (1%) 72 63	10, 81, 141, 215	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASP	4.2
1	A	24	SER	3.5
10	L	146	ASP	3.4
1	A	18	ASN	3.3
2	B	497	ASN	3.3
2	B	312	THR	3.2
1	A	22	PRO	3.1
2	B	87	ALA	3.1
6	F	95	ASN	3.1
1	A	21	VAL	3.0
1	A	515	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	34	PHE	2.8
5	E	52	ALA	2.8
2	B	309	PHE	2.7
1	A	234	LYS	2.7
1	A	17	ASP	2.7
2	B	90	ILE	2.7
2	B	489	SER	2.6
1	A	40	ARG	2.6
1	A	33	HIS	2.5
1	A	244	LEU	2.5
2	B	672	SER	2.5
2	B	313	LYS	2.5
1	A	692	SER	2.5
1	A	516	ASP	2.4
1	A	182	LYS	2.4
1	A	289	THR	2.4
1	A	183	ARG	2.3
1	A	521	GLY	2.3
1	A	522	GLY	2.2
1	A	20	PRO	2.2
1	A	627	PRO	2.1
2	B	97	LYS	2.1
12	X	8	THR	2.0
1	A	499	GLY	2.0
2	B	407	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(\AA^2)	Q<0.9
13	CLA	A	844	41/65	0.67	0.40	116,136,148,281	0
13	CLA	A	815	45/65	0.73	0.64	111,150,177,185	0
15	BCR	A	847	40/40	0.73	0.82	98,140,151,162	0
13	CLA	M	1202	45/65	0.73	0.73	51,149,183,198	0
15	BCR	A	848	40/40	0.74	0.95	112,132,147,157	0
15	BCR	A	849	40/40	0.75	1.28	95,136,179,183	0
13	CLA	A	816	49/65	0.76	0.85	119,163,187,193	0
13	CLA	A	812	54/65	0.77	0.63	136,181,240,396	0
15	BCR	B	841	40/40	0.77	0.84	65,105,151,155	0
13	CLA	J	1102	45/65	0.78	0.38	75,111,128,280	0
13	CLA	A	836	45/65	0.79	0.47	63,96,163,234	0
13	CLA	A	810	45/65	0.79	0.50	109,136,151,223	0
16	LHG	X	101	23/49	0.80	0.40	78,81,207,208	0
15	BCR	B	850	40/40	0.80	0.42	83,107,144,146	0
13	CLA	A	827	65/65	0.81	0.72	68,103,137,248	0
15	BCR	A	850	40/40	0.81	0.90	56,96,126,139	0
13	CLA	A	807	51/65	0.81	0.51	87,100,151,177	0
13	CLA	B	834	45/65	0.81	0.54	91,118,151,158	0
13	CLA	A	822	49/65	0.82	0.47	102,126,157,235	0
18	LMG	B	848	55/55	0.82	0.67	42,51,67,114	0
13	CLA	A	813	60/65	0.82	0.60	115,146,178,366	0
13	CLA	B	819	45/65	0.82	0.50	98,131,171,173	0
13	CLA	A	820	61/65	0.83	0.76	119,135,166,198	0
13	CLA	A	855	45/65	0.83	0.40	95,118,140,153	0
13	CLA	A	845	52/65	0.83	0.44	56,78,188,214	0
13	CLA	A	817	54/65	0.83	0.45	83,104,164,172	0
15	BCR	F	1302	40/40	0.83	0.66	70,94,125,128	0
13	CLA	B	814	55/65	0.83	0.70	77,122,182,325	0
13	CLA	A	821	65/65	0.84	0.56	72,100,164,266	0
15	BCR	J	1105	40/40	0.84	0.43	63,67,71,71	0
13	CLA	A	835	54/65	0.85	0.50	54,79,117,204	0
13	CLA	B	831	58/65	0.85	0.46	80,101,148,333	0
13	CLA	B	810	45/65	0.85	0.49	47,84,145,182	0
16	LHG	A	853	49/49	0.86	0.69	57,74,107,127	0
15	BCR	B	843	40/40	0.86	0.60	45,59,82,86	0
13	CLA	B	828	45/65	0.86	0.43	70,80,132,193	0
13	CLA	B	833	45/65	0.86	0.47	77,104,141,148	0
13	CLA	B	820	55/65	0.86	0.49	77,105,141,146	0
13	CLA	B	818	47/65	0.86	0.61	56,99,146,292	0
13	CLA	B	813	45/65	0.86	0.40	51,86,132,141	0
13	CLA	A	823	51/65	0.86	0.51	74,129,153,156	0
13	CLA	B	829	49/65	0.87	0.47	80,85,125,141	0
15	BCR	A	852	40/40	0.87	0.82	78,107,149,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	A	840	65/65	0.87	0.44	77,87,117,198	0
13	CLA	A	842	65/65	0.88	0.57	62,82,149,162	0
13	CLA	B	835	60/65	0.88	0.32	65,106,240,292	0
13	CLA	M	1201	54/65	0.88	0.51	34,42,121,127	0
13	CLA	J	1103	37/65	0.88	0.31	85,117,155,158	0
13	CLA	B	836	65/65	0.88	0.42	69,98,146,234	0
13	CLA	A	825	65/65	0.88	0.32	74,102,152,193	0
15	BCR	J	1104	40/40	0.88	0.82	64,78,113,120	0
15	BCR	A	851	40/40	0.88	0.71	50,58,118,132	0
13	CLA	A	829	65/65	0.88	0.60	83,108,179,197	0
13	CLA	A	811	65/65	0.88	0.65	95,134,173,321	0
15	BCR	M	1203	40/40	0.88	0.53	43,48,87,92	0
13	CLA	B	809	45/65	0.88	0.45	39,95,125,308	0
13	CLA	A	841	51/65	0.88	0.38	80,105,182,204	0
15	BCR	B	842	40/40	0.88	0.66	48,76,129,134	0
13	CLA	A	809	65/65	0.88	0.49	78,117,148,152	0
13	CLA	A	819	65/65	0.88	0.59	97,140,181,328	0
13	CLA	A	824	59/65	0.88	0.54	59,101,164,321	0
13	CLA	A	818	54/65	0.88	0.47	92,136,168,207	0
13	CLA	A	802	65/65	0.88	0.59	40,77,110,230	0
13	CLA	A	828	65/65	0.89	0.49	59,74,127,289	0
13	CLA	B	806	65/65	0.89	0.45	33,63,107,170	0
13	CLA	B	803	65/65	0.89	0.64	40,68,95,180	0
13	CLA	A	804	59/65	0.89	0.59	83,99,117,144	0
13	CLA	A	826	65/65	0.89	0.61	53,80,112,127	0
13	CLA	B	807	65/65	0.89	0.63	38,65,106,122	0
13	CLA	B	832	45/65	0.89	0.39	71,121,142,247	0
13	CLA	F	1301	45/65	0.89	0.45	94,137,167,175	0
13	CLA	A	805	65/65	0.89	0.58	85,98,117,126	0
15	BCR	B	845	40/40	0.90	0.40	60,66,78,82	0
15	BCR	B	844	25/40	0.90	0.44	65,68,113,118	0
13	CLA	A	843	65/65	0.90	0.49	56,83,169,197	0
15	BCR	B	846	40/40	0.90	0.70	75,91,131,137	0
13	CLA	A	833	65/65	0.90	0.56	39,45,110,121	0
13	CLA	B	817	65/65	0.90	0.48	57,65,113,125	0
13	CLA	A	831	50/65	0.90	0.39	45,76,105,144	0
13	CLA	A	814	45/65	0.90	0.32	108,150,172,174	0
13	CLA	B	838	65/65	0.90	0.54	35,45,102,125	0
13	CLA	L	1004	65/65	0.90	0.44	21,31,64,72	0
13	CLA	B	839	65/65	0.91	0.49	35,49,151,215	0
13	CLA	J	1101	65/65	0.91	0.52	77,129,178,357	0
13	CLA	A	832	65/65	0.91	0.34	42,45,81,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	A	806	65/65	0.91	0.57	63,80,155,164	0
16	LHG	A	854	27/49	0.91	0.37	49,58,88,122	0
13	CLA	B	802	65/65	0.91	0.53	61,82,112,165	0
13	CLA	A	808	65/65	0.91	0.40	72,89,172,177	0
13	CLA	A	830	65/65	0.91	0.51	59,71,105,119	0
13	CLA	B	804	65/65	0.91	0.57	45,51,117,199	0
13	CLA	B	824	65/65	0.91	0.38	58,65,88,96	0
14	PQN	B	840	33/33	0.91	0.73	56,84,105,121	0
13	CLA	X	102	45/65	0.91	0.26	67,104,127,283	0
13	CLA	B	821	45/65	0.92	0.35	63,69,105,191	0
13	CLA	A	838	65/65	0.92	0.37	45,81,109,114	0
13	CLA	A	837	51/65	0.92	0.43	52,56,96,147	0
15	BCR	B	847	40/40	0.92	0.70	40,51,116,126	0
13	CLA	A	803	65/65	0.92	0.57	76,100,142,222	0
14	PQN	A	846	33/33	0.92	0.56	55,64,82,82	0
13	CLA	B	837	47/65	0.92	0.27	65,71,119,193	0
13	CLA	B	815	59/65	0.92	0.48	55,58,76,293	0
13	CLA	B	812	65/65	0.92	0.41	37,42,111,117	0
13	CLA	B	830	65/65	0.92	0.61	82,91,129,139	0
13	CLA	B	808	65/65	0.92	0.60	36,41,97,103	0
15	BCR	I	102	40/40	0.92	0.38	19,20,48,52	0
13	CLA	L	1002	65/65	0.92	0.36	29,65,103,148	0
13	CLA	I	101	65/65	0.92	0.38	33,57,85,338	0
13	CLA	B	826	65/65	0.92	0.51	42,47,127,149	0
13	CLA	L	1003	65/65	0.92	0.35	16,52,179,216	0
13	CLA	B	825	65/65	0.93	0.47	40,60,136,157	0
13	CLA	B	801	65/65	0.93	0.42	57,68,123,322	0
13	CLA	B	811	65/65	0.93	0.58	48,71,108,145	0
15	BCR	L	1005	40/40	0.93	0.45	11,16,81,93	0
13	CLA	B	827	65/65	0.93	0.47	44,66,95,108	0
13	CLA	A	834	65/65	0.93	0.44	39,40,92,96	0
15	BCR	L	1006	40/40	0.93	0.29	16,24,64,78	0
15	BCR	B	849	40/40	0.93	0.41	12,43,147,152	0
13	CLA	B	823	46/65	0.94	0.28	59,68,120,137	0
13	CLA	A	839	47/65	0.94	0.31	48,51,119,202	0
13	CLA	B	816	60/65	0.94	0.54	46,53,111,221	0
19	CA	L	1001	1/1	0.94	0.14	22,22,22,22	0
13	CLA	B	822	54/65	0.94	0.44	61,86,118,158	0
13	CLA	B	805	65/65	0.94	0.41	41,48,97,150	0
13	CLA	A	801	65/65	0.94	0.49	44,53,82,89	0
17	SF4	C	102	8/8	0.99	0.16	47,48,122,359	0
17	SF4	A	856	8/8	0.99	0.22	49,50,150,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	SF4	C	101	8/8	0.99	0.20	48,48,49,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.