Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:36 AM GMT

PDB ID	:	3PCQ
Title	:	Femtosecond X-ray protein Nanocrystallography
Authors	:	Chapman, H.N.; Fromme, P.; Barty, A.; White, T.A.; Kirian, R.A.; Aquila, A.; Hunter, M.S.; Schulz, J.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Maia, F.R.N.C.; Martin, A.V.; Schlichting, I.; Lomb, L.; Coppola, N.; Shoeman, R.L.; Epp, S.W.; Hartmann, R.; Rolles, D.; Rudenko, A.; Foucar, L.; Kimmel, N.; Weidenspointner, G.; Holl, P.; Liang, M.; Barthelmess, M.; Caleman, C.; Boutet, S.; Bogan, M.J.; Krzywinski, J.; Bostedt, C.; Bajt, S.; Gumprecht, L.; Rudek, B.; Erk, B.; Schmidt, C.; Homke, A.; Reich, C.; Pietschner, D.; Struder, L.; Hauser, G.; Gorke, H.; Ullrich, J.; Herrmann, S.; Schaller, G.; Schopper, F.; Soltau, H.; Kuhnel, K.-U.; Messerschmidt, M.; Bozek, J.D.; Hau-Riege, S.P.; Frank, M.; Hampton, C.Y.; Sierra, R.; Starodub, D.; Williams, G.J.; Hajdu, J.; Timneanu, N.; Seibert, M.M.; Andreasson, J.; Rocker, A.; Jonsson, O.; Svenda, M.; Stern, S.; Nass, K.; Andritschke, R.; Schroter, C.-D.; Krasniqi, F.; Bott, M.; Schmidt, K.E.; Wang, X.; Grotjohann, I.; Holton, J.M.; Barends, T.R.M.; Neutze, R.; Marchesini, S.; Fromme, R.; Schorb, S.; Rupp, D.; Adolph, M.; Gorkhover, T.; Andersson, I.; Hirsemann, H.; Potdevin, G.; Graafsma, H.; Nilsson, B.; Spence, J.C.H.
Deposited on	:	2010-10-21
Resolution	:	8.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

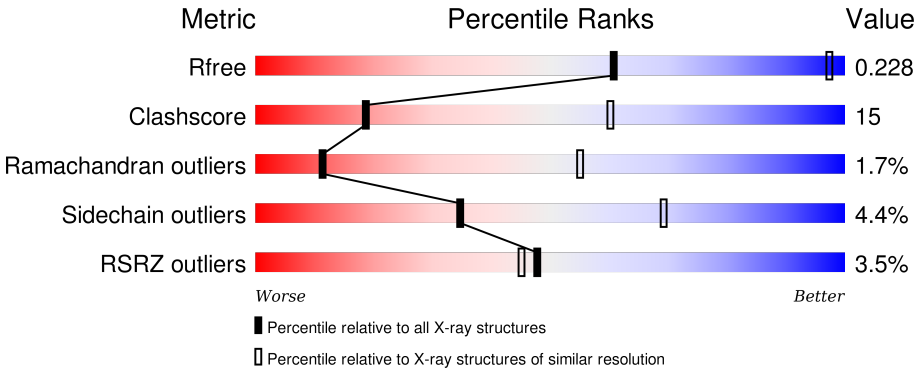
MolProbity : 4.02b-467

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 8.98 Å.

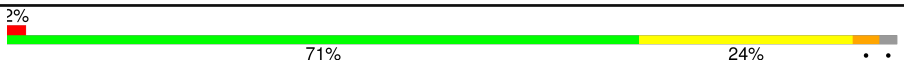
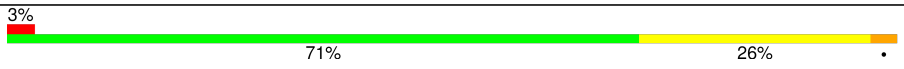
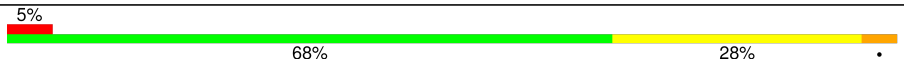
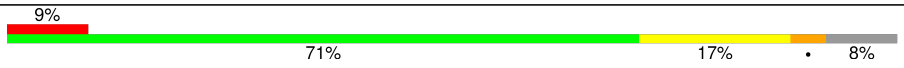
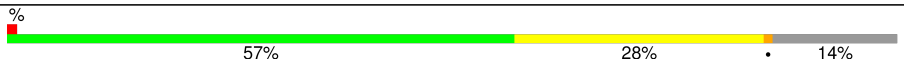
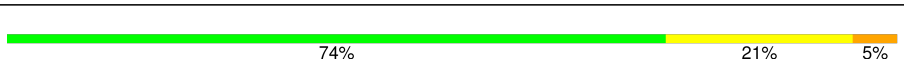
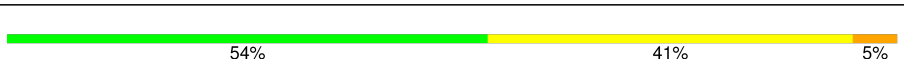
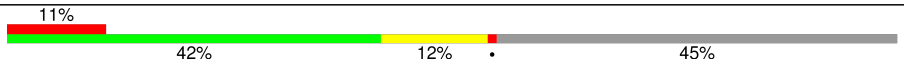
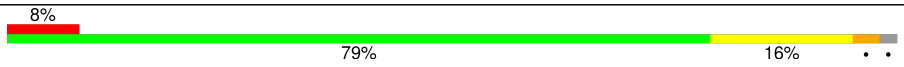
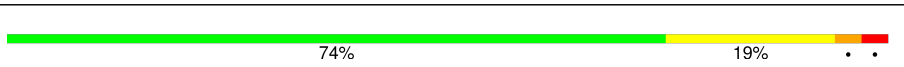
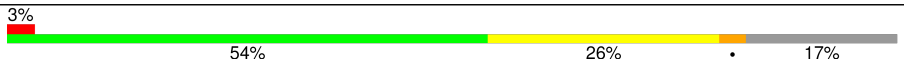
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 <=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.

Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	
5	E	75	
6	F	164	
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	-	-	X
13	CLA	A	803	X	-	-	X
13	CLA	A	804	X	-	-	X
13	CLA	A	805	X	-	-	X
13	CLA	A	806	X	-	-	X
13	CLA	A	807	X	-	-	X
13	CLA	A	808	X	-	-	X
13	CLA	A	809	X	-	-	X
13	CLA	A	810	X	-	-	X
13	CLA	A	812	X	-	-	X
13	CLA	A	813	X	-	-	X
13	CLA	A	814	X	-	-	X
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	X
13	CLA	A	818	X	-	-	X
13	CLA	A	819	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	820	X	-	-	X
13	CLA	A	821	X	-	-	X
13	CLA	A	822	X	-	-	X
13	CLA	A	823	X	-	-	X
13	CLA	A	824	X	-	-	X
13	CLA	A	825	X	-	-	X
13	CLA	A	826	X	-	-	X
13	CLA	A	827	X	-	-	X
13	CLA	A	828	X	-	-	X
13	CLA	A	829	X	-	-	X
13	CLA	A	830	X	-	-	X
13	CLA	A	831	X	-	-	X
13	CLA	A	832	X	-	-	X
13	CLA	A	833	X	-	-	X
13	CLA	A	834	-	-	-	X
13	CLA	A	835	X	-	-	X
13	CLA	A	836	X	-	-	X
13	CLA	A	837	X	-	-	X
13	CLA	A	838	X	-	-	X
13	CLA	A	839	X	-	-	X
13	CLA	A	840	X	-	-	X
13	CLA	A	841	X	-	-	X
13	CLA	A	842	X	-	-	X
13	CLA	A	843	X	-	-	X
13	CLA	A	844	X	-	-	X
13	CLA	A	845	X	-	-	X
13	CLA	A	846	X	-	-	X
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	X
13	CLA	B	803	X	-	-	X
13	CLA	B	804	X	-	-	X
13	CLA	B	805	X	-	-	X
13	CLA	B	806	X	-	-	X
13	CLA	B	807	X	-	-	X
13	CLA	B	808	X	-	-	X
13	CLA	B	809	X	-	-	X
13	CLA	B	810	X	-	-	X
13	CLA	B	811	X	-	-	X
13	CLA	B	812	X	-	-	X
13	CLA	B	813	X	-	-	X
13	CLA	B	814	X	-	-	X
13	CLA	B	815	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	816	X	-	-	X
13	CLA	B	817	X	-	-	X
13	CLA	B	818	X	-	-	X
13	CLA	B	819	X	-	-	X
13	CLA	B	820	X	-	-	X
13	CLA	B	821	X	-	-	X
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	X
13	CLA	B	825	X	-	-	X
13	CLA	B	826	X	-	-	X
13	CLA	B	827	X	-	-	X
13	CLA	B	828	X	-	-	X
13	CLA	B	829	X	-	-	X
13	CLA	B	830	X	-	-	X
13	CLA	B	831	X	-	-	X
13	CLA	B	832	X	-	-	X
13	CLA	B	833	X	-	-	X
13	CLA	B	834	X	-	-	X
13	CLA	B	835	X	-	-	X
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	X
13	CLA	B	839	-	-	-	X
13	CLA	B	840	X	-	-	X
13	CLA	B	841	X	-	-	X
13	CLA	F	1301	X	-	-	X
13	CLA	J	101	X	-	-	X
13	CLA	J	102	X	-	-	-
13	CLA	K	1401	X	-	-	X
13	CLA	L	1002	X	-	-	X
13	CLA	L	1003	X	-	-	X
13	CLA	L	1004	X	-	-	X
13	CLA	M	1601	X	-	-	X
13	CLA	X	1701	X	-	-	X
14	PQN	A	847	-	-	-	X
14	PQN	B	842	-	-	-	X
16	BCR	A	849	-	-	-	X
16	BCR	A	850	-	-	-	X
16	BCR	A	851	-	-	-	X
16	BCR	A	852	-	-	-	X
16	BCR	A	853	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	BCR	A	854	-	-	-	X
16	BCR	B	843	-	-	-	X
16	BCR	B	844	-	-	-	X
16	BCR	B	845	-	-	-	X
16	BCR	B	846	-	-	-	X
16	BCR	B	847	-	-	-	X
16	BCR	B	848	-	-	-	X
16	BCR	B	849	-	-	-	X
16	BCR	F	1302	-	-	-	X
16	BCR	I	101	-	-	-	X
16	BCR	I	102	-	-	-	X
16	BCR	J	103	-	-	-	X
16	BCR	J	104	-	-	-	X
16	BCR	J	105	-	-	-	X
16	BCR	L	1005	-	-	-	X
16	BCR	L	1006	-	-	-	X
16	BCR	M	1602	-	-	-	X
17	LHG	A	855	-	-	-	X
17	LHG	A	856	X	-	-	X
17	LHG	B	851	-	-	-	X
18	LMG	B	850	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24196 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

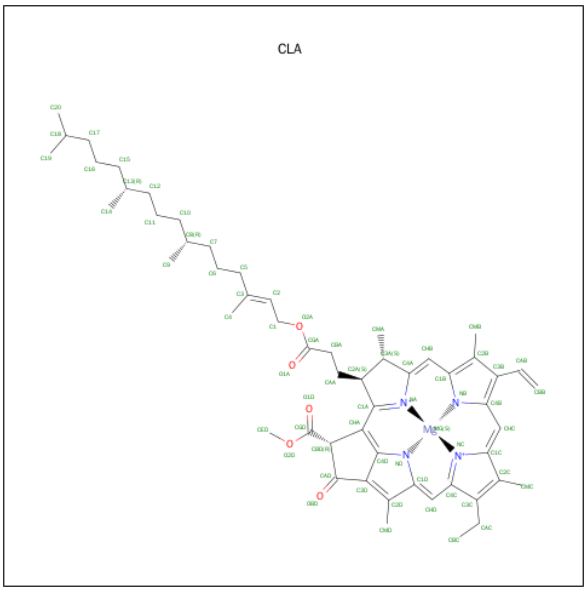
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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
			232	163	34	35			

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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
			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		
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		

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

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

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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
			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
			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		
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		

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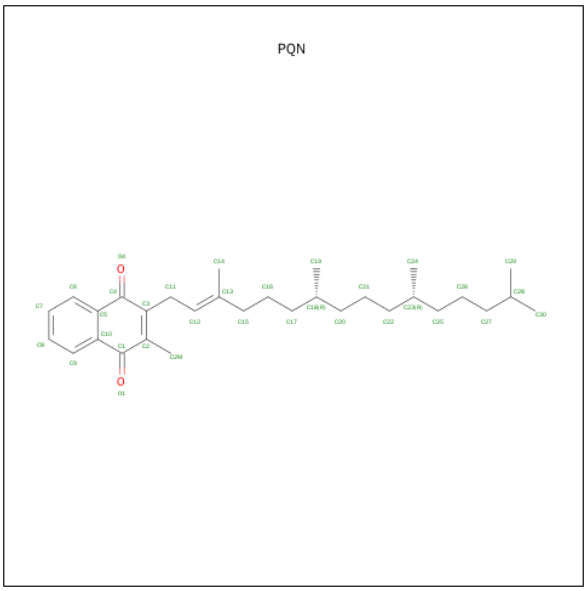
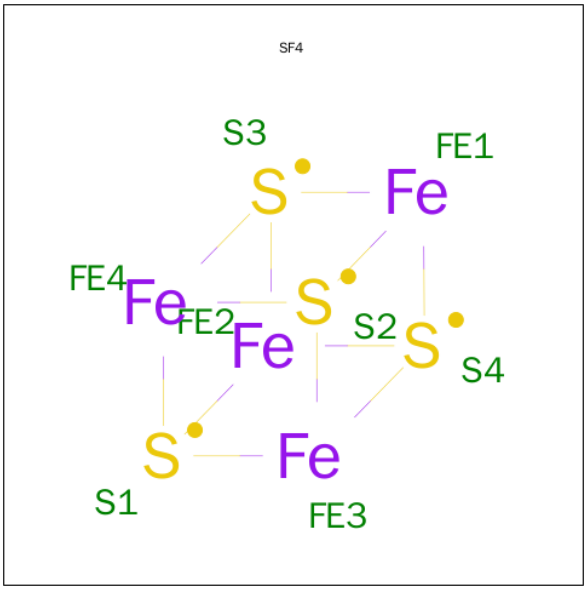
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
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	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	K	1	Total	C	Mg	N	O	0	0
			45	35	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	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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 33 31 2	0	0
14	B	1	Total C O 33 31 2	0	0

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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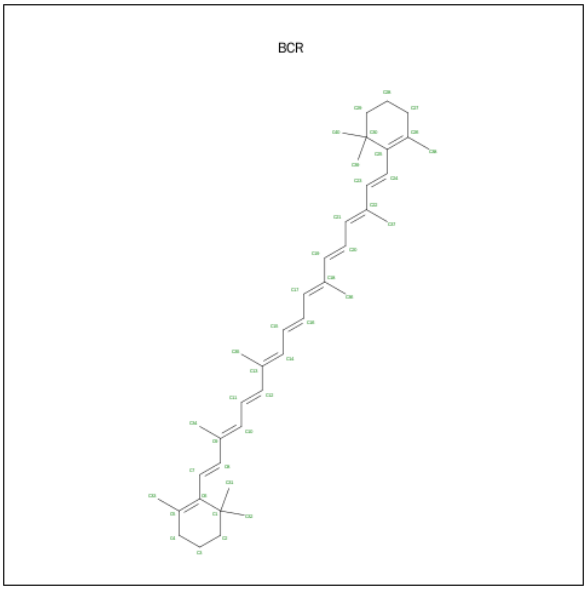
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total Fe S 8 4 4	0	0

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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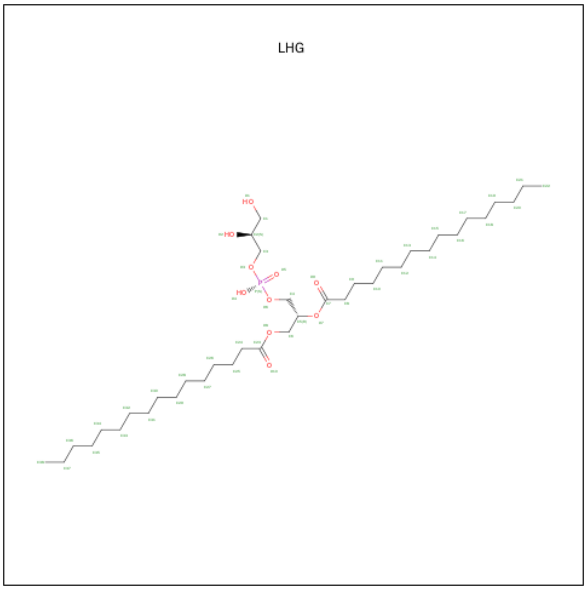
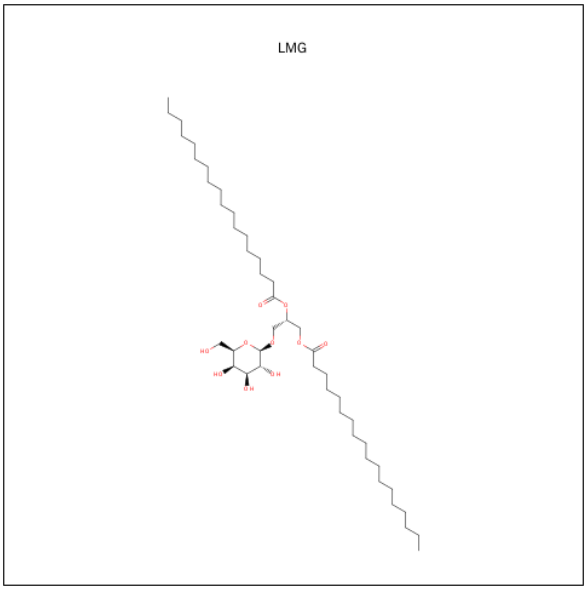
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total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

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		

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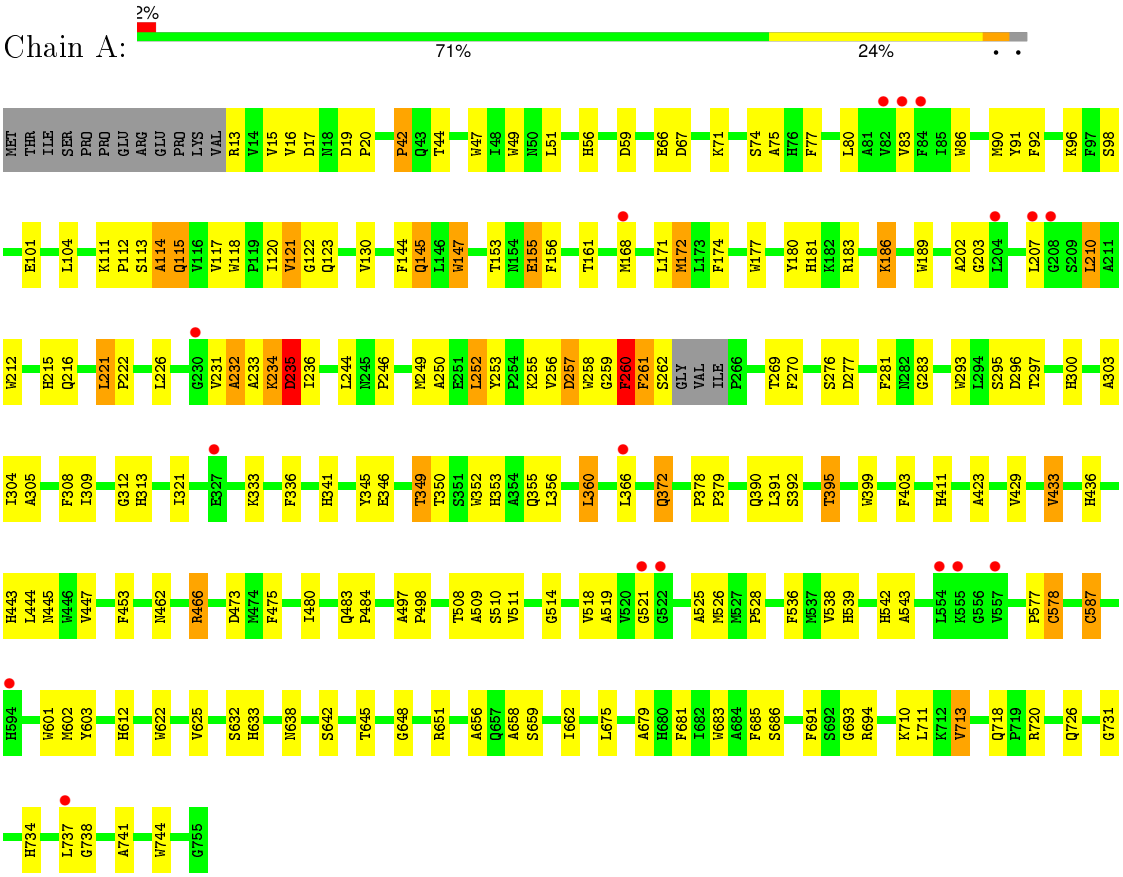
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	21	Total O 21 21	0	0
20	D	17	Total O 17 17	0	0
20	E	5	Total O 5 5	0	0
20	F	6	Total O 6 6	0	0
20	I	3	Total O 3 3	0	0
20	J	1	Total O 1 1	0	0
20	L	27	Total O 27 27	0	0
20	M	2	Total O 2 2	0	0

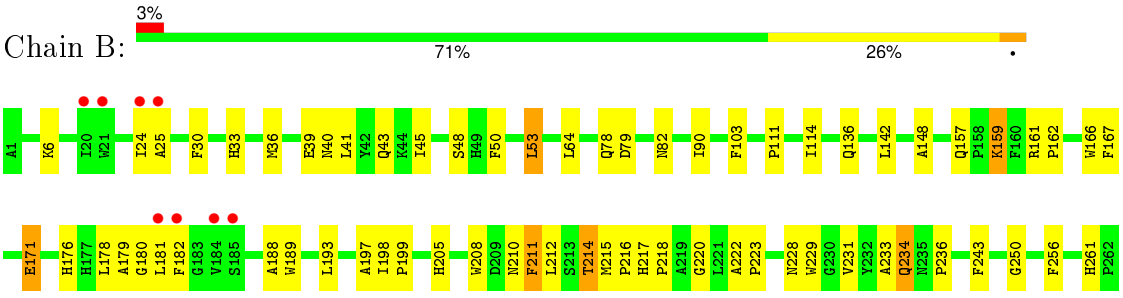
3 Residue-property plots (i)

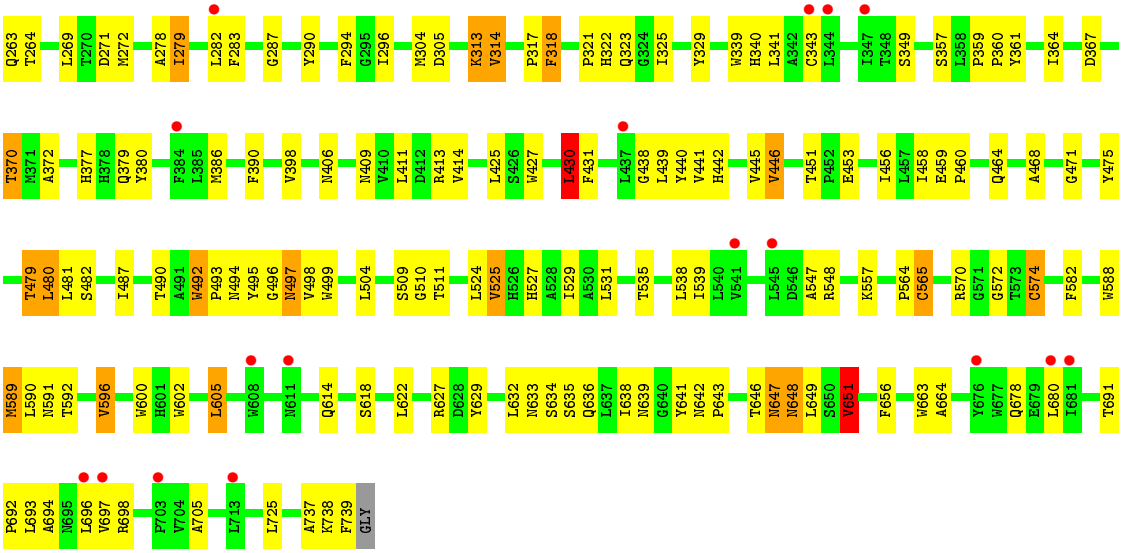
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

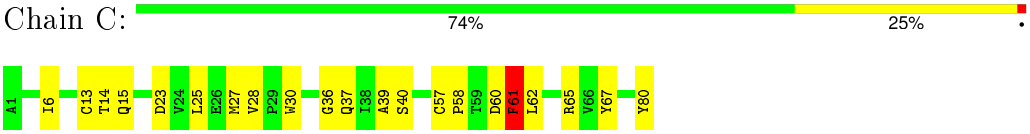


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

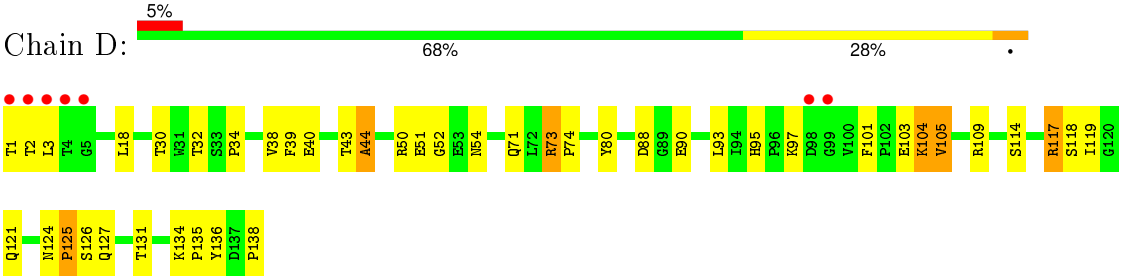




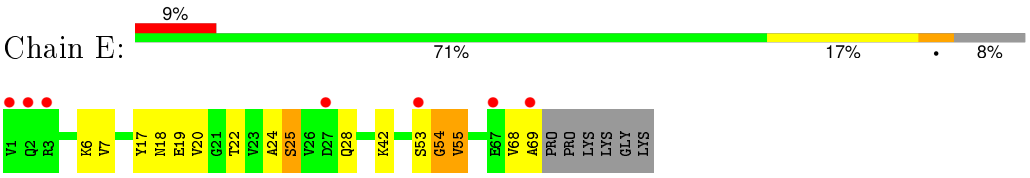
- Molecule 3: Photosystem I iron-sulfur center



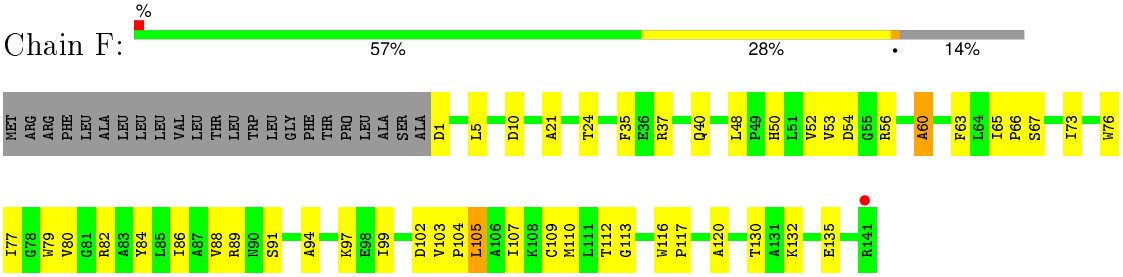
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I reaction center subunit IV

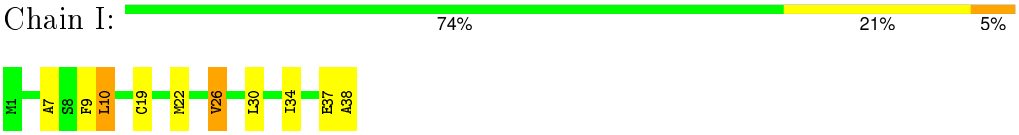


- Molecule 6: Photosystem I reaction center subunit III



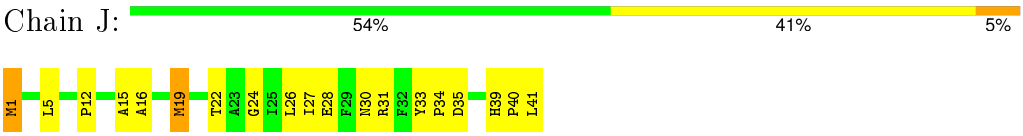
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



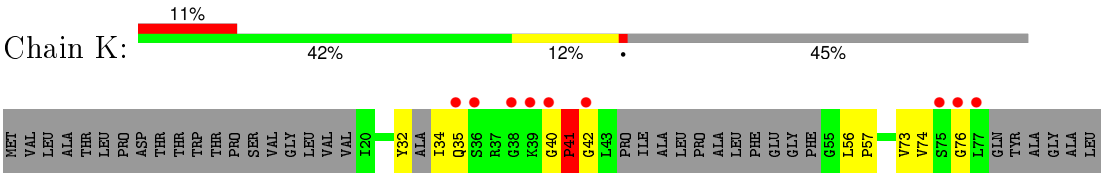
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:



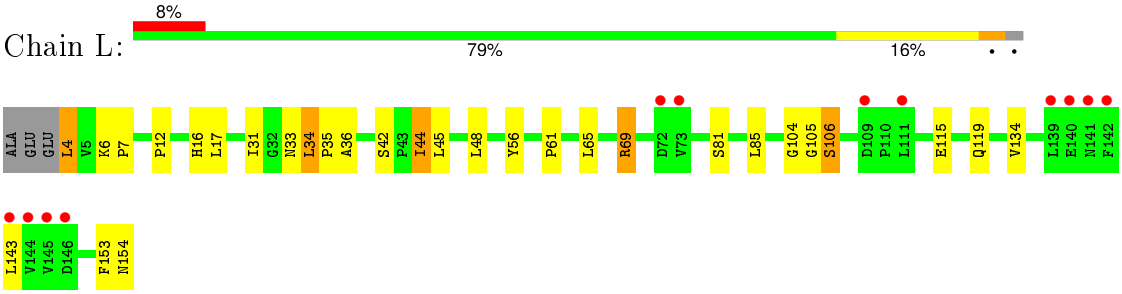
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



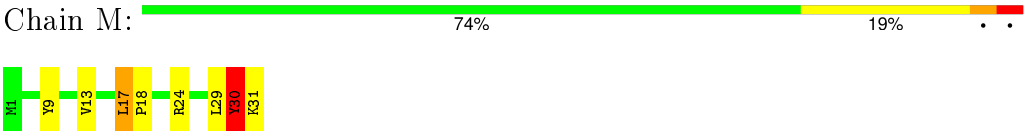
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:



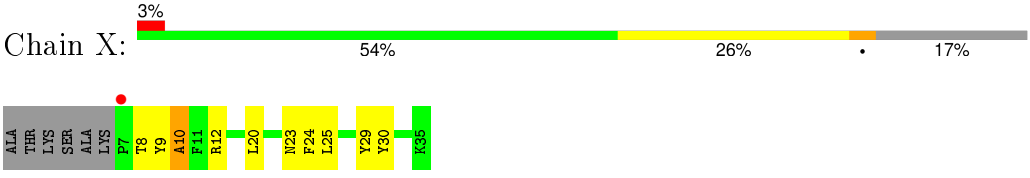
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:



- Molecule 12: Photosystem I 4.8K protein

Chain X:



4 Data and refinement statistics (i)

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)	81.12 – 8.98 81.12 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.12-8.98) 99.1 (81.12-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.6.0076	Depositor
R, R_{free}	0.252 , 0.232 0.246 , 0.228	Depositor DCC
R_{free} test set	187 reflections (3.46%)	DCC
Wilson B-factor (Å^2)	203.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.500 for H, K, L 0.500 for K, H, -L 0.499 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.16$, $< L^2 > = 0.04$	Xtriage
Outliers	0 of 5591 reflections	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	24196	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.67	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.54	0/241	0.67	0/330
All	All	0.55	0/17940	0.70	15/24451 (0.1%)

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
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	80	TYR	CA-C-O	9.93	140.96	120.10
11	M	30	TYR	N-CA-C	7.84	132.17	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.51	131.88	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	GLY	N-CA-C	-6.42	97.05	113.10
3	C	60	ASP	CA-C-N	-6.26	103.42	117.20
9	K	57	PRO	N-CA-CB	6.15	110.69	103.30
3	C	60	ASP	C-N-CA	5.90	136.45	121.70
3	C	61	PHE	N-CA-CB	5.87	121.16	110.60
1	A	114	ALA	N-CA-C	-5.85	95.21	111.00
9	K	41	PRO	N-CA-CB	5.73	110.17	103.30
9	K	35	GLN	N-CA-C	5.36	125.47	111.00
2	B	430	LEU	CA-CB-CG	5.11	127.05	115.30
2	B	651	VAL	CB-CA-C	-5.09	101.73	111.40
5	E	55	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	214	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	39	0
5	E	539	0	528	10	1
6	F	1065	0	1079	41	1
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	2
11	M	241	0	264	13	0
12	X	232	0	220	6	0
13	A	2687	0	2675	139	0
13	B	2349	0	2304	151	0
13	F	45	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	1
20	A	53	0	0	5	1
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	2
20	M	2	0	0	1	0
All	All	24196	0	23793	736	5

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 15.

All (736) 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)
8:J:31:ARG:HD3	16:J:104:BCR:H312	1.26	1.17
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.28	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.04
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01
2:B:243:PHE:H	2:B:263:GLN:HE22	1.07	1.01
2:B:231:VAL:O	2:B:234:GLN:HG2	1.62	0.99
1:A:536:PHE:HA	13:A:839:CLA:HED1	1.45	0.96
2:B:406:ASN:HD22	2:B:409:ASN:HD21	0.98	0.96
2:B:494:ASN:HD22	2:B:496:GLY:H	1.13	0.93
11:M:31:LYS:O	11:M:31:LYS:HG2	1.70	0.92
1:A:353:HIS:HD2	1:A:411:HIS:HD1	1.21	0.88
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.54	0.88
16:A:854:BCR:H362	13:B:802:CLA:H42	1.55	0.87
1:A:117:VAL:HG13	1:A:123:GLN:HE21	1.42	0.84
4:D:101:PHE:HB2	4:D:104:LYS:HE2	1.59	0.83
2:B:406:ASN:ND2	2:B:409:ASN:HD21	1.76	0.83
8:J:24:GLY:HA3	13:J:101:CLA:HBB1	1.61	0.83
8:J:31:ARG:HD3	16:J:104:BCR:C31	2.08	0.83
1:A:333:LYS:O	13:A:846:CLA:HBC3	1.81	0.81
2:B:509:SER:O	2:B:511:THR:N	2.12	0.81
1:A:203:GLY:HA2	13:A:821:CLA:HBC1	1.62	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.64	0.79
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.63	0.79
2:B:494:ASN:ND2	2:B:496:GLY:H	1.80	0.78
2:B:459:GLU:HG3	6:F:5:LEU:HD11	1.63	0.78
2:B:243:PHE:H	2:B:263:GLN:NE2	1.82	0.78
1:A:345:TYR:O	1:A:349:THR:HB	1.84	0.78
1:A:508:THR:HG22	1:A:510:SER:N	1.96	0.77
2:B:313:LYS:O	2:B:314:VAL:HG22	1.85	0.77
3:C:37:GLN:NE2	4:D:105:VAL:HG22	1.99	0.77
2:B:278:ALA:HB2	13:B:817:CLA:HBB1	1.66	0.77
2:B:339:TRP:HE1	13:B:824:CLA:C2B	1.99	0.76
2:B:25:ALA:HB2	18:B:850:LMG:H121	1.67	0.76
13:A:801:CLA:HBB1	13:B:802:CLA:HED1	1.67	0.75
1:A:231:VAL:O	1:A:232:ALA:HB3	1.87	0.75
2:B:367:ASP:CG	2:B:370:THR:HG23	2.06	0.75
13:A:829:CLA:H192	16:J:103:BCR:H14C	1.69	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
13:B:818:CLA:HBB1	13:B:818:CLA:HMB1	1.68	0.75
13:B:825:CLA:HAA2	13:B:826:CLA:OBD	1.87	0.74
13:A:829:CLA:H93	16:J:103:BCR:H361	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:O	13:A:835:CLA:HBB2	1.88	0.74
2:B:639:ASN:HD22	2:B:642:ASN:HD22	1.36	0.74
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
2:B:229:TRP:HB2	13:B:816:CLA:H12	1.70	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:CD	2:B:159:LYS:H	1.92	0.72
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:181:LEU:HG	13:B:813:CLA:H43	1.70	0.72
2:B:622:LEU:HD12	13:B:802:CLA:C1	2.15	0.72
2:B:425:LEU:HG	13:B:839:CLA:CBB	2.20	0.72
2:B:329:TYR:OH	2:B:340:HIS:HE1	1.71	0.72
11:M:31:LYS:O	11:M:31:LYS:CG	2.34	0.72
2:B:725:LEU:HD11	13:B:829:CLA:H203	1.70	0.72
2:B:343:CYS:HB3	13:B:824:CLA:H42	1.72	0.72
13:B:819:CLA:HAA2	13:B:824:CLA:HBB1	1.72	0.72
3:C:39:ALA:O	20:C:209:HOH:O	2.07	0.72
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.72	0.71
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.72	0.70
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.73	0.70
1:A:341:HIS:HE1	17:A:856:LHG:HC11	1.56	0.70
5:E:68:VAL:HG23	5:E:69:ALA:H	1.56	0.69
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.92	0.69
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.74	0.69
2:B:589:MET:HE1	2:B:590:LEU:HA	1.75	0.69
1:A:13:ARG:HE	1:A:15:VAL:CG2	2.05	0.68
2:B:602:TRP:HE1	2:B:614:GLN:HE21	1.40	0.68
13:A:839:CLA:H101	13:L:1003:CLA:H191	1.75	0.68
6:F:52:VAL:HG12	6:F:54:ASP:HB2	1.76	0.68
1:A:399:TRP:CD1	13:A:829:CLA:HAB	2.29	0.68
1:A:221:LEU:HD11	1:A:295:SER:HA	1.76	0.68
1:A:117:VAL:HG13	1:A:123:GLN:NE2	2.07	0.67
2:B:25:ALA:HA	13:B:829:CLA:H42	1.75	0.67
1:A:101:GLU:OE2	1:A:155:GLU:HG2	1.95	0.67
2:B:339:TRP:HZ2	13:B:824:CLA:HAB	1.58	0.66
6:F:102:ASP:OD2	6:F:105:LEU:HB2	1.94	0.66
1:A:336:PHE:HB2	17:A:856:LHG:HC41	1.78	0.66
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.31	0.66
9:K:73:VAL:HA	13:K:1401:CLA:HBB1	1.77	0.66
14:A:847:PQN:H172	16:B:848:BCR:H382	1.77	0.66
4:D:50:ARG:H	4:D:54:ASN:ND2	1.88	0.66
2:B:188:ALA:HA	13:B:815:CLA:CBB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:HB3	13:A:806:CLA:HAC1	1.77	0.65
2:B:318:PHE:CD1	13:B:822:CLA:HAB	2.32	0.65
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	0.65
2:B:210:ASN:O	2:B:214:THR:HG23	1.96	0.65
2:B:41:LEU:O	2:B:45:ILE:HG12	1.97	0.65
2:B:318:PHE:HB2	13:B:823:CLA:HMA1	1.78	0.65
1:A:257:ASP:OD1	1:A:262:SER:HB3	1.96	0.65
2:B:313:LYS:O	2:B:314:VAL:HG13	1.97	0.65
1:A:249:MET:O	1:A:252:LEU:O	2.15	0.65
1:A:269:THR:O	1:A:270:PHE:HB2	1.96	0.65
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.78	0.65
2:B:492:TRP:CE3	2:B:493:PRO:HD3	2.32	0.65
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.65
13:A:844:CLA:H191	13:L:1003:CLA:HBB1	1.78	0.64
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.64
13:B:829:CLA:HBB1	13:B:829:CLA:HMB1	1.78	0.64
2:B:647:ASN:ND2	2:B:649:LEU:H	1.95	0.64
10:L:61:PRO:HB3	13:L:1004:CLA:HBB1	1.78	0.64
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.31	0.64
8:J:12:PRO:HB2	16:J:104:BCR:H391	1.78	0.64
13:B:806:CLA:H162	13:B:828:CLA:HBB2	1.80	0.64
2:B:641:TYR:HB2	2:B:646:THR:HG22	1.79	0.64
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	0.63
3:C:23:ASP:OD2	4:D:95:HIS:HD2	1.81	0.63
13:B:803:CLA:H111	16:B:849:BCR:H362	1.79	0.63
6:F:63:PHE:O	6:F:66:PRO:HD2	1.97	0.63
2:B:318:PHE:HA	13:B:822:CLA:CAB	2.28	0.63
2:B:622:LEU:CD1	13:B:802:CLA:H11	2.16	0.63
4:D:117:ARG:HG2	4:D:118:SER:O	1.98	0.63
1:A:177:TRP:HB2	13:A:812:CLA:HMC3	1.80	0.63
13:A:801:CLA:HAB	13:B:801:CLA:NA	2.14	0.62
11:M:29:LEU:O	11:M:30:TYR:HB2	1.99	0.62
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.81	0.62
1:A:104:LEU:HD11	1:A:153:THR:HA	1.81	0.62
6:F:60:ALA:O	6:F:65:ILE:HG12	1.98	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	0.62
2:B:166:TRP:CZ2	13:B:811:CLA:HMA1	2.33	0.62
2:B:228:ASN:O	2:B:231:VAL:HG23	2.00	0.62
1:A:86:TRP:HA	13:A:808:CLA:HBB2	1.82	0.62
2:B:136:GLN:HE22	2:B:208:TRP:HE1	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:647:ASN:HD21	2:B:649:LEU:HB2	1.64	0.62
1:A:356:LEU:O	1:A:360:LEU:HB2	1.99	0.62
1:A:602:MET:HG2	13:A:827:CLA:HBC1	1.80	0.62
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.62
2:B:278:ALA:CB	13:B:817:CLA:HBB1	2.29	0.61
1:A:90:MET:HE3	13:A:809:CLA:HED2	1.82	0.61
1:A:429:VAL:O	1:A:433:VAL:HG13	1.99	0.61
13:A:827:CLA:HAA2	13:A:828:CLA:OBD	2.01	0.61
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
13:A:844:CLA:HMA1	2:B:694:ALA:CB	2.30	0.61
1:A:543:ALA:HB1	13:A:839:CLA:HMB3	1.83	0.61
1:A:726:GLN:HG3	17:A:855:LHG:O9	2.01	0.61
2:B:438:GLY:HA3	13:B:833:CLA:CBB	2.31	0.61
11:M:24:ARG:HG3	11:M:24:ARG:HH11	1.64	0.61
1:A:601:TRP:HH2	13:A:802:CLA:HBB1	1.66	0.61
13:A:846:CLA:HBD	13:A:846:CLA:H61	1.83	0.61
10:L:153:PHE:O	10:L:154:ASN:HB2	1.99	0.61
13:B:806:CLA:H151	13:B:806:CLA:H102	1.84	0.60
1:A:453:PHE:O	13:A:835:CLA:CBB	2.48	0.60
3:C:30:TRP:O	3:C:36:GLY:HA2	2.00	0.60
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	0.60
1:A:303:ALA:HB2	13:A:819:CLA:HBB1	1.83	0.60
13:B:837:CLA:HMB2	13:B:839:CLA:HED1	1.82	0.60
9:K:32:TYR:O	9:K:34:ILE:N	2.34	0.60
1:A:484:PRO:HB3	13:A:839:CLA:HED3	1.83	0.60
13:A:803:CLA:H71	13:A:843:CLA:HMC3	1.82	0.60
13:A:801:CLA:HBB1	13:B:802:CLA:CED	2.31	0.60
1:A:168:MET:CE	1:A:171:LEU:HD23	2.31	0.60
1:A:300:HIS:O	1:A:304:ILE:HG12	2.02	0.59
1:A:19:ASP:HA	1:A:181:HIS:O	2.02	0.59
1:A:210:LEU:HD21	16:A:849:BCR:H342	1.84	0.59
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.84	0.59
1:A:259:GLY:O	1:A:261:PHE:N	2.35	0.59
2:B:181:LEU:HD21	13:B:813:CLA:H12	1.85	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
2:B:589:MET:HE2	2:B:589:MET:O	2.02	0.59
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
13:B:830:CLA:HBC1	16:B:846:BCR:H23C	1.83	0.59
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.59
1:A:16:VAL:HG12	1:A:17:ASP:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
13:A:841:CLA:H43	13:B:832:CLA:HAA2	1.84	0.59
10:L:36:ALA:HB2	13:L:1003:CLA:HMD1	1.84	0.58
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.58
2:B:591:ASN:HB2	13:B:802:CLA:HBC2	1.83	0.58
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.58
2:B:438:GLY:HA3	13:B:833:CLA:HBB1	1.86	0.58
1:A:207:LEU:HD22	16:A:850:BCR:H361	1.85	0.58
1:A:145:GLN:NE2	1:A:145:GLN:H	2.02	0.58
13:A:809:CLA:HMC2	13:A:829:CLA:H142	1.84	0.58
1:A:86:TRP:HA	13:A:808:CLA:CBB	2.33	0.58
13:B:833:CLA:O1D	8:J:35:ASP:HA	2.02	0.58
2:B:243:PHE:N	2:B:263:GLN:HE22	1.90	0.58
13:A:824:CLA:HMA1	13:A:846:CLA:HAC2	1.85	0.58
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:N	2:B:648:ASN:HD22	2.02	0.58
1:A:744:TRP:HB2	13:A:829:CLA:HBB1	1.87	0.57
16:A:854:BCR:HC8	16:A:854:BCR:H321	1.84	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57
1:A:392:SER:HB3	13:A:829:CLA:HMA1	1.87	0.57
2:B:380:TYR:CD1	13:B:827:CLA:HBB1	2.39	0.57
6:F:82:ARG:O	6:F:86:ILE:HG12	2.04	0.57
13:A:803:CLA:H12	2:B:430:LEU:HD12	1.85	0.57
2:B:414:VAL:HG11	16:B:846:BCR:H401	1.85	0.57
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.04	0.57
1:A:542:HIS:HB3	13:A:838:CLA:HBB1	1.87	0.57
1:A:349:THR:HG22	1:A:350:THR:HG23	1.87	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.56
8:J:15:ALA:O	8:J:19:MET:HB2	2.05	0.56
2:B:678:GLN:NE2	2:B:705:ALA:H	2.03	0.56
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.86	0.56
13:A:809:CLA:H112	13:A:831:CLA:H203	1.87	0.56
1:A:355:GLN:HG3	13:A:826:CLA:H152	1.87	0.56
2:B:279:ILE:HD11	13:B:817:CLA:CBC	2.35	0.56
2:B:282:LEU:HD12	13:B:819:CLA:HMC1	1.87	0.56
1:A:67:ASP:O	1:A:71:LYS:HG3	2.05	0.56
6:F:37:ARG:O	6:F:40:GLN:HG2	2.04	0.56
2:B:234:GLN:OE1	2:B:234:GLN:HA	2.06	0.56
2:B:339:TRP:CZ2	13:B:824:CLA:HAB	2.39	0.56
2:B:480:LEU:O	2:B:482:SER:N	2.38	0.56
1:A:233:ALA:O	1:A:235:ASP:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:ILE:HG23	2:B:283:PHE:CE2	2.41	0.56
6:F:76:TRP:CE2	6:F:113:GLY:HA3	2.40	0.56
2:B:339:TRP:CH2	16:B:846:BCR:H372	2.40	0.56
1:A:189:TRP:CZ2	13:A:811:CLA:HMA1	2.40	0.56
12:X:9:TYR:O	12:X:10:ALA:HB2	2.05	0.56
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	0.56
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.04	0.56
1:A:366:LEU:HD11	13:A:820:CLA:H71	1.86	0.56
1:A:741:ALA:HB2	16:A:854:BCR:H323	1.88	0.56
13:A:801:CLA:HAB	13:B:801:CLA:C1A	2.37	0.55
1:A:297:THR:O	1:A:300:HIS:HB3	2.06	0.55
2:B:588:TRP:HH2	13:B:802:CLA:CBB	2.19	0.55
13:A:833:CLA:H12	13:L:1003:CLA:H93	1.86	0.55
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.33	0.55
13:A:805:CLA:HMC3	13:A:807:CLA:HED2	1.86	0.55
9:K:40:GLY:O	9:K:41:PRO:C	2.45	0.55
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55
2:B:589:MET:HE2	2:B:589:MET:C	2.27	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.37	0.55
1:A:681:PHE:CD2	16:A:854:BCR:H363	2.42	0.55
13:B:827:CLA:HBC3	18:B:850:LMG:H421	1.88	0.55
2:B:233:ALA:O	2:B:234:GLN:O	2.24	0.55
13:B:828:CLA:H51	16:B:845:BCR:H392	1.88	0.55
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.41	0.55
2:B:261:HIS:CD2	2:B:264:THR:H	2.25	0.55
2:B:525:VAL:HG13	13:B:801:CLA:H141	1.89	0.55
13:A:819:CLA:H41	13:A:836:CLA:HAA2	1.88	0.55
16:A:852:BCR:H333	16:A:853:BCR:H333	1.88	0.55
2:B:589:MET:HE1	2:B:590:LEU:CA	2.37	0.55
1:A:372:GLN:HG3	13:A:827:CLA:CED	2.37	0.54
13:B:840:CLA:H18	16:I:101:BCR:H362	1.89	0.54
1:A:681:PHE:CG	16:A:854:BCR:H363	2.43	0.54
13:A:844:CLA:HMA1	2:B:694:ALA:HB1	1.88	0.54
10:L:35:PRO:HG3	13:L:1003:CLA:HED2	1.88	0.54
2:B:205:HIS:ND1	20:B:947:HOH:O	2.23	0.54
1:A:244:LEU:O	1:A:246:PRO:HD3	2.06	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
1:A:390:GLN:HA	1:A:390:GLN:HE21	1.71	0.54
4:D:43:THR:O	4:D:44:ALA:HB3	2.07	0.54
1:A:403:PHE:HB3	13:A:807:CLA:H112	1.90	0.54
13:B:819:CLA:HMB2	13:B:824:CLA:HMA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:ARG:HD3	13:B:830:CLA:OBD	2.07	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	0.54
1:A:308:PHE:HE2	13:A:822:CLA:HAB	1.72	0.54
2:B:614:GLN:O	2:B:618:SER:HB2	2.07	0.54
12:X:25:LEU:O	12:X:29:TYR:HD1	1.89	0.54
2:B:318:PHE:HA	13:B:822:CLA:HAB	1.88	0.54
2:B:171:GLU:HB3	2:B:290:TYR:HB3	1.90	0.54
6:F:52:VAL:CG1	6:F:54:ASP:HB2	2.36	0.54
2:B:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54
2:B:212:LEU:HD21	16:B:845:BCR:H341	1.90	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.42	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.53
13:A:804:CLA:HED1	8:J:12:PRO:HA	1.90	0.53
1:A:305:ALA:O	1:A:309:ILE:HG12	2.08	0.53
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.90	0.53
13:A:802:CLA:OBD	13:B:801:CLA:HMB3	2.08	0.53
13:A:803:CLA:H142	16:A:854:BCR:H402	1.89	0.53
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.21	0.53
13:A:801:CLA:HMB3	13:B:802:CLA:OBD	2.09	0.53
13:A:828:CLA:HBB1	13:A:836:CLA:HMA2	1.90	0.53
6:F:88:VAL:HG11	6:F:97:LYS:CB	2.37	0.53
13:B:829:CLA:H143	18:B:850:LMG:H231	1.89	0.53
1:A:466:ARG:O	2:B:646:THR:HG21	2.09	0.53
8:J:19:MET:CE	8:J:19:MET:HA	2.38	0.53
1:A:13:ARG:HE	1:A:15:VAL:HG22	1.72	0.53
2:B:479:THR:O	2:B:480:LEU:O	2.27	0.53
10:L:16:HIS:CD2	10:L:17:LEU:H	2.27	0.53
13:A:822:CLA:HMB2	13:A:826:CLA:HMA3	1.91	0.53
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
13:A:803:CLA:O1A	2:B:531:LEU:HD11	2.09	0.53
1:A:296:ASP:HB3	13:A:819:CLA:HMA1	1.90	0.53
13:A:831:CLA:H111	17:A:855:LHG:H202	1.90	0.52
13:A:827:CLA:H162	16:A:852:BCR:H272	1.91	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
1:A:59:ASP:OD2	1:A:353:HIS:HE1	1.91	0.52
1:A:622:TRP:O	1:A:633:HIS:HD2	1.92	0.52
1:A:90:MET:CE	13:A:809:CLA:HED2	2.39	0.52
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.52
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.91	0.52
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.44	0.52
2:B:36:MET:HE2	2:B:41:LEU:N	2.24	0.52
1:A:578:CYS:HB3	1:A:587:CYS:HA	1.91	0.52
13:A:836:CLA:HMD2	13:A:837:CLA:HBB1	1.91	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	0.52
2:B:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52
2:B:430:LEU:HB3	13:B:832:CLA:HED3	1.90	0.52
1:A:744:TRP:CZ2	13:A:829:CLA:H43	2.44	0.52
2:B:634:SER:O	2:B:638:ILE:HB	2.10	0.52
2:B:294:PHE:HE1	13:B:812:CLA:HMA1	1.75	0.52
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.92	0.52
1:A:83:VAL:HG11	13:A:806:CLA:H72	1.92	0.51
1:A:16:VAL:HG11	1:A:183:ARG:HB3	1.92	0.51
1:A:77:PHE:CE2	13:A:811:CLA:HBB1	2.45	0.51
1:A:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
1:A:168:MET:HE1	1:A:171:LEU:HD23	1.92	0.51
1:A:259:GLY:C	1:A:261:PHE:H	2.13	0.51
1:A:71:LYS:NZ	20:A:931:HOH:O	2.43	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.08	0.51
2:B:279:ILE:HD11	13:B:817:CLA:HBC2	1.92	0.51
2:B:456:ILE:HG22	2:B:458:ILE:CD1	2.40	0.51
13:A:828:CLA:HMB3	13:A:836:CLA:H12	1.93	0.51
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.93	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.11	0.51
1:A:444:LEU:HB2	13:A:840:CLA:CBB	2.40	0.51
2:B:159:LYS:HD2	2:B:159:LYS:N	2.04	0.51
1:A:303:ALA:CB	13:A:819:CLA:HBB1	2.40	0.51
13:B:840:CLA:HBB2	14:B:842:PQN:H141	1.91	0.51
1:A:453:PHE:C	13:A:835:CLA:HBB2	2.31	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	0.51
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
1:A:118:TRP:CB	16:J:104:BCR:H323	2.41	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
13:B:819:CLA:HMD1	13:B:821:CLA:HBB1	1.93	0.50
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.46	0.50
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:30:TYR:O	11:M:31:LYS:OXT	2.29	0.50
13:B:823:CLA:HBB1	13:B:830:CLA:HMD2	1.94	0.50
3:C:14:THR:HG22	3:C:27:MET:HG3	1.94	0.50
2:B:588:TRP:HH2	13:B:802:CLA:HBB1	1.77	0.50
2:B:339:TRP:HE1	13:B:824:CLA:C3B	2.23	0.50
13:A:803:CLA:HBB1	13:B:802:CLA:NB	2.27	0.50
13:B:824:CLA:H61	13:B:826:CLA:H42	1.93	0.50
4:D:32:THR:HA	4:D:52:GLY:O	2.12	0.50
2:B:431:PHE:CZ	16:J:105:BCR:HC41	2.46	0.50
4:D:101:PHE:HB3	4:D:103:GLU:OE2	2.11	0.49
13:B:829:CLA:H8	18:B:850:LMG:H242	1.94	0.49
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.40	0.49
5:E:68:VAL:O	5:E:69:ALA:O	2.30	0.49
2:B:548:ARG:HH22	4:D:124:ASN:ND2	2.10	0.49
2:B:664:ALA:C	13:B:803:CLA:HBB1	2.31	0.49
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.49
13:A:844:CLA:H52	13:B:840:CLA:H43	1.93	0.49
2:B:340:HIS:HD2	13:B:805:CLA:OBD	1.96	0.49
1:A:691:PHE:HB2	13:A:803:CLA:HBC2	1.95	0.49
2:B:114:ILE:O	13:B:808:CLA:HMD3	2.12	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	0.49
13:A:820:CLA:HMB1	13:A:820:CLA:HBB1	1.93	0.49
6:F:80:VAL:HG22	6:F:109:CYS:O	2.13	0.49
6:F:84:TYR:O	6:F:88:VAL:HG23	2.12	0.49
2:B:458:ILE:HD12	2:B:458:ILE:N	2.28	0.49
5:E:7:VAL:O	5:E:20:VAL:HA	2.13	0.49
13:B:801:CLA:H72	13:B:802:CLA:CED	2.42	0.49
13:B:819:CLA:CMB	13:B:824:CLA:HMA3	2.41	0.49
4:D:30:THR:O	4:D:80:TYR:HA	2.13	0.49
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.48	0.49
2:B:261:HIS:CD2	2:B:263:GLN:H	2.31	0.49
2:B:182:PHE:CE2	13:B:813:CLA:H61	2.48	0.49
2:B:425:LEU:HG	13:B:839:CLA:HBB1	1.94	0.49
2:B:390:PHE:CE1	16:B:847:BCR:H373	2.48	0.49
2:B:294:PHE:O	2:B:296:ILE:HG22	2.13	0.49
2:B:446:VAL:HG13	2:B:451:THR:O	2.13	0.49
13:B:806:CLA:H143	13:B:828:CLA:HBB2	1.95	0.48
1:A:651:ARG:HG3	2:B:638:ILE:CG2	2.43	0.48
13:A:803:CLA:H71	13:A:843:CLA:CMC	2.42	0.48
2:B:261:HIS:HD2	2:B:263:GLN:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:TRP:O	1:A:296:ASP:HB2	2.13	0.48
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.95	0.48
10:L:143:LEU:HD12	10:L:143:LEU:HA	1.61	0.48
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.48
2:B:271:ASP:HB3	13:B:817:CLA:HMA1	1.95	0.48
2:B:487:ILE:HG12	13:B:835:CLA:HMD3	1.95	0.48
1:A:444:LEU:HB2	13:A:840:CLA:HBB1	1.96	0.48
13:A:810:CLA:HMA1	8:J:27:ILE:HD13	1.95	0.48
13:B:806:CLA:H91	18:B:850:LMG:H401	1.96	0.48
1:A:399:TRP:NE1	13:A:829:CLA:HAB	2.27	0.48
1:A:283:GLY:O	1:A:508:THR:O	2.32	0.48
6:F:109:CYS:O	6:F:112:THR:HB	2.13	0.48
8:J:33:TYR:N	8:J:34:PRO:HD3	2.28	0.48
1:A:118:TRP:HB3	16:J:104:BCR:H323	1.94	0.48
6:F:88:VAL:HG13	6:F:97:LYS:HD2	1.95	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.14	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
8:J:31:ARG:CD	16:J:104:BCR:H312	2.19	0.48
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.95	0.48
1:A:360:LEU:CD1	13:A:831:CLA:HBB1	2.44	0.48
2:B:180:GLY:HA3	13:B:813:CLA:HBB1	1.96	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.13	0.47
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.47
9:K:74:VAL:C	9:K:76:GLY:H	2.17	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47
11:M:24:ARG:NH1	20:M:1702:HOH:O	2.46	0.47
6:F:10:ASP:HB3	20:F:1406:HOH:O	2.14	0.47
13:B:824:CLA:H61	13:B:824:CLA:H41	1.68	0.47
13:B:814:CLA:HAB	13:B:828:CLA:H13	1.96	0.47
2:B:647:ASN:HD22	2:B:649:LEU:N	2.08	0.47
1:A:168:MET:O	1:A:172:MET:HB2	2.14	0.47
4:D:124:ASN:O	4:D:127:GLN:HB2	2.13	0.47
1:A:74:SER:OG	1:A:180:TYR:HB2	2.15	0.47
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.96	0.47
13:A:815:CLA:HBA2	13:A:817:CLA:HMB3	1.96	0.47
1:A:691:PHE:HB2	13:A:803:CLA:CBC	2.45	0.47
1:A:56:HIS:CG	13:A:806:CLA:HAB	2.49	0.47
1:A:121:VAL:HB	13:B:833:CLA:HMD1	1.96	0.47
2:B:525:VAL:CG1	13:B:801:CLA:H141	2.45	0.47
2:B:693:LEU:HD12	13:L:1003:CLA:H11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:808:CLA:H142	13:B:808:CLA:HMB2	1.97	0.47
13:A:804:CLA:H8	8:J:16:ALA:HA	1.97	0.47
1:A:399:TRP:HB3	13:A:829:CLA:HMC3	1.96	0.47
2:B:589:MET:CE	2:B:589:MET:C	2.83	0.47
8:J:40:PRO:O	8:J:41:LEU:HB2	2.14	0.47
1:A:447:VAL:HG21	13:A:840:CLA:C2C	2.44	0.47
1:A:174:PHE:HD2	13:A:811:CLA:CBC	2.28	0.47
13:A:806:CLA:HMC3	13:A:831:CLA:HMA1	1.97	0.47
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.47
2:B:313:LYS:O	2:B:314:VAL:CG2	2.60	0.47
1:A:379:PRO:HB2	13:A:820:CLA:HAA2	1.96	0.47
13:A:843:CLA:H172	8:J:19:MET:HG3	1.97	0.47
3:C:65:ARG:HG2	3:C:67:TYR:OH	2.14	0.47
2:B:641:TYR:CB	2:B:646:THR:HG22	2.42	0.47
11:M:24:ARG:NH1	11:M:24:ARG:CG	2.78	0.47
13:A:843:CLA:H2	13:A:843:CLA:O1A	2.15	0.46
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.97	0.46
13:B:810:CLA:H42	10:L:81:SER:HA	1.97	0.46
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	0.46
1:A:638:ASN:O	1:A:642:SER:HB2	2.16	0.46
13:B:820:CLA:HBB1	16:B:843:BCR:H14C	1.97	0.46
1:A:603:TYR:OH	13:A:801:CLA:HED1	2.15	0.46
13:A:822:CLA:CMB	13:A:826:CLA:HMA3	2.46	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
13:B:838:CLA:H203	6:F:67:SER:HB3	1.98	0.46
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
1:A:90:MET:HE1	13:A:809:CLA:HAA2	1.98	0.46
13:B:802:CLA:H41	13:B:802:CLA:H61	1.56	0.46
13:A:821:CLA:HBC2	13:A:821:CLA:HMC1	1.97	0.46
13:B:828:CLA:HBA2	13:B:828:CLA:H3A	1.64	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.46
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.96	0.46
2:B:386:MET:HE1	16:B:847:BCR:H361	1.98	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46
10:L:33:ASN:HB3	13:L:1002:CLA:HAC1	1.98	0.46
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.46	0.46
1:A:744:TRP:CG	16:A:854:BCR:HC22	2.51	0.46
1:A:445:ASN:ND2	13:B:803:CLA:HED2	2.31	0.46
2:B:642:ASN:HB2	2:B:643:PRO:HD3	1.95	0.46
3:C:23:ASP:OD2	4:D:95:HIS:CD2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:810:CLA:HBB1	13:B:810:CLA:HHC	1.96	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
2:B:738:LYS:O	2:B:739:PHE:CB	2.64	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
11:M:13:VAL:HG23	16:M:1602:BCR:H402	1.98	0.46
13:A:801:CLA:HED1	20:A:908:HOH:O	2.15	0.46
16:A:854:BCR:H381	13:B:832:CLA:HMA1	1.97	0.46
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.96	0.46
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.46
13:B:807:CLA:H102	16:I:101:BCR:HC31	1.98	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.31	0.46
1:A:508:THR:HG21	20:A:930:HOH:O	2.15	0.45
13:B:830:CLA:H3A	13:B:830:CLA:HBA2	1.49	0.45
2:B:189:TRP:CA	13:B:814:CLA:HBB1	2.45	0.45
13:B:828:CLA:H12	16:B:844:BCR:H393	1.97	0.45
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	0.45
2:B:479:THR:H	2:B:482:SER:HB3	1.79	0.45
1:A:475:PHE:HA	1:A:480:ILE:O	2.15	0.45
13:L:1002:CLA:C1B	13:L:1003:CLA:HED1	2.46	0.45
13:A:826:CLA:HAB	16:A:852:BCR:H341	1.98	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.45
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	0.45
2:B:468:ALA:O	2:B:482:SER:HB2	2.16	0.45
1:A:44:THR:HB	1:A:720:ARG:HG2	1.98	0.45
8:J:22:THR:O	8:J:26:LEU:HD13	2.15	0.45
13:A:823:CLA:H3A	13:A:823:CLA:HBA2	1.44	0.45
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.51	0.45
13:A:821:CLA:H3A	13:A:821:CLA:HBA2	1.83	0.45
13:B:818:CLA:H41	13:B:818:CLA:H62	1.69	0.45
2:B:220:GLY:HA3	13:B:815:CLA:HMD1	1.98	0.45
1:A:313:HIS:CE1	16:A:849:BCR:H363	2.51	0.45
1:A:539:HIS:CG	13:A:839:CLA:HED2	2.51	0.45
2:B:64:LEU:HD11	16:B:845:BCR:H271	1.98	0.45
13:B:820:CLA:HBA2	13:B:820:CLA:H3A	1.64	0.45
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.46	0.45
13:B:816:CLA:H41	13:B:816:CLA:H62	1.71	0.45
10:L:115:GLU:O	10:L:119:GLN:HG3	2.17	0.45
1:A:112:PRO:HB3	1:A:144:PHE:CD1	2.51	0.45
2:B:339:TRP:CZ3	16:B:846:BCR:H372	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:HB1	13:A:806:CLA:HBB1	1.98	0.45
2:B:445:VAL:HG21	13:B:833:CLA:HAC2	1.97	0.45
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:737:LEU:HD22	13:A:843:CLA:HMA1	1.99	0.45
13:B:832:CLA:HBB1	13:B:833:CLA:HMB2	1.98	0.45
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
1:A:508:THR:HG22	1:A:509:ALA:N	2.31	0.45
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.52	0.45
11:M:17:LEU:HB3	11:M:18:PRO:HD3	1.98	0.45
2:B:570:ARG:HH11	2:B:570:ARG:HG3	1.81	0.45
8:J:1:MET:O	8:J:1:MET:HE2	2.17	0.45
4:D:134:LYS:HG2	4:D:136:TYR:CZ	2.52	0.45
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.45
4:D:114:SER:N	20:D:206:HOH:O	2.50	0.45
1:A:86:TRP:HE1	13:A:809:CLA:HBA1	1.82	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.33	0.45
2:B:497:ASN:O	2:B:499:TRP:CE3	2.70	0.45
1:A:321:ILE:HD11	13:A:821:CLA:H2A	1.99	0.45
2:B:557:LYS:NZ	4:D:124:ASN:OD1	2.43	0.45
13:A:801:CLA:NA	13:B:801:CLA:HAB	2.31	0.44
13:B:827:CLA:CGA	13:B:827:CLA:H3A	2.47	0.44
2:B:48:SER:HB3	13:B:805:CLA:HBB1	1.98	0.44
2:B:480:LEU:C	2:B:482:SER:N	2.69	0.44
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.52	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
13:A:807:CLA:H3A	13:A:831:CLA:HAB	1.99	0.44
1:A:90:MET:HE2	13:A:829:CLA:HED1	1.99	0.44
2:B:531:LEU:HD21	13:B:802:CLA:HBB1	1.99	0.44
13:B:814:CLA:HBA1	16:B:845:BCR:H383	2.00	0.44
13:A:806:CLA:H71	16:A:851:BCR:H402	1.99	0.44
13:B:835:CLA:HMB1	16:B:847:BCR:HC31	1.98	0.44
13:M:1601:CLA:H3A	13:M:1601:CLA:HBA2	1.69	0.44
2:B:79:ASP:OD2	2:B:82:ASN:HB2	2.18	0.44
2:B:441:VAL:O	2:B:445:VAL:HG23	2.17	0.44
1:A:484:PRO:HB3	13:A:839:CLA:CED	2.46	0.44
2:B:370:THR:HG21	20:B:922:HOH:O	2.16	0.44
1:A:212:TRP:N	13:A:815:CLA:HBB1	2.32	0.44
13:B:810:CLA:CED	13:B:810:CLA:H43	2.47	0.44
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
3:C:6:ILE:HD12	3:C:6:ILE:N	2.33	0.44
13:B:831:CLA:HBC3	16:F:1302:BCR:H362	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:56:TYR:OH	13:L:1004:CLA:HED2	2.18	0.44
5:E:6:LYS:CD	5:E:22:THR:HG22	2.47	0.44
13:A:810:CLA:HBC2	13:A:829:CLA:H141	1.98	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	0.44
1:A:98:SER:HB2	1:A:113:SER:O	2.18	0.44
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.99	0.44
16:A:854:BCR:H23C	16:A:854:BCR:H403	1.99	0.44
1:A:642:SER:O	1:A:648:GLY:HA3	2.17	0.44
13:A:843:CLA:H62	13:A:843:CLA:H41	1.73	0.44
2:B:211:PHE:CE2	2:B:212:LEU:HG	2.53	0.44
13:B:809:CLA:H102	13:B:827:CLA:H193	1.98	0.44
2:B:181:LEU:HD13	13:B:813:CLA:HHB	2.00	0.44
1:A:462:ASN:HB3	1:A:645:THR:HG22	1.99	0.44
1:A:111:LYS:HB2	1:A:130:VAL:HB	2.00	0.44
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.43
13:B:806:CLA:H41	13:B:806:CLA:H61	1.60	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
8:J:1:MET:HE2	8:J:5:LEU:HG	2.00	0.43
2:B:317:PRO:HB3	20:B:949:HOH:O	2.18	0.43
1:A:519:ALA:HB2	1:A:625:VAL:HG21	2.00	0.43
2:B:427:TRP:CE2	13:B:831:CLA:HBB1	2.53	0.43
2:B:430:LEU:HB3	13:B:832:CLA:CED	2.48	0.43
2:B:531:LEU:HD21	13:B:802:CLA:CBB	2.48	0.43
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.43
2:B:234:GLN:O	2:B:236:PRO:HD3	2.18	0.43
2:B:339:TRP:CE2	13:B:826:CLA:H91	2.54	0.43
2:B:36:MET:HE1	2:B:41:LEU:N	2.33	0.43
13:A:820:CLA:HMB1	13:A:820:CLA:CBB	2.48	0.43
2:B:431:PHE:HD2	13:B:838:CLA:HBB2	1.84	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43
2:B:529:ILE:HG21	13:B:837:CLA:HAB	1.99	0.43
13:B:839:CLA:HBC2	13:X:1701:CLA:HBC3	2.00	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.45	0.43
13:B:835:CLA:HBA2	13:B:836:CLA:HMB3	2.00	0.43
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	0.43
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
1:A:91:TYR:CE2	1:A:147:TRP:CZ3	3.07	0.43
2:B:439:LEU:HD11	16:J:105:BCR:H342	2.00	0.43
1:A:215:HIS:HB2	13:A:815:CLA:C1C	2.48	0.43
1:A:443:HIS:CD2	13:A:832:CLA:HMB1	2.53	0.43
6:F:21:ALA:HB2	6:F:35:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
1:A:261:PHE:CD2	1:A:261:PHE:O	2.72	0.43
1:A:212:TRP:CA	13:A:815:CLA:HBB1	2.49	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
13:A:844:CLA:H41	13:A:844:CLA:H62	1.62	0.43
2:B:325:ILE:HD12	2:B:409:ASN:ND2	2.34	0.43
16:J:105:BCR:H20C	16:J:105:BCR:H361	1.89	0.43
2:B:360:PRO:HG3	13:B:818:CLA:HBA1	2.00	0.43
2:B:36:MET:HE1	2:B:40:ASN:C	2.39	0.43
13:A:820:CLA:O1A	13:A:830:CLA:HMD1	2.19	0.43
4:D:18:LEU:HA	4:D:18:LEU:HD23	1.86	0.43
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.43
1:A:683:TRP:CE3	13:A:801:CLA:HMA1	2.54	0.42
13:B:832:CLA:H61	16:F:1302:BCR:H312	2.00	0.42
13:A:845:CLA:HBA2	13:A:845:CLA:H3A	1.74	0.42
13:B:808:CLA:O1A	13:B:827:CLA:HBD	2.20	0.42
1:A:257:ASP:OD1	1:A:262:SER:CB	2.66	0.42
8:J:39:HIS:HA	16:J:105:BCR:H21C	2.00	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.92	0.42
13:B:810:CLA:CBB	7:I:19:CYS:HB3	2.50	0.42
2:B:24:ILE:HA	13:B:804:CLA:HMD3	2.01	0.42
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.01	0.42
1:A:711:LEU:O	1:A:713:VAL:HG22	2.20	0.42
13:B:817:CLA:H3A	13:B:817:CLA:HBA2	1.39	0.42
10:L:4:LEU:HD22	10:L:4:LEU:N	2.35	0.42
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.35	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
4:D:95:HIS:HA	4:D:97:LYS:N	2.34	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.83	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.19	0.42
2:B:357:SER:C	2:B:359:PRO:HD3	2.40	0.42
1:A:403:PHE:CB	13:A:807:CLA:H112	2.49	0.42
2:B:588:TRP:CH2	13:B:802:CLA:CBB	3.02	0.42
13:A:810:CLA:H11	16:J:103:BCR:H19C	2.02	0.42
13:B:829:CLA:CBB	13:B:829:CLA:HMB1	2.48	0.42
1:A:256:VAL:HG12	1:A:257:ASP:N	2.34	0.42
2:B:492:TRP:CZ3	13:B:836:CLA:HMD3	2.54	0.42
2:B:458:ILE:CD1	2:B:458:ILE:N	2.82	0.42
1:A:120:ILE:O	1:A:122:GLY:N	2.52	0.42
1:A:360:LEU:HD11	13:A:831:CLA:HBB1	2.02	0.42
16:A:854:BCR:H362	13:B:802:CLA:C4	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:19:MET:HE2	8:J:19:MET:HA	2.00	0.42
1:A:542:HIS:HD2	20:A:926:HOH:O	2.03	0.42
13:A:825:CLA:H92	16:A:852:BCR:H14C	2.01	0.42
2:B:341:LEU:HD21	13:B:829:CLA:HAB	2.02	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.20	0.42
1:A:234:LYS:H	1:A:234:LYS:HG2	1.69	0.42
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
13:A:827:CLA:H51	13:A:838:CLA:H43	2.00	0.42
13:B:806:CLA:H143	13:B:828:CLA:CBB	2.50	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.42
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:145:GLN:CD	1:A:145:GLN:H	2.22	0.42
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.42
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
2:B:261:HIS:HD2	2:B:264:THR:H	1.67	0.42
1:A:741:ALA:CB	16:A:854:BCR:H323	2.50	0.42
2:B:414:VAL:HG11	16:B:846:BCR:C40	2.50	0.42
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.42
1:A:336:PHE:CD2	10:L:4:LEU:HD21	2.55	0.42
13:A:811:CLA:H3A	13:A:811:CLA:HBA2	1.63	0.42
2:B:527:HIS:CD2	16:J:105:BCR:H322	2.55	0.42
1:A:156:PHE:CE2	13:A:817:CLA:HAA2	2.55	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42
13:A:829:CLA:H93	16:J:103:BCR:H20C	2.02	0.41
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
17:B:851:LHG:HC5	12:X:12:ARG:HB3	2.02	0.41
1:A:744:TRP:NE1	13:A:829:CLA:H11	2.35	0.41
1:A:685:PHE:HA	13:A:803:CLA:HAB	2.01	0.41
13:A:837:CLA:HBA2	13:A:837:CLA:H3A	1.72	0.41
13:A:846:CLA:H12	13:A:846:CLA:HBA2	1.85	0.41
2:B:189:TRP:HA	13:B:814:CLA:HBB1	2.02	0.41
3:C:25:LEU:HA	3:C:40:SER:O	2.20	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	0.41
11:M:9:TYR:HB3	16:M:1602:BCR:H401	2.02	0.41
1:A:346:GLU:N	1:A:346:GLU:OE1	2.47	0.41
1:A:49:TRP:CZ3	17:A:855:LHG:H121	2.56	0.41
2:B:663:TRP:CE3	13:B:801:CLA:HMA1	2.56	0.41
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.41
1:A:203:GLY:HA3	13:A:814:CLA:HBB1	2.02	0.41
2:B:136:GLN:HE21	13:B:814:CLA:HAA1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
1:A:710:LYS:O	1:A:710:LYS:HD2	2.20	0.41
1:A:49:TRP:HZ3	17:A:855:LHG:H121	1.86	0.41
1:A:202:ALA:C	13:A:821:CLA:HBC3	2.41	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
1:A:212:TRP:HA	13:A:815:CLA:HBB1	2.01	0.41
4:D:50:ARG:HG3	4:D:50:ARG:NH1	2.35	0.41
13:L:1003:CLA:H111	13:L:1003:CLA:H152	1.99	0.41
13:B:816:CLA:H3A	13:B:816:CLA:HBA2	1.68	0.41
2:B:529:ILE:HG21	13:B:837:CLA:CAB	2.51	0.41
3:C:13:CYS:SG	3:C:15:GLN:HB2	2.60	0.41
2:B:691:THR:HA	2:B:692:PRO:HD3	1.90	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
1:A:161:THR:HG22	16:A:850:BCR:HC32	2.02	0.41
13:B:825:CLA:HBA2	13:B:825:CLA:H3A	1.69	0.41
13:B:805:CLA:H3A	13:B:805:CLA:HBA1	1.74	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
13:A:820:CLA:HBA2	13:A:820:CLA:H3A	1.89	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
13:A:802:CLA:O1A	13:A:802:CLA:H3A	2.21	0.41
13:B:803:CLA:H122	16:I:101:BCR:H281	2.03	0.41
4:D:104:LYS:H	4:D:104:LYS:HG2	1.51	0.41
13:A:822:CLA:HMD1	13:A:823:CLA:HBB1	2.02	0.41
13:B:818:CLA:H3A	13:B:818:CLA:CGA	2.51	0.41
13:B:814:CLA:HMA2	16:B:845:BCR:H282	2.03	0.41
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
1:A:260:PHE:O	1:A:261:PHE:HB2	2.21	0.41
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.41
1:A:713:VAL:HG11	13:A:841:CLA:HMB3	2.03	0.41
13:A:843:CLA:H203	13:F:1301:CLA:CBB	2.52	0.41
6:F:80:VAL:HG21	6:F:110:MET:HA	2.03	0.41
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.56	0.41
13:A:843:CLA:H52	13:A:843:CLA:NC	2.36	0.40
13:A:803:CLA:C14	16:A:854:BCR:H402	2.51	0.40
13:B:809:CLA:H203	7:I:26:VAL:CG2	2.51	0.40
13:A:835:CLA:HED2	10:L:65:LEU:O	2.21	0.40
20:A:944:HOH:O	10:L:16:HIS:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.40
13:B:810:CLA:O2A	13:B:810:CLA:H2A	2.20	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
1:A:118:TRP:HB3	16:J:104:BCR:C32	2.51	0.40
1:A:360:LEU:HA	1:A:360:LEU:HD12	1.93	0.40
2:B:459:GLU:HA	2:B:460:PRO:HD3	1.82	0.40
2:B:313:LYS:O	2:B:314:VAL:CG1	2.68	0.40
2:B:589:MET:HE1	2:B:590:LEU:N	2.36	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
10:L:44:ILE:HB	20:L:1123:HOH:O	2.20	0.40
2:B:629:TYR:O	2:B:633:ASN:HB2	2.21	0.40
1:A:114:ALA:O	1:A:115:GLN:O	2.39	0.40
2:B:490:THR:O	2:B:495:TYR:HA	2.21	0.40
13:A:810:CLA:CBB	13:B:833:CLA:HMD2	2.51	0.40
13:A:825:CLA:HHB	13:A:846:CLA:HBB1	2.02	0.40
13:B:817:CLA:O1D	13:B:818:CLA:HMA1	2.21	0.40
2:B:318:PHE:H	13:B:822:CLA:C2B	2.34	0.40
8:J:30:ASN:O	8:J:34:PRO:HG3	2.21	0.40
2:B:33:HIS:HE1	13:B:804:CLA:HED1	1.85	0.40
2:B:269:LEU:HD23	2:B:272:MET:HE3	2.02	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
16:L:1006:BCR:H361	16:L:1006:BCR:H20C	1.88	0.40
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.40
2:B:279:ILE:HD11	13:B:817:CLA:HBC3	2.02	0.40
13:B:823:CLA:CBB	13:B:830:CLA:HMD2	2.51	0.40
2:B:377:HIS:HE2	13:B:828:CLA:C1B	2.35	0.40
2:B:176:HIS:CG	13:B:813:CLA:HMC2	2.56	0.40
2:B:36:MET:HE3	2:B:40:ASN:CB	2.47	0.40
20:C:210:HOH:O	4:D:138:PRO:HG3	2.21	0.40
2:B:605:LEU:HA	2:B:605:LEU:HD12	1.80	0.40
1:A:120:ILE:HG12	1:A:121:VAL:N	2.36	0.40
1:A:741:ALA:CB	16:A:854:BCR:C32	2.99	0.40
2:B:642:ASN:CB	2:B:643:PRO:CD	2.88	0.40
3:C:40:SER:HA	20:C:209:HOH:O	2.21	0.40
4:D:88:ASP:HB3	4:D:90:GLU:H	1.86	0.40
2:B:53:LEU:HA	2:B:53:LEU:HD12	1.83	0.40

All (5) 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)
20:L:1126:HOH:O	20:L:1126:HOH:O[2_655]	1.08	1.12
10:L:153:PHE:O	19:L:1001:CA:CA[3_665]	1.57	0.63
5:E:28:GLN:OE1	6:F:1:ASP:N[4_664]	2.00	0.20
10:L:154:ASN:OXT	20:A:950:HOH:O[3_665]	2.07	0.13
20:L:1108:HOH:O	20:L:1117:HOH:O[2_655]	2.07	0.13

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%)	695 (94%)	31 (4%)	10 (1%)	14 58
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	16 61
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	15 60
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	8 49
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	2 26
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	8 49
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	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1 21
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	15 60
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	5 40
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	4 38
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	11 55

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE

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Mol	Chain	Res	Type
1	A	261	PHE
2	B	234	GLN
2	B	313	LYS
2	B	314	VAL
2	B	480	LEU
2	B	492	TRP
2	B	497	ASN
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	91	SER
9	K	41	PRO
9	K	42	GLY
11	M	30	TYR
12	X	10	ALA
1	A	121	VAL
1	A	578	CYS
2	B	565	CYS
4	D	3	LEU
6	F	60	ALA
6	F	89	ARG
10	L	106	SER
1	A	234	LYS
4	D	44	ALA
5	E	53	SER
10	L	104	GLY
1	A	42	PRO
1	A	232	ALA
2	B	481	LEU
5	E	25	SER
5	E	54	GLY
1	A	276	SER
5	E	55	VAL
9	K	56	LEU

5.3.2 Protein sidechains (i)

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%)	565 (96%)	24 (4%)	37 71
2	B	595/597 (100%)	567 (95%)	28 (5%)	32 68
3	C	67/67 (100%)	66 (98%)	1 (2%)	72 88
4	D	115/115 (100%)	107 (93%)	8 (7%)	19 56
5	E	59/64 (92%)	59 (100%)	0	100 100
6	F	109/128 (85%)	107 (98%)	2 (2%)	66 87
7	I	32/32 (100%)	30 (94%)	2 (6%)	22 59
8	J	36/36 (100%)	34 (94%)	2 (6%)	26 62
10	L	117/119 (98%)	109 (93%)	8 (7%)	20 57
11	M	26/26 (100%)	25 (96%)	1 (4%)	40 73
12	X	20/27 (74%)	18 (90%)	2 (10%)	9 38
All	All	1765/1814 (97%)	1687 (96%)	78 (4%)	35 69

All (78) 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	253	TYR
1	A	257	ASP
1	A	260	PHE
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
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

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Mol	Chain	Res	Type
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	211	PHE
2	B	214	THR
2	B	256	PHE
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	635	SER
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
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
4	D	125	PRO
4	D	126	SER
6	F	56	ARG
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL

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Mol	Chain	Res	Type
8	J	1	MET
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	42	SER
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	145	GLN
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	426	GLN
1	A	445	ASN
1	A	542	HIS
1	A	633	HIS
1	A	647	ASN
1	A	718	GLN
2	B	33	HIS
2	B	136	GLN
2	B	261	HIS
2	B	263	GLN
2	B	336	GLN
2	B	340	HIS
2	B	406	ASN
2	B	494	ASN
2	B	611	ASN
2	B	614	GLN
2	B	616	ASN
2	B	639	ASN

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Mol	Chain	Res	Type
2	B	647	ASN
2	B	648	ASN
2	B	678	GLN
2	B	688	HIS
3	C	37	GLN
4	D	54	ASN
4	D	71	GLN
4	D	95	HIS
5	E	18	ASN
6	F	40	GLN
6	F	95	ASN
10	L	16	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	-	55,73,73	0.88	1 (1%)	61,113,113	2.24	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	802	20	55,73,73	0.86	3 (5%)	61,113,113	1.41	10 (16%)
13	CLA	A	803	-	55,73,73	0.96	4 (7%)	61,113,113	1.46	11 (18%)
13	CLA	A	804	-	55,73,73	0.84	3 (5%)	61,113,113	1.49	8 (13%)
13	CLA	A	805	13	49,67,73	0.89	2 (4%)	53,105,113	1.69	12 (22%)
13	CLA	A	806	-	55,73,73	0.84	2 (3%)	61,113,113	1.60	11 (18%)
13	CLA	A	807	-	55,73,73	0.87	2 (3%)	61,113,113	1.66	14 (22%)
13	CLA	A	808	-	41,59,73	1.07	3 (7%)	44,96,113	1.63	9 (20%)
13	CLA	A	809	1	55,73,73	1.06	4 (7%)	61,113,113	1.57	11 (18%)
13	CLA	A	810	1	55,73,73	0.79	1 (1%)	61,113,113	1.54	11 (18%)
13	CLA	A	811	-	32,53,73	0.99	3 (9%)	37,89,113	1.63	8 (21%)
13	CLA	A	812	13	55,73,73	0.88	3 (5%)	61,113,113	1.38	9 (14%)
13	CLA	A	813	-	44,62,73	1.02	4 (9%)	47,99,113	1.62	9 (19%)
13	CLA	A	814	-	50,68,73	0.86	2 (4%)	55,107,113	1.58	10 (18%)
13	CLA	A	815	-	32,53,73	1.07	3 (9%)	37,89,113	1.72	8 (21%)
13	CLA	A	816	-	32,53,73	0.86	1 (3%)	37,89,113	1.84	9 (24%)
13	CLA	A	817	20	39,57,73	0.94	2 (5%)	43,93,113	1.70	8 (18%)
13	CLA	A	818	-	44,62,73	0.99	3 (6%)	47,99,113	1.55	8 (17%)
13	CLA	A	819	-	44,62,73	1.08	4 (9%)	47,99,113	1.67	12 (25%)
13	CLA	A	820	-	55,73,73	0.99	4 (7%)	61,113,113	1.57	13 (21%)
13	CLA	A	821	-	51,69,73	0.99	4 (7%)	56,108,113	1.62	12 (21%)
13	CLA	A	822	20	55,73,73	0.89	4 (7%)	61,113,113	1.57	14 (22%)
13	CLA	A	823	-	39,57,73	0.98	2 (5%)	43,93,113	1.83	12 (27%)
13	CLA	A	824	-	41,59,73	1.03	3 (7%)	44,96,113	1.72	8 (18%)
13	CLA	A	825	-	49,67,73	0.90	2 (4%)	53,105,113	1.53	12 (22%)
13	CLA	A	826	20	55,73,73	0.90	2 (3%)	61,113,113	1.50	9 (14%)
13	CLA	A	827	20	55,73,73	0.86	2 (3%)	61,113,113	1.43	10 (16%)
13	CLA	A	828	-	55,73,73	0.94	2 (3%)	61,113,113	1.51	9 (14%)
13	CLA	A	829	-	55,73,73	0.83	2 (3%)	61,113,113	1.38	11 (18%)
13	CLA	A	830	-	55,73,73	0.78	1 (1%)	61,113,113	1.51	9 (14%)
13	CLA	A	831	-	55,73,73	0.97	4 (7%)	61,113,113	1.50	11 (18%)
13	CLA	A	832	-	40,58,73	1.08	3 (7%)	44,95,113	1.88	13 (29%)
13	CLA	A	833	-	55,73,73	0.78	0	61,113,113	1.50	11 (18%)
13	CLA	A	834	-	55,73,73	0.73	0	61,113,113	1.43	10 (16%)
13	CLA	A	835	-	55,73,73	0.98	3 (5%)	61,113,113	1.60	11 (18%)
13	CLA	A	836	-	44,62,73	1.00	4 (9%)	47,99,113	1.67	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	A	837	1	32,53,73	0.95	2 (6%)	37,89,113	1.72	9 (24%)
13	CLA	A	838	-	41,59,73	0.84	0	44,96,113	1.69	11 (25%)
13	CLA	A	839	-	55,73,73	0.95	3 (5%)	61,113,113	1.32	7 (11%)
13	CLA	A	840	-	37,55,73	1.05	3 (8%)	42,91,113	1.74	10 (23%)
13	CLA	A	841	-	55,73,73	0.87	4 (7%)	61,113,113	1.43	12 (19%)
13	CLA	A	842	20	41,59,73	1.04	4 (9%)	44,96,113	1.63	10 (22%)
13	CLA	A	843	-	55,73,73	0.99	2 (3%)	61,113,113	1.51	11 (18%)
13	CLA	A	844	20	55,73,73	1.02	5 (9%)	61,113,113	1.44	11 (18%)
13	CLA	A	845	-	29,49,73	1.08	3 (10%)	32,83,113	1.44	3 (9%)
13	CLA	A	846	17	42,60,73	1.15	5 (11%)	45,97,113	1.88	11 (24%)
14	PQN	A	847	-	34,34,34	3.59	17 (50%)	44,45,45	2.21	3 (6%)
15	SF4	A	848	1,2	0,12,12	0.00	-	0,24,24	0.00	-
16	BCR	A	849	-	41,41,41	1.33	5 (12%)	56,56,56	1.92	16 (28%)
16	BCR	A	850	-	41,41,41	1.24	4 (9%)	56,56,56	1.81	16 (28%)
16	BCR	A	851	-	41,41,41	1.38	6 (14%)	56,56,56	1.98	18 (32%)
16	BCR	A	852	-	41,41,41	1.34	6 (14%)	56,56,56	1.82	15 (26%)
16	BCR	A	853	-	41,41,41	1.25	7 (17%)	56,56,56	1.94	17 (30%)
16	BCR	A	854	-	41,41,41	1.34	6 (14%)	56,56,56	2.07	21 (37%)
17	LHG	A	855	-	48,48,48	1.67	6 (12%)	49,54,54	1.25	3 (6%)
17	LHG	A	856	13	26,26,48	2.19	5 (19%)	27,32,54	1.51	4 (14%)
13	CLA	B	801	-	55,73,73	0.91	3 (5%)	61,113,113	1.38	10 (16%)
13	CLA	B	802	20	55,73,73	0.85	1 (1%)	61,113,113	1.59	9 (14%)
13	CLA	B	803	-	55,73,73	1.09	4 (7%)	61,113,113	1.37	10 (16%)
13	CLA	B	804	-	44,62,73	1.04	2 (4%)	47,99,113	1.77	9 (19%)
13	CLA	B	805	-	55,73,73	0.87	3 (5%)	61,113,113	1.47	9 (14%)
13	CLA	B	806	-	55,73,73	0.80	1 (1%)	61,113,113	1.34	9 (14%)
13	CLA	B	807	-	55,73,73	0.95	3 (5%)	61,113,113	1.50	9 (14%)
13	CLA	B	808	-	55,73,73	0.91	3 (5%)	61,113,113	1.66	11 (18%)
13	CLA	B	809	2	55,73,73	0.70	0	61,113,113	1.42	10 (16%)
13	CLA	B	810	2	55,73,73	0.82	1 (1%)	61,113,113	1.39	10 (16%)
13	CLA	B	811	-	32,53,73	1.04	4 (12%)	37,89,113	1.64	8 (21%)
13	CLA	B	812	-	32,53,73	0.88	1 (3%)	37,89,113	1.71	9 (24%)
13	CLA	B	813	-	55,73,73	0.84	2 (3%)	61,113,113	1.49	9 (14%)
13	CLA	B	814	-	55,73,73	0.94	4 (7%)	61,113,113	1.53	9 (14%)
13	CLA	B	815	-	32,53,73	1.02	3 (9%)	37,89,113	1.76	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLA	B	816	-	45,63,73	1.11	6 (13%)	49,101,113	1.61	11 (22%)
13	CLA	B	817	-	49,67,73	1.01	4 (8%)	53,105,113	1.58	11 (20%)
13	CLA	B	818	-	50,68,73	1.01	3 (6%)	55,107,113	1.67	12 (21%)
13	CLA	B	819	20	55,73,73	0.90	3 (5%)	61,113,113	1.43	10 (16%)
13	CLA	B	820	-	37,55,73	0.89	2 (5%)	42,91,113	1.88	12 (28%)
13	CLA	B	821	-	32,53,73	0.97	1 (3%)	37,89,113	1.85	10 (27%)
13	CLA	B	822	20	45,63,73	1.03	2 (4%)	49,101,113	1.55	12 (24%)
13	CLA	B	823	-	32,53,73	0.97	2 (6%)	37,89,113	1.64	8 (21%)
13	CLA	B	824	2	44,62,73	1.15	5 (11%)	47,99,113	1.71	11 (23%)
13	CLA	B	825	20	36,54,73	0.85	2 (5%)	41,90,113	1.84	11 (26%)
13	CLA	B	826	-	55,73,73	0.82	2 (3%)	61,113,113	1.50	10 (16%)
13	CLA	B	827	-	55,73,73	1.03	3 (5%)	61,113,113	1.64	12 (19%)
13	CLA	B	828	-	55,73,73	1.11	6 (10%)	61,113,113	1.53	11 (18%)
13	CLA	B	829	-	55,73,73	0.86	3 (5%)	61,113,113	1.61	10 (16%)
13	CLA	B	830	-	32,53,73	1.08	4 (12%)	37,89,113	1.81	10 (27%)
13	CLA	B	831	-	39,57,73	1.06	3 (7%)	43,93,113	1.70	10 (23%)
13	CLA	B	832	-	55,73,73	0.94	2 (3%)	61,113,113	1.53	9 (14%)
13	CLA	B	833	-	48,66,73	1.02	4 (8%)	52,104,113	1.67	11 (21%)
13	CLA	B	834	-	32,53,73	1.10	3 (9%)	37,89,113	1.70	10 (27%)
13	CLA	B	835	20	32,53,73	1.14	4 (12%)	37,89,113	1.63	8 (21%)
13	CLA	B	836	20	32,53,73	0.88	2 (6%)	37,89,113	1.60	8 (21%)
13	CLA	B	837	-	50,68,73	1.03	3 (6%)	55,107,113	1.53	9 (16%)
13	CLA	B	838	-	55,73,73	0.93	3 (5%)	61,113,113	1.55	14 (22%)
13	CLA	B	839	-	37,55,73	1.00	3 (8%)	42,91,113	1.60	10 (23%)
13	CLA	B	840	20	55,73,73	0.93	2 (3%)	61,113,113	1.33	8 (13%)
13	CLA	B	841	-	55,73,73	0.83	4 (7%)	61,113,113	1.48	11 (18%)
14	PQN	B	842	-	34,34,34	3.52	15 (44%)	44,45,45	2.07	3 (6%)
16	BCR	B	843	-	41,41,41	1.49	5 (12%)	56,56,56	2.08	16 (28%)
16	BCR	B	844	-	41,41,41	1.54	8 (19%)	56,56,56	2.14	18 (32%)
16	BCR	B	845	-	41,41,41	1.24	5 (12%)	56,56,56	2.05	20 (35%)
16	BCR	B	846	-	25,25,41	1.35	4 (16%)	33,33,56	1.89	11 (33%)
16	BCR	B	847	-	41,41,41	1.22	5 (12%)	56,56,56	1.92	19 (33%)
16	BCR	B	848	-	41,41,41	1.22	4 (9%)	56,56,56	2.03	20 (35%)
16	BCR	B	849	-	41,41,41	1.26	6 (14%)	56,56,56	1.77	17 (30%)
18	LMG	B	850	-	55,55,55	0.86	2 (3%)	63,63,63	1.26	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	LHG	B	851	-	22,22,48	2.63	4 (18%)	23,28,54	1.05	1 (4%)
15	SF4	C	101	3	0,12,12	0.00	-	0,24,24	0.00	-
15	SF4	C	102	3	0,12,12	0.00	-	0,24,24	0.00	-
13	CLA	F	1301	20	32,53,73	0.92	1 (3%)	37,89,113	1.64	9 (24%)
16	BCR	F	1302	-	41,41,41	1.25	3 (7%)	56,56,56	1.85	14 (25%)
16	BCR	I	101	-	41,41,41	1.29	7 (17%)	56,56,56	1.83	15 (26%)
16	BCR	I	102	-	41,41,41	1.26	6 (14%)	56,56,56	1.85	16 (28%)
13	CLA	J	101	8	32,53,73	1.01	3 (9%)	37,89,113	1.81	9 (24%)
13	CLA	J	102	-	27,45,73	1.11	2 (7%)	29,78,113	1.67	9 (31%)
16	BCR	J	103	-	41,41,41	1.26	5 (12%)	56,56,56	1.93	16 (28%)
16	BCR	J	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.85	21 (37%)
16	BCR	J	105	-	41,41,41	1.39	6 (14%)	56,56,56	1.92	13 (23%)
13	CLA	K	1401	-	32,53,73	1.03	3 (9%)	37,89,113	1.68	8 (21%)
13	CLA	L	1002	10	55,73,73	0.88	2 (3%)	61,113,113	1.57	10 (16%)
13	CLA	L	1003	-	55,73,73	1.02	5 (9%)	61,113,113	1.45	11 (18%)
13	CLA	L	1004	20	55,73,73	0.90	1 (1%)	61,113,113	1.47	9 (14%)
16	BCR	L	1005	-	41,41,41	1.39	6 (14%)	56,56,56	1.85	15 (26%)
16	BCR	L	1006	-	41,41,41	1.56	8 (19%)	56,56,56	1.77	11 (19%)
13	CLA	M	1601	20	32,53,73	0.99	2 (6%)	37,89,113	1.81	10 (27%)
16	BCR	M	1602	-	41,41,41	1.30	6 (14%)	56,56,56	1.82	13 (23%)
13	CLA	X	1701	12	32,53,73	0.88	1 (3%)	37,89,113	1.72	10 (27%)

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	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	802	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	803	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	804	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	805	13	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	806	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	807	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	808	-	2/2/17/25	0/21/119/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	809	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	810	1	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	811	-	-	0/11/111/135	0/0/9/9
13	CLA	A	812	13	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	813	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	814	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	A	815	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	816	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	817	20	3/3/16/25	1/18/116/135	0/0/9/9
13	CLA	A	818	-	1/1/17/25	0/24/122/135	0/0/9/9
13	CLA	A	819	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	820	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	821	-	3/3/19/25	0/33/131/135	0/0/9/9
13	CLA	A	822	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	823	-	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	A	824	-	2/2/17/25	0/21/119/135	0/0/9/9
13	CLA	A	825	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	A	826	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	827	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	828	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	829	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	A	830	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	831	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	832	-	3/3/17/25	0/19/117/135	0/0/9/9
13	CLA	A	833	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	834	-	-	0/37/135/135	0/0/9/9
13	CLA	A	835	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	836	-	3/3/17/25	0/24/122/135	0/0/9/9
13	CLA	A	837	1	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	A	838	-	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	839	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	A	840	-	1/1/16/25	0/16/114/135	0/0/9/9
13	CLA	A	841	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	842	20	3/3/17/25	0/21/119/135	0/0/9/9
13	CLA	A	843	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	844	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	A	845	-	3/3/14/25	0/5/101/135	0/0/9/9
13	CLA	A	846	17	3/3/17/25	0/22/120/135	0/0/9/9
14	PQN	A	847	-	-	0/23/43/43	0/2/2/2
15	SF4	A	848	1,2	-	0/0/48/48	0/6/5/5
16	BCR	A	849	-	-	0/29/63/63	0/2/2/2
16	BCR	A	850	-	-	0/29/63/63	0/2/2/2
16	BCR	A	851	-	-	0/29/63/63	0/2/2/2
16	BCR	A	852	-	-	0/29/63/63	0/2/2/2
16	BCR	A	853	-	-	0/29/63/63	0/2/2/2
16	BCR	A	854	-	-	0/29/63/63	0/2/2/2
17	LHG	A	855	-	-	0/53/53/53	0/0/0/0
17	LHG	A	856	13	1/1/5/5	0/31/31/53	0/0/0/0
13	CLA	B	801	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	802	20	2/2/20/25	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	-	2/2/17/25	0/24/122/135	0/0/9/9
13	CLA	B	805	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	806	-	3/3/20/25	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	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	809	2	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	810	2	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	811	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	812	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	813	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	814	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	815	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	B	816	-	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	817	-	3/3/18/25	0/30/128/135	0/0/9/9
13	CLA	B	818	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	819	20	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	820	-	3/3/16/25	0/16/114/135	0/0/9/9
13	CLA	B	821	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	822	20	3/3/18/25	0/25/123/135	0/0/9/9
13	CLA	B	823	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	824	2	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	825	20	3/3/16/25	0/15/113/135	0/0/9/9
13	CLA	B	826	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	827	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	828	-	1/1/20/25	0/37/135/135	0/0/9/9
13	CLA	B	829	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	830	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	831	-	3/3/16/25	0/18/116/135	0/0/9/9
13	CLA	B	832	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	833	-	3/3/18/25	0/29/127/135	0/0/9/9
13	CLA	B	834	-	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	835	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	836	20	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	B	837	-	3/3/19/25	0/31/129/135	0/0/9/9
13	CLA	B	838	-	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	B	839	-	-	0/16/114/135	0/0/9/9
13	CLA	B	840	20	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	B	841	-	2/2/20/25	0/37/135/135	0/0/9/9
14	PQN	B	842	-	-	0/23/43/43	0/2/2/2
16	BCR	B	843	-	-	0/29/63/63	0/2/2/2
16	BCR	B	844	-	-	0/29/63/63	0/2/2/2
16	BCR	B	845	-	-	0/29/63/63	0/2/2/2
16	BCR	B	846	-	-	0/18/35/63	0/1/1/2
16	BCR	B	847	-	-	0/29/63/63	0/2/2/2
16	BCR	B	848	-	-	0/29/63/63	0/2/2/2
16	BCR	B	849	-	-	0/29/63/63	0/2/2/2
18	LMG	B	850	-	-	0/50/70/70	0/1/1/1
17	LHG	B	851	-	-	0/26/26/53	0/0/0/0
15	SF4	C	101	3	-	0/0/48/48	0/6/5/5
15	SF4	C	102	3	-	0/0/48/48	0/6/5/5
13	CLA	F	1301	20	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	F	1302	-	-	0/29/63/63	0/2/2/2
16	BCR	I	101	-	-	0/29/63/63	0/2/2/2
16	BCR	I	102	-	-	0/29/63/63	0/2/2/2
13	CLA	J	101	8	3/3/16/25	0/11/111/135	0/0/9/9
13	CLA	J	102	-	3/3/13/25	0/2/96/135	0/0/9/9
16	BCR	J	103	-	-	0/29/63/63	0/2/2/2
16	BCR	J	104	-	-	0/29/63/63	0/2/2/2
16	BCR	J	105	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	K	1401	-	2/2/16/25	0/11/111/135	0/0/9/9
13	CLA	L	1002	10	3/3/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1003	-	2/2/20/25	0/37/135/135	0/0/9/9
13	CLA	L	1004	20	3/3/20/25	0/37/135/135	0/0/9/9
16	BCR	L	1005	-	-	0/29/63/63	0/2/2/2
16	BCR	L	1006	-	-	0/29/63/63	0/2/2/2
13	CLA	M	1601	20	3/3/16/25	0/11/111/135	0/0/9/9
16	BCR	M	1602	-	-	0/29/63/63	0/2/2/2
13	CLA	X	1701	12	3/3/16/25	0/11/111/135	0/0/9/9

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	C2M-C2	-6.92	1.36	1.50
14	B	842	PQN	C2M-C2	-6.60	1.37	1.50
14	B	842	PQN	C16-C15	-4.52	1.35	1.52
14	A	847	PQN	C16-C15	-4.38	1.35	1.52
13	B	807	CLA	C3B-C2B	-3.76	1.35	1.40
13	A	835	CLA	C3B-C2B	-3.54	1.35	1.40
13	B	830	CLA	C3B-C2B	-3.50	1.35	1.40
13	B	837	CLA	C3B-C2B	-3.21	1.36	1.40
13	B	838	CLA	C3B-C2B	-3.20	1.36	1.40
13	B	831	CLA	C3B-C2B	-3.17	1.36	1.40
13	B	832	CLA	C3B-C2B	-3.12	1.36	1.40
13	A	819	CLA	C3B-C2B	-3.06	1.36	1.40
13	A	826	CLA	C3B-C2B	-2.98	1.36	1.40
13	A	809	CLA	C3B-C2B	-2.97	1.36	1.40
13	A	832	CLA	C3B-C2B	-2.96	1.36	1.40
13	B	811	CLA	C3B-C2B	-2.89	1.36	1.40
13	B	803	CLA	C3B-C2B	-2.84	1.36	1.40
13	B	808	CLA	C3B-C2B	-2.81	1.36	1.40
13	A	831	CLA	C3B-C2B	-2.80	1.36	1.40
13	A	808	CLA	C3B-C2B	-2.77	1.36	1.40
13	A	839	CLA	C3B-C2B	-2.76	1.36	1.40
13	A	811	CLA	C3B-C2B	-2.70	1.36	1.40
13	B	834	CLA	C3B-C2B	-2.69	1.36	1.40
13	A	824	CLA	C3B-C2B	-2.67	1.36	1.40
13	B	835	CLA	C3B-C2B	-2.67	1.36	1.40
13	B	819	CLA	C3B-C2B	-2.66	1.36	1.40
13	B	839	CLA	C3B-C2B	-2.65	1.36	1.40
14	A	847	PQN	C10-C1	-2.62	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	840	CLA	C3B-C2B	-2.62	1.36	1.40
13	B	828	CLA	C3B-C2B	-2.61	1.36	1.40
13	A	815	CLA	C3B-C2B	-2.57	1.36	1.40
13	B	808	CLA	C1B-CHB	-2.54	1.32	1.39
13	A	844	CLA	C3B-C2B	-2.53	1.37	1.40
13	B	810	CLA	C3B-C2B	-2.51	1.37	1.40
13	B	824	CLA	C3B-C2B	-2.51	1.37	1.40
13	A	823	CLA	C3B-C2B	-2.51	1.37	1.40
13	B	831	CLA	C1B-CHB	-2.50	1.32	1.39
13	B	817	CLA	C3B-C2B	-2.50	1.37	1.40
13	A	802	CLA	C3B-C2B	-2.50	1.37	1.40
16	A	854	BCR	C23-C22	-2.48	1.40	1.45
13	A	804	CLA	C3B-C2B	-2.48	1.37	1.40
13	A	812	CLA	C3B-C2B	-2.48	1.37	1.40
13	A	822	CLA	C1B-CHB	-2.44	1.33	1.39
13	B	816	CLA	C3B-C2B	-2.42	1.37	1.40
18	B	850	LMG	O7-C8	-2.41	1.40	1.46
13	A	846	CLA	C3B-C2B	-2.41	1.37	1.40
13	A	832	CLA	C1B-CHB	-2.40	1.33	1.39
13	A	813	CLA	C3B-C2B	-2.40	1.37	1.40
13	A	803	CLA	C1B-CHB	-2.40	1.33	1.39
13	A	840	CLA	C3B-C2B	-2.38	1.37	1.40
13	B	815	CLA	C3B-C2B	-2.37	1.37	1.40
13	K	1401	CLA	C3B-C2B	-2.37	1.37	1.40
16	M	1602	BCR	C23-C22	-2.36	1.40	1.45
13	A	821	CLA	C3B-C2B	-2.36	1.37	1.40
16	L	1005	BCR	C19-C18	-2.36	1.40	1.45
13	B	803	CLA	C1B-CHB	-2.36	1.33	1.39
13	B	807	CLA	C1B-CHB	-2.35	1.33	1.39
13	B	801	CLA	C1B-CHB	-2.32	1.33	1.39
13	A	827	CLA	C1B-CHB	-2.32	1.33	1.39
16	B	846	BCR	C23-C22	-2.31	1.40	1.45
16	B	849	BCR	C23-C22	-2.30	1.40	1.45
13	A	842	CLA	C3B-C2B	-2.29	1.37	1.40
16	B	848	BCR	C23-C22	-2.29	1.40	1.45
13	A	841	CLA	C1B-CHB	-2.28	1.33	1.39
13	A	809	CLA	C1B-CHB	-2.28	1.33	1.39
13	B	817	CLA	C1B-CHB	-2.27	1.33	1.39
13	B	811	CLA	C1B-CHB	-2.27	1.33	1.39
13	B	839	CLA	C1B-CHB	-2.25	1.33	1.39
13	L	1003	CLA	C1B-CHB	-2.25	1.33	1.39
14	B	842	PQN	C5-C4	-2.25	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	824	CLA	C1B-CHB	-2.24	1.33	1.39
13	B	814	CLA	C3B-C2B	-2.24	1.37	1.40
13	A	818	CLA	C3B-C2B	-2.23	1.37	1.40
13	A	804	CLA	C1B-CHB	-2.22	1.33	1.39
13	B	823	CLA	C3B-C2B	-2.21	1.37	1.40
13	A	836	CLA	C3B-C2B	-2.20	1.37	1.40
13	A	815	CLA	C1B-CHB	-2.19	1.33	1.39
14	B	842	PQN	C10-C1	-2.19	1.43	1.48
13	A	806	CLA	C1B-CHB	-2.18	1.33	1.39
16	I	102	BCR	C19-C18	-2.18	1.41	1.45
13	B	813	CLA	C1B-CHB	-2.17	1.33	1.39
13	A	818	CLA	C1B-CHB	-2.17	1.33	1.39
13	B	841	CLA	C3B-C2B	-2.16	1.37	1.40
13	A	817	CLA	C3B-C2B	-2.16	1.37	1.40
16	I	101	BCR	C19-C18	-2.15	1.41	1.45
13	B	838	CLA	C1B-CHB	-2.15	1.33	1.39
13	A	825	CLA	C1B-CHB	-2.15	1.33	1.39
13	A	839	CLA	C1B-CHB	-2.15	1.33	1.39
13	A	814	CLA	C1B-CHB	-2.15	1.33	1.39
13	A	835	CLA	C1B-CHB	-2.15	1.33	1.39
13	A	812	CLA	C1B-CHB	-2.14	1.34	1.39
13	B	835	CLA	C1B-CHB	-2.13	1.34	1.39
13	B	819	CLA	C1B-CHB	-2.12	1.34	1.39
13	B	834	CLA	C1B-CHB	-2.10	1.34	1.39
14	A	847	PQN	C5-C4	-2.09	1.44	1.48
13	B	830	CLA	C1B-CHB	-2.09	1.34	1.39
13	B	814	CLA	C1B-CHB	-2.09	1.34	1.39
13	A	802	CLA	C1B-CHB	-2.09	1.34	1.39
16	L	1006	BCR	C23-C22	-2.08	1.41	1.45
13	K	1401	CLA	C1B-CHB	-2.07	1.34	1.39
13	A	829	CLA	C1B-CHB	-2.06	1.34	1.39
16	B	844	BCR	C29-C28	-2.05	1.47	1.52
16	A	853	BCR	C19-C18	-2.05	1.41	1.45
13	B	836	CLA	C3B-C2B	-2.04	1.37	1.40
13	B	841	CLA	CAA-CBA	-2.04	1.45	1.52
13	A	844	CLA	C1B-CHB	-2.03	1.34	1.39
13	B	815	CLA	C1B-CHB	-2.02	1.34	1.39
13	L	1003	CLA	C3B-C2B	-2.02	1.37	1.40
16	I	101	BCR	C2-C3	-2.02	1.47	1.52
13	B	841	CLA	C1C-NC	-2.01	1.34	1.37
17	A	855	LHG	O8-C6	-2.01	1.40	1.45
13	J	101	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	808	CLA	C1-C2	2.00	1.55	1.49
13	A	842	CLA	C4-C3	2.01	1.55	1.50
13	B	816	CLA	C2-C3	2.01	1.36	1.33
13	B	801	CLA	CHC-C1C	2.01	1.41	1.35
13	B	801	CLA	C4-C3	2.01	1.55	1.50
13	A	841	CLA	C4-C3	2.01	1.55	1.50
13	A	822	CLA	C1-C2	2.01	1.55	1.49
13	A	836	CLA	C1-C2	2.02	1.55	1.49
13	A	820	CLA	C3B-CAB	2.02	1.52	1.47
13	B	824	CLA	C1-C2	2.03	1.55	1.49
13	A	842	CLA	CHC-C1C	2.03	1.41	1.35
13	B	829	CLA	OBD-CAD	2.03	1.25	1.22
13	B	830	CLA	CAA-C2A	2.03	1.58	1.54
13	A	841	CLA	CAA-C2A	2.04	1.58	1.54
16	B	849	BCR	C5-C6	2.04	1.37	1.34
13	A	845	CLA	CAA-C2A	2.04	1.58	1.54
13	B	804	CLA	CAA-C2A	2.04	1.58	1.54
13	B	806	CLA	CHC-C1C	2.05	1.41	1.35
13	B	825	CLA	CAA-C2A	2.05	1.58	1.54
13	A	831	CLA	CAA-C2A	2.05	1.58	1.54
13	B	841	CLA	CHC-C1C	2.06	1.41	1.35
13	B	805	CLA	CMD-C2D	2.07	1.56	1.51
13	A	837	CLA	CAA-C2A	2.08	1.58	1.54
16	A	853	BCR	C2-C1	2.08	1.59	1.54
13	B	805	CLA	CHC-C1C	2.09	1.41	1.35
13	A	807	CLA	C4-C3	2.09	1.55	1.50
13	J	101	CLA	CAA-C2A	2.09	1.58	1.54
13	B	840	CLA	CAA-C2A	2.09	1.58	1.54
13	A	803	CLA	C2-C3	2.09	1.37	1.33
13	B	818	CLA	CHC-C1C	2.09	1.41	1.35
13	A	835	CLA	C2-C3	2.09	1.37	1.33
16	B	844	BCR	C5-C6	2.10	1.37	1.34
13	B	837	CLA	C4-C3	2.10	1.55	1.50
13	B	811	CLA	CAA-C2A	2.10	1.58	1.54
13	B	814	CLA	C5-C3	2.11	1.56	1.51
13	A	827	CLA	CAA-C2A	2.11	1.58	1.54
16	L	1005	BCR	C38-C26	2.11	1.54	1.51
16	J	105	BCR	C26-C25	2.11	1.37	1.34
16	M	1602	BCR	C26-C25	2.11	1.37	1.34
13	B	833	CLA	C4-C3	2.12	1.55	1.50
16	B	849	BCR	C26-C25	2.12	1.37	1.34
16	A	853	BCR	C33-C5	2.13	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	805	CLA	C5-C3	2.13	1.56	1.51
13	L	1003	CLA	CMD-C2D	2.13	1.56	1.51
16	A	851	BCR	C5-C6	2.13	1.37	1.34
13	B	829	CLA	CHC-C1C	2.14	1.42	1.35
13	B	826	CLA	C3B-CAB	2.15	1.52	1.47
13	B	828	CLA	C1-C2	2.15	1.56	1.49
13	A	829	CLA	C4-C3	2.15	1.55	1.50
13	A	813	CLA	C4-C3	2.15	1.55	1.50
13	B	803	CLA	C4-C3	2.16	1.56	1.50
13	A	846	CLA	C5-C3	2.16	1.56	1.51
13	B	833	CLA	CAA-C2A	2.17	1.58	1.54
16	A	852	BCR	C26-C25	2.18	1.37	1.34
13	B	828	CLA	CHC-C1C	2.18	1.42	1.35
16	A	852	BCR	C14-C13	2.18	1.38	1.35
13	A	813	CLA	CAA-C2A	2.21	1.58	1.54
13	L	1002	CLA	CAA-C2A	2.21	1.58	1.54
14	B	842	PQN	C8-C7	2.21	1.43	1.38
14	A	847	PQN	C7-C6	2.21	1.43	1.38
13	B	807	CLA	CAA-C2A	2.21	1.58	1.54
13	A	813	CLA	CHC-C1C	2.22	1.42	1.35
13	A	824	CLA	CAA-C2A	2.22	1.58	1.54
13	A	821	CLA	CAA-C2A	2.22	1.58	1.54
16	A	851	BCR	C29-C30	2.23	1.59	1.54
14	B	842	PQN	C8-C9	2.23	1.43	1.38
16	I	102	BCR	C33-C5	2.23	1.54	1.51
13	A	820	CLA	CAA-C2A	2.24	1.58	1.54
13	A	846	CLA	C4-C3	2.24	1.56	1.50
13	B	828	CLA	CAA-C2A	2.25	1.58	1.54
13	A	820	CLA	C1-C2	2.25	1.56	1.49
13	A	842	CLA	C5-C3	2.26	1.58	1.51
13	L	1003	CLA	CAA-C2A	2.26	1.58	1.54
13	A	803	CLA	CAA-C2A	2.26	1.58	1.54
16	I	101	BCR	C30-C25	2.26	1.57	1.53
14	A	847	PQN	C8-C9	2.27	1.43	1.38
14	A	847	PQN	C9-C10	2.27	1.43	1.39
13	A	821	CLA	C5-C3	2.27	1.56	1.51
13	A	811	CLA	CAA-C2A	2.28	1.58	1.54
13	A	845	CLA	CHC-C1C	2.28	1.42	1.35
13	A	830	CLA	CHC-C1C	2.28	1.42	1.35
16	L	1006	BCR	C5-C6	2.28	1.37	1.34
16	B	847	BCR	C29-C30	2.29	1.59	1.54
14	A	847	PQN	C11-C3	2.29	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	847	BCR	C5-C6	2.29	1.38	1.34
13	A	811	CLA	CHC-C1C	2.30	1.42	1.35
13	A	836	CLA	C5-C3	2.30	1.56	1.51
13	A	831	CLA	C5-C3	2.30	1.56	1.51
16	A	853	BCR	C26-C25	2.31	1.38	1.34
13	B	816	CLA	C4-C3	2.31	1.56	1.50
16	I	101	BCR	C26-C25	2.31	1.38	1.34
13	B	825	CLA	CHC-C1C	2.31	1.42	1.35
13	A	814	CLA	CHC-C1C	2.31	1.42	1.35
13	M	1601	CLA	CAA-C2A	2.32	1.58	1.54
13	A	819	CLA	C5-C3	2.32	1.56	1.51
16	L	1006	BCR	C38-C26	2.32	1.54	1.51
16	L	1005	BCR	C2-C1	2.32	1.59	1.54
14	A	847	PQN	C8-C7	2.33	1.44	1.38
13	B	820	CLA	CAA-C2A	2.33	1.58	1.54
16	B	846	BCR	C14-C13	2.34	1.40	1.34
13	A	803	CLA	CHC-C1C	2.34	1.42	1.35
13	A	812	CLA	CHC-C1C	2.35	1.42	1.35
13	B	818	CLA	C3B-CAB	2.35	1.52	1.47
16	B	844	BCR	C38-C26	2.36	1.54	1.51
16	B	844	BCR	C29-C30	2.36	1.59	1.54
13	B	833	CLA	CHC-C1C	2.36	1.42	1.35
16	I	101	BCR	C2-C1	2.36	1.59	1.54
13	A	817	CLA	CHC-C1C	2.36	1.42	1.35
16	I	101	BCR	C33-C5	2.37	1.54	1.51
13	B	813	CLA	CHC-C1C	2.37	1.42	1.35
13	B	808	CLA	CHC-C1C	2.38	1.42	1.35
13	A	843	CLA	C1-C2	2.39	1.56	1.49
13	A	836	CLA	CHC-C1C	2.39	1.42	1.35
13	A	844	CLA	C4-C3	2.40	1.56	1.50
13	A	804	CLA	CHC-C1C	2.40	1.42	1.35
14	B	842	PQN	C9-C10	2.40	1.43	1.39
16	B	845	BCR	C5-C6	2.40	1.38	1.34
13	A	844	CLA	CAA-C2A	2.40	1.58	1.54
13	A	824	CLA	CHC-C1C	2.40	1.42	1.35
16	A	853	BCR	C29-C30	2.40	1.59	1.54
16	A	851	BCR	C26-C25	2.41	1.38	1.34
13	A	816	CLA	CHC-C1C	2.41	1.42	1.35
13	B	836	CLA	CHC-C1C	2.42	1.42	1.35
13	A	801	CLA	CHC-C1C	2.42	1.42	1.35
13	B	828	CLA	C5-C3	2.43	1.56	1.51
13	B	818	CLA	CAA-C2A	2.43	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	805	CLA	CAA-C2A	2.44	1.59	1.54
16	B	847	BCR	C1-C6	2.45	1.57	1.53
14	A	847	PQN	C11-C12	2.46	1.54	1.50
13	B	811	CLA	CHC-C1C	2.47	1.43	1.35
13	B	819	CLA	CHC-C1C	2.47	1.43	1.35
13	J	102	CLA	CBD-CAD	2.47	1.57	1.51
16	I	102	BCR	C26-C25	2.47	1.38	1.34
13	K	1401	CLA	CHC-C1C	2.47	1.43	1.35
13	A	810	CLA	CHC-C1C	2.48	1.43	1.35
13	B	833	CLA	C5-C3	2.48	1.56	1.51
13	B	816	CLA	CHC-C1C	2.48	1.43	1.35
17	A	855	LHG	O7-C7	2.48	1.41	1.34
14	A	847	PQN	C15-C13	2.49	1.56	1.51
16	A	854	BCR	C14-C13	2.49	1.39	1.35
13	B	814	CLA	CHC-C1C	2.49	1.43	1.35
16	B	848	BCR	C5-C6	2.49	1.38	1.34
16	A	852	BCR	C2-C1	2.49	1.60	1.54
16	L	1005	BCR	C26-C25	2.50	1.38	1.34
13	B	839	CLA	CHC-C1C	2.50	1.43	1.35
13	A	844	CLA	CMD-C2D	2.51	1.57	1.51
16	B	848	BCR	C2-C1	2.51	1.60	1.54
13	B	812	CLA	CHC-C1C	2.52	1.43	1.35
13	A	802	CLA	CHC-C1C	2.52	1.43	1.35
16	J	103	BCR	C26-C25	2.53	1.38	1.34
13	B	832	CLA	CHC-C1C	2.54	1.43	1.35
16	A	852	BCR	C1-C6	2.54	1.57	1.53
13	A	837	CLA	CHC-C1C	2.54	1.43	1.35
13	A	825	CLA	CHC-C1C	2.55	1.43	1.35
13	A	807	CLA	CHC-C1C	2.56	1.43	1.35
13	B	820	CLA	CHC-C1C	2.56	1.43	1.35
13	B	830	CLA	CHC-C1C	2.56	1.43	1.35
13	J	102	CLA	CHC-C1C	2.56	1.43	1.35
13	B	835	CLA	CAA-C2A	2.56	1.59	1.54
16	A	850	BCR	C1-C6	2.57	1.57	1.53
14	B	842	PQN	C11-C3	2.57	1.56	1.51
13	A	818	CLA	CHC-C1C	2.59	1.43	1.35
13	B	817	CLA	CAA-C2A	2.59	1.59	1.54
16	L	1006	BCR	C29-C30	2.59	1.60	1.54
13	B	822	CLA	CHC-C1C	2.60	1.43	1.35
16	M	1602	BCR	C30-C25	2.61	1.57	1.53
13	B	817	CLA	CHC-C1C	2.61	1.43	1.35
13	A	819	CLA	CHC-C1C	2.61	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	849	BCR	C2-C1	2.61	1.60	1.54
13	M	1601	CLA	CHC-C1C	2.62	1.43	1.35
16	B	846	BCR	C30-C25	2.62	1.57	1.53
16	I	102	BCR	C29-C30	2.62	1.60	1.54
17	A	855	LHG	O8-C23	2.62	1.41	1.33
13	B	829	CLA	CAA-C2A	2.64	1.59	1.54
13	A	806	CLA	CHC-C1C	2.64	1.43	1.35
13	B	831	CLA	CHC-C1C	2.64	1.43	1.35
13	A	822	CLA	CAA-C2A	2.64	1.59	1.54
16	L	1006	BCR	C26-C25	2.64	1.38	1.34
13	A	846	CLA	CAA-C2A	2.65	1.59	1.54
13	A	808	CLA	CHC-C1C	2.65	1.43	1.35
13	A	843	CLA	CHC-C1C	2.66	1.43	1.35
16	I	101	BCR	C29-C30	2.66	1.60	1.54
16	J	103	BCR	C2-C1	2.66	1.60	1.54
13	B	827	CLA	CAA-C2A	2.66	1.59	1.54
13	B	804	CLA	CHC-C1C	2.66	1.43	1.35
13	B	816	CLA	CAA-C2A	2.66	1.59	1.54
13	A	840	CLA	CAA-C2A	2.67	1.59	1.54
13	B	826	CLA	CHC-C1C	2.67	1.43	1.35
13	B	816	CLA	C5-C3	2.68	1.57	1.51
18	B	850	LMG	O8-C28	2.69	1.41	1.33
13	B	824	CLA	C5-C3	2.69	1.57	1.51
16	L	1005	BCR	C29-C30	2.69	1.60	1.54
16	A	853	BCR	C30-C25	2.69	1.57	1.53
13	A	845	CLA	CBD-CAD	2.69	1.57	1.51
13	A	805	CLA	CHC-C1C	2.70	1.43	1.35
16	A	849	BCR	C26-C25	2.70	1.38	1.34
13	B	822	CLA	CAA-C2A	2.70	1.59	1.54
16	I	102	BCR	C2-C1	2.70	1.60	1.54
13	B	827	CLA	OBD-CAD	2.70	1.26	1.22
13	F	1301	CLA	CHC-C1C	2.71	1.43	1.35
16	B	845	BCR	C1-C6	2.71	1.57	1.53
16	J	103	BCR	C30-C25	2.72	1.57	1.53
13	A	840	CLA	CHC-C1C	2.72	1.43	1.35
16	A	854	BCR	C29-C30	2.73	1.60	1.54
13	J	101	CLA	CHC-C1C	2.74	1.43	1.35
13	A	839	CLA	CHC-C1C	2.74	1.43	1.35
16	B	845	BCR	C29-C30	2.75	1.60	1.54
16	B	849	BCR	C30-C25	2.75	1.57	1.53
16	B	847	BCR	C2-C1	2.76	1.60	1.54
16	J	105	BCR	C29-C30	2.77	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	1004	CLA	CHC-C1C	2.77	1.44	1.35
16	F	1302	BCR	C29-C30	2.78	1.60	1.54
16	J	105	BCR	C5-C6	2.78	1.38	1.34
16	B	849	BCR	C29-C30	2.79	1.60	1.54
16	B	845	BCR	C2-C1	2.79	1.60	1.54
13	A	832	CLA	CHC-C1C	2.79	1.44	1.35
16	B	844	BCR	C30-C25	2.79	1.57	1.53
13	B	837	CLA	CHC-C1C	2.80	1.44	1.35
14	A	847	PQN	C6-C5	2.80	1.44	1.39
13	A	819	CLA	CAA-C2A	2.81	1.59	1.54
16	B	846	BCR	C29-C30	2.81	1.60	1.54
13	A	828	CLA	C5-C3	2.81	1.57	1.51
17	A	856	LHG	O8-C23	2.81	1.41	1.33
16	B	843	BCR	C29-C30	2.81	1.60	1.54
16	B	845	BCR	C30-C25	2.81	1.57	1.53
13	A	826	CLA	CHC-C1C	2.82	1.44	1.35
16	M	1602	BCR	C2-C1	2.82	1.60	1.54
13	B	815	CLA	CHC-C1C	2.82	1.44	1.35
16	B	844	BCR	C2-C1	2.83	1.60	1.54
13	B	802	CLA	CHC-C1C	2.83	1.44	1.35
13	A	823	CLA	CHC-C1C	2.83	1.44	1.35
13	B	835	CLA	CHC-C1C	2.83	1.44	1.35
13	A	809	CLA	CAA-C2A	2.83	1.59	1.54
13	A	821	CLA	CHC-C1C	2.83	1.44	1.35
16	A	850	BCR	C29-C30	2.84	1.60	1.54
16	A	849	BCR	C29-C30	2.84	1.60	1.54
16	M	1602	BCR	C29-C30	2.84	1.60	1.54
16	B	848	BCR	C29-C30	2.86	1.61	1.54
13	A	822	CLA	CHC-C1C	2.87	1.44	1.35
16	J	103	BCR	C1-C6	2.88	1.57	1.53
13	A	815	CLA	CHC-C1C	2.89	1.44	1.35
16	A	851	BCR	C2-C1	2.89	1.61	1.54
13	B	823	CLA	CHC-C1C	2.90	1.44	1.35
14	B	842	PQN	C6-C5	2.91	1.44	1.39
13	A	828	CLA	CHC-C1C	2.91	1.44	1.35
13	B	834	CLA	CHC-C1C	2.91	1.44	1.35
13	L	1003	CLA	CHC-C1C	2.91	1.44	1.35
13	A	846	CLA	CHC-C1C	2.92	1.44	1.35
13	B	827	CLA	CHC-C1C	2.94	1.44	1.35
13	B	824	CLA	CHC-C1C	2.94	1.44	1.35
13	X	1701	CLA	CHC-C1C	2.94	1.44	1.35
13	A	809	CLA	CHC-C1C	2.94	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	849	BCR	C2-C1	2.95	1.61	1.54
16	J	105	BCR	C2-C1	2.96	1.61	1.54
16	A	852	BCR	C29-C30	2.97	1.61	1.54
13	A	831	CLA	CHC-C1C	2.97	1.44	1.35
16	A	850	BCR	C2-C1	2.97	1.61	1.54
16	J	104	BCR	C30-C25	2.98	1.58	1.53
16	A	854	BCR	C2-C1	2.99	1.61	1.54
16	J	103	BCR	C29-C30	2.99	1.61	1.54
16	B	847	BCR	C30-C25	3.00	1.58	1.53
16	F	1302	BCR	C30-C25	3.00	1.58	1.53
13	A	841	CLA	CHC-C1C	3.01	1.44	1.35
13	B	803	CLA	CHC-C1C	3.04	1.44	1.35
13	B	821	CLA	CHC-C1C	3.07	1.44	1.35
13	A	820	CLA	C2-C3	3.08	1.39	1.33
16	I	102	BCR	C30-C25	3.11	1.58	1.53
16	B	843	BCR	C1-C6	3.12	1.58	1.53
16	B	843	BCR	C2-C1	3.14	1.61	1.54
16	A	854	BCR	C1-C6	3.14	1.58	1.53
14	B	842	PQN	C11-C12	3.16	1.55	1.50
13	L	1002	CLA	CHC-C1C	3.17	1.45	1.35
16	A	853	BCR	C1-C6	3.20	1.58	1.53
16	B	844	BCR	C26-C25	3.21	1.39	1.34
13	B	838	CLA	CHC-C1C	3.22	1.45	1.35
16	M	1602	BCR	C1-C6	3.22	1.58	1.53
16	J	105	BCR	C1-C6	3.23	1.58	1.53
16	A	850	BCR	C30-C25	3.27	1.58	1.53
16	L	1006	BCR	C2-C1	3.28	1.62	1.54
16	A	854	BCR	C30-C25	3.35	1.58	1.53
16	F	1302	BCR	C2-C1	3.36	1.62	1.54
16	A	849	BCR	C1-C6	3.36	1.58	1.53
17	B	851	LHG	O7-C7	3.38	1.44	1.34
16	A	849	BCR	C30-C25	3.39	1.58	1.53
16	J	104	BCR	C2-C1	3.41	1.62	1.54
14	A	847	PQN	C10-C5	3.41	1.46	1.40
16	J	105	BCR	C30-C25	3.44	1.58	1.53
16	A	851	BCR	C1-C6	3.55	1.58	1.53
16	A	851	BCR	C30-C25	3.56	1.58	1.53
16	B	843	BCR	C26-C25	3.57	1.40	1.34
16	J	104	BCR	C29-C30	3.58	1.62	1.54
17	A	856	LHG	O7-C7	3.59	1.45	1.34
17	A	855	LHG	P-O6	3.69	1.75	1.59
13	B	828	CLA	C2-C3	3.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	842	PQN	C10-C5	3.96	1.46	1.40
17	A	856	LHG	P-O3	4.04	1.77	1.59
16	A	852	BCR	C30-C25	4.23	1.59	1.53
16	L	1006	BCR	C30-C25	4.36	1.60	1.53
17	A	856	LHG	P-O6	4.42	1.79	1.59
16	B	843	BCR	C30-C25	4.50	1.60	1.53
16	L	1005	BCR	C30-C25	4.57	1.60	1.53
16	B	844	BCR	C1-C6	4.58	1.60	1.53
17	A	855	LHG	P-O3	4.68	1.80	1.59
16	L	1006	BCR	C1-C6	4.70	1.60	1.53
17	B	851	LHG	P-O3	4.75	1.80	1.59
14	A	847	PQN	C3-C2	4.88	1.46	1.35
14	B	842	PQN	C3-C2	4.90	1.46	1.35
17	B	851	LHG	P-O6	5.26	1.83	1.59
17	A	856	LHG	P-O5	7.35	1.78	1.51
17	A	855	LHG	P-O5	7.91	1.80	1.51
17	B	851	LHG	P-O5	8.29	1.81	1.51
14	B	842	PQN	O1-C1	8.35	1.41	1.23
14	A	847	PQN	O1-C1	8.86	1.42	1.23
14	B	842	PQN	O4-C4	8.87	1.42	1.23
14	A	847	PQN	O4-C4	9.19	1.42	1.23
14	B	842	PQN	C12-C13	10.12	1.52	1.33
14	A	847	PQN	C12-C13	10.16	1.52	1.33

All (1335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	842	PQN	C11-C12-C13	-7.97	113.20	126.70
14	A	847	PQN	C11-C12-C13	-7.86	113.38	126.70
14	A	847	PQN	C15-C13-C12	-7.70	106.45	121.05
13	A	801	CLA	O1D-CGD-CBD	-7.61	113.72	124.62
14	B	842	PQN	C15-C13-C12	-6.52	108.68	121.05
13	A	801	CLA	C3D-CAD-CBD	-6.21	98.82	107.60
13	A	807	CLA	CAA-C2A-C3A	-4.64	99.87	113.22
13	B	808	CLA	O1D-CGD-CBD	-4.53	118.12	124.62
13	A	822	CLA	CMB-C2B-C1B	-4.10	121.58	128.36
13	B	818	CLA	CMB-C2B-C1B	-4.00	121.75	128.36
13	B	813	CLA	O1D-CGD-CBD	-4.00	118.89	124.62
13	A	820	CLA	CMB-C2B-C1B	-3.99	121.76	128.36
16	A	853	BCR	C38-C26-C27	-3.97	105.90	113.43
13	A	805	CLA	O1D-CGD-CBD	-3.93	118.99	124.62
13	A	846	CLA	O1D-CGD-CBD	-3.90	119.03	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	814	CLA	O1D-CGD-CBD	-3.87	119.07	124.62
13	B	833	CLA	O1D-CGD-CBD	-3.87	119.07	124.62
13	A	814	CLA	O1D-CGD-CBD	-3.86	119.09	124.62
16	B	843	BCR	C38-C26-C27	-3.86	106.12	113.43
13	A	809	CLA	O1D-CGD-CBD	-3.85	119.11	124.62
13	A	826	CLA	O1D-CGD-CBD	-3.85	119.11	124.62
13	A	832	CLA	O1D-CGD-CBD	-3.84	119.12	124.62
13	B	830	CLA	O1D-CGD-CBD	-3.83	119.13	124.62
13	B	829	CLA	CMB-C2B-C1B	-3.74	122.17	128.36
13	B	815	CLA	O1D-CGD-CBD	-3.73	119.28	124.62
13	B	821	CLA	O1D-CGD-CBD	-3.70	119.31	124.62
13	A	830	CLA	CMB-C2B-C1B	-3.68	122.27	128.36
13	A	828	CLA	O1D-CGD-CBD	-3.68	119.34	124.62
13	L	1002	CLA	O1D-CGD-CBD	-3.68	119.35	124.62
13	B	829	CLA	O1D-CGD-CBD	-3.62	119.43	124.62
16	B	844	BCR	C38-C26-C27	-3.62	106.57	113.43
13	A	835	CLA	O1D-CGD-CBD	-3.61	119.44	124.62
16	B	848	BCR	C33-C5-C4	-3.59	106.62	113.43
13	B	804	CLA	O1D-CGD-CBD	-3.59	119.48	124.62
13	A	806	CLA	O1D-CGD-CBD	-3.57	119.51	124.62
13	B	802	CLA	OBD-CAD-CBD	-3.57	120.56	125.94
13	A	802	CLA	OBD-CAD-CBD	-3.56	120.56	125.94
13	A	816	CLA	O1D-CGD-CBD	-3.55	119.54	124.62
16	A	851	BCR	C38-C26-C27	-3.55	106.70	113.43
13	B	825	CLA	O1D-CGD-CBD	-3.53	119.56	124.62
16	B	844	BCR	C30-C25-C26	-3.53	117.48	122.66
16	J	103	BCR	C38-C26-C27	-3.51	106.77	113.43
13	B	820	CLA	O1D-CGD-CBD	-3.51	119.60	124.62
16	A	849	BCR	C38-C26-C27	-3.50	106.80	113.43
16	B	845	BCR	C38-C26-C27	-3.47	106.84	113.43
13	B	837	CLA	O1D-CGD-CBD	-3.46	119.66	124.62
13	B	826	CLA	CMB-C2B-C1B	-3.44	122.68	128.36
16	I	102	BCR	C33-C5-C4	-3.43	106.93	113.43
16	A	850	BCR	C38-C26-C27	-3.41	106.97	113.43
16	I	102	BCR	C38-C26-C27	-3.40	106.98	113.43
13	A	807	CLA	CMB-C2B-C1B	-3.35	122.81	128.36
13	A	823	CLA	O1D-CGD-CBD	-3.34	119.84	124.62
13	B	841	CLA	OBD-CAD-CBD	-3.34	120.90	125.94
16	L	1005	BCR	C33-C5-C4	-3.34	107.10	113.43
13	B	824	CLA	O1D-CGD-CBD	-3.33	119.85	124.62
13	B	805	CLA	OBD-CAD-CBD	-3.31	120.94	125.94
13	B	827	CLA	O1D-CGD-CBD	-3.30	119.89	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	847	BCR	C33-C5-C4	-3.30	107.18	113.43
13	A	821	CLA	O1D-CGD-CBD	-3.30	119.90	124.62
13	B	835	CLA	CMB-C2B-C1B	-3.29	122.93	128.36
16	B	846	BCR	C38-C26-C27	-3.28	107.20	113.43
16	B	845	BCR	C33-C5-C4	-3.28	107.22	113.43
16	J	105	BCR	C38-C26-C27	-3.27	107.22	113.43
13	B	809	CLA	CMB-C2B-C1B	-3.27	122.96	128.36
13	A	815	CLA	O1D-CGD-CBD	-3.27	119.94	124.62
13	B	807	CLA	OBD-CAD-CBD	-3.26	121.02	125.94
16	I	101	BCR	C38-C26-C27	-3.25	107.26	113.43
16	J	105	BCR	C33-C5-C4	-3.25	107.27	113.43
13	B	828	CLA	C4-C3-C5	-3.25	110.45	115.41
13	B	826	CLA	O1D-CGD-CBD	-3.22	120.00	124.62
16	B	843	BCR	C33-C5-C4	-3.21	107.34	113.43
13	A	838	CLA	O1D-CGD-CBD	-3.20	120.03	124.62
13	B	813	CLA	CMB-C2B-C1B	-3.20	123.07	128.36
13	A	835	CLA	C3B-CAB-CBB	-3.19	119.79	126.32
16	B	848	BCR	C38-C26-C27	-3.18	107.39	113.43
13	A	827	CLA	CMB-C2B-C1B	-3.18	123.10	128.36
16	B	843	BCR	C30-C25-C26	-3.17	118.00	122.66
16	L	1006	BCR	C33-C5-C4	-3.17	107.42	113.43
16	A	852	BCR	C38-C26-C27	-3.17	107.42	113.43
16	F	1302	BCR	C33-C5-C4	-3.17	107.43	113.43
13	B	802	CLA	O1D-CGD-CBD	-3.16	120.09	124.62
13	B	810	CLA	O1D-CGD-CBD	-3.16	120.09	124.62
16	A	851	BCR	C33-C5-C4	-3.15	107.46	113.43
16	A	849	BCR	C33-C5-C4	-3.14	107.48	113.43
16	F	1302	BCR	C38-C26-C27	-3.14	107.48	113.43
13	A	832	CLA	C2C-C1C-NC	-3.14	107.91	110.24
16	L	1005	BCR	C38-C26-C27	-3.13	107.50	113.43
13	A	844	CLA	O2A-CGA-O1A	-3.12	115.44	123.49
13	J	101	CLA	O1D-CGD-CBD	-3.10	120.17	124.62
13	B	817	CLA	OBD-CAD-CBD	-3.10	121.26	125.94
16	B	844	BCR	C33-C5-C4	-3.10	107.56	113.43
13	B	838	CLA	O1D-CGD-CBD	-3.09	120.20	124.62
13	B	825	CLA	CMB-C2B-C1B	-3.08	123.27	128.36
16	A	849	BCR	C30-C25-C26	-3.07	118.15	122.66
16	A	854	BCR	C33-C5-C4	-3.07	107.61	113.43
13	A	816	CLA	CMB-C2B-C1B	-3.06	123.29	128.36
13	A	806	CLA	CAA-C2A-C3A	-3.04	104.47	113.22
16	M	1602	BCR	C38-C26-C27	-3.03	107.69	113.43
13	A	810	CLA	CMB-C2B-C1B	-3.03	123.36	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	847	BCR	C38-C26-C27	-3.02	107.70	113.43
13	A	842	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
16	A	850	BCR	C33-C5-C4	-2.99	107.75	113.43
13	B	838	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
13	B	832	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
13	J	102	CLA	CAA-C2A-C3A	-2.99	109.04	116.20
13	B	822	CLA	CMB-C2B-C1B	-2.99	123.42	128.36
13	A	803	CLA	O2A-CGA-O1A	-2.98	115.79	123.49
13	L	1002	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
13	B	805	CLA	CMB-C2B-C1B	-2.98	123.44	128.36
13	B	818	CLA	O1D-CGD-CBD	-2.97	120.36	124.62
13	B	827	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
17	A	856	LHG	C6-C5-C4	-2.97	105.13	112.07
16	J	103	BCR	C30-C25-C26	-2.97	118.30	122.66
13	A	806	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
16	B	849	BCR	C38-C26-C27	-2.96	107.81	113.43
13	A	832	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
16	J	105	BCR	C1-C6-C5	-2.95	118.32	122.66
13	A	831	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
16	A	853	BCR	C30-C25-C26	-2.95	118.32	122.66
16	A	854	BCR	C38-C26-C27	-2.95	107.83	113.43
13	A	822	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
13	A	834	CLA	O1D-CGD-CBD	-2.95	120.40	124.62
13	B	805	CLA	O1D-CGD-CBD	-2.94	120.41	124.62
13	A	840	CLA	O1D-CGD-CBD	-2.93	120.42	124.62
13	A	806	CLA	CMB-C2B-C1B	-2.93	123.52	128.36
13	A	815	CLA	OBD-CAD-CBD	-2.93	121.52	125.94
13	A	834	CLA	CMB-C2B-C1B	-2.92	123.53	128.36
13	A	803	CLA	CMB-C2B-C1B	-2.91	123.54	128.36
13	B	803	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
13	A	819	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
13	A	836	CLA	O1D-CGD-CBD	-2.91	120.45	124.62
13	A	829	CLA	CMB-C2B-C1B	-2.90	123.56	128.36
13	A	838	CLA	O2A-CGA-O1A	-2.90	116.00	123.49
13	B	808	CLA	CAA-C2A-C3A	-2.90	104.87	113.22
16	J	104	BCR	C33-C5-C4	-2.90	107.93	113.43
16	B	848	BCR	C8-C9-C10	-2.89	114.33	118.98
16	B	844	BCR	C1-C6-C5	-2.89	118.42	122.66
13	B	840	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
13	L	1004	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
13	B	823	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
13	B	824	CLA	OBD-CAD-CBD	-2.88	121.59	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	843	BCR	C1-C6-C5	-2.88	118.43	122.66
16	B	849	BCR	C33-C5-C4	-2.87	107.98	113.43
13	A	817	CLA	CMB-C2B-C1B	-2.87	123.62	128.36
13	A	805	CLA	CMB-C2B-C1B	-2.87	123.62	128.36
16	A	852	BCR	C33-C5-C4	-2.86	108.00	113.43
13	B	816	CLA	OBD-CAD-CBD	-2.86	121.62	125.94
13	B	840	CLA	C3B-CAB-CBB	-2.86	120.47	126.32
13	A	829	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
13	A	846	CLA	C2C-C1C-NC	-2.84	108.13	110.24
13	A	830	CLA	O1D-CGD-CBD	-2.84	120.55	124.62
16	J	103	BCR	C33-C5-C4	-2.84	108.05	113.43
13	B	834	CLA	OBD-CAD-CBD	-2.84	121.66	125.94
13	K	1401	CLA	O1D-CGD-CBD	-2.83	120.57	124.62
13	A	824	CLA	O1D-CGD-CBD	-2.82	120.58	124.62
13	B	814	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
13	A	839	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
13	B	801	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
13	A	838	CLA	CMB-C2B-C1B	-2.81	123.71	128.36
13	L	1003	CLA	OBD-CAD-CBD	-2.81	121.69	125.94
13	B	835	CLA	OBD-CAD-CBD	-2.81	121.69	125.94
13	A	833	CLA	O1D-CGD-CBD	-2.81	120.59	124.62
13	A	821	CLA	OBD-CAD-CBD	-2.81	121.70	125.94
16	A	852	BCR	C30-C25-C26	-2.81	118.53	122.66
16	M	1602	BCR	C1-C6-C5	-2.81	118.53	122.66
16	I	101	BCR	C33-C5-C4	-2.81	108.11	113.43
13	A	811	CLA	CMB-C2B-C1B	-2.81	123.72	128.36
13	A	840	CLA	O2A-CGA-O1A	-2.81	116.25	123.49
13	A	835	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
13	A	843	CLA	CMB-C2B-C1B	-2.80	123.74	128.36
13	A	811	CLA	OBD-CAD-CBD	-2.79	121.72	125.94
13	M	1601	CLA	O1D-CGD-CBD	-2.79	120.62	124.62
13	B	818	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
13	A	837	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
16	B	845	BCR	C1-C6-C5	-2.78	118.58	122.66
13	A	809	CLA	C2C-C1C-NC	-2.77	108.18	110.24
13	B	809	CLA	OBD-CAD-CBD	-2.77	121.75	125.94
13	B	827	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
13	B	839	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
13	A	804	CLA	O1D-CGD-CBD	-2.76	120.66	124.62
16	M	1602	BCR	C33-C5-C4	-2.76	108.19	113.43
16	B	848	BCR	C12-C13-C14	-2.76	114.53	118.98
13	B	801	CLA	C7-C6-C5	-2.76	104.91	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	101	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
13	B	832	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
16	L	1006	BCR	C38-C26-C27	-2.76	108.20	113.43
13	A	822	CLA	CAA-C2A-C3A	-2.75	105.31	113.22
13	B	821	CLA	C2C-C1C-NC	-2.75	108.20	110.24
13	A	814	CLA	CMB-C2B-C1B	-2.75	123.82	128.36
13	A	837	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
13	B	811	CLA	CAA-C2A-C3A	-2.74	105.35	113.22
13	B	832	CLA	CMB-C2B-C1B	-2.73	123.85	128.36
16	A	849	BCR	C1-C6-C5	-2.73	118.65	122.66
13	A	809	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
13	A	829	CLA	O1D-CGD-CBD	-2.72	120.72	124.62
16	J	104	BCR	C38-C26-C27	-2.71	108.28	113.43
13	B	815	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
13	A	814	CLA	OBD-CAD-CBD	-2.71	121.85	125.94
13	A	823	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
13	A	838	CLA	C4-C3-C5	-2.71	112.62	115.68
13	B	808	CLA	O2A-CGA-O1A	-2.71	116.51	123.49
13	B	841	CLA	C3B-CAB-CBB	-2.70	120.79	126.32
13	B	821	CLA	CMB-C2B-C1B	-2.70	123.89	128.36
13	A	841	CLA	O1D-CGD-CBD	-2.70	120.75	124.62
13	B	806	CLA	CMB-C2B-C1B	-2.70	123.90	128.36
13	A	820	CLA	C4-C3-C5	-2.70	111.29	115.41
13	A	836	CLA	CMB-C2B-C1B	-2.70	123.90	128.36
13	B	819	CLA	O1D-CGD-CBD	-2.69	120.76	124.62
13	B	819	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
13	A	834	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
13	A	804	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
16	A	850	BCR	C30-C25-C26	-2.69	118.71	122.66
13	A	818	CLA	CMB-C2B-C1B	-2.69	123.92	128.36
16	B	845	BCR	C30-C25-C26	-2.69	118.71	122.66
13	A	844	CLA	CAA-C2A-C3A	-2.69	105.49	113.22
13	B	817	CLA	CMB-C2B-C1B	-2.68	123.93	128.36
13	A	825	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
13	B	841	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
13	A	841	CLA	C2C-C1C-NC	-2.68	108.25	110.24
13	A	823	CLA	OBD-CAD-CBD	-2.68	121.90	125.94
13	A	846	CLA	CMB-C2B-C1B	-2.67	123.94	128.36
13	A	817	CLA	OBD-CAD-CBD	-2.67	121.90	125.94
13	J	101	CLA	CMB-C2B-C1B	-2.67	123.94	128.36
13	A	804	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
16	L	1005	BCR	C30-C25-C26	-2.67	118.74	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	823	CLA	C2C-C1C-NC	-2.67	108.26	110.24
13	A	831	CLA	CMB-C2B-C1B	-2.67	123.95	128.36
13	A	831	CLA	OBD-CAD-CBD	-2.66	121.92	125.94
16	J	105	BCR	C30-C25-C26	-2.66	118.75	122.66
13	A	810	CLA	O1D-CGD-CBD	-2.66	120.81	124.62
13	B	812	CLA	CMB-C2B-C1B	-2.66	123.97	128.36
13	B	804	CLA	CMB-C2B-C1B	-2.65	123.97	128.36
16	I	102	BCR	C30-C25-C26	-2.65	118.77	122.66
13	A	820	CLA	O1D-CGD-CBD	-2.64	120.83	124.62
16	A	851	BCR	C1-C6-C5	-2.64	118.78	122.66
13	X	1701	CLA	CMB-C2B-C1B	-2.63	124.01	128.36
13	B	823	CLA	CMB-C2B-C1B	-2.62	124.02	128.36
13	A	824	CLA	CMB-C2B-C1B	-2.62	124.02	128.36
13	A	832	CLA	CAA-C2A-C3A	-2.62	105.67	113.22
13	B	839	CLA	C3B-CAB-CBB	-2.62	120.95	126.32
13	B	816	CLA	O1D-CGD-CBD	-2.62	120.87	124.62
13	A	826	CLA	OBD-CAD-CBD	-2.62	121.99	125.94
16	L	1006	BCR	C30-C25-C26	-2.62	118.81	122.66
13	X	1701	CLA	O1D-CGD-CBD	-2.62	120.87	124.62
13	B	820	CLA	CMB-C2B-C1B	-2.62	124.04	128.36
13	B	816	CLA	CMB-C2B-C1B	-2.61	124.04	128.36
13	L	1003	CLA	CAA-C2A-C3A	-2.61	105.72	113.22
13	B	807	CLA	O1D-CGD-CBD	-2.61	120.89	124.62
13	M	1601	CLA	OBD-CAD-CBD	-2.61	122.01	125.94
13	A	819	CLA	O1D-CGD-CBD	-2.60	120.89	124.62
13	B	839	CLA	CMB-C2B-C1B	-2.60	124.06	128.36
13	L	1004	CLA	CMB-C2B-C1B	-2.60	124.06	128.36
13	A	831	CLA	CAA-C2A-C3A	-2.60	105.75	113.22
13	A	835	CLA	CAA-C2A-C3A	-2.60	105.75	113.22
13	A	817	CLA	O1D-CGD-CBD	-2.60	120.90	124.62
13	B	808	CLA	OBD-CAD-CBD	-2.59	122.02	125.94
13	X	1701	CLA	OBD-CAD-CBD	-2.59	122.02	125.94
13	A	844	CLA	OBD-CAD-CBD	-2.59	122.02	125.94
16	B	848	BCR	C30-C25-C26	-2.59	118.85	122.66
13	A	819	CLA	CMB-C2B-C1B	-2.59	124.07	128.36
13	A	840	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	B	811	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
13	B	821	CLA	OBD-CAD-CBD	-2.59	122.03	125.94
16	F	1302	BCR	C1-C6-C5	-2.59	118.86	122.66
13	A	807	CLA	O2A-CGA-O1A	-2.58	116.82	123.49
13	B	828	CLA	CMB-C2B-C1B	-2.58	124.10	128.36
13	B	812	CLA	O1D-CGD-CBD	-2.58	120.93	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	847	BCR	C30-C25-C26	-2.57	118.88	122.66
13	B	819	CLA	CAA-C2A-C3A	-2.57	105.82	113.22
13	B	802	CLA	CMB-C2B-C1B	-2.57	124.11	128.36
13	B	841	CLA	CMB-C2B-C1B	-2.57	124.12	128.36
13	A	843	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
13	B	814	CLA	CMB-C2B-C1B	-2.56	124.12	128.36
13	A	815	CLA	CMB-C2B-C1B	-2.56	124.13	128.36
13	A	827	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
13	A	802	CLA	C2C-C1C-NC	-2.56	108.34	110.24
13	B	828	CLA	O1D-CGD-CBD	-2.55	120.96	124.62
13	A	821	CLA	C2C-C1C-NC	-2.55	108.34	110.24
13	K	1401	CLA	CMB-C2B-C1B	-2.54	124.15	128.36
13	B	819	CLA	OBD-CAD-CBD	-2.54	122.10	125.94
13	A	811	CLA	O1D-CGD-CBD	-2.54	120.98	124.62
13	F	1301	CLA	OBD-CAD-CBD	-2.54	122.11	125.94
13	A	825	CLA	OBD-CAD-CBD	-2.54	122.11	125.94
13	A	802	CLA	CMB-C2B-C1B	-2.54	124.17	128.36
13	M	1601	CLA	CMB-C2B-C1B	-2.53	124.18	128.36
16	F	1302	BCR	C30-C25-C26	-2.53	118.94	122.66
13	A	841	CLA	CMB-C2B-C1B	-2.53	124.18	128.36
13	A	830	CLA	OBD-CAD-CBD	-2.53	122.12	125.94
13	B	837	CLA	OBD-CAD-CBD	-2.53	122.12	125.94
13	B	808	CLA	CMB-C2B-C1B	-2.53	124.19	128.36
16	A	851	BCR	C30-C25-C26	-2.52	118.95	122.66
16	B	849	BCR	C8-C9-C10	-2.52	114.92	118.98
13	B	836	CLA	OBD-CAD-CBD	-2.52	122.13	125.94
13	B	823	CLA	O1D-CGD-CBD	-2.52	121.01	124.62
16	J	103	BCR	C1-C6-C5	-2.52	118.96	122.66
13	A	824	CLA	OBD-CAD-CBD	-2.52	122.14	125.94
13	A	825	CLA	CMB-C2B-C1B	-2.51	124.21	128.36
16	A	854	BCR	C30-C25-C26	-2.51	118.97	122.66
13	B	831	CLA	O1D-CGD-CBD	-2.51	121.02	124.62
13	A	808	CLA	O1D-CGD-CBD	-2.51	121.02	124.62
16	M	1602	BCR	C30-C25-C26	-2.51	118.97	122.66
13	B	831	CLA	C2C-C1C-NC	-2.51	108.37	110.24
13	B	833	CLA	CMB-C2B-C1B	-2.51	124.21	128.36
13	B	810	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
13	A	844	CLA	CMB-C2B-C1B	-2.51	124.22	128.36
16	J	104	BCR	C30-C25-C26	-2.50	118.99	122.66
13	A	833	CLA	CMB-C2B-C1B	-2.50	124.23	128.36
16	L	1006	BCR	C1-C6-C5	-2.49	119.00	122.66
13	B	831	CLA	OBD-CAD-CBD	-2.49	122.17	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	822	CLA	C2C-C1C-NC	-2.49	108.39	110.24
13	A	818	CLA	O1D-CGD-CBD	-2.49	121.05	124.62
13	B	820	CLA	OBD-CAD-CBD	-2.49	122.19	125.94
13	A	831	CLA	C2C-C1C-NC	-2.49	108.39	110.24
13	B	824	CLA	CMB-C2B-C1B	-2.49	124.25	128.36
13	B	831	CLA	CMB-C2B-C1B	-2.48	124.25	128.36
16	A	853	BCR	C33-C5-C4	-2.48	108.72	113.43
13	F	1301	CLA	CMB-C2B-C1B	-2.48	124.26	128.36
13	A	820	CLA	OBD-CAD-CBD	-2.48	122.19	125.94
13	A	838	CLA	OBD-CAD-CBD	-2.48	122.20	125.94
16	J	104	BCR	C1-C6-C5	-2.48	119.03	122.66
13	X	1701	CLA	C2C-C1C-NC	-2.47	108.40	110.24
13	A	836	CLA	O2A-CGA-O1A	-2.46	117.14	123.49
13	A	829	CLA	CAA-C2A-C3A	-2.46	106.15	113.22
13	A	819	CLA	C2C-C1C-NC	-2.46	108.42	110.24
13	B	838	CLA	C2C-C1C-NC	-2.45	108.42	110.24
13	B	811	CLA	C2C-C1C-NC	-2.45	108.42	110.24
13	J	102	CLA	CMB-C2B-C1B	-2.45	124.31	128.36
13	A	825	CLA	C3B-CAB-CBB	-2.45	121.31	126.32
13	A	801	CLA	CMB-C2B-C1B	-2.44	124.33	128.36
16	A	850	BCR	C1-C6-C5	-2.44	119.08	122.66
13	A	813	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
13	A	828	CLA	CMB-C2B-C1B	-2.43	124.35	128.36
13	A	837	CLA	OBD-CAD-CBD	-2.42	122.28	125.94
13	B	829	CLA	O2A-CGA-O1A	-2.42	117.24	123.49
13	A	819	CLA	C3B-CAB-CBB	-2.42	121.37	126.32
16	I	101	BCR	C1-C6-C5	-2.42	119.11	122.66
13	B	830	CLA	C3B-CAB-CBB	-2.41	121.38	126.32
16	B	846	BCR	C30-C25-C26	-2.41	119.13	122.66
13	B	824	CLA	C2C-C1C-NC	-2.41	108.45	110.24
13	A	839	CLA	CMB-C2B-C1B	-2.40	124.39	128.36
13	B	809	CLA	O1D-CGD-CBD	-2.40	121.18	124.62
13	B	825	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
13	A	812	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
13	A	805	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
13	A	845	CLA	CMB-C2B-C1B	-2.40	124.40	128.36
13	A	828	CLA	C2C-C1C-NC	-2.39	108.46	110.24
13	B	802	CLA	O2A-CGA-O1A	-2.39	117.31	123.49
13	A	813	CLA	CMB-C2B-C1B	-2.39	124.40	128.36
13	A	808	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
13	A	812	CLA	CMB-C2B-C1B	-2.39	124.41	128.36
13	B	801	CLA	CAA-C2A-C3A	-2.39	106.34	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	854	BCR	C1-C6-C5	-2.39	119.16	122.66
13	B	803	CLA	CMB-C2B-C1B	-2.38	124.42	128.36
13	A	820	CLA	O2A-CGA-O1A	-2.38	117.35	123.49
16	I	101	BCR	C30-C25-C26	-2.38	119.17	122.66
13	A	836	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
13	A	809	CLA	O2A-CGA-O1A	-2.37	117.37	123.49
13	B	815	CLA	C2C-C1C-NC	-2.37	108.48	110.24
13	A	808	CLA	CMB-C2B-C1B	-2.37	124.44	128.36
13	A	822	CLA	O1D-CGD-CBD	-2.37	121.23	124.62
13	A	829	CLA	O2A-CGA-O1A	-2.37	117.38	123.49
13	B	816	CLA	O2A-CGA-O1A	-2.36	117.39	123.49
13	B	840	CLA	CMB-C2B-C1B	-2.36	124.45	128.36
13	L	1003	CLA	O1D-CGD-CBD	-2.36	121.24	124.62
13	A	846	CLA	O2A-CGA-O1A	-2.36	117.40	123.49
13	A	833	CLA	CAA-C2A-C3A	-2.36	106.44	113.22
13	A	810	CLA	OBD-CAD-CBD	-2.36	122.38	125.94
13	B	836	CLA	CMB-C2B-C1B	-2.35	124.47	128.36
13	A	816	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
13	A	821	CLA	CMB-C2B-C1B	-2.35	124.47	128.36
13	B	822	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
13	A	818	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
13	B	811	CLA	CMB-C2B-C1B	-2.35	124.48	128.36
16	A	854	BCR	C23-C22-C21	-2.34	115.21	118.98
13	B	817	CLA	O1D-CGD-CBD	-2.34	121.26	124.62
13	A	842	CLA	CMB-C2B-C1B	-2.34	124.49	128.36
16	B	847	BCR	C1-C6-C5	-2.33	119.23	122.66
13	A	833	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
13	A	825	CLA	CAA-C2A-C3A	-2.33	106.51	113.22
13	A	842	CLA	C3B-CAB-CBB	-2.33	121.55	126.32
13	B	833	CLA	C2C-C1C-NC	-2.33	108.51	110.24
13	A	821	CLA	O2A-CGA-O1A	-2.33	117.48	123.49
13	A	807	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
13	L	1002	CLA	CMB-C2B-C1B	-2.32	124.52	128.36
13	A	826	CLA	CMB-C2B-C1B	-2.32	124.53	128.36
13	L	1003	CLA	CMB-C2B-C1B	-2.32	124.53	128.36
13	A	803	CLA	CAA-C2A-C3A	-2.32	106.55	113.22
13	B	836	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
13	A	841	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
13	A	840	CLA	CMB-C2B-C1B	-2.31	124.54	128.36
13	A	837	CLA	C2C-C1C-NC	-2.31	108.52	110.24
13	L	1003	CLA	C2C-C1C-NC	-2.31	108.53	110.24
13	B	818	CLA	O2A-CGA-O1A	-2.30	117.54	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	842	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
13	B	826	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
13	B	837	CLA	CMB-C2B-C1B	-2.30	124.56	128.36
13	A	801	CLA	CAA-C2A-C3A	-2.29	106.63	113.22
13	B	827	CLA	C2C-C1C-NC	-2.29	108.54	110.24
16	A	853	BCR	C8-C9-C10	-2.29	115.30	118.98
13	B	825	CLA	CAA-C2A-C3A	-2.29	106.65	113.22
16	A	852	BCR	C1-C6-C5	-2.28	119.31	122.66
13	J	101	CLA	C2C-C1C-NC	-2.28	108.55	110.24
13	B	814	CLA	CAA-C2A-C3A	-2.28	106.67	113.22
13	A	832	CLA	CMB-C2B-C1B	-2.27	124.60	128.36
13	A	805	CLA	C2C-C1C-NC	-2.27	108.55	110.24
13	B	830	CLA	C2C-C1C-NC	-2.27	108.55	110.24
13	B	817	CLA	CAA-C2A-C3A	-2.27	106.70	113.22
16	I	102	BCR	C1-C6-C5	-2.27	119.33	122.66
13	B	813	CLA	OBD-CAD-CBD	-2.26	122.52	125.94
13	B	823	CLA	C2C-C1C-NC	-2.26	108.56	110.24
13	A	813	CLA	O2A-CGA-O1A	-2.26	117.65	123.49
13	B	812	CLA	OBD-CAD-CBD	-2.26	122.53	125.94
13	B	838	CLA	CMB-C2B-C1B	-2.26	124.62	128.36
13	B	830	CLA	CMB-C2B-C1B	-2.25	124.64	128.36
13	B	834	CLA	CMB-C2B-C1B	-2.25	124.64	128.36
13	A	827	CLA	O1D-CGD-CBD	-2.25	121.40	124.62
13	L	1002	CLA	C2C-C1C-NC	-2.25	108.57	110.24
13	A	832	CLA	O2A-CGA-O1A	-2.25	117.70	123.49
13	A	807	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
13	B	838	CLA	C4-C3-C5	-2.24	111.99	115.41
13	A	846	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
13	B	803	CLA	C2C-C1C-NC	-2.23	108.58	110.24
13	B	828	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
13	A	822	CLA	C12-C11-C10	-2.23	101.94	112.99
13	B	833	CLA	OBD-CAD-CBD	-2.22	122.58	125.94
13	B	834	CLA	C2C-C1C-NC	-2.22	108.59	110.24
16	L	1005	BCR	C1-C6-C5	-2.22	119.40	122.66
13	A	833	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
13	A	831	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
13	B	829	CLA	OBD-CAD-CBD	-2.22	122.59	125.94
13	A	828	CLA	OBD-CAD-CBD	-2.22	122.59	125.94
13	L	1004	CLA	O1D-CGD-CBD	-2.22	121.45	124.62
13	B	822	CLA	O1D-CGD-CBD	-2.21	121.45	124.62
13	A	809	CLA	CMB-C2B-C1B	-2.21	124.70	128.36
13	F	1301	CLA	O1D-CGD-CBD	-2.21	121.45	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	835	CLA	O1D-CGD-CBD	-2.21	121.45	124.62
13	A	812	CLA	O1D-CGD-CBD	-2.21	121.46	124.62
13	B	830	CLA	OBD-CAD-CBD	-2.20	122.62	125.94
13	B	819	CLA	C3B-CAB-CBB	-2.20	121.82	126.32
13	J	102	CLA	CMA-C3A-C2A	-2.20	110.94	116.20
16	B	849	BCR	C30-C25-C26	-2.19	119.44	122.66
13	A	813	CLA	O1D-CGD-CBD	-2.19	121.48	124.62
13	A	843	CLA	C2C-C1C-NC	-2.19	108.61	110.24
13	K	1401	CLA	C3B-CAB-CBB	-2.19	121.84	126.32
16	A	853	BCR	C23-C22-C21	-2.18	115.47	118.98
13	B	806	CLA	OBD-CAD-CBD	-2.18	122.65	125.94
13	A	824	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
16	J	103	BCR	C32-C1-C2	-2.17	101.01	108.79
13	A	825	CLA	O2A-CGA-O1A	-2.16	117.91	123.49
13	B	834	CLA	CAA-C2A-C3A	-2.16	106.99	113.22
16	A	853	BCR	C1-C6-C5	-2.16	119.48	122.66
13	B	837	CLA	O2A-CGA-O1A	-2.16	117.91	123.49
13	B	809	CLA	C12-C11-C10	-2.16	102.27	112.99
13	A	828	CLA	O2A-CGA-O1A	-2.16	117.92	123.49
16	I	102	BCR	C19-C18-C17	-2.15	115.51	118.98
13	B	839	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
16	I	101	BCR	C19-C18-C17	-2.15	115.52	118.98
13	A	804	CLA	C2C-C1C-NC	-2.15	108.64	110.24
13	B	822	CLA	C2C-C1C-NC	-2.15	108.65	110.24
16	B	849	BCR	C23-C22-C21	-2.14	115.53	118.98
13	A	844	CLA	CMA-C3A-C2A	-2.14	104.88	114.35
13	L	1004	CLA	C2C-C1C-NC	-2.14	108.65	110.24
13	B	820	CLA	O2A-CGA-O1A	-2.13	117.99	123.49
13	B	840	CLA	O1D-CGD-CBD	-2.13	121.57	124.62
13	A	834	CLA	C3B-CAB-CBB	-2.13	121.96	126.32
13	L	1003	CLA	O2A-CGA-O1A	-2.13	118.00	123.49
13	B	804	CLA	CAA-C2A-C3A	-2.12	107.11	113.22
13	A	823	CLA	O2A-CGA-O1A	-2.12	118.02	123.49
13	B	832	CLA	C12-C11-C10	-2.12	102.47	112.99
13	A	810	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
13	B	839	CLA	O2A-CGA-O1A	-2.11	118.03	123.49
13	B	808	CLA	C7-C6-C5	-2.11	106.82	113.06
13	A	810	CLA	C2C-C1C-NC	-2.11	108.67	110.24
13	A	805	CLA	O2A-CGA-O1A	-2.11	118.05	123.49
16	A	852	BCR	C40-C30-C29	-2.11	101.23	108.79
13	A	805	CLA	C12-C11-C10	-2.11	106.17	113.66
13	B	809	CLA	CAA-C2A-C3A	-2.11	107.16	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	840	CLA	C3B-CAB-CBB	-2.11	122.01	126.32
13	B	834	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
13	B	808	CLA	C3B-CAB-CBB	-2.10	122.01	126.32
16	B	849	BCR	C1-C6-C5	-2.10	119.57	122.66
16	B	848	BCR	C1-C6-C5	-2.10	119.58	122.66
13	L	1002	CLA	C4-C3-C5	-2.10	112.20	115.41
13	L	1002	CLA	O2A-CGA-O1A	-2.10	118.08	123.49
13	B	838	CLA	CAA-C2A-C3A	-2.10	107.19	113.22
13	A	843	CLA	O1D-CGD-CBD	-2.09	121.62	124.62
13	B	810	CLA	C3B-CAB-CBB	-2.09	122.05	126.32
13	A	802	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
13	A	834	CLA	O2A-CGA-O1A	-2.08	118.11	123.49
13	K	1401	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
13	A	812	CLA	O2A-CGA-O1A	-2.08	118.12	123.49
13	A	816	CLA	CAA-C2A-C3A	-2.08	107.24	113.22
13	B	807	CLA	CMB-C2B-C1B	-2.08	124.92	128.36
13	B	817	CLA	O2A-CGA-O1A	-2.08	118.13	123.49
13	A	841	CLA	CAA-C2A-C3A	-2.08	107.25	113.22
13	A	842	CLA	O2A-CGA-O1A	-2.07	118.15	123.49
13	B	804	CLA	C2C-C1C-NC	-2.06	108.71	110.24
13	B	838	CLA	C3B-CAB-CBB	-2.06	122.10	126.32
13	A	803	CLA	OBD-CAD-CBD	-2.06	122.83	125.94
16	A	854	BCR	C32-C1-C2	-2.06	101.41	108.79
13	B	832	CLA	C2C-C1C-NC	-2.06	108.71	110.24
13	A	835	CLA	CMB-C2B-C1B	-2.06	124.96	128.36
13	B	810	CLA	CMB-C2B-C1B	-2.05	124.97	128.36
13	A	819	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
13	A	826	CLA	C2C-C1C-NC	-2.05	108.72	110.24
13	A	802	CLA	C6-C5-C3	-2.05	107.98	112.48
13	F	1301	CLA	C3B-CAB-CBB	-2.05	122.12	126.32
13	B	815	CLA	OBD-CAD-CBD	-2.05	122.85	125.94
13	M	1601	CLA	C2C-C1C-NC	-2.05	108.72	110.24
13	B	803	CLA	C12-C11-C10	-2.05	102.84	112.99
13	B	816	CLA	C2C-C1C-NC	-2.04	108.72	110.24
16	J	104	BCR	C40-C30-C29	-2.04	101.48	108.79
16	J	104	BCR	C19-C18-C17	-2.04	115.70	118.98
13	B	817	CLA	C2C-C1C-NC	-2.04	108.73	110.24
13	J	102	CLA	OBD-CAD-CBD	-2.04	121.68	125.98
13	B	812	CLA	C2C-C1C-NC	-2.04	108.73	110.24
16	B	847	BCR	C19-C18-C17	-2.03	115.71	118.98
13	X	1701	CLA	C3B-CAB-CBB	-2.03	122.16	126.32
13	B	804	CLA	O2A-CGA-O1A	-2.03	118.25	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	847	BCR	C40-C30-C29	-2.03	101.52	108.79
13	B	826	CLA	C2C-C1C-NC	-2.03	108.73	110.24
13	B	820	CLA	C2C-C1C-NC	-2.02	108.74	110.24
13	J	102	CLA	C2C-C1C-NC	-2.02	108.74	110.24
13	B	810	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
13	A	841	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
13	B	827	CLA	O2A-CGA-O1A	-2.02	118.29	123.49
13	A	803	CLA	O1D-CGD-CBD	-2.01	121.73	124.62
13	B	806	CLA	O1D-CGD-CBD	-2.01	121.74	124.62
13	A	815	CLA	C2C-C1C-NC	-2.01	108.75	110.24
13	A	827	CLA	CAA-C2A-C3A	-2.01	107.45	113.22
13	A	808	CLA	C4-C3-C5	-2.00	113.42	115.68
13	B	801	CLA	CMB-C2B-C1B	-2.00	125.05	128.36
16	B	847	BCR	C34-C9-C8	2.00	121.43	118.10
16	A	851	BCR	C32-C1-C6	2.00	113.44	110.30
13	A	827	CLA	CED-O2D-CGD	2.00	120.69	115.99
13	A	814	CLA	C2A-C1A-CHA	2.00	127.58	123.89
13	B	818	CLA	CBA-CAA-C2A	2.01	119.39	113.73
16	A	851	BCR	C8-C7-C6	2.01	133.35	127.32
13	M	1601	CLA	C1C-NC-C4C	2.01	108.71	106.27
13	B	827	CLA	CED-O2D-CGD	2.01	120.70	115.99
13	A	823	CLA	C2A-C1A-CHA	2.01	127.59	123.89
13	A	838	CLA	C2A-C1A-CHA	2.01	127.59	123.89
16	L	1005	BCR	C23-C24-C25	2.01	133.37	127.32
16	B	843	BCR	C40-C30-C25	2.02	113.46	110.30
16	B	843	BCR	C37-C22-C23	2.02	121.45	118.10
13	J	102	CLA	C1C-NC-C4C	2.02	108.72	106.27
16	A	854	BCR	C3-C4-C5	2.02	117.08	113.87
16	A	854	BCR	C37-C22-C23	2.02	121.46	118.10
13	A	801	CLA	CGD-CBD-CAD	2.03	117.49	110.62
16	J	104	BCR	C35-C13-C12	2.03	121.47	118.10
13	A	805	CLA	CMB-C2B-C3B	2.03	129.06	125.09
13	M	1601	CLA	C2A-C1A-CHA	2.03	127.62	123.89
13	A	825	CLA	CED-O2D-CGD	2.03	120.75	115.99
13	B	833	CLA	C1C-NC-C4C	2.03	108.73	106.27
16	L	1005	BCR	C37-C22-C23	2.03	121.48	118.10
13	B	816	CLA	CBA-CAA-C2A	2.03	119.47	113.73
13	A	811	CLA	CBA-CAA-C2A	2.04	119.48	113.55
13	A	834	CLA	CED-O2D-CGD	2.04	120.77	115.99
16	B	849	BCR	C30-C25-C24	2.04	121.53	115.82
16	J	104	BCR	C34-C9-C8	2.04	121.49	118.10
13	B	841	CLA	CMB-C2B-C3B	2.04	129.08	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	809	CLA	CBA-CAA-C2A	2.05	119.50	113.73
13	A	814	CLA	CMB-C2B-C3B	2.05	129.09	125.09
13	A	802	CLA	CED-O2D-CGD	2.05	120.79	115.99
13	A	842	CLA	C1D-CHD-C4C	2.05	125.70	122.60
13	A	821	CLA	C2A-C1A-CHA	2.05	127.67	123.89
13	B	831	CLA	C1C-NC-C4C	2.06	108.77	106.27
16	A	851	BCR	C15-C14-C13	2.06	130.17	127.20
16	B	849	BCR	C23-C24-C25	2.06	133.49	127.32
13	A	837	CLA	C1C-NC-C4C	2.06	108.77	106.27
16	A	849	BCR	C30-C25-C24	2.06	121.59	115.82
16	M	1602	BCR	C32-C1-C6	2.06	113.53	110.30
13	A	820	CLA	C5-C3-C2	2.06	124.96	121.05
16	B	847	BCR	C20-C21-C22	2.06	130.18	127.20
16	B	844	BCR	C15-C14-C13	2.07	130.18	127.20
13	X	1701	CLA	C1C-NC-C4C	2.07	108.78	106.27
13	A	806	CLA	CBA-CAA-C2A	2.07	119.57	113.73
16	M	1602	BCR	C30-C25-C24	2.07	121.61	115.82
16	B	848	BCR	C40-C30-C25	2.07	113.55	110.30
16	B	848	BCR	C11-C10-C9	2.07	130.19	127.20
13	J	102	CLA	OBD-CAD-C3D	2.07	130.76	127.55
13	B	836	CLA	C2A-C1A-CHA	2.07	127.70	123.89
13	B	841	CLA	CED-O2D-CGD	2.07	120.85	115.99
16	B	845	BCR	C36-C18-C19	2.07	121.55	118.10
13	B	818	CLA	C6-C5-C3	2.08	117.04	112.48
13	A	809	CLA	CED-O2D-CGD	2.08	120.86	115.99
16	B	846	BCR	C36-C18-C19	2.08	121.55	118.10
16	J	105	BCR	C40-C30-C25	2.08	113.56	110.30
16	A	854	BCR	C34-C9-C8	2.08	121.56	118.10
13	B	823	CLA	C1C-NC-C4C	2.08	108.80	106.27
16	A	851	BCR	C35-C13-C12	2.08	121.56	118.10
13	B	825	CLA	O2A-CGA-CBA	2.08	121.03	112.36
13	A	844	CLA	CBA-CAA-C2A	2.08	119.61	113.73
13	L	1004	CLA	CBA-CAA-C2A	2.08	119.61	113.73
16	J	103	BCR	C37-C22-C23	2.09	121.57	118.10
16	A	850	BCR	C32-C1-C6	2.09	113.58	110.30
16	B	845	BCR	C20-C21-C22	2.09	130.21	127.20
13	A	813	CLA	CED-O2D-CGD	2.09	120.90	115.99
16	F	1302	BCR	C40-C30-C25	2.09	113.59	110.30
13	A	825	CLA	C1C-NC-C4C	2.10	108.81	106.27
16	I	101	BCR	C34-C9-C8	2.10	121.59	118.10
16	F	1302	BCR	C1-C6-C7	2.10	121.71	115.82
13	A	835	CLA	C5-C3-C2	2.10	125.04	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	843	BCR	C8-C7-C6	2.10	133.64	127.32
16	A	852	BCR	C23-C24-C25	2.11	133.64	127.32
16	B	845	BCR	C34-C9-C8	2.11	121.60	118.10
13	B	808	CLA	CED-O2D-CGD	2.11	120.93	115.99
13	B	807	CLA	C1C-NC-C4C	2.11	108.84	106.27
16	B	843	BCR	C20-C21-C22	2.12	130.25	127.20
13	B	826	CLA	CED-O2D-CGD	2.12	120.95	115.99
16	J	104	BCR	C15-C14-C13	2.12	130.26	127.20
13	B	827	CLA	CAA-CBA-CGA	2.12	119.53	113.32
16	A	850	BCR	C15-C14-C13	2.12	130.26	127.20
16	A	851	BCR	C28-C27-C26	2.12	117.24	113.87
13	B	803	CLA	C1C-NC-C4C	2.12	108.85	106.27
16	B	849	BCR	C11-C10-C9	2.12	130.27	127.20
13	B	834	CLA	C1C-NC-C4C	2.13	108.85	106.27
13	B	838	CLA	CBA-CAA-C2A	2.13	119.73	113.73
16	A	850	BCR	C23-C24-C25	2.13	133.71	127.32
13	B	822	CLA	CBA-CAA-C2A	2.13	119.75	113.73
16	A	849	BCR	C37-C22-C23	2.13	121.64	118.10
13	A	802	CLA	C1D-CHD-C4C	2.13	125.83	122.60
13	B	835	CLA	C2A-C1A-CHA	2.13	127.82	123.89
16	B	845	BCR	C32-C1-C6	2.14	113.65	110.30
13	A	838	CLA	CMB-C2B-C3B	2.14	129.27	125.09
13	X	1701	CLA	CED-O2D-CGD	2.14	121.01	115.99
16	A	849	BCR	C35-C13-C12	2.14	121.66	118.10
16	B	844	BCR	C36-C18-C19	2.14	121.67	118.10
13	A	841	CLA	C1C-NC-C4C	2.15	108.88	106.27
13	A	832	CLA	C1C-NC-C4C	2.15	108.88	106.27
13	L	1003	CLA	C1D-CHD-C4C	2.15	125.85	122.60
16	B	847	BCR	C1-C6-C7	2.15	121.84	115.82
13	B	820	CLA	C2A-C1A-CHA	2.15	127.85	123.89
16	B	844	BCR	C34-C9-C8	2.15	121.68	118.10
13	A	836	CLA	C6-C5-C3	2.15	117.21	112.48
16	A	853	BCR	C7-C8-C9	2.15	129.50	126.22
16	I	101	BCR	C1-C6-C7	2.16	121.86	115.82
13	A	805	CLA	CED-O2D-CGD	2.16	121.05	115.99
13	B	821	CLA	C2A-C1A-CHA	2.17	127.87	123.89
16	L	1006	BCR	C32-C1-C6	2.17	113.70	110.30
16	J	105	BCR	C16-C17-C18	2.17	130.33	127.20
13	A	846	CLA	C2A-C1A-CHA	2.17	127.88	123.89
13	B	838	CLA	C1C-NC-C4C	2.17	108.90	106.27
16	B	848	BCR	C24-C23-C22	2.17	129.52	126.22
13	F	1301	CLA	C2A-C1A-CHA	2.17	127.88	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	829	CLA	CED-O2D-CGD	2.17	121.09	115.99
13	B	801	CLA	C6-C5-C3	2.18	117.26	112.48
13	B	824	CLA	C2A-C1A-CHA	2.18	127.90	123.89
13	L	1003	CLA	C1C-NC-C4C	2.18	108.92	106.27
16	B	845	BCR	C30-C25-C24	2.18	121.92	115.82
16	B	845	BCR	C1-C6-C7	2.18	121.93	115.82
13	A	833	CLA	CMB-C2B-C3B	2.18	129.36	125.09
13	A	842	CLA	CED-O2D-CGD	2.18	121.11	115.99
16	I	101	BCR	C32-C1-C6	2.19	113.73	110.30
16	J	104	BCR	C1-C6-C7	2.19	121.95	115.82
16	B	844	BCR	C35-C13-C12	2.19	121.74	118.10
16	J	104	BCR	C24-C23-C22	2.20	129.56	126.22
13	B	820	CLA	C1C-NC-C4C	2.20	108.94	106.27
16	B	849	BCR	C15-C14-C13	2.20	130.37	127.20
13	J	101	CLA	C2A-C1A-CHA	2.20	127.94	123.89
16	B	843	BCR	C1-C6-C7	2.20	121.99	115.82
13	B	811	CLA	C1D-CHD-C4C	2.20	125.94	122.60
13	B	822	CLA	C1C-NC-C4C	2.20	108.95	106.27
16	B	846	BCR	C30-C25-C24	2.21	122.00	115.82
13	A	831	CLA	C1D-CHD-C4C	2.21	125.94	122.60
13	A	838	CLA	C1D-CHD-C4C	2.21	125.94	122.60
13	A	807	CLA	CAA-CBA-CGA	2.21	119.78	113.32
13	A	821	CLA	CED-O2D-CGD	2.21	121.17	115.99
16	F	1302	BCR	C30-C25-C24	2.21	122.01	115.82
16	B	848	BCR	C36-C18-C19	2.22	121.79	118.10
13	A	829	CLA	CMB-C2B-C3B	2.22	129.43	125.09
13	A	839	CLA	CED-O2D-CGD	2.23	121.21	115.99
16	A	853	BCR	C34-C9-C8	2.23	121.80	118.10
16	B	845	BCR	C40-C30-C25	2.23	113.79	110.30
16	J	104	BCR	C28-C27-C26	2.23	117.40	113.87
13	B	837	CLA	CED-O2D-CGD	2.23	121.22	115.99
13	A	810	CLA	CBA-CAA-C2A	2.23	120.02	113.73
16	I	102	BCR	C1-C6-C7	2.23	122.06	115.82
16	L	1006	BCR	C30-C25-C24	2.23	122.06	115.82
13	B	822	CLA	CMB-C2B-C3B	2.23	129.45	125.09
16	B	846	BCR	C15-C14-C13	2.24	129.75	127.42
16	A	850	BCR	C40-C30-C25	2.24	113.81	110.30
13	A	832	CLA	C1-C2-C3	2.24	130.38	126.71
13	B	825	CLA	CED-O2D-CGD	2.24	121.25	115.99
13	A	843	CLA	CBA-CAA-C2A	2.24	120.06	113.73
13	A	820	CLA	CBA-CAA-C2A	2.25	120.07	113.73
13	B	805	CLA	CMB-C2B-C3B	2.25	129.49	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	853	BCR	C37-C22-C23	2.25	121.84	118.10
16	A	849	BCR	C32-C1-C6	2.26	113.84	110.30
16	B	849	BCR	C24-C23-C22	2.26	129.66	126.22
13	B	830	CLA	CED-O2D-CGD	2.26	121.30	115.99
13	B	833	CLA	CBA-CAA-C2A	2.27	120.13	113.73
13	B	806	CLA	CMB-C2B-C3B	2.27	129.53	125.09
16	L	1005	BCR	C36-C18-C19	2.27	121.88	118.10
13	B	806	CLA	CED-O2D-CGD	2.27	121.33	115.99
13	B	828	CLA	C1D-CHD-C4C	2.28	126.05	122.60
16	A	850	BCR	C1-C6-C7	2.28	122.21	115.82
13	A	844	CLA	CED-O2D-CGD	2.28	121.34	115.99
13	B	803	CLA	C1D-CHD-C4C	2.29	126.06	122.60
13	A	821	CLA	C1C-NC-C4C	2.29	109.05	106.27
13	A	806	CLA	CMB-C2B-C3B	2.29	129.57	125.09
16	J	103	BCR	C35-C13-C12	2.29	121.91	118.10
13	B	825	CLA	C1C-NC-C4C	2.29	109.06	106.27
16	B	848	BCR	C35-C13-C12	2.30	121.92	118.10
13	A	843	CLA	C6-C5-C3	2.30	117.54	112.48
16	B	848	BCR	C23-C24-C25	2.30	134.24	127.32
13	A	841	CLA	C1D-CHD-C4C	2.31	126.09	122.60
13	A	831	CLA	CED-O2D-CGD	2.31	121.40	115.99
13	B	806	CLA	C1D-CHD-C4C	2.31	126.09	122.60
16	B	845	BCR	C23-C24-C25	2.31	134.25	127.32
13	A	826	CLA	CED-O2D-CGD	2.31	121.41	115.99
13	B	805	CLA	C1D-CHD-C4C	2.31	126.10	122.60
13	B	809	CLA	C1D-CHD-C4C	2.32	126.11	122.60
13	A	830	CLA	CED-O2D-CGD	2.32	121.42	115.99
16	I	102	BCR	C29-C30-C25	2.32	114.03	110.36
13	B	812	CLA	C1C-NC-C4C	2.32	109.08	106.27
16	J	105	BCR	C30-C25-C24	2.32	122.31	115.82
13	B	836	CLA	CED-O2D-CGD	2.32	121.43	115.99
13	B	824	CLA	C6-C5-C3	2.32	117.58	112.48
13	A	822	CLA	C1C-NC-C4C	2.32	109.09	106.27
13	A	829	CLA	C1D-CHD-C4C	2.33	126.12	122.60
13	B	826	CLA	C1D-CHD-C4C	2.33	126.13	122.60
13	B	807	CLA	CED-O2D-CGD	2.33	121.45	115.99
13	B	841	CLA	CBA-CAA-C2A	2.33	120.31	113.73
16	A	849	BCR	C1-C6-C7	2.33	122.34	115.82
16	M	1602	BCR	C8-C7-C6	2.33	134.32	127.32
16	I	102	BCR	C36-C18-C19	2.33	121.98	118.10
16	J	103	BCR	C24-C23-C22	2.34	129.78	126.22
13	A	839	CLA	C1D-CHD-C4C	2.34	126.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	104	BCR	C36-C18-C19	2.34	121.99	118.10
13	A	805	CLA	C1D-CHD-C4C	2.34	126.14	122.60
13	B	839	CLA	C1D-CHD-C4C	2.34	126.15	122.60
13	A	823	CLA	C1C-NC-C4C	2.35	109.12	106.27
13	A	819	CLA	CBA-CAA-C2A	2.35	120.36	113.73
13	B	830	CLA	C1C-NC-C4C	2.35	109.12	106.27
13	A	829	CLA	CED-O2D-CGD	2.35	121.50	115.99
16	A	852	BCR	C1-C6-C7	2.36	122.42	115.82
13	K	1401	CLA	CED-O2D-CGD	2.36	121.52	115.99
13	A	835	CLA	CED-O2D-CGD	2.36	121.52	115.99
13	A	807	CLA	C2A-C1A-CHA	2.36	128.23	123.89
13	F	1301	CLA	CED-O2D-CGD	2.36	121.52	115.99
13	A	803	CLA	CMB-C2B-C3B	2.36	129.71	125.09
13	B	821	CLA	C1C-NC-C4C	2.37	109.14	106.27
13	A	808	CLA	C1D-CHD-C4C	2.37	126.18	122.60
13	A	827	CLA	C1D-CHD-C4C	2.37	126.18	122.60
16	F	1302	BCR	C7-C8-C9	2.37	129.83	126.22
13	B	814	CLA	CED-O2D-CGD	2.37	121.56	115.99
16	B	849	BCR	C34-C9-C8	2.37	122.05	118.10
16	J	104	BCR	C40-C30-C25	2.37	114.03	110.30
16	A	852	BCR	C40-C30-C25	2.38	114.03	110.30
13	B	839	CLA	CED-O2D-CGD	2.38	121.57	115.99
13	B	805	CLA	CED-O2D-CGD	2.38	121.57	115.99
13	B	816	CLA	CED-O2D-CGD	2.38	121.58	115.99
13	B	804	CLA	C1D-CHD-C4C	2.39	126.21	122.60
13	B	802	CLA	C2A-C1A-CHA	2.39	128.29	123.89
13	A	834	CLA	CMB-C2B-C3B	2.40	129.78	125.09
13	A	816	CLA	CMB-C2B-C3B	2.41	129.79	125.09
16	B	845	BCR	C35-C13-C12	2.41	122.10	118.10
13	A	812	CLA	C1D-CHD-C4C	2.41	126.25	122.60
13	A	823	CLA	CED-O2D-CGD	2.41	121.64	115.99
13	A	835	CLA	C1D-CHD-C4C	2.41	126.25	122.60
16	J	104	BCR	C23-C24-C25	2.41	134.56	127.32
13	A	816	CLA	CED-O2D-CGD	2.41	121.65	115.99
13	A	840	CLA	CED-O2D-CGD	2.42	121.66	115.99
13	B	815	CLA	C1D-CHD-C4C	2.42	126.26	122.60
16	A	850	BCR	C24-C23-C22	2.42	129.90	126.22
16	I	102	BCR	C30-C25-C24	2.42	122.59	115.82
13	B	831	CLA	CED-O2D-CGD	2.42	121.68	115.99
13	A	811	CLA	C1D-CHD-C4C	2.43	126.28	122.60
13	B	841	CLA	C1D-CHD-C4C	2.43	126.28	122.60
13	B	818	CLA	CED-O2D-CGD	2.43	121.70	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	840	CLA	C1D-CHD-C4C	2.44	126.29	122.60
13	A	824	CLA	C1D-CHD-C4C	2.44	126.29	122.60
16	A	851	BCR	C30-C25-C24	2.44	122.64	115.82
16	A	851	BCR	C1-C6-C7	2.44	122.65	115.82
16	A	850	BCR	C7-C8-C9	2.44	129.94	126.22
16	B	848	BCR	C34-C9-C8	2.45	122.17	118.10
13	L	1002	CLA	C1D-CHD-C4C	2.45	126.30	122.60
13	B	833	CLA	C1D-CHD-C4C	2.45	126.31	122.60
13	A	809	CLA	C1D-CHD-C4C	2.45	126.31	122.60
16	A	850	BCR	C30-C25-C24	2.45	122.69	115.82
16	A	852	BCR	C32-C1-C6	2.45	114.15	110.30
16	I	101	BCR	C23-C24-C25	2.46	134.69	127.32
16	B	846	BCR	C35-C13-C12	2.46	120.69	114.64
13	B	812	CLA	CED-O2D-CGD	2.46	121.76	115.99
13	A	828	CLA	C1D-CHD-C4C	2.46	126.33	122.60
13	A	843	CLA	C1D-CHD-C4C	2.47	126.34	122.60
13	A	825	CLA	C1D-CHD-C4C	2.48	126.35	122.60
16	A	853	BCR	C1-C6-C7	2.48	122.75	115.82
13	B	810	CLA	CED-O2D-CGD	2.48	121.80	115.99
13	B	816	CLA	C1D-CHD-C4C	2.48	126.35	122.60
13	A	808	CLA	CED-O2D-CGD	2.48	121.81	115.99
16	B	847	BCR	C36-C18-C19	2.48	122.23	118.10
13	A	832	CLA	CED-O2D-CGD	2.49	121.82	115.99
16	L	1005	BCR	C8-C7-C6	2.49	134.78	127.32
13	B	803	CLA	O2D-CGD-CBD	2.49	114.72	111.30
13	A	814	CLA	CED-O2D-CGD	2.50	121.86	115.99
16	A	854	BCR	C1-C6-C7	2.50	122.83	115.82
13	B	813	CLA	CMB-C2B-C3B	2.51	129.99	125.09
16	I	102	BCR	C37-C22-C23	2.51	122.27	118.10
13	A	803	CLA	C1D-CHD-C4C	2.51	126.39	122.60
13	A	844	CLA	C1D-CHD-C4C	2.51	126.40	122.60
13	B	838	CLA	C1D-CHD-C4C	2.51	126.40	122.60
13	B	828	CLA	CBA-CAA-C2A	2.51	120.83	113.73
13	A	826	CLA	C1D-CHD-C4C	2.51	126.41	122.60
18	B	850	LMG	C7-O1-C1	2.52	119.10	113.82
13	B	828	CLA	CED-O2D-CGD	2.52	121.90	115.99
13	A	818	CLA	C1D-CHD-C4C	2.52	126.42	122.60
13	A	810	CLA	C2A-C1A-CHA	2.53	128.54	123.89
13	B	831	CLA	C1D-CHD-C4C	2.53	126.42	122.60
13	B	825	CLA	CMB-C2B-C3B	2.53	130.03	125.09
13	B	801	CLA	C1D-CHD-C4C	2.53	126.43	122.60
16	A	853	BCR	C23-C24-C25	2.53	134.92	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	829	CLA	C1D-CHD-C4C	2.53	126.43	122.60
16	A	849	BCR	C8-C7-C6	2.53	134.92	127.32
13	A	846	CLA	CED-O2D-CGD	2.53	121.93	115.99
13	A	822	CLA	O2A-CGA-CBA	2.53	119.62	111.90
13	A	818	CLA	CED-O2D-CGD	2.53	121.94	115.99
13	B	819	CLA	CED-O2D-CGD	2.54	121.95	115.99
16	L	1006	BCR	C8-C7-C6	2.54	134.96	127.32
13	A	822	CLA	CAA-CBA-CGA	2.54	120.76	113.32
13	B	810	CLA	C2A-C1A-CHA	2.55	128.57	123.89
13	B	813	CLA	CED-O2D-CGD	2.55	121.96	115.99
13	A	837	CLA	CED-O2D-CGD	2.55	121.96	115.99
13	B	814	CLA	C1D-CHD-C4C	2.55	126.46	122.60
13	B	801	CLA	O2D-CGD-CBD	2.55	114.80	111.30
13	A	813	CLA	C1D-CHD-C4C	2.55	126.46	122.60
13	A	836	CLA	C1D-CHD-C4C	2.55	126.47	122.60
13	A	815	CLA	C1D-CHD-C4C	2.56	126.47	122.60
13	B	826	CLA	CMB-C2B-C3B	2.56	130.09	125.09
13	A	820	CLA	CMB-C2B-C3B	2.56	130.09	125.09
13	A	802	CLA	O2A-CGA-CBA	2.57	119.72	111.90
13	B	802	CLA	C1D-CHD-C4C	2.57	126.49	122.60
16	A	854	BCR	C15-C14-C13	2.57	130.91	127.20
13	B	809	CLA	CED-O2D-CGD	2.57	122.03	115.99
16	I	101	BCR	C36-C18-C19	2.58	122.39	118.10
16	L	1005	BCR	C29-C30-C25	2.58	114.45	110.36
13	B	813	CLA	C1D-CHD-C4C	2.58	126.51	122.60
16	B	844	BCR	C32-C1-C6	2.58	114.35	110.30
13	B	817	CLA	CED-O2D-CGD	2.59	122.05	115.99
13	A	807	CLA	C1D-CHD-C4C	2.59	126.52	122.60
13	A	827	CLA	CMB-C2B-C3B	2.59	130.15	125.09
16	B	847	BCR	C32-C1-C6	2.59	114.36	110.30
13	A	807	CLA	O2D-CGD-CBD	2.59	114.85	111.30
16	B	847	BCR	C30-C25-C24	2.59	123.08	115.82
13	A	830	CLA	C1D-CHD-C4C	2.60	126.53	122.60
13	A	811	CLA	CED-O2D-CGD	2.60	122.08	115.99
13	A	801	CLA	C1D-CHD-C4C	2.60	126.54	122.60
13	B	837	CLA	C1D-CHD-C4C	2.61	126.55	122.60
13	A	807	CLA	CMB-C2B-C3B	2.61	130.20	125.09
13	A	819	CLA	C1D-CHD-C4C	2.62	126.56	122.60
13	A	836	CLA	CED-O2D-CGD	2.62	122.13	115.99
16	B	847	BCR	C16-C17-C18	2.62	130.99	127.20
13	A	819	CLA	CED-O2D-CGD	2.63	122.15	115.99
13	B	834	CLA	C1D-CHD-C4C	2.63	126.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	812	CLA	CED-O2D-CGD	2.64	122.17	115.99
13	A	833	CLA	CED-O2D-CGD	2.64	122.18	115.99
13	B	827	CLA	C1D-CHD-C4C	2.64	126.60	122.60
16	I	102	BCR	C3-C4-C5	2.64	118.06	113.87
16	J	103	BCR	C1-C6-C7	2.64	123.22	115.82
13	A	843	CLA	CED-O2D-CGD	2.64	122.19	115.99
13	B	823	CLA	C1D-CHD-C4C	2.65	126.61	122.60
13	A	815	CLA	CED-O2D-CGD	2.65	122.20	115.99
13	B	840	CLA	O2A-CGA-CBA	2.65	119.98	111.90
16	J	103	BCR	C8-C7-C6	2.65	135.28	127.32
13	A	817	CLA	C1D-CHD-C4C	2.65	126.62	122.60
16	A	849	BCR	C23-C24-C25	2.66	135.30	127.32
16	I	101	BCR	C29-C30-C25	2.66	114.58	110.36
13	A	804	CLA	C1D-CHD-C4C	2.67	126.64	122.60
13	B	835	CLA	C1D-CHD-C4C	2.67	126.64	122.60
16	J	103	BCR	C36-C18-C19	2.67	122.54	118.10
13	A	806	CLA	CED-O2D-CGD	2.67	122.26	115.99
13	B	818	CLA	C1D-CHD-C4C	2.67	126.65	122.60
16	A	853	BCR	C11-C10-C9	2.67	131.06	127.20
16	B	844	BCR	C23-C24-C25	2.69	135.38	127.32
13	K	1401	CLA	C1D-CHD-C4C	2.69	126.67	122.60
13	B	821	CLA	CED-O2D-CGD	2.69	122.29	115.99
13	B	801	CLA	CED-O2D-CGD	2.69	122.30	115.99
13	A	820	CLA	C1D-CHD-C4C	2.69	126.67	122.60
13	B	819	CLA	C1D-CHD-C4C	2.69	126.68	122.60
13	B	835	CLA	CED-O2D-CGD	2.70	122.33	115.99
16	B	847	BCR	C29-C30-C25	2.70	114.64	110.36
13	A	820	CLA	CED-O2D-CGD	2.71	122.34	115.99
13	B	834	CLA	CED-O2D-CGD	2.72	122.36	115.99
13	B	824	CLA	C1D-CHD-C4C	2.72	126.71	122.60
16	A	854	BCR	C30-C25-C24	2.72	123.44	115.82
13	A	830	CLA	CMB-C2B-C3B	2.72	130.42	125.09
13	J	101	CLA	CED-O2D-CGD	2.73	122.38	115.99
13	A	845	CLA	C1D-CHD-C4C	2.73	126.73	122.60
13	B	822	CLA	C1D-CHD-C4C	2.73	126.73	122.60
13	B	822	CLA	CED-O2D-CGD	2.73	122.40	115.99
13	A	831	CLA	O2A-CGA-CBA	2.73	120.23	111.90
13	B	833	CLA	CED-O2D-CGD	2.74	122.41	115.99
13	A	814	CLA	C1D-CHD-C4C	2.74	126.75	122.60
16	B	848	BCR	C32-C1-C6	2.75	114.61	110.30
16	L	1005	BCR	C40-C30-C25	2.75	114.61	110.30
13	B	817	CLA	C1D-CHD-C4C	2.75	126.76	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	845	BCR	C28-C27-C26	2.75	118.23	113.87
13	B	807	CLA	C1D-CHD-C4C	2.76	126.77	122.60
16	B	844	BCR	C1-C6-C7	2.76	123.54	115.82
13	B	824	CLA	CED-O2D-CGD	2.76	122.46	115.99
13	B	836	CLA	C1D-CHD-C4C	2.76	126.78	122.60
16	B	844	BCR	C20-C21-C22	2.76	131.18	127.20
13	B	821	CLA	C1D-CHD-C4C	2.76	126.78	122.60
16	I	102	BCR	C7-C8-C9	2.78	130.44	126.22
16	L	1006	BCR	C29-C30-C25	2.78	114.76	110.36
13	B	837	CLA	O2A-CGA-CBA	2.78	120.38	111.90
13	A	823	CLA	C1D-CHD-C4C	2.79	126.83	122.60
13	B	811	CLA	CED-O2D-CGD	2.79	122.54	115.99
13	B	806	CLA	O2A-CGA-CBA	2.79	120.42	111.90
13	A	822	CLA	C1D-CHD-C4C	2.80	126.83	122.60
13	B	820	CLA	CED-O2D-CGD	2.80	122.56	115.99
13	B	832	CLA	C1D-CHD-C4C	2.81	126.85	122.60
13	A	816	CLA	C1D-CHD-C4C	2.82	126.87	122.60
16	A	852	BCR	C30-C25-C24	2.82	123.72	115.82
17	A	856	LHG	O7-C7-C8	2.83	117.67	111.53
13	B	803	CLA	CED-O2D-CGD	2.83	122.63	115.99
13	A	835	CLA	O2A-CGA-CBA	2.83	120.53	111.90
16	A	853	BCR	C2-C1-C6	2.84	114.86	110.36
13	A	806	CLA	C1D-CHD-C4C	2.84	126.90	122.60
16	A	854	BCR	C32-C1-C6	2.84	114.76	110.30
13	A	846	CLA	C1D-CHD-C4C	2.84	126.91	122.60
16	A	849	BCR	C24-C23-C22	2.85	130.56	126.22
16	A	851	BCR	C7-C8-C9	2.85	130.56	126.22
16	F	1302	BCR	C24-C23-C22	2.85	130.56	126.22
16	J	104	BCR	C30-C25-C24	2.86	123.82	115.82
16	B	846	BCR	C40-C30-C25	2.86	114.78	110.30
13	A	807	CLA	CED-O2D-CGD	2.86	122.69	115.99
13	B	838	CLA	CED-O2D-CGD	2.87	122.71	115.99
13	M	1601	CLA	CED-O2D-CGD	2.87	122.72	115.99
13	A	810	CLA	C1D-CHD-C4C	2.87	126.95	122.60
13	X	1701	CLA	C1D-CHD-C4C	2.87	126.95	122.60
16	I	101	BCR	C7-C8-C9	2.88	130.60	126.22
13	B	818	CLA	CMB-C2B-C3B	2.88	130.71	125.09
16	B	848	BCR	C15-C14-C13	2.88	131.36	127.20
16	M	1602	BCR	C1-C6-C7	2.89	123.90	115.82
13	F	1301	CLA	C1D-CHD-C4C	2.89	126.98	122.60
16	I	102	BCR	C32-C1-C6	2.89	114.84	110.30
16	A	850	BCR	C29-C30-C25	2.90	114.96	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	803	CLA	O2D-CGD-CBD	2.91	115.29	111.30
16	B	849	BCR	C29-C30-C25	2.91	114.98	110.36
13	A	817	CLA	CED-O2D-CGD	2.92	122.83	115.99
13	L	1004	CLA	C1D-CHD-C4C	2.92	127.02	122.60
17	A	855	LHG	O7-C7-C8	2.92	117.87	111.53
16	L	1005	BCR	C30-C25-C24	2.93	124.01	115.82
16	B	845	BCR	C24-C23-C22	2.93	130.68	126.22
13	A	834	CLA	O2A-CGA-CBA	2.93	120.84	111.90
16	B	847	BCR	C24-C23-C22	2.94	130.70	126.22
17	B	851	LHG	O7-C7-C8	2.95	117.93	111.53
13	J	102	CLA	C1D-CHD-C4C	2.95	127.06	122.60
16	L	1005	BCR	C2-C1-C6	2.95	115.03	110.36
16	A	854	BCR	C16-C17-C18	2.95	131.46	127.20
16	B	846	BCR	C24-C23-C22	2.95	130.71	126.22
13	B	820	CLA	C1D-CHD-C4C	2.95	127.07	122.60
13	B	830	CLA	C1D-CHD-C4C	2.96	127.07	122.60
13	B	825	CLA	C1D-CHD-C4C	2.96	127.08	122.60
13	B	814	CLA	O2A-CGA-CBA	2.96	120.92	111.90
13	A	827	CLA	O2A-CGA-CBA	2.96	120.92	111.90
13	A	803	CLA	CED-O2D-CGD	2.96	122.94	115.99
13	A	841	CLA	CED-O2D-CGD	2.99	122.99	115.99
16	B	846	BCR	C29-C30-C25	2.99	115.10	110.36
13	A	839	CLA	O2D-CGD-CBD	2.99	115.41	111.30
16	B	844	BCR	C2-C1-C6	3.00	115.11	110.36
13	J	101	CLA	C1D-CHD-C4C	3.00	127.14	122.60
13	A	818	CLA	O2A-CGA-CBA	3.00	121.03	111.90
13	M	1601	CLA	C1D-CHD-C4C	3.01	127.15	122.60
16	A	849	BCR	C2-C1-C6	3.01	115.13	110.36
13	B	829	CLA	CMB-C2B-C3B	3.01	130.98	125.09
13	A	822	CLA	CED-O2D-CGD	3.01	123.06	115.99
13	L	1004	CLA	O2A-CGA-CBA	3.02	121.09	111.90
13	L	1003	CLA	O2A-CGA-CBA	3.02	121.09	111.90
16	B	849	BCR	C7-C8-C9	3.02	130.82	126.22
13	A	807	CLA	CBA-CAA-C2A	3.03	122.27	113.73
13	B	828	CLA	C5-C3-C2	3.03	126.80	121.05
16	L	1005	BCR	C24-C23-C22	3.04	130.84	126.22
16	A	851	BCR	C40-C30-C25	3.04	115.07	110.30
13	A	825	CLA	O2A-CGA-CBA	3.04	121.17	111.90
16	A	851	BCR	C2-C1-C6	3.05	115.19	110.36
13	B	840	CLA	CED-O2D-CGD	3.05	123.14	115.99
13	A	821	CLA	C1D-CHD-C4C	3.05	127.21	122.60
13	B	833	CLA	O2A-CGA-CBA	3.05	121.19	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	809	CLA	O2A-CGA-CBA	3.05	121.19	111.90
16	B	843	BCR	C23-C24-C25	3.05	136.49	127.32
16	B	843	BCR	C7-C8-C9	3.05	130.87	126.22
13	B	831	CLA	O2A-CGA-CBA	3.06	121.21	111.90
13	A	837	CLA	C1D-CHD-C4C	3.06	127.24	122.60
13	B	819	CLA	O2A-CGA-CBA	3.07	121.25	111.90
13	B	812	CLA	C1D-CHD-C4C	3.08	127.26	122.60
16	J	103	BCR	C23-C24-C25	3.08	136.57	127.32
13	B	822	CLA	O2A-CGA-CBA	3.08	121.29	111.90
13	B	841	CLA	O2A-CGA-CBA	3.09	121.31	111.90
16	A	852	BCR	C2-C1-C6	3.10	115.28	110.36
13	B	824	CLA	O2A-CGA-CBA	3.10	121.36	111.90
13	A	801	CLA	OBD-CAD-C3D	3.11	134.70	128.35
13	B	801	CLA	O2A-CGA-CBA	3.13	121.44	111.90
13	A	822	CLA	CMB-C2B-C3B	3.13	131.21	125.09
13	B	829	CLA	O2A-CGA-CBA	3.13	121.44	111.90
16	F	1302	BCR	C29-C30-C25	3.13	115.32	110.36
16	J	104	BCR	C7-C8-C9	3.14	130.99	126.22
13	A	826	CLA	O2A-CGA-CBA	3.14	121.47	111.90
13	A	833	CLA	C1D-CHD-C4C	3.15	127.37	122.60
18	B	850	LMG	O8-C28-C29	3.16	121.52	111.90
16	A	852	BCR	C29-C30-C25	3.16	115.36	110.36
16	B	843	BCR	C29-C30-C25	3.16	115.37	110.36
13	B	803	CLA	O2A-CGA-CBA	3.16	121.54	111.90
13	B	839	CLA	O2A-CGA-CBA	3.17	121.55	111.90
16	M	1602	BCR	C29-C30-C25	3.18	115.40	110.36
16	A	853	BCR	C29-C30-C25	3.20	115.43	110.36
16	F	1302	BCR	C2-C1-C6	3.22	115.46	110.36
16	B	843	BCR	C24-C23-C22	3.22	131.12	126.22
13	B	835	CLA	O2D-CGD-CBD	3.22	115.72	111.30
13	B	802	CLA	O2A-CGA-CBA	3.22	121.72	111.90
13	A	841	CLA	O2D-CGD-CBD	3.23	115.72	111.30
16	L	1006	BCR	C2-C1-C6	3.23	115.47	110.36
13	B	813	CLA	O2A-CGA-CBA	3.23	121.73	111.90
13	B	832	CLA	O2A-CGA-CBA	3.24	121.76	111.90
13	A	814	CLA	O2A-CGA-CBA	3.24	121.78	111.90
13	A	806	CLA	O2A-CGA-CBA	3.25	121.79	111.90
13	B	805	CLA	O2A-CGA-CBA	3.25	121.80	111.90
13	A	822	CLA	O2D-CGD-CBD	3.25	115.76	111.30
13	A	832	CLA	C1D-CHD-C4C	3.26	127.53	122.60
16	J	105	BCR	C29-C30-C25	3.26	115.53	110.36
17	A	856	LHG	O8-C23-C24	3.26	120.52	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	826	CLA	O2A-CGA-CBA	3.27	121.85	111.90
13	A	839	CLA	O2A-CGA-CBA	3.27	121.86	111.90
16	B	847	BCR	C2-C1-C6	3.28	115.55	110.36
16	B	849	BCR	C2-C1-C6	3.28	115.56	110.36
13	A	836	CLA	O2A-CGA-CBA	3.29	121.93	111.90
13	A	841	CLA	O2A-CGA-CBA	3.30	121.96	111.90
16	B	848	BCR	C2-C1-C6	3.30	115.59	110.36
17	A	855	LHG	O8-C23-C24	3.31	121.97	111.90
16	M	1602	BCR	C2-C1-C6	3.31	115.60	110.36
13	B	807	CLA	O2A-CGA-CBA	3.31	122.00	111.90
13	B	810	CLA	O2A-CGA-CBA	3.32	122.01	111.90
13	A	833	CLA	O2A-CGA-CBA	3.32	122.02	111.90
16	A	850	BCR	C2-C1-C6	3.33	115.63	110.36
16	A	849	BCR	C29-C30-C25	3.33	115.64	110.36
13	A	829	CLA	O2A-CGA-CBA	3.34	122.08	111.90
13	B	808	CLA	C4A-NA-C1A	3.34	110.68	106.36
13	A	817	CLA	O2A-CGA-CBA	3.34	122.09	111.90
13	A	801	CLA	O2A-CGA-CBA	3.35	122.10	111.90
13	A	804	CLA	O2A-CGA-CBA	3.35	122.11	111.90
16	B	845	BCR	C2-C1-C6	3.35	115.67	110.36
13	A	832	CLA	O2A-CGA-CBA	3.35	122.12	111.90
16	B	848	BCR	C29-C30-C25	3.36	115.68	110.36
13	B	828	CLA	C4A-NA-C1A	3.36	110.71	106.36
16	A	854	BCR	C29-C30-C25	3.36	115.69	110.36
16	J	103	BCR	C2-C1-C6	3.37	115.70	110.36
16	A	853	BCR	C24-C23-C22	3.39	131.38	126.22
16	F	1302	BCR	C15-C14-C13	3.41	132.12	127.20
13	B	838	CLA	O2A-CGA-CBA	3.41	122.29	111.90
13	A	812	CLA	O2D-CGD-CBD	3.41	115.98	111.30
16	B	846	BCR	C20-C21-C22	3.42	132.13	127.20
16	B	844	BCR	C29-C30-C25	3.42	115.78	110.36
13	L	1002	CLA	O2A-CGA-CBA	3.42	122.33	111.90
13	A	801	CLA	C4A-NA-C1A	3.43	110.79	106.36
13	B	840	CLA	O2D-CGD-CBD	3.43	116.00	111.30
13	A	805	CLA	O2A-CGA-CBA	3.44	122.37	111.90
13	A	802	CLA	C4A-NA-C1A	3.45	110.82	106.36
13	A	812	CLA	O2A-CGA-CBA	3.48	122.49	111.90
13	B	813	CLA	C4A-NA-C1A	3.50	110.88	106.36
13	A	803	CLA	C4A-NA-C1A	3.50	110.89	106.36
16	A	851	BCR	C24-C23-C22	3.52	131.58	126.22
13	A	828	CLA	O2A-CGA-CBA	3.53	122.64	111.90
16	J	104	BCR	C29-C30-C25	3.53	115.95	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	844	CLA	O2D-CGD-CBD	3.54	116.15	111.30
16	J	105	BCR	C24-C23-C22	3.54	131.61	126.22
13	A	840	CLA	C4A-NA-C1A	3.54	110.94	106.36
16	B	847	BCR	C7-C8-C9	3.54	131.62	126.22
16	J	104	BCR	C2-C1-C6	3.55	115.98	110.36
13	B	839	CLA	C4A-NA-C1A	3.55	110.95	106.36
13	B	828	CLA	O2D-CGD-CBD	3.56	116.18	111.30
16	A	852	BCR	C24-C23-C22	3.56	131.64	126.22
13	B	805	CLA	C4A-NA-C1A	3.56	110.97	106.36
13	A	835	CLA	C4A-NA-C1A	3.57	110.98	106.36
13	B	816	CLA	O2A-CGA-CBA	3.58	122.81	111.90
16	J	104	BCR	C38-C26-C25	3.59	128.13	124.61
13	B	802	CLA	C4A-NA-C1A	3.59	111.01	106.36
13	A	829	CLA	O2D-CGD-CBD	3.60	116.24	111.30
16	B	844	BCR	C24-C23-C22	3.62	131.72	126.22
13	B	804	CLA	O2A-CGA-CBA	3.62	122.92	111.90
13	A	844	CLA	C4A-NA-C1A	3.62	111.04	106.36
13	B	806	CLA	C4A-NA-C1A	3.63	111.05	106.36
13	A	808	CLA	O2A-CGA-CBA	3.63	122.96	111.90
13	A	829	CLA	C4A-NA-C1A	3.63	111.05	106.36
13	A	809	CLA	O2A-CGA-CBA	3.63	122.96	111.90
16	A	851	BCR	C29-C30-C25	3.63	116.11	110.36
13	B	803	CLA	C4A-NA-C1A	3.64	111.06	106.36
13	A	834	CLA	C4A-NA-C1A	3.65	111.08	106.36
13	A	831	CLA	C4A-NA-C1A	3.67	111.10	106.36
13	B	829	CLA	C4A-NA-C1A	3.67	111.10	106.36
16	J	103	BCR	C29-C30-C25	3.67	116.17	110.36
16	B	843	BCR	C2-C1-C6	3.68	116.19	110.36
13	B	806	CLA	O2D-CGD-CBD	3.68	116.35	111.30
13	A	806	CLA	C4A-NA-C1A	3.69	111.12	106.36
13	B	817	CLA	O2D-CGD-CBD	3.69	116.36	111.30
13	A	819	CLA	O2A-CGA-CBA	3.70	123.16	111.90
13	B	811	CLA	O2D-CGD-CBD	3.70	116.37	111.30
13	A	813	CLA	O2A-CGA-CBA	3.70	123.16	111.90
13	B	840	CLA	C4A-NA-C1A	3.70	111.14	106.36
13	A	843	CLA	O2D-CGD-CBD	3.70	116.38	111.30
13	A	820	CLA	O2D-CGD-CBD	3.71	116.39	111.30
13	B	817	CLA	O2A-CGA-CBA	3.72	123.25	111.90
16	J	105	BCR	C8-C7-C6	3.73	138.51	127.32
16	A	854	BCR	C2-C1-C6	3.73	116.27	110.36
16	B	848	BCR	C7-C8-C9	3.73	131.90	126.22
13	B	837	CLA	C4A-NA-C1A	3.74	111.19	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	839	CLA	C4A-NA-C1A	3.74	111.20	106.36
13	L	1004	CLA	C4A-NA-C1A	3.74	111.20	106.36
13	B	820	CLA	O2A-CGA-CBA	3.74	123.31	111.90
13	A	818	CLA	C4A-NA-C1A	3.75	111.21	106.36
13	A	830	CLA	O2A-CGA-CBA	3.76	123.35	111.90
13	A	824	CLA	C4A-NA-C1A	3.77	111.24	106.36
16	M	1602	BCR	C24-C23-C22	3.79	131.99	126.22
13	A	824	CLA	O2A-CGA-CBA	3.79	123.44	111.90
13	B	816	CLA	C4A-NA-C1A	3.79	111.26	106.36
13	A	807	CLA	C4A-NA-C1A	3.79	111.26	106.36
16	J	105	BCR	C2-C1-C6	3.80	116.38	110.36
13	B	835	CLA	C4A-NA-C1A	3.81	111.29	106.36
13	K	1401	CLA	C4A-NA-C1A	3.82	111.30	106.36
13	A	826	CLA	C4A-NA-C1A	3.83	111.31	106.36
13	B	839	CLA	O2D-CGD-CBD	3.83	116.55	111.30
13	A	842	CLA	O2A-CGA-CBA	3.83	123.57	111.90
16	A	854	BCR	C24-C23-C22	3.83	132.06	126.22
13	A	811	CLA	C4A-NA-C1A	3.84	111.32	106.36
13	B	809	CLA	C4A-NA-C1A	3.84	111.33	106.36
13	A	811	CLA	O2D-CGD-CBD	3.85	116.58	111.30
13	A	830	CLA	C4A-NA-C1A	3.85	111.34	106.36
16	A	854	BCR	C40-C30-C25	3.85	116.34	110.30
13	B	827	CLA	C4A-NA-C1A	3.86	111.35	106.36
13	A	843	CLA	C4A-NA-C1A	3.86	111.35	106.36
16	B	844	BCR	C7-C8-C9	3.86	132.10	126.22
13	L	1002	CLA	C4A-NA-C1A	3.87	111.36	106.36
13	A	819	CLA	O2D-CGD-CBD	3.87	116.61	111.30
13	A	846	CLA	O2A-CGA-CBA	3.88	123.72	111.90
13	L	1003	CLA	C4A-NA-C1A	3.89	111.39	106.36
13	B	832	CLA	C4A-NA-C1A	3.89	111.39	106.36
13	B	822	CLA	O2D-CGD-CBD	3.89	116.64	111.30
13	A	815	CLA	C4A-NA-C1A	3.89	111.39	106.36
13	B	818	CLA	O2A-CGA-CBA	3.90	123.77	111.90
13	A	823	CLA	O2A-CGA-CBA	3.90	123.77	111.90
13	B	811	CLA	C4A-NA-C1A	3.90	111.40	106.36
13	A	804	CLA	C4A-NA-C1A	3.90	111.40	106.36
13	A	842	CLA	C4A-NA-C1A	3.90	111.40	106.36
13	A	844	CLA	O2A-CGA-CBA	3.90	123.78	111.90
13	B	808	CLA	O2A-CGA-CBA	3.90	123.79	111.90
13	B	824	CLA	C4A-NA-C1A	3.90	111.41	106.36
13	A	820	CLA	O2A-CGA-CBA	3.91	123.81	111.90
13	A	821	CLA	O2A-CGA-CBA	3.91	123.81	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	825	CLA	C4A-NA-C1A	3.92	111.43	106.36
13	B	815	CLA	C4A-NA-C1A	3.93	111.44	106.36
13	A	810	CLA	O2A-CGA-CBA	3.93	123.88	111.90
13	A	843	CLA	O2A-CGA-CBA	3.94	123.89	111.90
13	B	834	CLA	C4A-NA-C1A	3.94	111.45	106.36
13	B	801	CLA	C4A-NA-C1A	3.94	111.46	106.36
13	A	822	CLA	C4A-NA-C1A	3.94	111.46	106.36
13	B	819	CLA	O2D-CGD-CBD	3.95	116.71	111.30
16	I	102	BCR	C24-C23-C22	3.95	132.24	126.22
13	A	827	CLA	C4A-NA-C1A	3.95	111.47	106.36
13	A	825	CLA	O2D-CGD-CBD	3.96	116.73	111.30
13	B	814	CLA	C4A-NA-C1A	3.97	111.49	106.36
13	B	823	CLA	C4A-NA-C1A	3.97	111.49	106.36
13	B	810	CLA	O2D-CGD-CBD	3.97	116.75	111.30
13	B	817	CLA	C4A-NA-C1A	3.98	111.50	106.36
16	A	853	BCR	C33-C5-C6	3.98	128.52	124.61
13	B	831	CLA	C4A-NA-C1A	3.99	111.52	106.36
13	A	819	CLA	C4A-NA-C1A	3.99	111.52	106.36
13	B	841	CLA	C4A-NA-C1A	4.01	111.54	106.36
13	A	805	CLA	C4A-NA-C1A	4.01	111.54	106.36
13	B	819	CLA	C4A-NA-C1A	4.03	111.57	106.36
13	F	1301	CLA	O2D-CGD-CBD	4.03	116.82	111.30
16	I	101	BCR	C2-C1-C6	4.03	116.75	110.36
13	B	827	CLA	CBA-CAA-C2A	4.04	125.12	113.73
13	B	838	CLA	C4A-NA-C1A	4.04	111.58	106.36
16	M	1602	BCR	C33-C5-C6	4.05	128.58	124.61
13	A	838	CLA	C4A-NA-C1A	4.05	111.59	106.36
13	B	809	CLA	O2D-CGD-CBD	4.05	116.86	111.30
16	I	102	BCR	C33-C5-C6	4.06	128.59	124.61
13	A	810	CLA	O2D-CGD-CBD	4.06	116.87	111.30
13	A	828	CLA	C4A-NA-C1A	4.07	111.62	106.36
13	A	809	CLA	C4A-NA-C1A	4.07	111.62	106.36
13	B	828	CLA	O2A-CGA-CBA	4.08	124.32	111.90
13	B	810	CLA	C4A-NA-C1A	4.08	111.64	106.36
13	B	826	CLA	C4A-NA-C1A	4.08	111.64	106.36
13	A	836	CLA	C4A-NA-C1A	4.09	111.64	106.36
13	A	832	CLA	C4A-NA-C1A	4.09	111.65	106.36
13	A	841	CLA	C4A-NA-C1A	4.09	111.65	106.36
16	J	104	BCR	C33-C5-C6	4.10	128.63	124.61
13	A	845	CLA	C4A-NA-C1A	4.10	111.67	106.36
13	A	808	CLA	C4A-NA-C1A	4.11	111.68	106.36
13	A	810	CLA	C4A-NA-C1A	4.13	111.70	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	833	CLA	C4A-NA-C1A	4.13	111.70	106.36
13	B	836	CLA	O2D-CGD-CBD	4.14	116.97	111.30
13	B	825	CLA	C4A-NA-C1A	4.14	111.71	106.36
13	A	814	CLA	C4A-NA-C1A	4.15	111.72	106.36
13	A	820	CLA	C4A-NA-C1A	4.15	111.72	106.36
13	A	803	CLA	O2A-CGA-CBA	4.15	124.54	111.90
13	B	804	CLA	C4A-NA-C1A	4.15	111.73	106.36
13	A	840	CLA	O2A-CGA-CBA	4.16	124.56	111.90
13	B	807	CLA	C4A-NA-C1A	4.17	111.75	106.36
13	A	823	CLA	C4A-NA-C1A	4.18	111.76	106.36
13	A	818	CLA	O2D-CGD-CBD	4.18	117.03	111.30
13	A	838	CLA	O2A-CGA-CBA	4.18	124.65	111.90
13	J	102	CLA	C4A-NA-C1A	4.18	111.77	106.36
13	B	822	CLA	C4A-NA-C1A	4.19	111.78	106.36
16	B	845	BCR	C29-C30-C25	4.20	117.02	110.36
13	A	813	CLA	O2D-CGD-CBD	4.21	117.07	111.30
13	F	1301	CLA	C4A-NA-C1A	4.21	111.81	106.36
13	A	836	CLA	O2D-CGD-CBD	4.21	117.08	111.30
13	A	817	CLA	C4A-NA-C1A	4.22	111.81	106.36
13	A	808	CLA	O2D-CGD-CBD	4.23	117.10	111.30
13	B	818	CLA	C4A-NA-C1A	4.24	111.84	106.36
13	B	830	CLA	C4A-NA-C1A	4.25	111.85	106.36
13	A	837	CLA	C4A-NA-C1A	4.26	111.87	106.36
13	A	812	CLA	C4A-NA-C1A	4.26	111.87	106.36
13	B	836	CLA	C4A-NA-C1A	4.27	111.89	106.36
16	A	854	BCR	C7-C8-C9	4.28	132.74	126.22
13	A	837	CLA	O2D-CGD-CBD	4.29	117.18	111.30
16	A	852	BCR	C33-C5-C6	4.30	128.82	124.61
13	A	846	CLA	C4A-NA-C1A	4.32	111.94	106.36
13	A	802	CLA	O2D-CGD-CBD	4.33	117.24	111.30
13	J	101	CLA	C4A-NA-C1A	4.35	111.98	106.36
16	B	849	BCR	C38-C26-C25	4.37	128.90	124.61
13	B	821	CLA	C4A-NA-C1A	4.38	112.02	106.36
13	X	1701	CLA	C4A-NA-C1A	4.38	112.03	106.36
13	B	812	CLA	C4A-NA-C1A	4.38	112.03	106.36
13	B	823	CLA	O2D-CGD-CBD	4.39	117.31	111.30
13	A	838	CLA	O2D-CGD-CBD	4.39	117.32	111.30
13	A	816	CLA	C4A-NA-C1A	4.39	112.04	106.36
13	B	818	CLA	O2D-CGD-CBD	4.39	117.32	111.30
13	A	821	CLA	C4A-NA-C1A	4.40	112.06	106.36
16	B	845	BCR	C7-C8-C9	4.41	132.93	126.22
16	B	847	BCR	C38-C26-C25	4.41	128.93	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	841	CLA	O2D-CGD-CBD	4.41	117.35	111.30
13	A	813	CLA	C4A-NA-C1A	4.41	112.06	106.36
13	A	842	CLA	O2D-CGD-CBD	4.41	117.35	111.30
16	A	854	BCR	C38-C26-C25	4.42	128.94	124.61
13	B	827	CLA	O2D-CGD-CBD	4.42	117.36	111.30
16	B	849	BCR	C33-C5-C6	4.43	128.96	124.61
13	A	827	CLA	O2D-CGD-CBD	4.44	117.39	111.30
13	B	838	CLA	O2D-CGD-CBD	4.45	117.41	111.30
13	A	815	CLA	O2D-CGD-CBD	4.46	117.41	111.30
16	F	1302	BCR	C33-C5-C6	4.46	128.98	124.61
16	A	850	BCR	C33-C5-C6	4.46	128.98	124.61
13	M	1601	CLA	C4A-NA-C1A	4.47	112.14	106.36
13	A	834	CLA	O2D-CGD-CBD	4.47	117.44	111.30
13	L	1003	CLA	O2D-CGD-CBD	4.49	117.46	111.30
13	B	827	CLA	O2A-CGA-CBA	4.50	125.61	111.90
13	A	833	CLA	C4A-NA-C1A	4.51	112.19	106.36
17	A	856	LHG	C25-C24-C23	4.53	137.56	114.17
13	A	833	CLA	O2D-CGD-CBD	4.53	117.52	111.30
16	A	854	BCR	C33-C5-C6	4.54	129.06	124.61
13	B	812	CLA	O2D-CGD-CBD	4.54	117.52	111.30
16	I	102	BCR	C38-C26-C25	4.55	129.07	124.61
13	X	1701	CLA	O2D-CGD-CBD	4.55	117.54	111.30
13	B	816	CLA	O2D-CGD-CBD	4.56	117.55	111.30
16	J	103	BCR	C33-C5-C6	4.57	129.09	124.61
13	B	820	CLA	C4A-NA-C1A	4.57	112.27	106.36
13	A	821	CLA	O2D-CGD-CBD	4.58	117.58	111.30
13	L	1004	CLA	O2D-CGD-CBD	4.59	117.60	111.30
13	A	817	CLA	O2D-CGD-CBD	4.59	117.60	111.30
16	B	846	BCR	C38-C26-C25	4.61	129.13	124.61
16	B	844	BCR	C33-C5-C6	4.63	129.15	124.61
13	A	840	CLA	O2D-CGD-CBD	4.63	117.65	111.30
13	A	830	CLA	O2D-CGD-CBD	4.65	117.68	111.30
13	B	807	CLA	O2D-CGD-CBD	4.66	117.69	111.30
16	L	1005	BCR	C38-C26-C25	4.71	129.22	124.61
13	B	834	CLA	O2D-CGD-CBD	4.80	117.88	111.30
13	A	807	CLA	O2A-CGA-CBA	4.80	126.53	111.90
13	B	831	CLA	O2D-CGD-CBD	4.84	117.94	111.30
16	A	849	BCR	C33-C5-C6	4.85	129.37	124.61
16	B	845	BCR	C38-C26-C25	4.85	129.37	124.61
16	A	851	BCR	C33-C5-C6	4.88	129.39	124.61
16	A	852	BCR	C38-C26-C25	4.89	129.40	124.61
13	A	814	CLA	O2D-CGD-CBD	4.89	118.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	823	CLA	O2D-CGD-CBD	4.90	118.02	111.30
16	B	848	BCR	C38-C26-C25	4.90	129.42	124.61
16	I	101	BCR	C38-C26-C25	4.91	129.42	124.61
13	B	824	CLA	O2D-CGD-CBD	4.91	118.04	111.30
16	M	1602	BCR	C38-C26-C25	4.93	129.44	124.61
13	A	806	CLA	O2D-CGD-CBD	4.99	118.15	111.30
13	K	1401	CLA	O2D-CGD-CBD	5.00	118.16	111.30
16	L	1006	BCR	C38-C26-C25	5.01	129.52	124.61
13	B	805	CLA	O2D-CGD-CBD	5.03	118.20	111.30
13	J	101	CLA	O2D-CGD-CBD	5.05	118.22	111.30
13	B	826	CLA	O2D-CGD-CBD	5.05	118.23	111.30
16	A	850	BCR	C38-C26-C25	5.06	129.57	124.61
16	F	1302	BCR	C38-C26-C25	5.07	129.59	124.61
13	B	813	CLA	O2D-CGD-CBD	5.09	118.29	111.30
13	A	824	CLA	O2D-CGD-CBD	5.09	118.29	111.30
13	B	821	CLA	O2D-CGD-CBD	5.10	118.30	111.30
13	B	830	CLA	O2D-CGD-CBD	5.13	118.34	111.30
13	B	837	CLA	O2D-CGD-CBD	5.15	118.36	111.30
16	J	105	BCR	C38-C26-C25	5.16	129.68	124.61
13	A	832	CLA	O2D-CGD-CBD	5.22	118.47	111.30
16	B	847	BCR	C33-C5-C6	5.24	129.75	124.61
16	B	843	BCR	C33-C5-C6	5.24	129.75	124.61
16	A	851	BCR	C38-C26-C25	5.24	129.75	124.61
13	M	1601	CLA	O2D-CGD-CBD	5.25	118.50	111.30
13	B	832	CLA	O2D-CGD-CBD	5.25	118.50	111.30
16	I	101	BCR	C33-C5-C6	5.28	129.79	124.61
13	B	820	CLA	O2D-CGD-CBD	5.30	118.58	111.30
16	B	845	BCR	C33-C5-C6	5.32	129.83	124.61
16	J	105	BCR	C33-C5-C6	5.33	129.84	124.61
13	A	831	CLA	O2D-CGD-CBD	5.34	118.62	111.30
13	A	809	CLA	O2D-CGD-CBD	5.36	118.65	111.30
13	A	804	CLA	O2D-CGD-CBD	5.39	118.69	111.30
13	A	826	CLA	O2D-CGD-CBD	5.42	118.73	111.30
13	A	816	CLA	O2D-CGD-CBD	5.46	118.80	111.30
13	B	825	CLA	O2D-CGD-CBD	5.48	118.82	111.30
13	A	828	CLA	O2D-CGD-CBD	5.51	118.85	111.30
16	L	1005	BCR	C33-C5-C6	5.51	130.01	124.61
13	B	815	CLA	O2D-CGD-CBD	5.57	118.94	111.30
18	B	850	LMG	C30-C29-C28	5.68	135.91	113.59
17	A	855	LHG	C25-C24-C23	5.74	136.17	113.59
13	B	814	CLA	O2D-CGD-CBD	5.75	119.19	111.30
16	L	1006	BCR	C33-C5-C6	5.76	130.26	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	103	BCR	C38-C26-C25	5.76	130.26	124.61
16	B	848	BCR	C33-C5-C6	5.77	130.27	124.61
16	A	849	BCR	C38-C26-C25	5.77	130.27	124.61
13	B	833	CLA	O2D-CGD-CBD	5.78	119.23	111.30
13	A	846	CLA	O2D-CGD-CBD	5.79	119.24	111.30
13	B	808	CLA	O2D-CGD-CBD	5.85	119.33	111.30
13	A	805	CLA	O2D-CGD-CBD	5.89	119.39	111.30
13	L	1002	CLA	O2D-CGD-CBD	6.02	119.56	111.30
13	B	804	CLA	O2D-CGD-CBD	6.12	119.69	111.30
13	A	835	CLA	O2D-CGD-CBD	6.25	119.87	111.30
16	A	853	BCR	C38-C26-C25	6.27	130.76	124.61
13	B	829	CLA	O2D-CGD-CBD	6.29	119.93	111.30
13	B	802	CLA	O2D-CGD-CBD	6.29	119.93	111.30
16	B	844	BCR	C38-C26-C25	6.54	131.02	124.61
16	B	843	BCR	C38-C26-C25	6.71	131.20	124.61
14	B	842	PQN	C14-C13-C15	6.93	125.98	115.41
14	A	847	PQN	C14-C13-C15	8.07	127.74	115.41
13	A	801	CLA	O2D-CGD-CBD	11.00	126.39	111.30

All (249) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	1004	CLA	NC
13	L	1004	CLA	ND
13	L	1004	CLA	NA
13	A	829	CLA	ND
13	A	820	CLA	NC
13	A	820	CLA	ND
13	A	820	CLA	NA
13	A	818	CLA	NA
13	A	804	CLA	NC
13	A	804	CLA	ND
13	A	804	CLA	NA
13	A	843	CLA	NC
13	A	843	CLA	ND
13	A	843	CLA	NA
13	B	806	CLA	NA
13	B	806	CLA	NC
13	B	806	CLA	ND
13	B	811	CLA	ND
13	B	811	CLA	NA
13	J	101	CLA	NC

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Mol	Chain	Res	Type	Atom
13	J	101	CLA	ND
13	J	101	CLA	NA
13	B	836	CLA	NC
13	B	836	CLA	ND
13	B	836	CLA	NA
13	B	804	CLA	ND
13	B	804	CLA	NA
13	A	845	CLA	NC
13	A	845	CLA	ND
13	A	845	CLA	NA
13	B	825	CLA	NC
13	B	825	CLA	ND
13	B	825	CLA	NA
13	F	1301	CLA	NC
13	F	1301	CLA	ND
13	F	1301	CLA	NA
13	B	838	CLA	NC
13	B	838	CLA	ND
13	B	838	CLA	NA
13	M	1601	CLA	NC
13	M	1601	CLA	ND
13	M	1601	CLA	NA
13	A	839	CLA	ND
13	A	839	CLA	NA
13	A	815	CLA	NC
13	A	815	CLA	ND
13	A	815	CLA	NA
13	B	826	CLA	NC
13	B	826	CLA	ND
13	B	826	CLA	NA
13	B	823	CLA	NC
13	B	823	CLA	ND
13	B	823	CLA	NA
13	A	836	CLA	NC
13	A	836	CLA	ND
13	A	836	CLA	NA
13	A	835	CLA	NC
13	A	835	CLA	ND
13	A	835	CLA	NA
13	A	830	CLA	NC
13	A	830	CLA	ND
13	B	835	CLA	NC

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Mol	Chain	Res	Type	Atom
13	B	835	CLA	ND
13	B	835	CLA	NA
13	A	823	CLA	NC
13	A	823	CLA	ND
13	A	823	CLA	NA
13	B	829	CLA	NC
13	B	829	CLA	ND
13	B	829	CLA	NA
13	A	801	CLA	NC
13	A	801	CLA	ND
13	A	801	CLA	NA
13	B	801	CLA	ND
13	A	826	CLA	NC
13	A	826	CLA	ND
13	A	826	CLA	NA
13	A	825	CLA	NC
13	A	825	CLA	ND
13	A	825	CLA	NA
13	A	846	CLA	NC
13	A	846	CLA	ND
13	A	846	CLA	NA
13	B	822	CLA	NC
13	B	822	CLA	ND
13	B	822	CLA	NA
13	A	806	CLA	NA
13	A	806	CLA	NC
13	A	806	CLA	ND
13	B	813	CLA	NA
13	B	813	CLA	NC
13	B	813	CLA	ND
13	B	831	CLA	NC
13	B	831	CLA	ND
13	B	831	CLA	NA
13	J	102	CLA	NC
13	J	102	CLA	ND
13	J	102	CLA	NA
13	B	820	CLA	NC
13	B	820	CLA	ND
13	B	820	CLA	NA
13	B	810	CLA	NC
13	B	810	CLA	ND
13	B	810	CLA	NA

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Mol	Chain	Res	Type	Atom
13	A	816	CLA	NC
13	A	816	CLA	ND
13	A	816	CLA	NA
13	A	819	CLA	NC
13	A	819	CLA	ND
13	A	819	CLA	NA
13	A	813	CLA	NC
13	A	813	CLA	ND
13	A	813	CLA	NA
13	B	833	CLA	NC
13	B	833	CLA	ND
13	B	833	CLA	NA
13	A	833	CLA	NC
13	A	833	CLA	ND
13	A	833	CLA	NA
13	B	817	CLA	NC
13	B	817	CLA	ND
13	B	817	CLA	NA
13	A	832	CLA	NC
13	A	832	CLA	ND
13	A	832	CLA	NA
13	B	814	CLA	NC
13	B	814	CLA	ND
13	B	814	CLA	NA
13	B	830	CLA	NC
13	B	830	CLA	ND
13	B	830	CLA	NA
13	A	821	CLA	NC
13	A	821	CLA	ND
13	A	821	CLA	NA
13	B	803	CLA	NA
13	B	805	CLA	NA
13	B	805	CLA	NC
13	B	805	CLA	ND
13	B	828	CLA	NA
13	B	827	CLA	ND
13	A	803	CLA	ND
13	A	803	CLA	NA
13	B	808	CLA	ND
13	B	808	CLA	NA
13	L	1002	CLA	NC
13	L	1002	CLA	ND

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Mol	Chain	Res	Type	Atom
13	L	1002	CLA	NA
13	B	807	CLA	NC
13	B	807	CLA	ND
13	B	807	CLA	NA
13	A	814	CLA	NC
13	A	814	CLA	ND
13	A	814	CLA	NA
13	A	837	CLA	NC
13	A	837	CLA	ND
13	A	837	CLA	NA
13	B	824	CLA	NC
13	B	824	CLA	ND
13	B	824	CLA	NA
13	A	840	CLA	ND
13	B	840	CLA	NC
13	B	840	CLA	ND
13	A	844	CLA	NC
13	A	844	CLA	ND
13	A	844	CLA	NA
13	A	812	CLA	NC
13	A	812	CLA	ND
13	A	812	CLA	NA
13	B	812	CLA	NC
13	B	812	CLA	ND
13	B	812	CLA	NA
13	B	818	CLA	NC
13	B	818	CLA	ND
13	B	818	CLA	NA
13	A	838	CLA	NC
13	A	838	CLA	ND
13	A	838	CLA	NA
13	A	824	CLA	ND
13	A	824	CLA	NA
13	B	802	CLA	ND
13	B	802	CLA	NA
13	L	1003	CLA	NC
13	L	1003	CLA	NA
13	A	807	CLA	NC
13	A	807	CLA	ND
13	A	807	CLA	NA
13	A	808	CLA	ND
13	A	808	CLA	NA

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Mol	Chain	Res	Type	Atom
13	A	831	CLA	NC
13	A	831	CLA	ND
13	A	831	CLA	NA
13	B	837	CLA	NC
13	B	837	CLA	ND
13	B	837	CLA	NA
13	B	816	CLA	NC
13	B	816	CLA	ND
13	B	816	CLA	NA
13	A	822	CLA	NC
13	A	822	CLA	ND
13	A	822	CLA	NA
13	B	841	CLA	NC
13	B	841	CLA	NA
13	B	821	CLA	NC
13	B	821	CLA	ND
13	B	821	CLA	NA
13	A	805	CLA	NC
13	A	805	CLA	ND
13	A	805	CLA	NA
13	A	841	CLA	NC
13	A	841	CLA	ND
13	A	841	CLA	NA
13	B	819	CLA	NC
13	B	819	CLA	ND
13	B	819	CLA	NA
13	A	810	CLA	NC
13	A	810	CLA	ND
13	A	810	CLA	NA
13	B	832	CLA	NC
13	B	832	CLA	ND
13	B	832	CLA	NA
13	K	1401	CLA	NC
13	K	1401	CLA	NA
13	A	802	CLA	ND
13	A	802	CLA	NA
13	B	809	CLA	ND
13	A	828	CLA	NC
13	A	828	CLA	ND
13	A	828	CLA	NA
13	A	817	CLA	NC
13	A	817	CLA	ND

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Mol	Chain	Res	Type	Atom
13	A	817	CLA	NA
13	B	815	CLA	NC
13	B	815	CLA	NA
13	B	834	CLA	NC
13	B	834	CLA	ND
13	B	834	CLA	NA
13	A	809	CLA	NC
13	A	809	CLA	ND
13	A	809	CLA	NA
13	A	842	CLA	NC
13	A	842	CLA	ND
13	A	842	CLA	NA
17	A	856	LHG	C2
13	A	827	CLA	NC
13	A	827	CLA	ND
13	A	827	CLA	NA
13	X	1701	CLA	NC
13	X	1701	CLA	ND
13	X	1701	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	817	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

114 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	801	CLA	9	0
13	A	802	CLA	3	0
13	A	803	CLA	10	0
13	A	804	CLA	2	0
13	A	805	CLA	1	0
13	A	806	CLA	6	0
13	A	807	CLA	4	0
13	A	808	CLA	2	0
13	A	809	CLA	6	0
13	A	810	CLA	4	0
13	A	811	CLA	4	0
13	A	812	CLA	1	0
13	A	814	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	815	CLA	5	0
13	A	817	CLA	2	0
13	A	819	CLA	4	0
13	A	820	CLA	6	0
13	A	821	CLA	5	0
13	A	822	CLA	4	0
13	A	823	CLA	2	0
13	A	824	CLA	1	0
13	A	825	CLA	2	0
13	A	826	CLA	4	0
13	A	827	CLA	5	0
13	A	828	CLA	3	0
13	A	829	CLA	13	0
13	A	830	CLA	1	0
13	A	831	CLA	6	0
13	A	832	CLA	1	0
13	A	833	CLA	1	0
13	A	835	CLA	4	0
13	A	836	CLA	4	0
13	A	837	CLA	2	0
13	A	838	CLA	2	0
13	A	839	CLA	6	0
13	A	840	CLA	3	0
13	A	841	CLA	2	0
13	A	843	CLA	8	0
13	A	844	CLA	5	0
13	A	845	CLA	1	0
13	A	846	CLA	5	0
14	A	847	PQN	1	0
16	A	849	BCR	2	0
16	A	850	BCR	2	0
16	A	851	BCR	1	0
16	A	852	BCR	4	0
16	A	853	BCR	1	0
16	A	854	BCR	13	0
17	A	855	LHG	4	0
17	A	856	LHG	2	0
13	B	801	CLA	8	0
13	B	802	CLA	17	0
13	B	803	CLA	4	0
13	B	804	CLA	2	0
13	B	805	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	806	CLA	6	0
13	B	807	CLA	1	0
13	B	808	CLA	3	0
13	B	809	CLA	2	0
13	B	810	CLA	5	0
13	B	811	CLA	1	0
13	B	812	CLA	1	0
13	B	813	CLA	6	0
13	B	814	CLA	6	0
13	B	815	CLA	2	0
13	B	816	CLA	3	0
13	B	817	CLA	8	0
13	B	818	CLA	5	0
13	B	819	CLA	5	0
13	B	820	CLA	2	0
13	B	821	CLA	1	0
13	B	822	CLA	4	0
13	B	823	CLA	3	0
13	B	824	CLA	10	0
13	B	825	CLA	2	0
13	B	826	CLA	3	0
13	B	827	CLA	5	0
13	B	828	CLA	8	0
13	B	829	CLA	7	0
13	B	830	CLA	5	0
13	B	831	CLA	2	0
13	B	832	CLA	6	0
13	B	833	CLA	7	0
13	B	835	CLA	3	0
13	B	836	CLA	2	0
13	B	837	CLA	3	0
13	B	838	CLA	2	0
13	B	839	CLA	4	0
13	B	840	CLA	3	0
14	B	842	PQN	1	0
16	B	843	BCR	1	0
16	B	844	BCR	1	0
16	B	845	BCR	5	0
16	B	846	BCR	5	0
16	B	847	BCR	3	0
16	B	848	BCR	1	0
16	B	849	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	850	LMG	5	0
17	B	851	LHG	1	0
13	F	1301	CLA	1	0
16	F	1302	BCR	2	0
16	I	101	BCR	3	0
13	J	101	CLA	1	0
16	J	103	BCR	4	0
16	J	104	BCR	7	0
16	J	105	BCR	5	0
13	K	1401	CLA	1	0
13	L	1002	CLA	2	0
13	L	1003	CLA	8	0
13	L	1004	CLA	2	0
16	L	1006	BCR	1	0
13	M	1601	CLA	1	0
16	M	1602	BCR	2	0
13	X	1701	CLA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.20	17 (2%) 64 59	22, 45, 71, 93	0
2	B	739/740 (99%)	-0.09	25 (3%) 49 46	20, 38, 71, 89	0
3	C	80/80 (100%)	-0.59	0 100 100	22, 33, 45, 54	0
4	D	138/138 (100%)	-0.03	7 (5%) 32 32	27, 41, 56, 84	0
5	E	69/75 (92%)	0.48	7 (10%) 9 14	29, 46, 62, 76	0
6	F	141/164 (85%)	-0.20	1 (0%) 89 85	37, 57, 68, 72	0
7	I	38/38 (100%)	0.41	0 100 100	20, 33, 47, 53	0
8	J	41/41 (100%)	0.07	0 100 100	53, 60, 77, 86	0
9	K	46/83 (55%)	1.08	9 (19%) 1 7	72, 81, 96, 99	0
10	L	151/154 (98%)	0.31	12 (7%) 15 19	19, 26, 47, 67	0
11	M	31/31 (100%)	0.32	0 100 100	30, 38, 52, 62	0
12	X	29/35 (82%)	-0.00	1 (3%) 49 46	58, 63, 81, 88	0
All	All	2243/2334 (96%)	-0.06	79 (3%) 48 45	19, 42, 74, 99	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	THR	7.8
4	D	3	LEU	6.3
4	D	4	THR	5.9
1	A	207	LEU	5.8
10	L	144	VAL	4.8
5	E	1	VAL	4.4
10	L	141	ASN	4.4
4	D	1	THR	4.2
1	A	521	GLY	4.1
2	B	24	ILE	4.0
2	B	697	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	181	LEU	3.8
2	B	680	LEU	3.7
10	L	142	PHE	3.6
9	K	38	GLY	3.5
10	L	72	ASP	3.4
2	B	713	LEU	3.4
1	A	82	VAL	3.4
9	K	36	SER	3.3
5	E	2	GLN	3.3
2	B	696	LEU	3.3
1	A	168	MET	3.3
2	B	184	VAL	3.3
9	K	77	LEU	3.3
1	A	554	LEU	3.2
2	B	21	TRP	3.2
2	B	347	ILE	3.1
9	K	35	GLN	3.1
2	B	608	TRP	3.1
1	A	208	GLY	3.1
1	A	555	LYS	3.1
1	A	83	VAL	3.1
10	L	145	VAL	3.0
2	B	676	TYR	2.9
2	B	541	VAL	2.9
2	B	344	LEU	2.9
10	L	139	LEU	2.9
1	A	522	GLY	2.8
2	B	185	SER	2.8
5	E	53	SER	2.8
4	D	99	GLY	2.8
9	K	76	GLY	2.8
10	L	140	GLU	2.8
2	B	545	LEU	2.7
1	A	204	LEU	2.7
2	B	182	PHE	2.7
1	A	737	LEU	2.7
1	A	84	PHE	2.7
2	B	25	ALA	2.6
12	X	7	PRO	2.6
10	L	143	LEU	2.6
5	E	69	ALA	2.6
10	L	109	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	594	HIS	2.5
10	L	73	VAL	2.5
9	K	42	GLY	2.5
4	D	5	GLY	2.5
9	K	39	LYS	2.4
1	A	327	GLU	2.4
9	K	75	SER	2.4
1	A	366	LEU	2.4
10	L	111	LEU	2.4
2	B	681	ILE	2.3
1	A	557	VAL	2.3
2	B	20	ILE	2.3
2	B	703	PRO	2.3
2	B	611	ASN	2.3
9	K	40	GLY	2.2
2	B	437	LEU	2.2
5	E	67	GLU	2.2
2	B	282	LEU	2.2
5	E	27	ASP	2.2
4	D	98	ASP	2.2
2	B	384	PHE	2.1
1	A	230	GLY	2.1
2	B	343	CYS	2.1
6	F	141	ARG	2.1
10	L	146	ASP	2.1
5	E	3	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	BCR	B	845	40/40	0.74	1.29	9.49	33,51,87,88	0
13	CLA	A	843	65/65	0.90	1.48	6.80	29,35,60,60	0
13	CLA	B	831	49/65	0.83	0.82	6.19	36,40,63,65	0
16	BCR	J	104	40/40	0.86	0.87	5.98	61,69,75,76	0
13	CLA	M	1601	45/65	0.78	0.87	5.20	96,97,99,100	0
13	CLA	A	836	54/65	0.92	0.59	4.88	46,50,64,64	0
16	BCR	B	844	40/40	0.69	1.82	4.71	56,68,93,93	0
16	BCR	A	852	40/40	0.57	1.14	4.68	47,60,96,96	0
16	BCR	A	854	40/40	0.93	1.45	4.64	29,39,50,53	0
16	BCR	M	1602	40/40	0.83	0.88	4.54	28,37,59,62	0
13	CLA	A	837	45/65	0.87	0.56	4.43	60,68,76,80	0
16	BCR	I	101	40/40	0.86	0.78	4.29	19,27,40,40	0
13	CLA	B	809	65/65	0.94	0.72	4.13	20,26,61,62	0
13	CLA	A	804	65/65	0.92	0.83	4.12	45,50,80,83	0
13	CLA	A	825	59/65	0.85	0.74	3.98	34,43,76,76	0
13	CLA	J	101	45/65	0.72	0.70	3.89	98,99,100,100	0
13	CLA	B	841	65/65	0.85	1.15	3.79	22,29,44,50	0
16	BCR	B	847	40/40	0.88	0.97	3.73	46,53,61,61	0
16	BCR	B	843	40/40	0.77	0.86	3.64	88,90,97,98	0
16	BCR	F	1302	40/40	0.88	0.77	3.57	43,49,60,60	0
16	BCR	J	103	40/40	0.89	1.37	3.53	55,58,60,60	0
16	BCR	L	1006	40/40	0.89	0.45	3.48	26,35,66,67	0
16	BCR	J	105	40/40	0.73	0.78	3.46	53,67,93,94	0
14	PQN	A	847	33/33	0.92	0.77	3.39	41,43,67,68	0
13	CLA	A	809	65/65	0.94	0.75	3.39	33,40,66,67	0
13	CLA	B	830	45/65	0.83	0.69	3.31	51,54,67,72	0
16	BCR	B	848	40/40	0.92	0.96	3.27	40,52,58,58	0
13	CLA	A	839	65/65	0.87	0.70	3.09	32,38,58,59	0
16	BCR	L	1005	40/40	0.84	1.37	2.97	20,24,29,30	0
13	CLA	A	845	41/65	0.73	0.82	2.61	87,90,92,93	0
13	CLA	B	828	65/65	0.90	1.11	2.57	31,35,48,52	0
13	CLA	B	840	65/65	0.74	1.10	2.56	13,18,41,42	0
13	CLA	B	834	45/65	0.96	0.47	2.56	40,47,53,56	0
13	CLA	B	839	47/65	0.84	0.55	2.56	41,47,55,60	0
13	CLA	B	832	65/65	0.88	0.63	2.53	37,43,65,66	0
16	BCR	A	853	40/40	0.76	1.16	2.53	30,37,59,60	0
13	CLA	A	844	65/65	0.78	0.93	2.48	17,22,43,47	0
13	CLA	B	833	58/65	0.77	0.70	2.45	36,47,77,78	0
16	BCR	B	849	40/40	0.84	1.07	2.42	23,27,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	CLA	B	815	45/65	0.76	0.55	2.40	57,62,73,77	0
13	CLA	A	834	65/65	0.84	1.04	2.40	24,28,43,44	0
13	CLA	X	1701	45/65	0.89	0.46	2.39	77,83,86,88	0
13	CLA	A	819	54/65	0.93	0.39	2.36	44,50,54,56	0
13	CLA	A	829	65/65	0.98	0.61	2.36	38,46,74,75	0
13	CLA	B	811	45/65	0.80	0.39	2.34	42,49,62,66	0
13	CLA	A	810	65/65	0.85	0.90	2.31	39,43,77,78	0
18	LMG	B	850	55/55	0.69	1.11	2.30	34,40,57,60	0
17	LHG	A	856	27/49	0.92	0.40	2.29	51,56,60,61	0
13	CLA	A	846	52/65	0.82	0.54	2.24	69,75,97,99	0
17	LHG	A	855	49/49	0.79	0.76	2.21	39,50,60,63	0
13	CLA	B	814	65/65	0.82	0.65	2.21	34,43,68,69	0
13	CLA	A	827	65/65	0.79	0.64	2.16	24,31,83,85	0
13	CLA	B	806	65/65	0.94	0.98	2.15	30,34,53,54	0
13	CLA	A	833	65/65	0.87	0.80	2.15	20,31,85,88	0
13	CLA	B	807	65/65	0.92	0.52	2.06	21,24,50,53	0
13	CLA	A	838	51/65	0.86	0.34	2.05	30,35,45,46	0
13	CLA	B	804	54/65	0.92	0.84	1.92	20,29,48,52	0
13	CLA	B	829	65/65	0.94	0.89	1.91	18,29,63,65	0
13	CLA	B	821	45/65	0.80	0.49	1.84	80,81,90,93	0
13	CLA	A	803	65/65	0.94	0.71	1.83	33,41,51,54	0
13	CLA	A	841	65/65	0.97	0.42	1.80	33,38,55,55	0
13	CLA	B	808	65/65	0.96	0.56	1.79	21,28,49,50	0
13	CLA	A	802	65/65	0.92	0.53	1.78	23,26,35,39	0
13	CLA	B	827	65/65	0.96	0.64	1.74	24,31,77,80	0
16	BCR	A	851	40/40	0.73	1.46	1.74	47,61,89,89	0
16	BCR	A	850	40/40	0.76	1.29	1.73	57,61,79,79	0
13	CLA	A	816	45/65	0.79	0.63	1.70	78,82,83,83	0
13	CLA	B	816	55/65	0.74	0.63	1.61	54,60,85,87	0
13	CLA	B	835	45/65	0.93	0.46	1.59	58,61,70,75	0
14	PQN	B	842	33/33	0.94	0.96	1.58	24,29,36,36	0
13	CLA	A	835	65/65	0.95	0.49	1.56	14,19,36,40	0
13	CLA	B	825	46/65	0.89	0.49	1.54	29,36,46,48	0
13	CLA	A	817	49/65	0.85	0.47	1.52	87,90,92,94	0
13	CLA	A	822	65/65	0.76	0.83	1.52	41,45,55,57	0
13	CLA	B	813	65/65	0.92	0.90	1.49	49,59,68,70	0
13	CLA	B	818	60/65	0.94	0.86	1.48	33,39,64,66	0
13	CLA	F	1301	45/65	0.82	0.53	1.48	75,77,82,83	0
13	CLA	A	830	65/65	0.93	0.72	1.47	33,40,52,55	0
16	BCR	B	846	25/40	0.82	0.98	1.46	64,66,69,70	0
16	BCR	A	849	40/40	0.83	0.80	1.46	62,69,79,79	0
13	CLA	B	802	65/65	0.96	0.53	1.41	28,39,55,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	CLA	B	819	65/65	0.84	0.74	1.40	78,82,99,100	0
13	CLA	A	842	51/65	0.94	0.45	1.34	38,43,70,71	0
13	CLA	L	1004	65/65	0.84	0.82	1.32	22,31,61,62	0
13	CLA	B	838	65/65	0.92	0.46	1.30	38,44,74,78	0
13	CLA	B	820	47/65	0.74	0.67	1.20	88,92,97,97	0
13	CLA	B	822	55/65	0.93	0.35	1.20	69,70,88,89	0
13	CLA	B	826	65/65	0.85	0.65	1.19	31,39,63,65	0
13	CLA	A	828	65/65	0.84	0.56	1.19	32,42,66,68	0
13	CLA	B	817	59/65	0.92	0.54	1.15	39,47,66,70	0
13	CLA	B	812	45/65	0.62	0.57	1.12	66,69,80,85	0
13	CLA	A	840	47/65	0.85	0.70	1.07	30,35,52,57	0
13	CLA	A	818	54/65	0.84	0.51	1.06	63,66,68,69	0
13	CLA	L	1003	65/65	0.89	0.79	1.05	17,23,66,67	0
13	CLA	A	820	65/65	0.93	0.59	1.04	43,48,56,58	0
13	CLA	A	824	51/65	0.78	0.66	1.03	53,59,77,77	0
13	CLA	A	812	65/65	0.81	0.45	1.00	63,65,72,74	0
16	BCR	I	102	40/40	0.92	0.59	0.96	19,26,31,32	0
13	CLA	A	807	65/65	0.91	0.77	0.96	38,43,51,52	0
13	CLA	A	821	61/65	0.82	0.74	0.95	56,62,85,85	0
13	CLA	A	831	65/65	0.94	0.53	0.93	35,43,52,53	0
13	CLA	B	837	60/65	0.95	0.33	0.91	42,48,70,71	0
13	CLA	B	803	65/65	0.86	0.62	0.87	24,29,35,36	0
13	CLA	L	1002	65/65	0.92	0.57	0.85	21,27,58,61	0
13	CLA	A	814	60/65	0.88	0.69	0.85	49,53,80,81	0
13	CLA	A	801	65/65	0.93	0.39	0.83	22,27,36,38	0
13	CLA	B	805	65/65	0.92	0.65	0.82	28,37,66,69	0
13	CLA	A	806	65/65	0.90	0.61	0.80	33,39,68,70	0
13	CLA	B	823	45/65	0.93	0.36	0.79	58,62,70,73	0
13	CLA	K	1401	45/65	0.80	0.66	0.78	70,74,81,84	0
13	CLA	A	808	51/65	0.81	0.46	0.75	55,58,79,79	0
15	SF4	C	101	8/8	0.97	0.24	0.74	24,25,26,26	0
13	CLA	A	805	59/65	0.89	0.46	0.71	40,46,85,86	0
17	LHG	B	851	23/49	0.83	0.47	0.66	79,89,92,93	0
13	CLA	A	832	50/65	0.94	0.43	0.64	32,37,58,59	0
13	CLA	A	826	65/65	0.90	0.45	0.60	45,49,62,63	0
13	CLA	B	810	65/65	0.90	0.53	0.59	15,23,43,44	0
13	CLA	A	811	45/65	0.77	0.39	0.56	68,71,75,76	0
13	CLA	A	815	45/65	0.89	0.36	0.53	64,66,67,68	0
13	CLA	A	813	54/65	0.84	0.56	0.39	44,47,76,77	0
13	CLA	B	801	65/65	0.92	0.31	0.35	22,30,38,46	0
13	CLA	B	824	54/65	0.91	0.51	0.18	54,59,69,71	0
13	CLA	A	823	49/65	0.71	0.50	0.08	64,68,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	SF4	C	102	8/8	0.93	0.21	-0.06	33,34,35,35	0
19	CA	L	1001	1/1	0.79	0.17	-0.88	27,27,27,27	0
15	SF4	A	848	8/8	0.99	0.18	-1.54	25,26,27,27	0
13	CLA	J	102	37/65	0.61	0.94	-	95,96,97,97	0
13	CLA	B	836	45/65	0.81	0.41	-	78,82,85,87	0

6.5 Other polymers

There are no such residues in this entry.