



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:27 am GMT

PDB ID : 3A0H
Title : Crystal structure of I-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-17
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

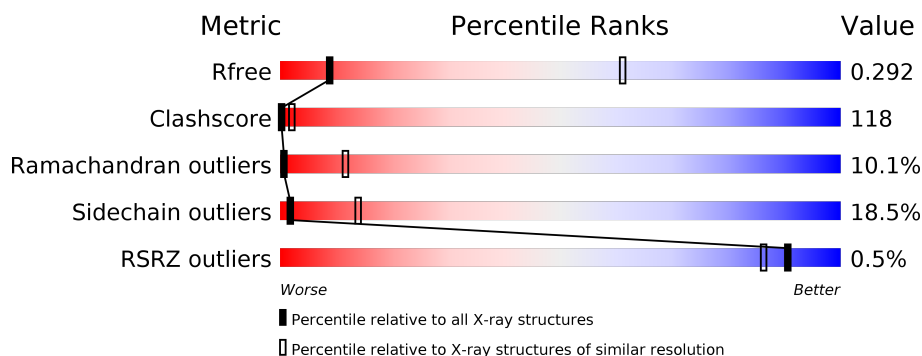
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	488	
2	b	488	
3	C	447	
3	c	447	


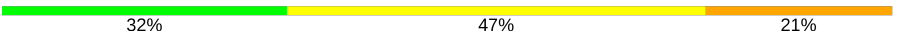







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Mol	Chain	Length	Quality of chain
4	D	340	
4	d	340	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	35	
8	i	35	
9	J	40	
9	j	40	
10	K	36	
10	k	36	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	242	
13	o	242	
14	T	30	
14	t	30	
15	U	98	
15	u	98	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	34	
17	x	34	
18	Y	28	
18	y	28	
19	N	23	
19	n	23	
20	Z	62	
20	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	1003	X	-	X	-
23	CLA	A	1006	X	-	X	X
23	CLA	A	1007	X	-	X	X
23	CLA	B	1009	X	-	X	-
23	CLA	B	1010	X	-	X	-
23	CLA	B	1011	X	-	X	-
23	CLA	B	1012	X	-	X	-
23	CLA	B	1013	X	-	X	-
23	CLA	B	1014	X	-	X	-
23	CLA	B	1015	X	-	X	-
23	CLA	B	1016	X	-	X	-
23	CLA	B	1018	X	-	X	X
23	CLA	B	1019	X	-	X	-
23	CLA	B	1020	X	-	X	-
23	CLA	B	1021	X	-	X	-
23	CLA	B	1022	X	-	X	-
23	CLA	B	1023	X	-	X	-
23	CLA	B	1024	X	-	X	X
23	CLA	C	1025	X	-	X	-
23	CLA	C	1026	X	-	X	X
23	CLA	C	1027	X	-	X	X
23	CLA	C	1028	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	1029	X	-	X	-
23	CLA	C	1030	X	-	X	-
23	CLA	C	1031	X	-	X	-
23	CLA	C	1032	X	-	X	-
23	CLA	C	1033	X	-	X	-
23	CLA	C	1035	X	-	X	-
23	CLA	C	1036	X	-	X	-
23	CLA	C	1037	X	-	X	X
23	CLA	D	1004	X	-	X	-
23	CLA	D	1005	X	-	X	X
23	CLA	D	1008	X	-	X	X
23	CLA	H	1017	X	-	X	X
23	CLA	K	1034	X	-	X	X
23	CLA	a	6003	X	-	-	-
23	CLA	a	6006	X	-	-	-
23	CLA	a	6007	X	-	-	X
23	CLA	b	6009	X	-	-	X
23	CLA	b	6010	X	-	-	-
23	CLA	b	6011	X	-	-	-
23	CLA	b	6012	X	-	-	X
23	CLA	b	6013	X	-	-	-
23	CLA	b	6014	X	-	-	X
23	CLA	b	6015	X	-	-	-
23	CLA	b	6016	X	-	-	-
23	CLA	b	6018	X	-	-	-
23	CLA	b	6019	X	-	-	-
23	CLA	b	6020	X	-	-	-
23	CLA	b	6021	X	-	-	X
23	CLA	b	6022	X	-	-	-
23	CLA	b	6023	X	-	-	-
23	CLA	b	6024	X	-	-	-
23	CLA	c	6025	X	-	-	-
23	CLA	c	6026	X	-	-	X
23	CLA	c	6027	X	-	-	X
23	CLA	c	6028	X	-	-	X
23	CLA	c	6029	X	-	-	X
23	CLA	c	6030	X	-	-	-
23	CLA	c	6031	X	-	-	X
23	CLA	c	6032	X	-	-	-
23	CLA	c	6033	X	-	-	-
23	CLA	c	6035	X	-	-	X
23	CLA	c	6036	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6037	X	-	-	X
23	CLA	d	6004	X	-	-	-
23	CLA	d	6005	X	-	-	X
23	CLA	d	6008	X	-	-	X
23	CLA	h	6017	X	-	-	X
23	CLA	k	6034	X	-	-	X
24	PHO	A	1038	X	-	X	-
24	PHO	D	1039	X	-	X	X
24	PHO	a	6038	X	-	-	X
24	PHO	d	6039	X	-	-	-
25	PQ9	A	1043	-	-	X	X
25	PQ9	D	1042	-	-	X	X
25	PQ9	d	6042	-	-	-	X
26	BCR	A	1044	-	-	X	X
26	BCR	B	1045	-	-	X	X
26	BCR	B	1047	-	-	X	X
26	BCR	B	1048	-	-	X	X
26	BCR	C	1052	-	-	X	-
26	BCR	C	1054	-	-	X	X
26	BCR	D	1050	-	-	X	X
26	BCR	H	1049	-	-	X	X
26	BCR	K	1051	-	-	X	X
26	BCR	T	6046	-	-	X	X
26	BCR	T	6048	-	-	-	X
26	BCR	Z	1053	-	-	-	X
26	BCR	a	6044	-	-	-	X
26	BCR	b	6045	-	-	-	X
26	BCR	b	6047	-	-	-	X
26	BCR	c	6054	-	-	-	X
26	BCR	d	6050	-	-	-	X
26	BCR	h	6049	-	-	-	X
26	BCR	k	6051	-	-	-	X
26	BCR	k	6052	-	-	-	X
26	BCR	t	1046	-	-	-	X
26	BCR	z	6053	-	-	-	X
27	LHG	A	1063	-	-	X	X
27	LHG	a	6063	-	-	-	X
28	IOD	B	1067	-	-	X	-
28	IOD	D	1064	-	-	X	-
28	IOD	D	1068	-	-	X	X
28	IOD	T	1066	-	-	X	-
28	IOD	d	6068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	DGD	B	1058	-	-	X	-
29	DGD	C	1055	-	-	X	X
29	DGD	C	1056	-	-	X	X
29	DGD	C	1057	-	-	X	-
29	DGD	b	6058	-	-	-	X
29	DGD	c	6055	-	-	-	X
29	DGD	c	6056	-	-	-	X
30	MGE	B	1060	-	-	X	X
30	MGE	D	1059	-	-	X	X
30	MGE	D	1062	-	-	X	X
30	MGE	L	1061	-	-	X	X
30	MGE	b	6060	-	-	-	X
30	MGE	d	6059	-	-	-	X
30	MGE	d	6062	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 48060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			
2	b	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			
3	c	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			
8	i	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			278	195	38	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			278	195	38	45			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1860	1162	314	380	4			
13	o	242	Total	C	N	O	S	0	0	0
			1860	1162	314	380	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			783	496	130	157			
15	u	98	Total	C	N	O	0	0	0
			783	496	130	157			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	X	34	Total	C	N	O		0	0	0
			246	166	36	44				
17	x	34	Total	C	N	O		0	0	0
			246	166	36	44				

- Molecule 18 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			
18	y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			

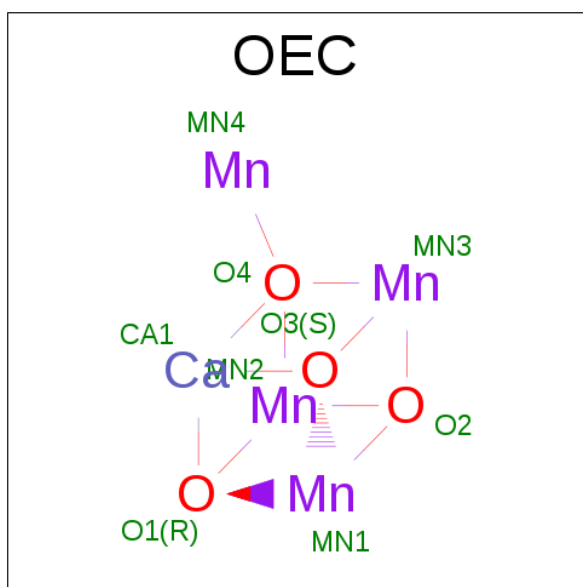
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	23	Total	C	N	O		0	0	0
			116	69	23	24				
19	n	23	Total	C	N	O		0	0	0
			116	69	23	24				

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

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

- Molecule 21 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

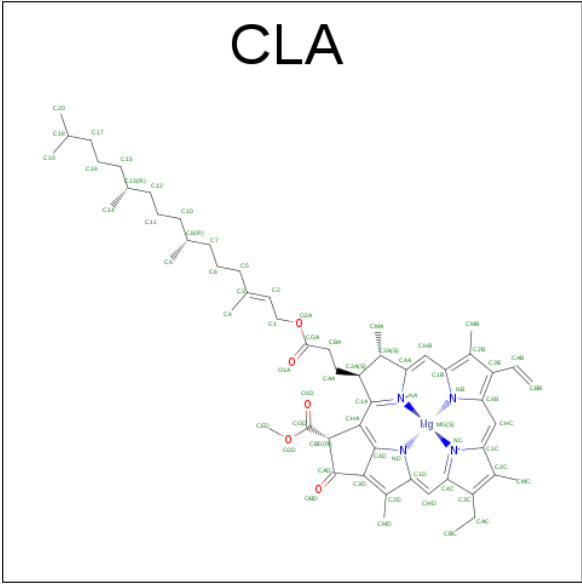


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	0	0
			5	1	4		
21	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Fe	0	0
			1	1		
22	D	1	Total	Fe	0	0
			1	1		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	h	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

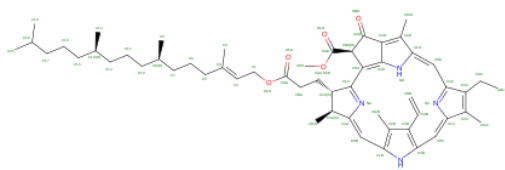
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

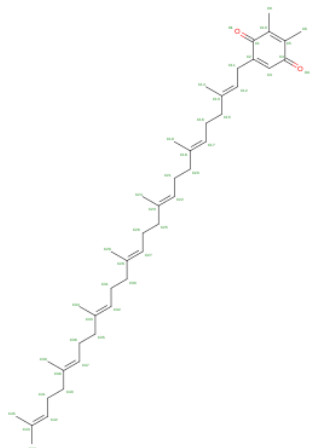
PHO



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

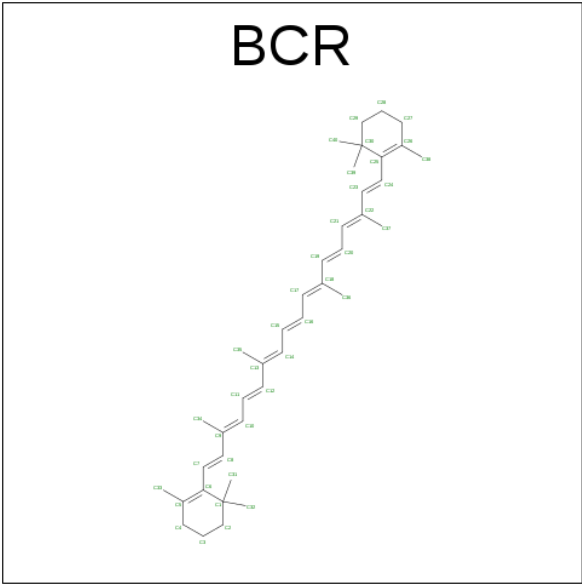
- Molecule 25 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: C₄₃H₆₄O₂).

PQ9



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			45	43	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			45	43	2		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



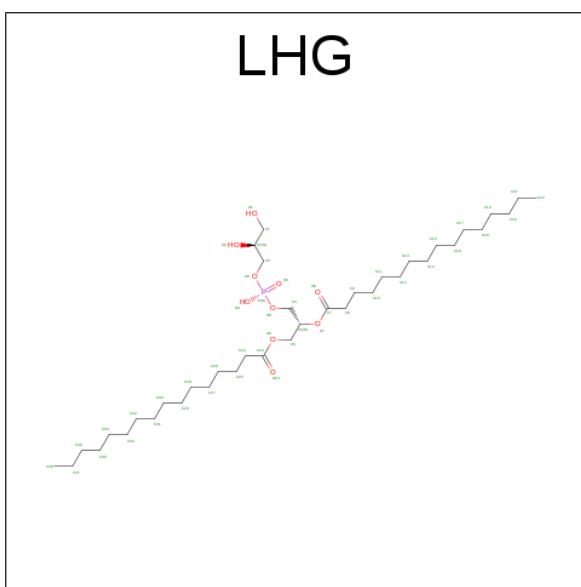
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	Z	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	H	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).

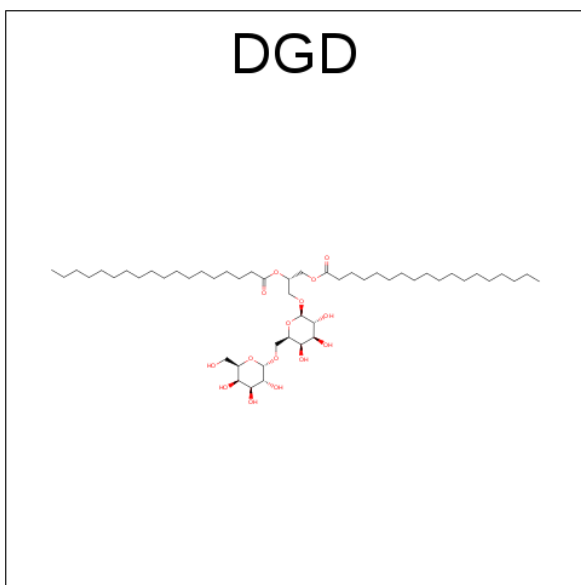


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is IODIDE ION (three-letter code: IOD) (formula: I).

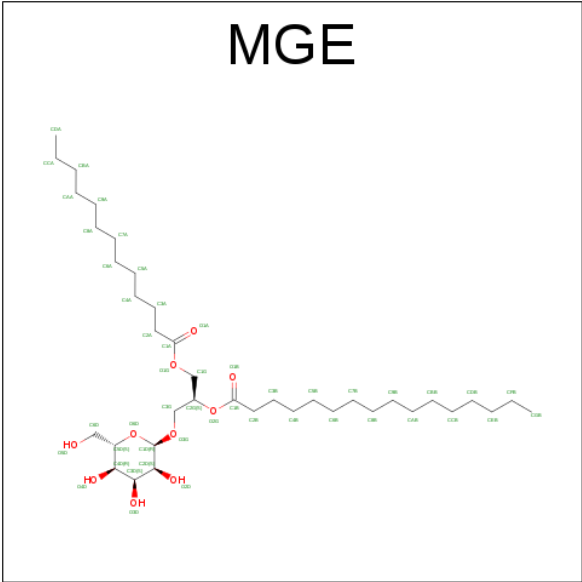
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	d	2	Total	I	0	0
			2	2		
28	B	1	Total	I	0	0
			1	1		
28	a	1	Total	I	0	0
			1	1		
28	A	1	Total	I	0	0
			1	1		
28	T	1	Total	I	0	0
			1	1		
28	D	2	Total	I	0	0
			2	2		
28	t	1	Total	I	0	0
			1	1		
28	b	1	Total	I	0	0
			1	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



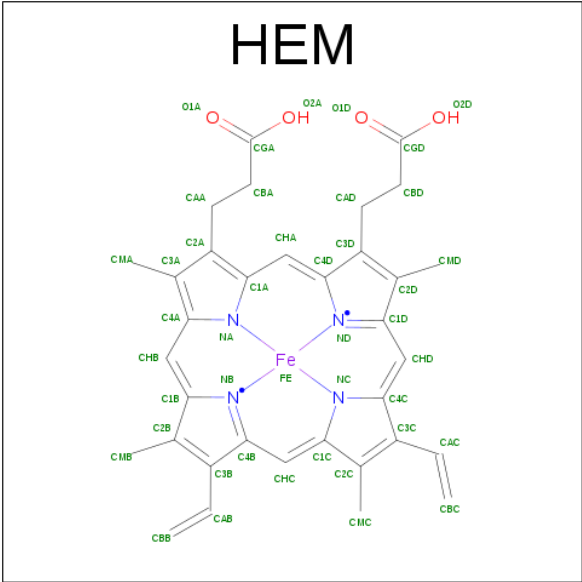
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	B	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	b	1	Total	C	O	0	0
			66	51	15		

- Molecule 30 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total	C	O	0	0
			48	38	10		
30	B	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			48	38	10		
30	L	1	Total	C	O	0	0
			48	38	10		
30	d	1	Total	C	O	0	0
			48	38	10		
30	b	1	Total	C	O	0	0
			48	38	10		
30	d	1	Total	C	O	0	0
			48	38	10		
30	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

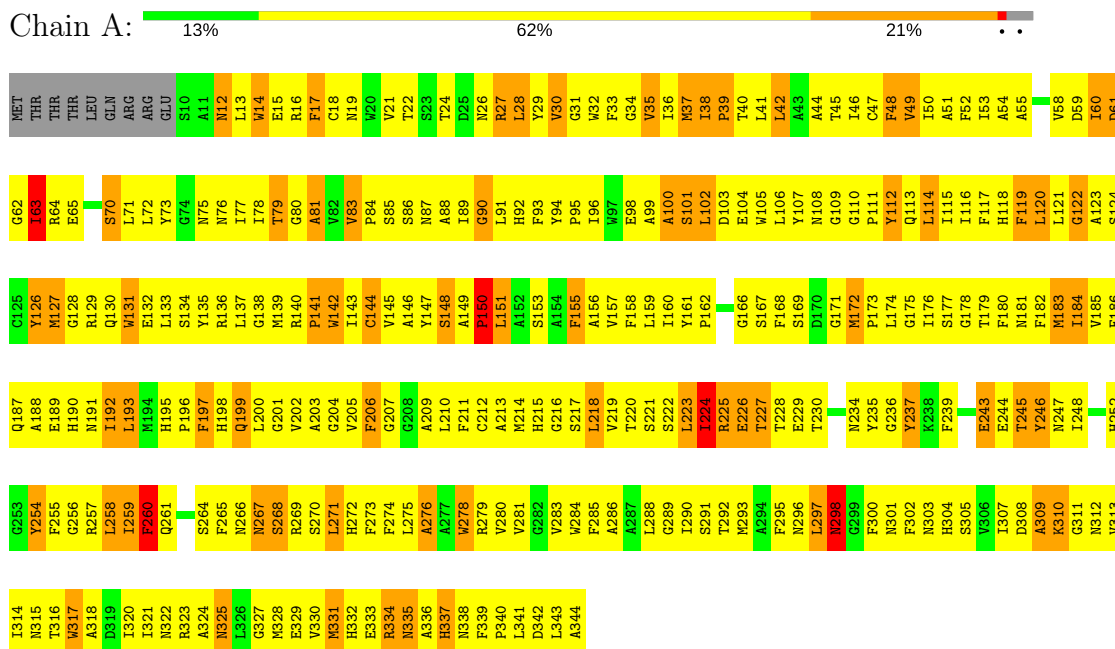


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

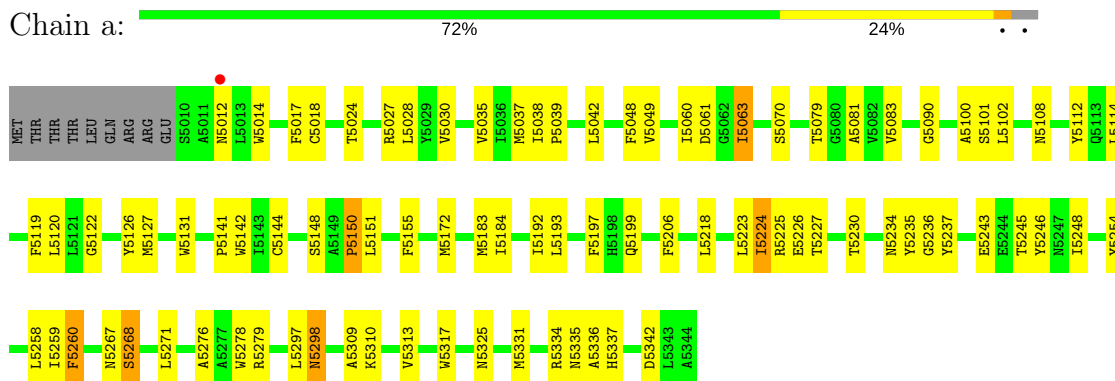
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein

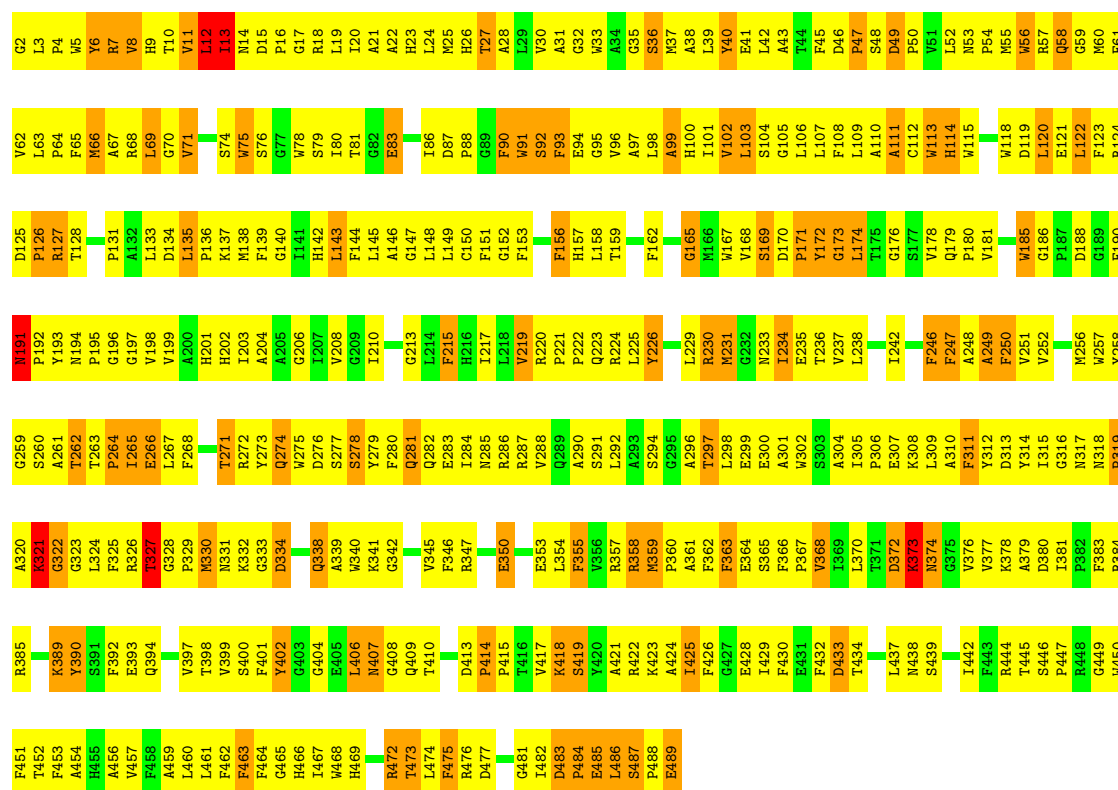


• Molecule 1: Photosystem Q(B) protein



• Molecule 2: Photosystem II core light harvesting protein





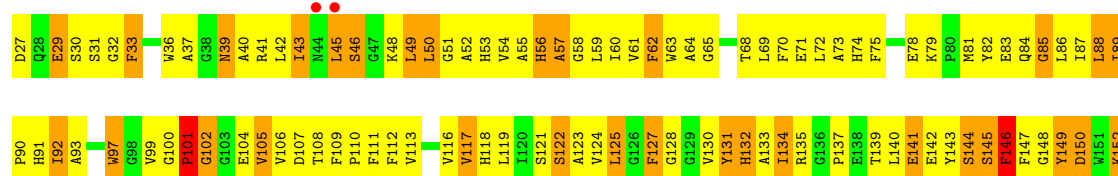
• Molecule 2: Photosystem II core light harvesting protein

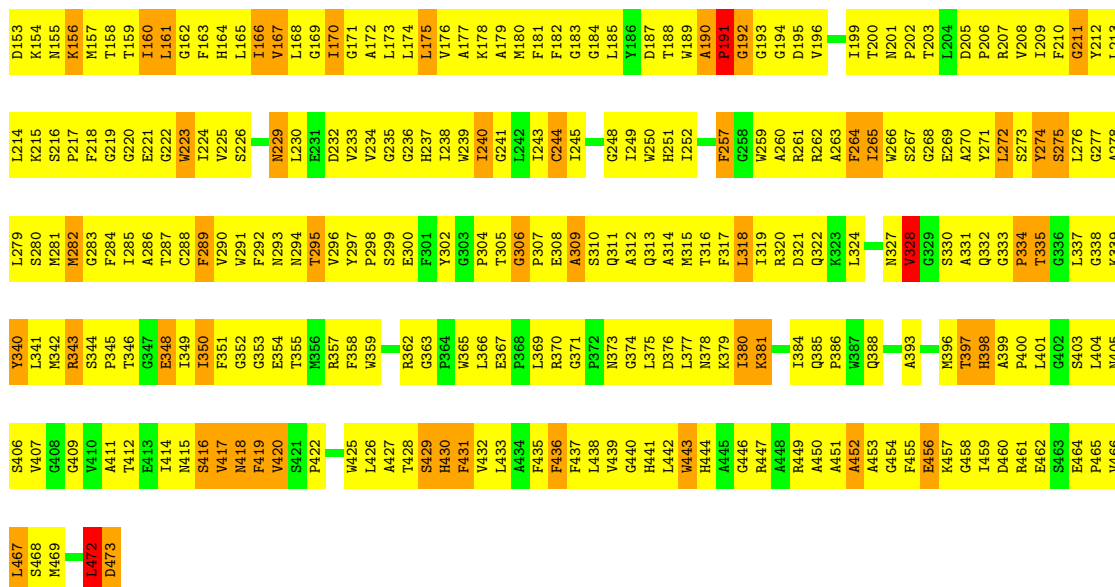
Chain b: 77% 22%



• Molecule 3: Photosystem II CP43 protein

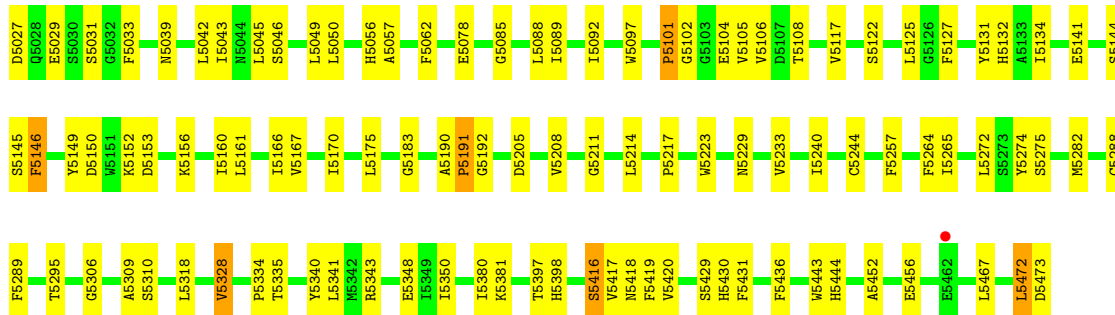
Chain C: 17% 64% 18%





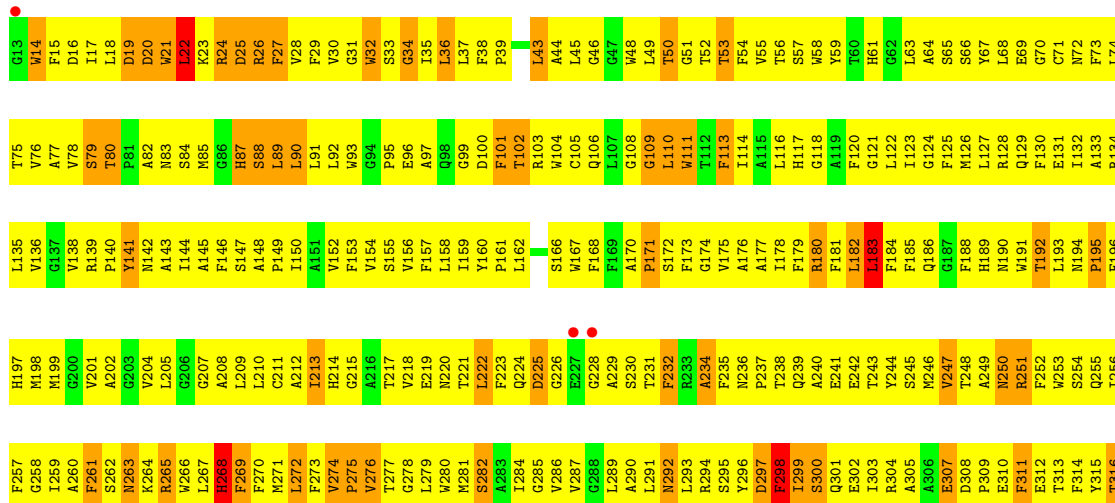
• Molecule 3: Photosystem II CP43 protein

Chain c: 77% 22%



• Molecule 4: Photosystem II D2 protein

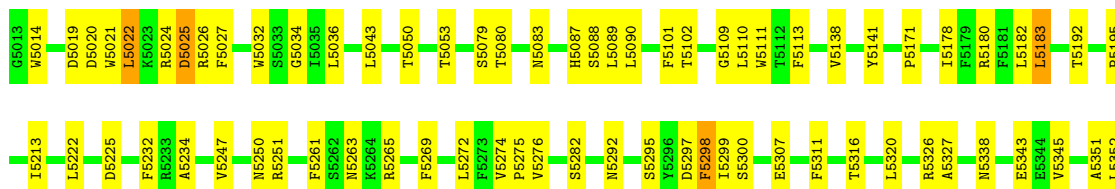
Chain D: 11% 69% 18%





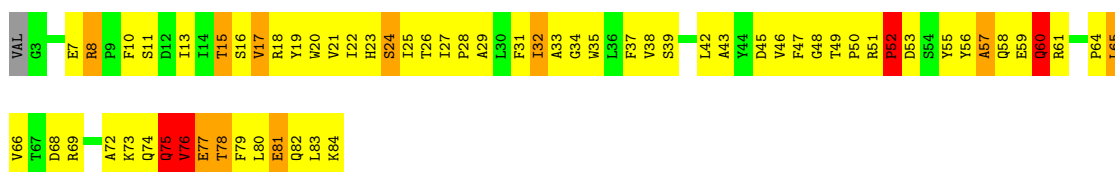
• Molecule 4: Photosystem II D2 protein

Chain d: 79% 20% •



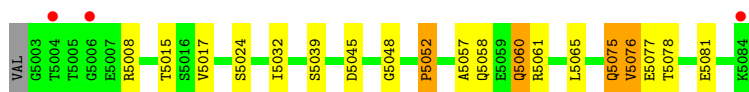
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 22% 60% 12% 5% •



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 4% 76% 18% 5% •



• Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 11% 48% 18% 20% •



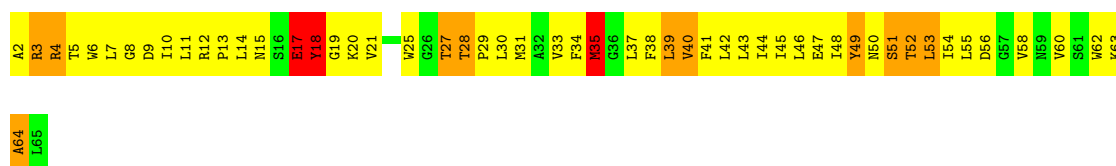
• Molecule 6: Cytochrome b559 subunit beta

Chain f: 5% 59% 18% 20% •

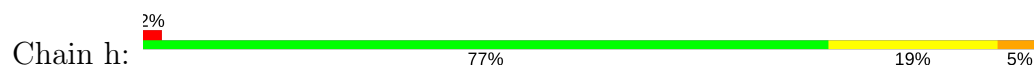


• Molecule 7: Photosystem II reaction center protein H

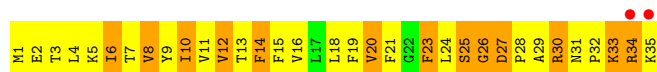
Chain H: 17% 61% 17% 5% •



- Molecule 7: Photosystem II reaction center protein H



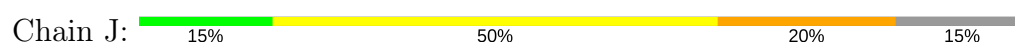
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



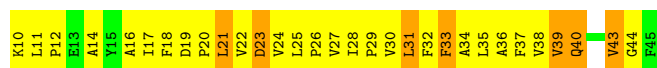
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



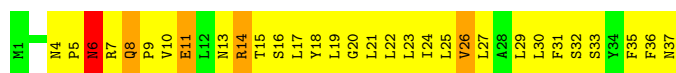
- Molecule 10: Photosystem II reaction center protein K

Chain k:  67% 31% .



- Molecule 11: Photosystem II reaction center protein L

Chain L:  16% 70% 11% .



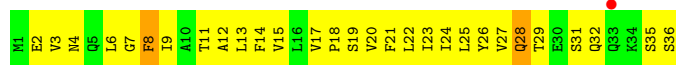
- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 81% 16% .



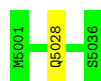
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 19% 75% 6% .



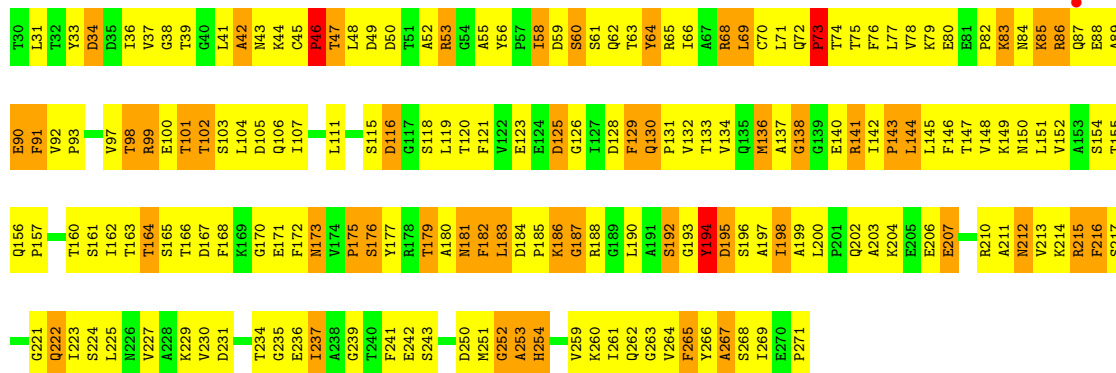
- Molecule 12: Photosystem II reaction center protein M

Chain m:  97% .

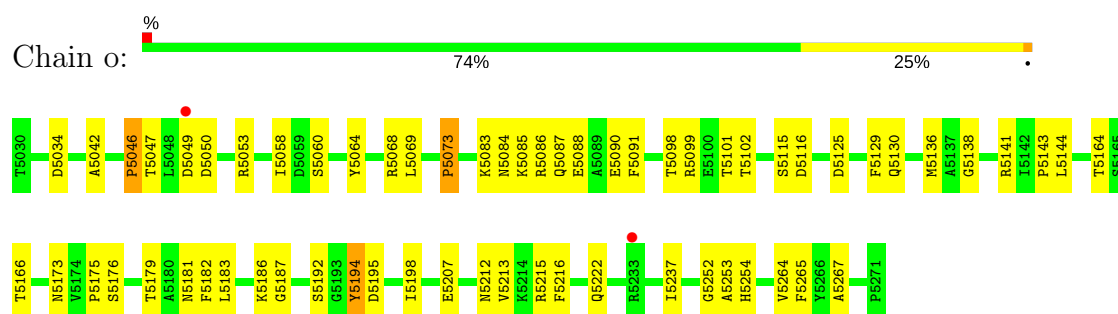


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

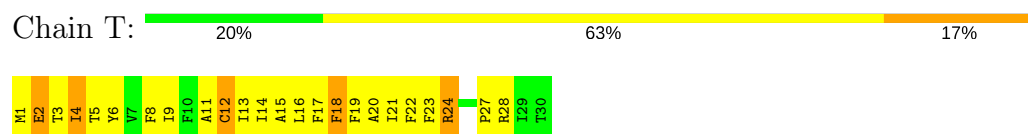
Chain O:  23% 55% 21% .



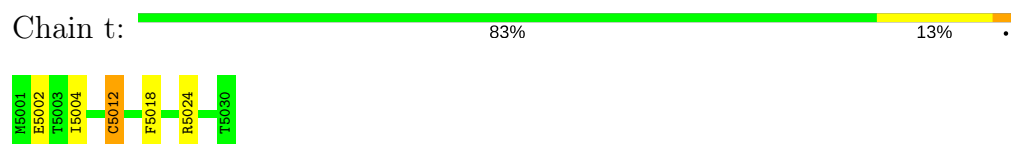
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



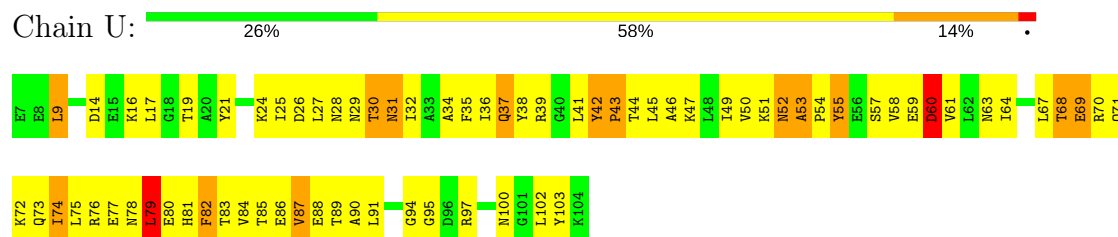
- Molecule 14: Photosystem II reaction center protein T



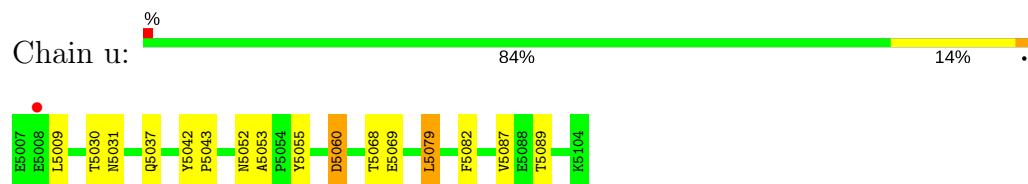
- Molecule 14: Photosystem II reaction center protein T



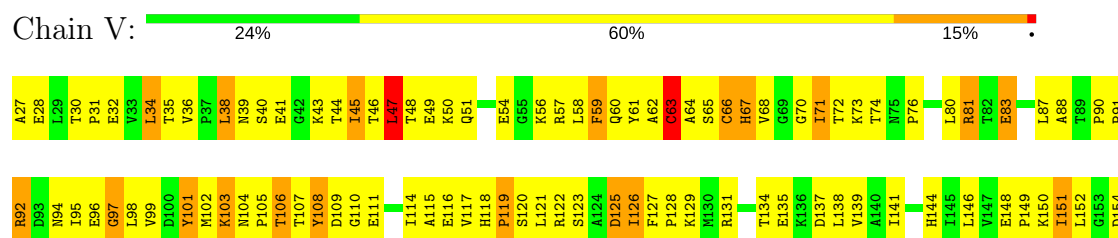
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550





• Molecule 16: Cytochrome c-550

Chain v: 79% 20%



• Molecule 17: Photosystem II reaction center protein X

Chain X: 32% 47% 21%



• Molecule 17: Photosystem II reaction center protein X

Chain x: 3% 71% 29%



• Molecule 18: Photosystem II reaction center protein ycf12

Chain Y: 29% 29% 36% 7%



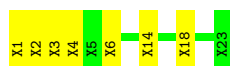
• Molecule 18: Photosystem II reaction center protein ycf12

Chain y: 57% 36% 7%



• Molecule 19: Photosystem II reaction center protein Y

Chain N: 70% 30%

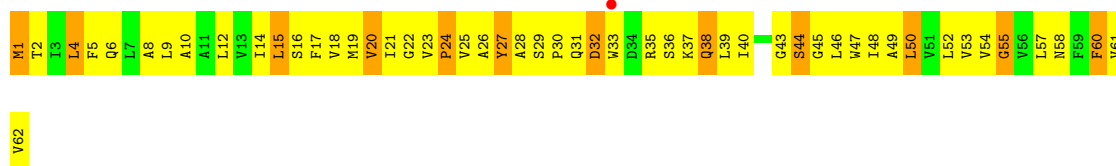
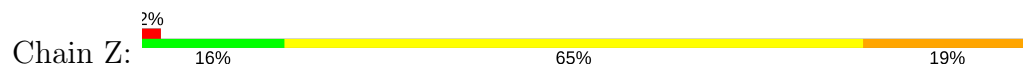


• Molecule 19: Photosystem II reaction center protein Y

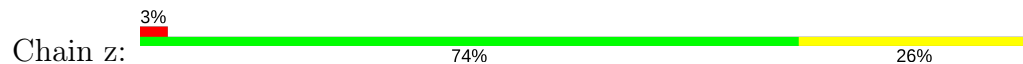
Chain n: 100%

There are no outlier residues recorded for this chain.

● Molecule 20: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 224.70Å 304.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-4.00) 94.8 (20.00-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 4.07Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.326 0.290 , 0.292	Depositor DCC
R_{free} test set	3592 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	148.7	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48060	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, MGE, DGD, CLA, FE2, PQ9, OEC, HEM, IOD, BCR

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	0.53	0/2714	0.74	0/3699
1	a	0.53	0/2714	0.74	0/3699
2	B	0.55	0/3971	0.80	2/5411 (0.0%)
2	b	0.55	0/3971	0.80	2/5411 (0.0%)
3	C	0.50	0/3568	0.80	2/4858 (0.0%)
3	c	0.50	0/3568	0.80	2/4858 (0.0%)
4	D	0.52	0/2801	0.78	0/3818
4	d	0.52	0/2801	0.78	0/3818
5	E	0.58	0/685	0.79	0/933
5	e	0.58	0/685	0.79	0/933
6	F	0.62	0/291	0.72	0/397
6	f	0.62	0/291	0.72	0/397
7	H	0.54	0/520	0.88	0/708
7	h	0.53	0/520	0.88	0/708
8	I	0.67	0/294	0.75	0/395
8	i	0.67	0/294	0.75	0/395
9	J	0.57	0/255	0.72	0/346
9	j	0.57	0/255	0.71	0/346
10	K	0.52	0/287	0.82	0/394
10	k	0.51	0/287	0.84	0/394
11	L	0.50	0/311	0.76	0/422
11	l	0.50	0/311	0.76	0/422
12	M	0.57	0/287	0.73	0/388
12	m	0.57	0/287	0.73	0/388
13	O	0.51	0/1891	0.83	1/2564 (0.0%)
13	o	0.51	0/1891	0.83	1/2564 (0.0%)
14	T	0.69	0/266	0.83	0/359
14	t	0.66	0/266	0.81	0/359
15	U	0.50	0/794	0.81	0/1076
15	u	0.50	0/794	0.80	0/1076
16	V	0.45	0/1085	0.77	1/1473 (0.1%)
16	v	0.45	0/1085	0.77	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.49	0/249	0.73	0/337
17	x	0.50	0/249	0.73	0/337
18	Y	0.63	0/209	0.94	0/279
18	y	0.63	0/209	0.94	0/279
20	Z	0.61	0/490	0.78	0/669
20	z	0.61	0/490	0.78	0/669
All	All	0.53	0/41936	0.79	12/57052 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	5327	THR	N-CA-C	5.91	126.96	111.00
2	B	327	THR	N-CA-C	5.89	126.91	111.00
3	c	5341	LEU	CA-CB-CG	-5.60	102.43	115.30
3	C	341	LEU	CA-CB-CG	-5.59	102.44	115.30
16	V	110	GLY	N-CA-C	-5.46	99.44	113.10
13	o	5187	GLY	N-CA-C	5.46	126.75	113.10
16	v	5110	GLY	N-CA-C	-5.44	99.49	113.10
13	O	187	GLY	N-CA-C	5.44	126.70	113.10
2	B	173	GLY	N-CA-C	-5.26	99.94	113.10
2	b	5173	GLY	N-CA-C	-5.25	99.97	113.10
3	C	214	LEU	CA-CB-CG	5.11	127.06	115.30
3	c	5214	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2528	733	0
1	a	2630	0	2528	0	0
2	B	3835	0	3700	797	0
2	b	3835	0	3700	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3455	0	3376	844	0
3	c	3455	0	3376	0	0
4	D	2706	0	2607	750	0
4	d	2706	0	2608	0	0
5	E	666	0	651	109	0
5	e	666	0	651	0	0
6	F	282	0	291	80	0
6	f	282	0	291	0	0
7	H	507	0	529	142	0
7	h	507	0	529	0	0
8	I	287	0	308	65	0
8	i	287	0	305	0	0
9	J	249	0	262	62	0
9	j	249	0	262	0	0
10	K	278	0	289	84	0
10	k	278	0	289	0	0
11	L	304	0	316	76	0
11	l	304	0	313	0	0
12	M	283	0	297	50	0
12	m	283	0	294	0	0
13	O	1860	0	1833	305	0
13	o	1860	0	1833	0	0
14	T	257	0	261	55	0
14	t	257	0	259	0	0
15	U	783	0	779	137	0
15	u	783	0	779	0	0
16	V	1064	0	1072	206	0
16	v	1064	0	1072	0	0
17	X	246	0	269	39	0
17	x	246	0	269	0	0
18	Y	208	0	237	77	0
18	y	208	0	237	0	0
19	N	116	0	26	6	0
19	n	116	0	26	0	0
20	Z	479	0	516	73	0
20	z	479	0	513	0	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	D	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	139	0
23	B	975	0	1080	668	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	780	0	864	488	0
23	D	195	0	216	157	0
23	H	65	0	72	45	0
23	K	65	0	72	87	0
23	a	195	0	216	0	0
23	b	975	0	1080	0	0
23	c	780	0	864	0	0
23	d	195	0	216	0	0
23	h	65	0	72	0	0
23	k	65	0	72	0	0
24	A	64	0	74	63	0
24	D	64	0	74	53	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	45	0	64	39	0
25	D	45	0	64	52	0
25	a	45	0	64	0	0
25	d	45	0	64	0	0
26	A	40	0	47	25	0
26	B	120	0	142	74	0
26	C	80	0	96	81	0
26	D	40	0	48	40	0
26	H	40	0	48	36	0
26	K	40	0	47	27	0
26	T	80	0	95	40	0
26	Z	40	0	47	18	0
26	a	40	0	47	0	0
26	b	80	0	95	0	0
26	c	40	0	48	0	0
26	d	40	0	48	0	0
26	h	40	0	48	0	0
26	k	80	0	95	0	0
26	t	40	0	48	0	0
26	z	40	0	47	0	0
27	A	49	0	74	36	0
27	a	49	0	74	0	0
28	A	1	0	0	1	0
28	B	1	0	0	3	0
28	D	2	0	0	10	0
28	T	1	0	0	2	0
28	a	1	0	0	0	0
28	b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	2	0	0	0	0
28	t	1	0	0	0	0
29	B	66	0	96	32	0
29	C	198	0	288	118	0
29	b	66	0	96	0	0
29	c	198	0	288	0	0
30	B	48	0	72	39	0
30	D	96	0	144	66	0
30	L	48	0	72	29	0
30	b	48	0	72	0	0
30	d	96	0	144	0	0
30	l	48	0	72	0	0
31	F	43	0	30	17	0
31	V	43	0	30	12	0
31	f	43	0	30	0	0
31	v	43	0	30	0	0
All	All	48060	0	48531	5652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 118.

All (5652) 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)
2:B:65:PHE:CE2	23:B:1012:CLA:HMA2	1.39	1.55
23:B:1011:CLA:HED2	23:B:1012:CLA:CED	1.31	1.53
26:C:1052:BCR:H371	26:C:1052:BCR:C26	1.34	1.50
23:B:1016:CLA:H162	23:D:1008:CLA:CMA	1.38	1.49
23:A:1003:CLA:CAA	23:A:1003:CLA:HED2	1.44	1.47
23:B:1009:CLA:CAD	23:B:1010:CLA:HBB2	1.46	1.45
23:A:1003:CLA:C2	24:A:1038:PHO:HBB1	1.50	1.41
23:B:1009:CLA:HBA1	23:B:1009:CLA:CGD	1.49	1.41
23:B:1022:CLA:H62	23:B:1022:CLA:C14	1.50	1.41
3:C:343:ARG:NH1	3:C:348:GLU:HG3	1.34	1.41
23:B:1016:CLA:H52	23:H:1017:CLA:C9	1.50	1.40
23:B:1022:CLA:H93	23:B:1022:CLA:C14	1.49	1.39
23:A:1003:CLA:H2	24:A:1038:PHO:CBB	1.52	1.39
23:B:1023:CLA:HED2	23:B:1024:CLA:CBB	1.55	1.37
23:B:1009:CLA:H8	23:B:1009:CLA:C14	1.52	1.36
23:B:1016:CLA:C5	23:H:1017:CLA:H91	1.56	1.36
23:C:1025:CLA:CMB	23:C:1025:CLA:H42	1.53	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1021:CLA:HED2	23:B:1021:CLA:C1A	1.54	1.35
23:B:1009:CLA:HAA1	23:B:1009:CLA:CED	1.54	1.35
23:A:1003:CLA:HAA2	23:A:1003:CLA:CED	1.56	1.34
23:B:1020:CLA:H161	23:B:1020:CLA:C10	1.57	1.34
23:B:1021:CLA:C10	23:B:1021:CLA:H142	1.57	1.34
26:A:1044:BCR:C39	26:A:1044:BCR:H371	1.59	1.33
26:B:1048:BCR:C40	26:B:1048:BCR:H371	1.59	1.33
25:D:1042:PQ9:C39	25:D:1042:PQ9:H42	1.58	1.33
26:T:6048:BCR:H371	26:T:6048:BCR:C39	1.59	1.33
26:T:6048:BCR:H371	26:T:6048:BCR:C40	1.59	1.33
23:B:1009:CLA:HED3	23:B:1009:CLA:C2A	1.58	1.32
23:B:1015:CLA:HBC1	26:B:1045:BCR:C34	1.55	1.32
26:A:1044:BCR:C40	26:A:1044:BCR:H371	1.59	1.32
25:D:1042:PQ9:H391	25:D:1042:PQ9:C42	1.49	1.32
23:C:1032:CLA:HAB	23:K:1034:CLA:CMC	1.57	1.32
23:D:1005:CLA:HAA2	25:D:1042:PQ9:C41	1.59	1.31
26:H:1049:BCR:H23C	26:H:1049:BCR:C39	1.51	1.31
23:D:1008:CLA:CMA	23:D:1008:CLA:HBA1	1.53	1.31
23:B:1010:CLA:H162	23:B:1010:CLA:C11	1.56	1.31
23:B:1011:CLA:CED	23:B:1012:CLA:HED1	1.61	1.30
26:B:1047:BCR:H371	26:B:1047:BCR:C39	1.59	1.30
26:B:1048:BCR:C39	26:B:1048:BCR:H371	1.59	1.30
26:B:1047:BCR:H371	26:B:1047:BCR:C40	1.59	1.30
26:C:1052:BCR:C38	26:C:1052:BCR:H371	1.61	1.30
4:D:160:TYR:OH	28:D:1068:IOD:I	2.20	1.29
23:C:1027:CLA:H171	23:C:1027:CLA:C12	1.59	1.28
26:C:1054:BCR:H23C	26:C:1054:BCR:C40	1.52	1.27
26:A:1044:BCR:H392	26:A:1044:BCR:C37	1.65	1.27
23:C:1032:CLA:H151	10:K:33:PHE:CZ	1.67	1.27
2:B:475:PHE:CE1	4:D:140:PRO:HG3	1.68	1.26
24:D:1039:PHO:CMA	24:D:1039:PHO:HBA2	1.51	1.26
23:C:1025:CLA:H12	23:C:1025:CLA:CHB	1.66	1.26
23:C:1029:CLA:C4C	23:C:1029:CLA:H42	1.62	1.26
16:V:64:ALA:O	16:V:68:VAL:HG12	1.35	1.25
26:A:1044:BCR:C37	26:A:1044:BCR:H403	1.65	1.25
26:B:1048:BCR:C37	26:B:1048:BCR:H392	1.66	1.25
26:A:1044:BCR:C30	26:A:1044:BCR:H371	1.65	1.25
23:B:1023:CLA:H13	23:B:1024:CLA:CMA	1.64	1.25
26:B:1047:BCR:H371	26:B:1047:BCR:C30	1.65	1.25
26:B:1048:BCR:C37	26:B:1048:BCR:H403	1.66	1.25
3:C:50:LEU:C	3:C:50:LEU:HD23	1.57	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:1008:CLA:C14	23:D:1008:CLA:H193	1.65	1.25
30:D:1059:MGE:H251	30:D:1059:MGE:CBB	1.60	1.25
23:B:1009:CLA:HBD	23:B:1010:CLA:CBB	1.65	1.25
26:B:1047:BCR:C37	26:B:1047:BCR:H392	1.66	1.25
26:T:6048:BCR:H371	26:T:6048:BCR:C30	1.65	1.25
23:B:1022:CLA:HBC3	23:B:1022:CLA:C9	1.65	1.24
29:B:1058:DGD:HB2	29:B:1058:DGD:CIB	1.65	1.24
23:D:1005:CLA:CAA	25:D:1042:PQ9:H412	1.66	1.24
24:D:1039:PHO:HMA3	24:D:1039:PHO:CBA	1.63	1.24
26:T:6048:BCR:H392	26:T:6048:BCR:C37	1.66	1.24
23:B:1022:CLA:H122	23:B:1022:CLA:C9	1.67	1.24
23:K:1034:CLA:O1D	23:K:1034:CLA:HAA2	1.35	1.24
23:C:1030:CLA:C12	23:C:1030:CLA:H172	1.64	1.24
26:T:6048:BCR:H403	26:T:6048:BCR:C37	1.66	1.23
26:B:1048:BCR:C30	26:B:1048:BCR:H371	1.65	1.23
30:B:1060:MGE:H212	30:B:1060:MGE:CFB	1.54	1.23
23:B:1022:CLA:CGD	23:B:1022:CLA:HAA1	1.70	1.22
26:B:1047:BCR:H403	26:B:1047:BCR:C37	1.66	1.22
3:C:265:ILE:CD1	3:C:452:ALA:HB2	1.68	1.22
23:D:1008:CLA:HMA2	23:D:1008:CLA:CBA	1.59	1.22
23:D:1008:CLA:C19	23:D:1008:CLA:H143	1.70	1.21
23:B:1020:CLA:H102	23:B:1020:CLA:H161	1.23	1.20
23:B:1021:CLA:C2A	23:B:1021:CLA:HED3	1.72	1.20
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.23	1.20
27:A:1063:LHG:H341	27:A:1063:LHG:C38	1.64	1.20
23:B:1009:CLA:HED3	23:B:1009:CLA:CAA	1.72	1.20
2:B:172:TYR:O	2:B:174:LEU:HA	1.41	1.20
23:A:1003:CLA:C4	23:A:1003:CLA:H71	1.68	1.19
23:B:1011:CLA:C19	23:H:1017:CLA:H101	1.72	1.19
30:B:1060:MGE:H251	30:B:1060:MGE:CBB	1.72	1.19
23:C:1025:CLA:HED3	23:C:1025:CLA:OBD	1.40	1.19
23:B:1023:CLA:C13	23:B:1024:CLA:HMA3	1.73	1.19
29:C:1056:DGD:CIB	29:C:1056:DGD:HB2	1.70	1.18
23:B:1009:CLA:CBD	23:B:1010:CLA:CBB	2.20	1.18
23:B:1016:CLA:H2	23:H:1017:CLA:H93	1.20	1.18
1:A:279:ARG:HH11	24:A:1038:PHO:CMC	1.54	1.18
23:C:1031:CLA:HMA2	23:C:1031:CLA:O2A	1.42	1.18
23:B:1011:CLA:H12	23:B:1013:CLA:H93	1.24	1.18
23:B:1009:CLA:C9	23:B:1009:CLA:H121	1.73	1.17
29:C:1057:DGD:HB2	29:C:1057:DGD:CIB	1.73	1.17
24:A:1038:PHO:H201	23:D:1005:CLA:C2B	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CGA	23:B:1011:CLA:H3A	1.60	1.17
23:B:1018:CLA:C10	23:B:1023:CLA:HAA1	1.74	1.17
23:C:1033:CLA:HMA2	23:K:1034:CLA:HAC1	1.25	1.17
29:C:1056:DGD:C3E	29:C:1056:DGD:HD61	1.73	1.17
3:C:46:SER:HB2	3:C:141:GLU:HB2	1.21	1.17
24:D:1039:PHO:HMA1	23:D:1004:CLA:C14	1.73	1.16
23:K:1034:CLA:CGD	23:K:1034:CLA:HAA2	1.76	1.16
23:C:1025:CLA:H141	23:C:1031:CLA:HMB3	1.18	1.16
31:F:1040:HEM:HBA2	31:F:1040:HEM:CMA	1.68	1.16
23:A:1003:CLA:C2A	23:A:1003:CLA:HED2	1.72	1.16
23:A:1003:CLA:C14	24:A:1038:PHO:H8	1.76	1.16
23:B:1009:CLA:H91	23:B:1009:CLA:C12	1.72	1.16
23:B:1010:CLA:C16	23:B:1010:CLA:H112	1.71	1.15
2:B:169:SER:HB3	2:B:176:GLY:HA2	1.24	1.15
29:C:1056:DGD:HBG2	29:C:1056:DGD:CEB	1.71	1.15
1:A:279:ARG:HD3	4:D:208:ALA:HB1	1.22	1.15
23:B:1021:CLA:H2A	23:B:1021:CLA:CED	1.76	1.15
29:C:1057:DGD:C8B	30:D:1059:MGE:H8B2	1.75	1.15
4:D:139:ARG:HH12	4:D:265:ARG:NH2	1.43	1.15
23:A:1006:CLA:HBC3	23:A:1006:CLA:HHD	1.24	1.15
23:B:1016:CLA:H193	23:H:1017:CLA:H191	1.21	1.15
23:C:1029:CLA:H51	23:C:1029:CLA:C4B	1.75	1.15
23:K:1034:CLA:H71	23:K:1034:CLA:C4	1.70	1.15
2:B:174:LEU:HD23	2:B:266:GLU:HG2	1.28	1.15
23:C:1030:CLA:H121	23:C:1030:CLA:C17	1.74	1.15
23:C:1025:CLA:C15	23:C:1031:CLA:H92	1.74	1.15
23:C:1035:CLA:H8	26:C:1052:BCR:H403	1.19	1.15
23:C:1035:CLA:H8	26:C:1052:BCR:C40	1.76	1.14
23:B:1015:CLA:C7	23:B:1015:CLA:H41	1.76	1.14
23:C:1031:CLA:HHD	23:C:1031:CLA:HBC2	1.24	1.14
26:D:1050:BCR:C37	30:D:1059:MGE:H3A1	1.78	1.14
1:A:321:ILE:HD11	4:D:176:ALA:HB1	1.25	1.14
23:B:1022:CLA:O1D	23:B:1022:CLA:HAA1	1.45	1.14
23:B:1009:CLA:CAD	23:B:1010:CLA:CBB	2.25	1.14
23:B:1014:CLA:HHD	23:B:1014:CLA:HBC2	1.24	1.14
2:B:149:LEU:HG	23:B:1011:CLA:HBC1	1.24	1.14
26:Z:1053:BCR:H372	26:Z:1053:BCR:H361	1.19	1.14
23:A:1007:CLA:OBD	23:A:1007:CLA:HED2	1.48	1.14
2:B:475:PHE:CD1	4:D:140:PRO:HG3	1.81	1.14
27:A:1063:LHG:C34	27:A:1063:LHG:H383	1.71	1.14
23:D:1005:CLA:CBC	23:D:1004:CLA:HBB2	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1038:PHO:HMB3	23:D:1005:CLA:H52	1.21	1.13
2:B:65:PHE:CE2	23:B:1012:CLA:CMA	2.31	1.13
23:A:1006:CLA:H172	26:D:1050:BCR:H282	1.29	1.13
3:C:49:LEU:HD21	23:C:1035:CLA:HMA1	1.21	1.13
23:C:1025:CLA:H12	23:C:1025:CLA:HHB	1.22	1.13
23:C:1025:CLA:HMB2	23:C:1025:CLA:C4	1.77	1.13
23:C:1031:CLA:OBD	23:C:1033:CLA:H122	1.47	1.13
23:K:1034:CLA:CGA	23:K:1034:CLA:H43	1.77	1.13
23:B:1015:CLA:HED2	23:B:1015:CLA:OBD	1.46	1.13
23:B:1011:CLA:O1A	23:B:1011:CLA:H3A	1.43	1.13
26:B:1045:BCR:H23C	26:B:1045:BCR:H383	1.30	1.13
23:C:1029:CLA:HMA2	23:C:1029:CLA:HBA2	1.21	1.13
23:B:1022:CLA:C4D	23:B:1022:CLA:H11	1.79	1.12
29:B:1058:DGD:CEB	29:B:1058:DGD:HBG2	1.74	1.12
23:B:1009:CLA:CMB	26:H:1049:BCR:H271	1.77	1.12
1:A:258:LEU:HD12	4:D:128:ARG:HH21	1.14	1.12
23:C:1037:CLA:HHD	23:C:1037:CLA:HBC2	1.25	1.12
6:F:45:ARG:HE	6:F:45:ARG:HA	1.13	1.12
2:B:65:PHE:CZ	23:B:1012:CLA:HMA2	1.85	1.12
1:A:337:HIS:O	4:D:351:ALA:HB2	1.50	1.12
23:B:1022:CLA:HHD	23:B:1022:CLA:HBC2	1.26	1.11
4:D:88:SER:HA	7:H:50:ASN:HD21	1.12	1.11
3:C:275:SER:HB3	23:C:1033:CLA:CED	1.79	1.11
3:C:49:LEU:HD22	3:C:52:ALA:H	1.01	1.11
4:D:261:PHE:H	25:D:1042:PQ9:H92	0.95	1.11
23:B:1011:CLA:C2D	23:B:1013:CLA:H42	1.79	1.11
23:B:1016:CLA:C16	23:D:1008:CLA:HMA1	1.81	1.11
26:K:1051:BCR:H403	26:K:1051:BCR:H23C	1.22	1.11
23:A:1003:CLA:H142	24:A:1038:PHO:H8	1.17	1.11
23:C:1026:CLA:H122	23:C:1026:CLA:H71	1.33	1.11
3:C:46:SER:CB	3:C:141:GLU:HB2	1.80	1.11
25:D:1042:PQ9:H342	25:D:1042:PQ9:H301	1.32	1.11
23:B:1015:CLA:HED2	23:B:1015:CLA:CAD	1.79	1.11
23:C:1025:CLA:H151	23:C:1031:CLA:C9	1.80	1.11
23:A:1006:CLA:H172	26:D:1050:BCR:C28	1.80	1.10
23:B:1015:CLA:HBC1	26:B:1045:BCR:H342	1.27	1.10
27:A:1063:LHG:H291	23:C:1032:CLA:C7	1.81	1.10
23:C:1032:CLA:C15	10:K:33:PHE:HZ	1.65	1.10
29:B:1058:DGD:HBT1	29:B:1058:DGD:HB61	1.20	1.10
2:B:5:TRP:HA	2:B:8:VAL:HG13	1.34	1.10
26:D:1050:BCR:H383	26:D:1050:BCR:H23C	1.11	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CMD	23:B:1013:CLA:H42	1.82	1.10
23:B:1014:CLA:H41	23:B:1014:CLA:C7	1.75	1.10
23:B:1016:CLA:C16	23:D:1008:CLA:CMA	2.30	1.10
23:B:1015:CLA:HBC1	26:B:1045:BCR:H343	1.28	1.10
23:B:1022:CLA:H142	23:B:1022:CLA:C9	1.82	1.10
23:C:1030:CLA:HBB1	23:C:1030:CLA:HHC	1.33	1.10
23:A:1003:CLA:H41	23:A:1003:CLA:H71	1.31	1.10
2:B:174:LEU:HD22	2:B:312:TYR:OH	1.48	1.09
23:C:1035:CLA:HBB1	23:C:1035:CLA:HHC	1.30	1.09
26:C:1052:BCR:C38	26:C:1052:BCR:C37	2.30	1.09
3:C:49:LEU:CD2	3:C:52:ALA:H	1.66	1.09
23:D:1008:CLA:HBB1	23:D:1008:CLA:HHC	1.29	1.09
23:B:1022:CLA:C6	23:B:1022:CLA:C14	2.31	1.09
3:C:171:GLY:HA2	3:C:174:LEU:HB2	1.35	1.09
23:D:1008:CLA:C19	23:D:1008:CLA:C14	2.30	1.09
23:B:1011:CLA:HMD2	23:B:1013:CLA:H42	1.35	1.09
23:B:1014:CLA:C4	23:B:1014:CLA:H72	1.82	1.09
23:B:1016:CLA:H2	23:H:1017:CLA:C9	1.81	1.09
23:C:1025:CLA:H122	26:C:1054:BCR:H351	1.12	1.09
23:C:1037:CLA:HHC	23:C:1037:CLA:HBB1	1.31	1.09
11:L:26:VAL:HG21	30:L:1061:MGE:H232	1.35	1.09
23:B:1009:CLA:C8	23:B:1009:CLA:C14	2.30	1.09
23:B:1009:CLA:CGD	23:B:1009:CLA:CBA	2.30	1.09
23:B:1018:CLA:HHC	23:B:1018:CLA:HBB1	1.31	1.09
26:C:1052:BCR:C37	26:C:1052:BCR:C26	2.30	1.09
26:D:1050:BCR:H372	30:D:1059:MGE:H3A1	1.16	1.09
2:B:5:TRP:HA	2:B:8:VAL:CG1	1.82	1.08
23:C:1025:CLA:C4	23:C:1025:CLA:C2B	2.30	1.08
23:C:1030:CLA:CBC	23:C:1030:CLA:HHD	1.82	1.08
26:T:6046:BCR:H331	26:T:6046:BCR:HC8	1.09	1.08
3:C:263:ALA:HB3	3:C:264:PHE:CE2	1.89	1.08
24:D:1039:PHO:HMA1	23:D:1004:CLA:H143	1.15	1.08
29:C:1057:DGD:HB81	30:D:1059:MGE:H8B2	1.32	1.08
23:C:1027:CLA:H171	23:C:1027:CLA:H122	1.10	1.08
23:K:1034:CLA:HHD	23:K:1034:CLA:HBC3	1.31	1.08
23:B:1021:CLA:C2A	23:B:1021:CLA:CED	2.30	1.08
29:C:1056:DGD:C6D	29:C:1056:DGD:HE5	1.83	1.08
29:C:1056:DGD:C5E	29:C:1056:DGD:HD62	1.84	1.08
23:D:1004:CLA:HBB1	23:D:1004:CLA:HHC	1.31	1.08
30:D:1059:MGE:H251	30:D:1059:MGE:H211	1.15	1.08
4:D:160:TYR:CZ	28:D:1068:IOD:I	2.77	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1021:CLA:CED	23:B:1021:CLA:C1A	2.30	1.08
23:B:1022:CLA:C9	23:B:1022:CLA:C14	2.30	1.08
23:C:1025:CLA:H122	26:C:1054:BCR:C35	1.84	1.08
23:A:1006:CLA:H172	26:D:1050:BCR:C27	1.83	1.08
23:B:1018:CLA:H101	23:B:1023:CLA:HAA1	1.36	1.07
13:O:179:THR:HG22	13:O:180:ALA:H	1.11	1.07
23:B:1021:CLA:H102	23:B:1021:CLA:C14	1.83	1.07
23:C:1030:CLA:HHD	23:C:1030:CLA:HBC2	1.32	1.07
26:C:1054:BCR:H403	26:C:1054:BCR:C23	1.74	1.07
29:C:1057:DGD:HAF2	30:D:1059:MGE:H222	1.08	1.07
23:B:1009:CLA:HHC	23:B:1009:CLA:HBB1	1.35	1.07
25:A:1043:PQ9:H451	30:D:1059:MGE:H101	1.08	1.07
26:Z:1053:BCR:H383	26:Z:1053:BCR:H23C	1.11	1.07
27:A:1063:LHG:H291	23:C:1032:CLA:H72	1.33	1.07
23:B:1012:CLA:C2D	23:B:1020:CLA:H201	1.84	1.07
23:B:1022:CLA:H92	23:B:1022:CLA:HBC3	1.07	1.07
23:C:1026:CLA:CBA	23:C:1027:CLA:HAC1	1.85	1.07
23:C:1026:CLA:HBA1	23:C:1027:CLA:CAC	1.85	1.07
3:C:417:VAL:HG12	16:V:68:VAL:HB	1.35	1.07
3:C:417:VAL:HG11	16:V:68:VAL:CG1	1.84	1.07
23:B:1009:CLA:HBD	23:B:1010:CLA:HBB1	1.11	1.07
23:B:1009:CLA:HAA1	23:B:1009:CLA:O2D	1.55	1.07
23:B:1010:CLA:H12	23:B:1010:CLA:HBD	1.35	1.07
23:C:1027:CLA:C17	23:C:1027:CLA:C12	2.31	1.07
2:B:362:PHE:CE1	28:D:1068:IOD:I	2.78	1.07
23:B:1011:CLA:CGA	23:B:1011:CLA:C3A	2.33	1.07
23:B:1012:CLA:HBB1	23:B:1015:CLA:CBB	1.85	1.06
23:B:1012:CLA:C2D	23:B:1020:CLA:C20	2.33	1.06
23:B:1022:CLA:H122	23:B:1022:CLA:H91	1.11	1.06
5:E:8:ARG:HE	6:F:13:TYR:HB2	1.18	1.06
23:K:1034:CLA:CGA	23:K:1034:CLA:C4	2.33	1.06
26:T:6048:BCR:C37	26:T:6048:BCR:C40	2.30	1.06
23:A:1003:CLA:H42	24:A:1038:PHO:C4B	1.85	1.06
23:B:1009:CLA:CAA	23:B:1009:CLA:CED	2.30	1.06
29:B:1058:DGD:HBT1	29:B:1058:DGD:C6B	1.84	1.06
30:D:1062:MGE:O1B	30:D:1062:MGE:H3G2	1.55	1.06
23:B:1011:CLA:CED	23:B:1012:CLA:CED	2.25	1.06
26:K:1051:BCR:H353	18:Y:32:GLY:HA3	1.32	1.06
25:A:1043:PQ9:H451	30:D:1059:MGE:CAA	1.86	1.06
23:B:1009:CLA:C8	23:B:1009:CLA:H143	1.84	1.06
23:B:1022:CLA:H142	23:B:1022:CLA:H62	1.06	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:GLY:HA3	3:C:41:ARG:HD3	1.37	1.06
23:B:1009:CLA:HED3	23:B:1009:CLA:H2A	1.08	1.06
23:C:1033:CLA:H171	23:C:1033:CLA:H143	1.10	1.06
23:D:1008:CLA:C18	23:D:1008:CLA:H143	1.86	1.06
30:D:1062:MGE:H1G1	11:L:19:LEU:HD21	1.37	1.06
3:C:49:LEU:HD22	3:C:52:ALA:N	1.71	1.05
2:B:362:PHE:HE1	28:D:1068:IOD:I	2.09	1.05
3:C:49:LEU:CD2	3:C:52:ALA:HB2	1.86	1.05
3:C:50:LEU:HD21	3:C:54:VAL:CG2	1.86	1.05
23:C:1032:CLA:CAB	23:K:1034:CLA:HMC3	1.85	1.05
26:B:1047:BCR:C39	26:B:1047:BCR:C37	2.30	1.05
2:B:5:TRP:CZ2	30:L:1061:MGE:H2A2	1.90	1.05
29:C:1056:DGD:C6D	29:C:1056:DGD:HE3	1.84	1.05
4:D:246:MET:HE3	4:D:264:LYS:HG2	1.39	1.05
3:C:42:LEU:HD11	3:C:49:LEU:CD1	1.86	1.05
16:V:103:LYS:HD2	16:V:121:LEU:HD12	1.37	1.05
26:B:1048:BCR:C37	26:B:1048:BCR:C39	2.30	1.05
3:C:343:ARG:HH12	3:C:348:GLU:CG	1.68	1.05
23:D:1005:CLA:H91	23:D:1005:CLA:H122	1.10	1.05
26:B:1047:BCR:H331	26:B:1047:BCR:HC8	1.37	1.05
23:D:1005:CLA:H91	23:D:1005:CLA:C12	1.83	1.05
16:V:103:LYS:HD2	16:V:121:LEU:CD1	1.87	1.05
26:H:1049:BCR:H392	26:H:1049:BCR:C23	1.76	1.04
10:K:39:VAL:CG2	18:Y:36:ILE:HD11	1.86	1.04
23:B:1009:CLA:H142	23:B:1009:CLA:H102	1.39	1.04
2:B:4:PRO:HG2	2:B:7:ARG:HG3	1.38	1.04
26:B:1047:BCR:HC8	26:B:1047:BCR:C33	1.82	1.04
23:D:1008:CLA:C14	23:D:1008:CLA:C18	2.36	1.04
14:T:18:PHE:HA	26:T:6046:BCR:H332	1.36	1.04
23:B:1010:CLA:H162	23:B:1010:CLA:H111	1.34	1.04
23:C:1030:CLA:H121	23:C:1030:CLA:H172	1.10	1.03
3:C:275:SER:HB3	23:C:1033:CLA:HED1	1.34	1.03
3:C:49:LEU:HD21	3:C:52:ALA:HB2	1.37	1.03
4:D:57:SER:HB2	4:D:79:SER:HB3	1.37	1.03
23:B:1015:CLA:CBC	26:B:1045:BCR:H342	1.88	1.03
29:C:1057:DGD:HBG2	29:C:1057:DGD:HBG2	1.35	1.03
26:T:6048:BCR:C39	26:T:6048:BCR:C37	2.30	1.03
23:A:1006:CLA:HBB1	23:A:1006:CLA:HHC	1.38	1.03
23:K:1034:CLA:H143	23:K:1034:CLA:H102	1.40	1.03
23:C:1029:CLA:HMD3	23:C:1031:CLA:HAB	1.37	1.03
23:A:1003:CLA:H42	24:A:1038:PHO:C1B	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH1	24:A:1038:PHO:HMC1	1.74	1.03
23:B:1021:CLA:C10	23:B:1021:CLA:C14	2.34	1.03
3:C:49:LEU:H	3:C:49:LEU:HD12	1.23	1.03
31:F:1040:HEM:HMA1	31:F:1040:HEM:HBA2	1.05	1.03
2:B:174:LEU:H	2:B:174:LEU:HD13	1.21	1.03
24:D:1039:PHO:CMA	23:D:1004:CLA:H143	1.87	1.03
23:B:1013:CLA:H122	23:B:1018:CLA:H42	1.38	1.02
23:B:1021:CLA:OBD	23:B:1022:CLA:HHC	1.59	1.02
2:B:105:GLY:CA	26:B:1047:BCR:H401	1.88	1.02
23:D:1005:CLA:C12	23:D:1005:CLA:C9	2.36	1.02
23:C:1025:CLA:C4	23:C:1025:CLA:CMB	2.34	1.02
23:B:1019:CLA:H93	30:L:1061:MGE:H9A2	1.41	1.02
3:C:343:ARG:NH1	3:C:348:GLU:CG	2.21	1.02
23:A:1007:CLA:C4	23:C:1029:CLA:H191	1.89	1.02
23:B:1014:CLA:H72	23:B:1014:CLA:H41	1.03	1.02
20:Z:55:GLY:HA2	26:Z:1053:BCR:C31	1.88	1.02
1:A:279:ARG:NH1	24:A:1038:PHO:CMC	2.22	1.02
3:C:265:ILE:HD11	3:C:452:ALA:HB2	1.05	1.02
27:A:1063:LHG:H161	27:A:1063:LHG:H122	1.42	1.02
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.20	1.02
26:B:1047:BCR:C40	26:B:1047:BCR:C37	2.30	1.02
23:B:1011:CLA:O1D	23:B:1013:CLA:H11	1.58	1.02
4:D:37:LEU:HD22	4:D:128:ARG:HD3	1.41	1.02
16:V:98:LEU:HD22	16:V:98:LEU:H	1.20	1.02
1:A:279:ARG:HH11	24:A:1038:PHO:HMC3	1.21	1.01
3:C:46:SER:HB2	3:C:141:GLU:CB	1.90	1.01
26:A:1044:BCR:C40	26:A:1044:BCR:C37	2.30	1.01
26:A:1044:BCR:C37	26:A:1044:BCR:C39	2.30	1.01
2:B:105:GLY:HA3	26:B:1047:BCR:H401	1.39	1.01
23:C:1033:CLA:HMA2	23:K:1034:CLA:CAC	1.90	1.01
23:B:1023:CLA:HED2	23:B:1024:CLA:HBB1	1.03	1.01
4:D:250:ASN:HB2	4:D:260:ALA:HB1	1.40	1.01
23:C:1035:CLA:HMD2	10:K:40:GLN:NE2	1.72	1.01
3:C:264:PHE:HD2	3:C:264:PHE:N	1.57	1.01
4:D:267:LEU:HD22	4:D:268:HIS:ND1	1.74	1.01
23:C:1029:CLA:H42	23:C:1029:CLA:NC	1.74	1.01
23:B:1019:CLA:H93	30:L:1061:MGE:C9A	1.90	1.01
3:C:229:ASN:HD22	3:C:229:ASN:H	1.03	1.01
2:B:326:ARG:HH11	4:D:297:ASP:HA	1.24	1.01
10:K:24:VAL:HG21	18:Y:25:ILE:HG22	1.41	1.01
23:D:1005:CLA:H122	23:D:1005:CLA:C9	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261:PHE:CZ	4:D:267:LEU:HA	1.96	1.01
23:B:1021:CLA:HED2	23:B:1021:CLA:CHA	1.91	1.00
23:C:1029:CLA:HMA2	23:C:1029:CLA:CBA	1.85	1.00
1:A:60:ILE:HD11	1:A:83:VAL:HB	1.41	1.00
27:A:1063:LHG:H292	23:C:1032:CLA:H52	1.41	1.00
3:C:50:LEU:C	3:C:50:LEU:CD2	2.30	1.00
7:H:13:PRO:HG2	7:H:14:LEU:HD12	1.39	1.00
23:B:1022:CLA:C9	23:B:1022:CLA:C12	2.32	1.00
23:C:1032:CLA:HAB	23:K:1034:CLA:HMC3	1.03	1.00
3:C:167:VAL:HG12	3:C:168:LEU:HD12	1.44	1.00
4:D:265:ARG:HG3	4:D:265:ARG:HH11	1.23	1.00
2:B:456:ALA:HB1	29:B:1058:DGD:HBV1	1.41	1.00
23:C:1027:CLA:C17	23:C:1027:CLA:H121	1.91	1.00
1:A:54:ALA:HB2	1:A:72:LEU:HD12	1.42	1.00
23:B:1016:CLA:C5	23:H:1017:CLA:H112	1.91	1.00
10:K:39:VAL:HG23	18:Y:36:ILE:HD11	1.00	1.00
3:C:265:ILE:HD11	3:C:452:ALA:CB	1.91	1.00
26:D:1050:BCR:HC8	26:D:1050:BCR:C33	1.91	1.00
23:B:1010:CLA:HBD	23:B:1010:CLA:C1	1.92	1.00
23:B:1015:CLA:CAD	23:B:1015:CLA:CED	2.40	1.00
3:C:166:ILE:HD12	3:C:249:ILE:HD12	1.44	1.00
4:D:91:LEU:HA	23:D:1008:CLA:CED	1.92	1.00
23:B:1011:CLA:H193	23:H:1017:CLA:H101	1.00	1.00
16:V:45:ILE:H	16:V:45:ILE:HD12	1.22	0.99
16:V:118:HIS:HD2	16:V:119:PRO:HD2	1.23	0.99
2:B:59:GLY:HA3	2:B:329:PRO:HB3	1.45	0.99
3:C:49:LEU:HB3	3:C:133:ALA:HA	1.40	0.99
23:A:1003:CLA:HAA2	23:A:1003:CLA:HED2	1.01	0.99
1:A:223:LEU:O	1:A:224:ILE:HB	1.60	0.99
23:C:1025:CLA:CHB	23:C:1025:CLA:C1	2.41	0.99
26:C:1052:BCR:H383	26:C:1052:BCR:C37	1.90	0.99
23:B:1016:CLA:H162	23:D:1008:CLA:HMA3	1.40	0.99
2:B:149:LEU:CG	23:B:1011:CLA:HBC1	1.92	0.99
12:M:29:THR:O	12:M:32:GLN:HG2	1.61	0.99
23:B:1012:CLA:CGA	23:B:1020:CLA:H141	1.91	0.99
23:C:1033:CLA:CMA	23:K:1034:CLA:C3C	2.41	0.99
2:B:278:SER:HB3	2:B:281:GLN:HG2	1.41	0.99
29:C:1056:DGD:HE5	29:C:1056:DGD:HD62	0.99	0.99
23:B:1012:CLA:C3B	23:B:1015:CLA:HBB2	1.91	0.99
2:B:341:LYS:HB3	2:B:406:LEU:HD22	1.45	0.99
4:D:91:LEU:HA	23:D:1008:CLA:HED1	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1009:CLA:C10	23:B:1009:CLA:H142	1.89	0.99
23:B:1015:CLA:H72	23:B:1015:CLA:H41	1.41	0.99
2:B:75:TRP:NE1	2:B:94:GLU:HB2	1.76	0.99
16:V:34:LEU:HD22	16:V:47:LEU:HB3	1.44	0.99
23:C:1030:CLA:HMB2	23:C:1031:CLA:NB	1.78	0.98
1:A:269:ARG:HD3	4:D:222:LEU:HD11	1.45	0.98
2:B:324:LEU:HA	4:D:293:LEU:HD22	1.43	0.98
23:C:1033:CLA:HMA3	23:K:1034:CLA:CMC	1.92	0.98
23:C:1025:CLA:C2B	23:C:1025:CLA:H42	1.93	0.98
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.43	0.98
23:C:1026:CLA:HBA1	23:C:1027:CLA:HAC1	0.98	0.98
3:C:417:VAL:HG11	16:V:68:VAL:HG11	1.40	0.98
3:C:91:HIS:CD2	23:C:1026:CLA:HED1	1.97	0.98
14:T:4:ILE:HD13	14:T:5:THR:N	1.78	0.98
23:B:1010:CLA:C16	23:B:1010:CLA:C11	2.30	0.98
23:B:1010:CLA:H162	23:B:1010:CLA:H112	1.31	0.98
23:B:1023:CLA:CED	23:B:1024:CLA:CBB	2.40	0.98
23:C:1030:CLA:HED2	23:C:1030:CLA:C3D	1.93	0.98
1:A:279:ARG:CD	4:D:208:ALA:HB1	1.93	0.98
3:C:348:GLU:HB3	13:O:42:ALA:HB1	1.43	0.98
30:D:1059:MGE:H211	30:D:1059:MGE:CFB	1.92	0.98
2:B:475:PHE:CD1	4:D:140:PRO:CG	2.45	0.98
23:C:1025:CLA:H151	23:C:1031:CLA:H92	1.34	0.98
23:C:1027:CLA:H152	26:Z:1053:BCR:H332	1.42	0.98
2:B:105:GLY:CA	26:B:1047:BCR:C40	2.42	0.98
23:D:1008:CLA:H172	23:D:1008:CLA:H141	1.46	0.97
23:C:1033:CLA:HED3	23:C:1033:CLA:OBD	1.62	0.97
25:A:1043:PQ9:C45	30:D:1059:MGE:H101	1.94	0.97
23:A:1003:CLA:H2A	23:A:1003:CLA:HED2	1.41	0.97
23:B:1020:CLA:HED1	23:B:1021:CLA:HMB2	1.46	0.97
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.43	0.97
23:D:1005:CLA:HBC2	23:D:1004:CLA:HBB2	1.42	0.97
23:C:1029:CLA:C4C	23:C:1029:CLA:C4	2.42	0.97
23:B:1014:CLA:HBA1	23:B:1014:CLA:CHA	1.95	0.97
23:B:1016:CLA:H52	23:H:1017:CLA:H91	0.97	0.97
23:B:1021:CLA:H102	23:B:1021:CLA:H142	0.99	0.97
3:C:271:TYR:CE1	23:C:1031:CLA:HAC1	1.99	0.97
23:D:1008:CLA:C17	23:D:1008:CLA:H141	1.95	0.97
1:A:159:LEU:HD21	29:C:1055:DGD:HA71	1.45	0.97
1:A:228:THR:HG22	1:A:229:GLU:H	1.27	0.97
7:H:6:TRP:CD1	7:H:10:ILE:HD11	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CAD	23:B:1013:CLA:H12	1.95	0.97
23:C:1033:CLA:CAD	23:C:1033:CLA:HED3	1.94	0.97
23:C:1032:CLA:H151	10:K:33:PHE:HZ	0.81	0.97
26:B:1048:BCR:C37	26:B:1048:BCR:C40	2.30	0.97
23:C:1033:CLA:H171	23:C:1033:CLA:C14	1.92	0.97
23:B:1009:CLA:C1A	23:B:1009:CLA:CGA	2.43	0.96
23:B:1020:CLA:C16	23:B:1020:CLA:C10	2.43	0.96
23:B:1022:CLA:C12	23:B:1022:CLA:H91	1.92	0.96
24:A:1038:PHO:H93	23:D:1005:CLA:H18	1.46	0.96
26:D:1050:BCR:H372	30:D:1059:MGE:C3A	1.95	0.96
23:B:1023:CLA:CED	23:B:1024:CLA:HBB1	1.94	0.96
23:C:1030:CLA:HBB2	23:C:1031:CLA:HED1	1.45	0.96
23:C:1033:CLA:C17	23:C:1033:CLA:H143	1.95	0.96
26:D:1050:BCR:HC8	26:D:1050:BCR:H331	1.43	0.96
2:B:174:LEU:N	2:B:174:LEU:HD13	1.79	0.96
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.43	0.96
2:B:103:LEU:HB2	23:B:1014:CLA:H92	1.45	0.96
23:C:1029:CLA:C5	23:C:1029:CLA:CHC	2.43	0.96
30:L:1061:MGE:H1G2	30:L:1061:MGE:O1B	1.63	0.96
16:V:38:LEU:HA	16:V:95:ILE:HG22	1.45	0.96
25:D:1042:PQ9:C24	30:L:1061:MGE:H263	1.95	0.96
23:B:1022:CLA:C8	23:B:1022:CLA:H143	1.95	0.96
23:C:1029:CLA:H52	23:C:1029:CLA:CHC	1.96	0.96
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.43	0.96
3:C:49:LEU:CD2	3:C:52:ALA:N	2.28	0.96
26:K:1051:BCR:C23	26:K:1051:BCR:H403	1.94	0.96
26:Z:1053:BCR:C38	26:Z:1053:BCR:H23C	1.91	0.96
23:B:1022:CLA:C7	23:B:1022:CLA:H143	1.96	0.95
23:B:1011:CLA:H2	23:B:1013:CLA:C9	1.95	0.95
23:B:1023:CLA:H91	23:B:1024:CLA:H151	1.47	0.95
29:C:1057:DGD:CEA	30:D:1059:MGE:H222	1.96	0.95
23:B:1011:CLA:HED2	23:B:1012:CLA:HED1	0.96	0.95
24:D:1039:PHO:CMA	23:D:1004:CLA:C14	2.41	0.95
23:B:1020:CLA:H161	23:B:1020:CLA:H101	1.47	0.95
3:C:155:ASN:HA	3:C:158:THR:HG22	1.49	0.95
26:Z:1053:BCR:H383	26:Z:1053:BCR:C23	1.97	0.95
23:C:1025:CLA:C12	26:C:1054:BCR:H351	1.96	0.95
23:A:1003:CLA:HBC2	23:A:1003:CLA:HHD	1.47	0.95
23:C:1030:CLA:H143	23:C:1030:CLA:H171	1.48	0.95
29:C:1055:DGD:CIB	29:C:1055:DGD:HBFI	1.97	0.95
3:C:46:SER:OG	3:C:149:TYR:HB3	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:348:GLU:HB3	13:O:42:ALA:CB	1.95	0.95
2:B:169:SER:HB3	2:B:176:GLY:CA	1.96	0.95
4:D:188:PHE:CE2	4:D:326:ARG:HG2	2.01	0.95
23:B:1021:CLA:H2A	23:B:1021:CLA:HED3	0.94	0.94
23:B:1011:CLA:H2	23:B:1013:CLA:H92	1.46	0.94
23:B:1018:CLA:H102	23:B:1023:CLA:CAA	1.97	0.94
23:B:1022:CLA:H143	23:B:1022:CLA:C10	1.97	0.94
3:C:264:PHE:CD2	3:C:264:PHE:N	2.30	0.94
23:B:1015:CLA:C7	23:B:1015:CLA:C4	2.41	0.94
23:C:1035:CLA:C2B	26:C:1052:BCR:H271	1.97	0.94
3:C:263:ALA:CB	3:C:264:PHE:CE2	2.51	0.94
13:O:80:GLU:O	13:O:82:PRO:HD3	1.68	0.94
23:B:1011:CLA:HED2	23:B:1012:CLA:HED3	1.46	0.94
7:H:12:ARG:HH12	7:H:15:ASN:HB3	1.30	0.94
23:B:1012:CLA:HBB1	23:B:1015:CLA:HBB2	1.46	0.94
5:E:8:ARG:NE	6:F:13:TYR:HB2	1.81	0.94
23:A:1006:CLA:H161	25:A:1043:PQ9:H443	1.47	0.94
2:B:8:VAL:O	2:B:11:VAL:HG23	1.67	0.94
23:C:1036:CLA:HBC2	23:C:1036:CLA:HMC1	1.48	0.94
23:C:1029:CLA:C4	23:C:1029:CLA:NC	2.30	0.94
23:C:1029:CLA:H11	23:C:1029:CLA:C4D	1.98	0.94
26:D:1050:BCR:H23C	26:D:1050:BCR:C38	1.91	0.94
23:B:1009:CLA:HMB1	26:H:1049:BCR:H271	1.46	0.94
23:B:1018:CLA:H102	23:B:1023:CLA:HAA1	1.50	0.94
23:C:1026:CLA:C7	23:C:1026:CLA:H122	1.95	0.94
23:D:1008:CLA:H193	23:D:1008:CLA:H143	1.33	0.94
14:T:18:PHE:HA	26:T:6046:BCR:C33	1.96	0.94
26:T:6046:BCR:C33	26:T:6046:BCR:HC8	1.96	0.94
26:T:6048:BCR:H371	26:T:6048:BCR:H403	1.33	0.94
2:B:65:PHE:HE2	23:B:1012:CLA:HMA2	1.32	0.94
31:F:1040:HEM:HMA1	31:F:1040:HEM:CBA	1.97	0.94
1:A:183:MET:HB3	23:A:1003:CLA:HBC3	1.48	0.94
3:C:333:GLY:H	3:C:338:GLY:HA2	1.33	0.94
27:A:1063:LHG:H321	23:K:1034:CLA:H151	1.50	0.94
10:K:33:PHE:O	10:K:33:PHE:HD2	1.51	0.94
3:C:117:VAL:HG11	23:C:1027:CLA:H42	1.50	0.93
3:C:179:ALA:HB1	3:C:199:ILE:HD13	1.49	0.93
3:C:263:ALA:HB3	3:C:264:PHE:CD2	2.03	0.93
23:A:1003:CLA:C7	23:A:1003:CLA:H41	1.91	0.93
23:B:1011:CLA:C3D	23:B:1013:CLA:H12	1.96	0.93
23:C:1033:CLA:HBB1	23:C:1033:CLA:HHC	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:ILE:HG23	26:C:1054:BCR:H381	1.47	0.93
29:C:1056:DGD:HE3	29:C:1056:DGD:HD61	0.94	0.93
26:D:1050:BCR:C22	30:D:1059:MGE:H3A1	1.97	0.93
16:V:148:GLU:HA	16:V:151:ILE:HD11	1.48	0.93
23:B:1022:CLA:H92	23:B:1022:CLA:CBC	1.98	0.93
23:C:1025:CLA:H152	23:C:1031:CLA:H92	1.49	0.93
1:A:187:GLN:HG3	1:A:325:ASN:HD21	1.32	0.93
23:B:1022:CLA:H142	23:B:1022:CLA:H93	0.95	0.93
23:C:1028:CLA:H2	29:C:1056:DGD:O1A	1.66	0.93
23:C:1029:CLA:CMD	23:C:1031:CLA:HAB	1.99	0.93
26:B:1047:BCR:H371	26:B:1047:BCR:H392	1.32	0.93
23:B:1016:CLA:H52	23:H:1017:CLA:H92	1.49	0.93
23:B:1022:CLA:H42	23:B:1022:CLA:O1A	1.68	0.93
15:U:68:THR:HG22	15:U:71:GLN:H	1.33	0.93
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.04	0.93
29:C:1055:DGD:HG31	29:C:1055:DGD:O2D	1.67	0.93
4:D:261:PHE:N	25:D:1042:PQ9:H92	1.81	0.93
23:B:1011:CLA:H193	23:H:1017:CLA:C10	1.95	0.93
23:B:1011:CLA:C1	23:B:1013:CLA:H93	1.99	0.93
23:B:1023:CLA:HMC1	23:B:1023:CLA:HBC2	1.47	0.93
30:B:1060:MGE:H8A2	11:L:23:LEU:HD21	1.47	0.93
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.48	0.93
9:J:10:LEU:H	9:J:10:LEU:HD13	1.34	0.93
10:K:39:VAL:HG23	18:Y:36:ILE:CD1	1.96	0.93
23:B:1014:CLA:C4	23:B:1014:CLA:C7	2.36	0.93
29:C:1057:DGD:HBG3	29:C:1057:DGD:HBF2	1.51	0.93
9:J:21:VAL:HG12	9:J:22:ILE:HD12	1.48	0.93
26:T:6046:BCR:H331	26:T:6046:BCR:C8	1.92	0.93
1:A:196:PRO:HB2	29:C:1057:DGD:HA81	1.47	0.92
23:B:1012:CLA:C1D	23:B:1020:CLA:C20	2.47	0.92
1:A:142:TRP:HB3	3:C:443:TRP:CH2	2.03	0.92
24:A:1038:PHO:C20	23:D:1005:CLA:CMB	2.48	0.92
26:B:1045:BCR:C8	26:B:1045:BCR:H331	1.98	0.92
2:B:370:LEU:HB2	2:B:379:ALA:HB3	1.47	0.92
23:C:1028:CLA:NC	29:C:1056:DGD:HA31	1.84	0.92
25:D:1042:PQ9:H242	30:L:1061:MGE:H212	1.46	0.92
2:B:83:GLU:HG2	2:B:86:ILE:HD11	1.51	0.92
23:A:1003:CLA:H42	24:A:1038:PHO:C3B	1.99	0.92
23:B:1021:CLA:O1A	23:B:1021:CLA:HED3	1.70	0.92
23:C:1030:CLA:HMB2	23:C:1031:CLA:C4B	1.99	0.92
23:A:1006:CLA:CBB	23:D:1004:CLA:H51	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1023:CLA:H101	23:B:1023:CLA:H161	1.51	0.92
24:A:1038:PHO:C20	23:D:1005:CLA:C2B	2.46	0.92
23:B:1016:CLA:H51	23:H:1017:CLA:H112	1.52	0.92
16:V:118:HIS:CD2	16:V:119:PRO:HD2	2.05	0.92
3:C:167:VAL:HA	3:C:170:ILE:HD12	1.50	0.92
4:D:139:ARG:HH12	4:D:265:ARG:HH21	1.15	0.92
25:A:1043:PQ9:H452	30:D:1059:MGE:H8A2	1.51	0.92
26:B:1045:BCR:H372	26:B:1045:BCR:H361	1.50	0.92
23:C:1031:CLA:HHD	23:C:1031:CLA:CBC	1.98	0.92
23:B:1014:CLA:HHD	23:B:1014:CLA:CBC	2.00	0.92
23:B:1021:CLA:O1A	23:B:1021:CLA:H2A	1.61	0.92
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.04	0.92
18:Y:44:GLY:O	18:Y:45:ASN:HB3	1.70	0.92
23:B:1015:CLA:CBC	26:B:1045:BCR:C34	2.45	0.91
3:C:167:VAL:O	3:C:170:ILE:HB	1.69	0.91
1:A:76:ASN:ND2	11:L:33:SER:HB3	1.85	0.91
23:B:1016:CLA:HHD	23:B:1016:CLA:HBC3	1.49	0.91
1:A:310:LYS:HB2	16:V:28:GLU:HB3	1.51	0.91
16:V:88:ALA:HA	16:V:108:TYR:CE2	2.05	0.91
23:A:1003:CLA:H42	24:A:1038:PHO:NB	1.85	0.91
2:B:174:LEU:CD2	2:B:266:GLU:HG2	2.01	0.91
23:C:1031:CLA:OBD	23:C:1033:CLA:H161	1.71	0.91
3:C:36:TRP:CZ3	3:C:37:ALA:HB2	2.06	0.91
23:B:1015:CLA:H71	23:B:1015:CLA:C4	2.00	0.91
23:D:1005:CLA:HBC1	23:D:1004:CLA:HBB2	1.48	0.91
23:B:1022:CLA:C2D	23:B:1022:CLA:H202	2.01	0.91
2:B:55:MET:HE3	2:B:80:ILE:HG21	1.51	0.91
20:Z:20:VAL:O	20:Z:24:PRO:HD2	1.69	0.91
29:C:1055:DGD:HAT1	29:C:1055:DGD:C6A	2.01	0.91
3:C:224:ILE:HD12	26:C:1054:BCR:H383	1.53	0.91
3:C:296:VAL:HG23	3:C:297:TYR:CD1	2.06	0.91
13:O:214:LYS:HE3	13:O:251:MET:HG3	1.53	0.91
23:A:1003:CLA:C4	24:A:1038:PHO:C1B	2.49	0.90
23:B:1013:CLA:HMB3	23:B:1014:CLA:H11	1.53	0.90
30:B:1060:MGE:H7B1	30:B:1060:MGE:H3B2	1.53	0.90
29:C:1057:DGD:CIB	29:C:1057:DGD:CEB	2.47	0.90
26:Z:1053:BCR:C37	26:Z:1053:BCR:H361	2.01	0.90
2:B:149:LEU:HB2	23:B:1012:CLA:H202	1.53	0.90
2:B:273:TYR:HA	2:B:276:ASP:OD1	1.71	0.90
23:C:1036:CLA:HBB1	23:C:1036:CLA:HHC	1.53	0.90
3:C:443:TRP:CD1	23:C:1032:CLA:HMD3	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1063:LHG:C29	23:C:1032:CLA:C7	2.50	0.90
23:B:1009:CLA:H2A	23:B:1009:CLA:CED	2.00	0.90
23:B:1022:CLA:H143	23:B:1022:CLA:H101	1.51	0.90
16:V:62:ALA:O	16:V:63:CYS:HB2	1.70	0.90
13:O:52:ALA:HB1	13:O:230:VAL:H	1.34	0.90
29:C:1057:DGD:HAF2	30:D:1059:MGE:CCB	1.99	0.90
3:C:100:GLY:HA2	3:C:196:VAL:HG12	1.50	0.90
3:C:61:VAL:HG11	3:C:125:LEU:HD13	1.53	0.90
23:C:1033:CLA:H2	23:C:1033:CLA:O1A	1.72	0.90
23:B:1009:CLA:HMB2	26:H:1049:BCR:H271	1.52	0.90
1:A:127:MET:O	1:A:130:GLN:HB3	1.72	0.90
1:A:224:ILE:H	2:B:482:ILE:HG23	1.34	0.90
3:C:56:HIS:C	3:C:58:GLY:H	1.72	0.90
1:A:184:ILE:HG12	4:D:186:GLN:NE2	1.87	0.90
1:A:180:PHE:CD1	4:D:192:THR:HB	2.07	0.90
23:B:1022:CLA:H43	23:B:1022:CLA:CGA	2.01	0.90
3:C:49:LEU:HD13	3:C:49:LEU:O	1.71	0.90
11:L:14:ARG:HA	12:M:26:TYR:HE1	1.36	0.90
3:C:199:ILE:HG21	3:C:234:VAL:HG11	1.54	0.89
3:C:449:ARG:HD3	23:C:1029:CLA:HED1	1.54	0.89
5:E:13:ILE:HG12	31:F:1040:HEM:HBC2	1.52	0.89
11:L:24:ILE:HD13	12:M:18:PRO:HG2	1.52	0.89
23:A:1006:CLA:CBC	23:A:1006:CLA:HHD	2.02	0.89
2:B:265:ILE:H	2:B:265:ILE:HD12	1.36	0.89
4:D:253:TRP:HA	4:D:256:ILE:CG2	2.02	0.89
25:A:1043:PQ9:H452	30:D:1059:MGE:C8A	2.01	0.89
23:C:1033:CLA:CMA	23:K:1034:CLA:C2C	2.51	0.89
30:B:1060:MGE:CBB	30:B:1060:MGE:CFB	2.32	0.89
3:C:48:LYS:HD2	23:C:1035:CLA:HED1	1.53	0.89
23:D:1008:CLA:H18	23:D:1008:CLA:H143	1.52	0.89
4:D:226:GLY:HA3	4:D:234:ALA:HB2	1.54	0.89
23:B:1009:CLA:H8	23:B:1009:CLA:H143	0.90	0.89
30:B:1060:MGE:H7B1	30:B:1060:MGE:C3B	2.03	0.89
8:I:31:ASN:HB2	8:I:32:PRO:HD2	1.55	0.89
26:A:1044:BCR:H403	26:A:1044:BCR:H372	1.55	0.89
23:C:1025:CLA:C12	26:C:1054:BCR:C35	2.49	0.89
27:A:1063:LHG:C29	23:C:1032:CLA:H72	2.01	0.89
6:F:41:GLN:NE2	9:J:28:PHE:HA	1.87	0.89
26:T:6046:BCR:H23C	26:T:6046:BCR:H392	1.54	0.89
23:B:1023:CLA:H91	23:B:1024:CLA:C15	2.03	0.89
2:B:127:ARG:HD3	2:B:128:THR:HG23	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:N	2:B:174:LEU:CD1	2.35	0.89
2:B:338:GLN:HA	2:B:338:GLN:HE21	1.36	0.89
2:B:460:LEU:HA	29:B:1058:DGD:HAG1	1.53	0.89
23:B:1013:CLA:HMC1	23:B:1013:CLA:HBC3	1.54	0.89
23:B:1012:CLA:H12	23:B:1013:CLA:H43	1.55	0.88
23:B:1013:CLA:HAB	23:B:1014:CLA:C5	2.03	0.88
2:B:191:ASN:ND2	7:H:60:VAL:HG12	1.88	0.88
23:B:1016:CLA:H162	23:D:1008:CLA:HMA1	0.89	0.88
3:C:223:TRP:CD1	3:C:224:ILE:HG12	2.08	0.88
25:D:1042:PQ9:O1	25:D:1042:PQ9:H143	1.72	0.88
1:A:314:ILE:HD12	4:D:58:TRP:HZ3	1.36	0.88
13:O:132:VAL:HG23	13:O:144:LEU:HD21	1.55	0.88
2:B:311:PHE:HE2	2:B:317:ASN:HD21	1.15	0.88
29:B:1058:DGD:HBF2	29:B:1058:DGD:HBF2	0.91	0.88
23:C:1035:CLA:C8	26:C:1052:BCR:C40	2.52	0.88
3:C:348:GLU:HG2	3:C:349:ILE:HG13	1.52	0.88
4:D:191:TRP:CE2	4:D:197:HIS:HB2	2.08	0.88
23:B:1021:CLA:H2	23:B:1021:CLA:CED	2.04	0.88
2:B:99:ALA:HB1	23:B:1014:CLA:C4	2.04	0.88
2:B:25:MET:HG3	26:B:1045:BCR:H401	1.55	0.88
23:C:1031:CLA:H141	26:C:1054:BCR:H362	1.54	0.88
3:C:117:VAL:HG12	3:C:118:HIS:N	1.87	0.88
3:C:56:HIS:HA	3:C:59:LEU:HD12	1.56	0.88
26:D:1050:BCR:H383	26:D:1050:BCR:C23	1.97	0.88
23:B:1012:CLA:CBB	23:B:1015:CLA:HBB2	2.04	0.88
2:B:105:GLY:HA3	26:B:1047:BCR:C40	2.02	0.88
2:B:7:ARG:HG2	2:B:7:ARG:NH1	1.83	0.88
4:D:183:LEU:HD23	4:D:183:LEU:H	1.38	0.88
10:K:31:LEU:HB3	26:K:1051:BCR:C14	2.03	0.88
1:A:265:PHE:CZ	27:A:1063:LHG:H151	2.07	0.87
1:A:220:THR:HA	1:A:223:LEU:HD23	1.53	0.87
26:B:1048:BCR:H372	26:B:1048:BCR:H403	1.56	0.87
4:D:124:GLY:HA2	4:D:127:LEU:HD12	1.54	0.87
11:L:29:LEU:HB2	14:T:9:ILE:HG21	1.54	0.87
15:U:31:ASN:HD22	15:U:32:ILE:N	1.70	0.87
18:Y:43:ARG:CG	18:Y:44:GLY:H	1.87	0.87
23:B:1020:CLA:H102	23:B:1020:CLA:C16	2.03	0.87
3:C:39:ASN:HB2	23:C:1032:CLA:HBA1	1.56	0.87
23:D:1008:CLA:HMC1	23:D:1008:CLA:CBC	2.05	0.87
18:Y:42:ARG:HB3	18:Y:43:ARG:HH11	1.40	0.87
23:B:1011:CLA:C19	23:H:1017:CLA:C10	2.51	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1018:CLA:H152	23:B:1020:CLA:O1A	1.75	0.87
3:C:63:TRP:HE1	23:C:1028:CLA:C2C	1.86	0.87
3:C:50:LEU:HD21	3:C:54:VAL:HG23	1.54	0.87
3:C:79:LYS:HB3	3:C:84:GLN:NE2	1.89	0.87
23:A:1003:CLA:HAA2	23:A:1003:CLA:HED3	1.54	0.87
4:D:258:GLY:O	4:D:259:ILE:HD13	1.73	0.87
23:B:1018:CLA:C10	23:B:1023:CLA:CAA	2.52	0.87
23:C:1029:CLA:C5	23:C:1029:CLA:C4B	2.52	0.87
26:H:1049:BCR:H311	26:H:1049:BCR:HC8	1.57	0.87
5:E:20:TRP:HZ2	9:J:13:VAL:HG23	1.40	0.87
3:C:417:VAL:CG1	16:V:68:VAL:HB	2.05	0.87
2:B:332:LYS:HB3	2:B:444:ARG:HH12	1.38	0.87
2:B:191:ASN:HD21	7:H:60:VAL:HA	1.39	0.87
26:B:1048:BCR:H392	26:B:1048:BCR:H373	1.56	0.87
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.09	0.87
5:E:73:LYS:O	5:E:76:VAL:HG23	1.74	0.87
15:U:45:LEU:O	15:U:49:ILE:HG13	1.74	0.87
15:U:68:THR:CG2	15:U:71:GLN:H	1.86	0.87
26:K:1051:BCR:C40	26:K:1051:BCR:H23C	2.01	0.87
7:H:44:ILE:HD11	17:X:19:PHE:CE2	2.10	0.87
23:B:1011:CLA:C2	23:B:1013:CLA:C9	2.53	0.86
23:B:1014:CLA:H111	26:B:1048:BCR:HC7	1.57	0.86
23:B:1023:CLA:H143	23:B:1024:CLA:H61	1.57	0.86
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.55	0.86
18:Y:32:GLY:O	18:Y:35:ILE:HG23	1.74	0.86
23:A:1003:CLA:C4	24:A:1038:PHO:C2B	2.52	0.86
1:A:44:ALA:HB2	1:A:118:HIS:HB3	1.57	0.86
23:C:1028:CLA:H102	29:C:1056:DGD:HAS2	1.57	0.86
29:C:1056:DGD:HA41	29:C:1056:DGD:O1A	1.73	0.86
6:F:40:MET:O	6:F:43:ILE:HG13	1.75	0.86
23:K:1034:CLA:C4	23:K:1034:CLA:C7	2.49	0.86
2:B:223:GLN:HE21	7:H:21:VAL:HG11	1.39	0.86
23:A:1003:CLA:H42	24:A:1038:PHO:C2B	2.06	0.86
2:B:456:ALA:CB	29:B:1058:DGD:HBV1	2.05	0.86
3:C:172:ALA:N	23:C:1025:CLA:HBC2	1.90	0.86
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.58	0.86
2:B:105:GLY:HA2	26:B:1047:BCR:C40	2.02	0.86
1:A:297:LEU:HD22	3:C:404:LEU:HD23	1.56	0.86
3:C:49:LEU:CD2	3:C:52:ALA:CB	2.53	0.86
26:T:6048:BCR:H403	26:T:6048:BCR:H372	1.57	0.86
26:A:1044:BCR:H392	26:A:1044:BCR:H373	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:1049:BCR:C39	26:H:1049:BCR:C23	2.30	0.86
7:H:54:ILE:O	7:H:55:LEU:HD13	1.75	0.86
23:B:1013:CLA:C12	23:B:1018:CLA:H42	2.05	0.86
23:C:1035:CLA:C9	26:C:1052:BCR:H402	2.06	0.86
3:C:140:LEU:HD21	3:C:146:PHE:HE1	1.38	0.86
3:C:223:TRP:NE1	3:C:224:ILE:HG12	1.90	0.86
3:C:49:LEU:N	3:C:49:LEU:HD12	1.91	0.86
23:K:1034:CLA:H71	23:K:1034:CLA:H43	1.57	0.86
1:A:103:ASP:HA	1:A:106:LEU:HD12	1.58	0.86
30:D:1059:MGE:H251	30:D:1059:MGE:H212	1.56	0.86
4:D:160:TYR:CE1	28:D:1068:IOD:I	2.98	0.86
4:D:95:PRO:HG3	17:X:15:SER:HB2	1.57	0.86
1:A:14:TRP:HH2	8:I:21:PHE:HB3	1.41	0.86
26:T:6048:BCR:H373	26:T:6048:BCR:H392	1.56	0.86
29:C:1056:DGD:C6D	29:C:1056:DGD:C3E	2.46	0.86
3:C:429:SER:HB3	29:C:1056:DGD:HA91	1.58	0.86
3:C:263:ALA:CB	3:C:264:PHE:CD2	2.59	0.86
3:C:50:LEU:HD23	3:C:51:GLY:N	1.91	0.86
13:O:55:ALA:HB1	13:O:161:SER:HB3	1.55	0.86
1:A:279:ARG:HD3	4:D:208:ALA:CB	2.06	0.85
3:C:50:LEU:O	3:C:50:LEU:HD23	1.76	0.85
4:D:213:ILE:HG12	25:D:1042:PQ9:H111	1.58	0.85
10:K:26:PRO:O	10:K:29:PRO:HD2	1.75	0.85
23:B:1019:CLA:CHA	23:B:1019:CLA:HBA1	2.07	0.85
3:C:42:LEU:CD1	3:C:49:LEU:CD1	2.54	0.85
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.58	0.85
23:A:1006:CLA:C17	26:D:1050:BCR:H282	2.07	0.85
1:A:258:LEU:HD12	4:D:128:ARG:NH2	1.91	0.85
23:B:1012:CLA:C1D	23:B:1020:CLA:H201	2.05	0.85
26:B:1047:BCR:H373	26:B:1047:BCR:H392	1.56	0.85
23:C:1027:CLA:HBC3	23:C:1027:CLA:HMC1	1.56	0.85
3:C:49:LEU:HD11	23:C:1035:CLA:HMA2	1.58	0.85
13:O:46:PRO:HB2	13:O:266:TYR:CD2	2.12	0.85
11:L:14:ARG:HA	12:M:26:TYR:CE1	2.10	0.85
23:B:1022:CLA:C13	23:B:1022:CLA:H93	2.05	0.85
13:O:179:THR:HG22	13:O:180:ALA:N	1.92	0.85
1:A:259:ILE:HD13	25:A:1043:PQ9:H242	1.58	0.85
23:C:1025:CLA:H141	23:C:1031:CLA:CMB	2.05	0.85
23:C:1033:CLA:HMA3	23:K:1034:CLA:C2C	2.07	0.85
2:B:52:LEU:HD22	2:B:311:PHE:HD1	1.41	0.85
13:O:132:VAL:HG23	13:O:144:LEU:CD2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CD2	1:A:71:LEU:HD11	2.11	0.85
29:C:1055:DGD:HGB2	29:C:1055:DGD:HBF1	1.58	0.85
6:F:15:ILE:HG13	6:F:16:PHE:HD1	1.41	0.85
3:C:50:LEU:CD2	3:C:51:GLY:N	2.40	0.85
23:B:1012:CLA:CBB	23:B:1015:CLA:CBB	2.55	0.85
2:B:3:LEU:HB3	11:L:9:PRO:O	1.77	0.85
23:B:1016:CLA:C16	23:D:1008:CLA:HMA3	2.02	0.84
23:B:1024:CLA:HMC1	23:B:1024:CLA:HBC2	1.59	0.84
13:O:176:SER:HB3	13:O:216:PHE:HE2	1.41	0.84
7:H:43:LEU:HD21	17:X:19:PHE:CE1	2.12	0.84
18:Y:42:ARG:CB	18:Y:43:ARG:HH11	1.90	0.84
23:C:1030:CLA:HED2	23:C:1030:CLA:CAD	2.07	0.84
10:K:33:PHE:O	10:K:33:PHE:CD2	2.30	0.84
2:B:149:LEU:HG	23:B:1011:CLA:CBC	2.05	0.84
3:C:406:SER:HB3	29:C:1056:DGD:HE1	1.59	0.84
23:D:1004:CLA:H201	30:D:1059:MGE:H8A1	1.58	0.84
6:F:19:ARG:HH22	31:F:1040:HEM:HAC	1.39	0.84
23:C:1025:CLA:H91	26:C:1054:BCR:H373	1.56	0.84
4:D:261:PHE:H	25:D:1042:PQ9:C9	1.85	0.84
23:C:1029:CLA:CBC	23:C:1029:CLA:HMC1	2.08	0.84
23:C:1037:CLA:HHD	23:C:1037:CLA:CBC	2.06	0.84
1:A:291:SER:HB3	3:C:431:PHE:CE1	2.13	0.84
1:A:338:ASN:O	1:A:339:PHE:CG	2.30	0.84
23:C:1031:CLA:C14	26:C:1054:BCR:H362	2.08	0.84
23:C:1033:CLA:H152	23:C:1033:CLA:H203	1.59	0.84
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.58	0.84
24:A:1038:PHO:H2A	24:A:1038:PHO:O1D	1.77	0.84
4:D:198:MET:HB3	23:D:1005:CLA:HED2	1.60	0.84
23:B:1016:CLA:C2	23:H:1017:CLA:C9	2.56	0.84
1:A:316:THR:C	4:D:63:LEU:HD21	1.97	0.84
23:B:1019:CLA:C19	23:B:1021:CLA:H72	2.07	0.84
23:B:1021:CLA:HED3	23:B:1021:CLA:H2	1.60	0.84
2:B:460:LEU:HD23	2:B:460:LEU:O	1.77	0.84
4:D:184:PHE:HE2	4:D:188:PHE:HD1	1.23	0.84
11:L:24:ILE:HD13	12:M:18:PRO:CG	2.08	0.84
25:D:1042:PQ9:H401	11:L:30:LEU:HD12	1.58	0.84
1:A:116:ILE:HD11	1:A:158:PHE:HB3	1.58	0.83
23:B:1011:CLA:H12	23:B:1013:CLA:C9	2.06	0.83
2:B:65:PHE:CZ	23:B:1012:CLA:CMA	2.58	0.83
2:B:463:PHE:CE1	23:B:1016:CLA:HBB1	2.12	0.83
23:B:1021:CLA:H41	30:B:1060:MGE:H242	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ARG:HD2	7:H:20:LYS:O	1.76	0.83
23:C:1033:CLA:C2	23:C:1033:CLA:H71	2.07	0.83
3:C:229:ASN:N	3:C:229:ASN:HD22	1.73	0.83
15:U:61:VAL:HG12	15:U:75:LEU:HD23	1.58	0.83
2:B:463:PHE:HE1	23:B:1016:CLA:HBB1	1.42	0.83
10:K:33:PHE:CD2	10:K:33:PHE:C	2.50	0.83
16:V:135:GLU:O	16:V:139:VAL:HG23	1.78	0.83
20:Z:23:VAL:HG13	20:Z:27:TYR:CE2	2.12	0.83
2:B:264:PRO:CG	2:B:267:LEU:HB2	2.09	0.83
1:A:160:ILE:HG21	3:C:431:PHE:HE1	1.44	0.83
7:H:6:TRP:O	7:H:10:ILE:HG13	1.79	0.83
9:J:31:GLY:O	9:J:35:GLY:HA3	1.78	0.83
1:A:301:ASN:HD22	3:C:407:VAL:HG11	1.41	0.83
23:B:1009:CLA:CAA	26:H:1049:BCR:H363	2.08	0.83
26:B:1047:BCR:H372	26:B:1047:BCR:H403	1.56	0.83
23:C:1025:CLA:C14	23:C:1031:CLA:HMB3	2.05	0.83
13:O:176:SER:HB3	13:O:216:PHE:CE2	2.13	0.83
14:T:1:MET:O	14:T:4:ILE:HG23	1.77	0.83
27:A:1063:LHG:H161	27:A:1063:LHG:C12	2.05	0.83
23:B:1022:CLA:H142	23:B:1022:CLA:C6	1.98	0.83
3:C:42:LEU:CD1	3:C:49:LEU:HD11	2.09	0.83
24:D:1039:PHO:HBC2	24:D:1039:PHO:CHD	2.06	0.83
23:K:1034:CLA:H41	23:K:1034:CLA:C7	2.08	0.83
2:B:12:LEU:HD13	23:B:1020:CLA:HMC2	1.60	0.83
25:D:1042:PQ9:H392	30:L:1061:MGE:H241	1.58	0.83
23:B:1011:CLA:HMD2	23:B:1014:CLA:HMB1	1.59	0.83
24:A:1038:PHO:H202	23:D:1005:CLA:CMB	2.08	0.83
9:J:21:VAL:CG1	9:J:22:ILE:HD12	2.09	0.83
23:C:1032:CLA:C15	10:K:33:PHE:CZ	2.48	0.83
23:C:1027:CLA:C15	26:Z:1053:BCR:H332	2.07	0.83
23:B:1022:CLA:H143	23:B:1022:CLA:C6	2.09	0.83
2:B:7:ARG:CG	2:B:7:ARG:HH11	1.91	0.83
3:C:185:LEU:HD12	3:C:230:LEU:HD22	1.59	0.83
1:A:184:ILE:HG12	4:D:186:GLN:HE21	1.44	0.83
14:T:4:ILE:HD13	14:T:5:THR:H	1.40	0.83
23:D:1008:CLA:C14	23:D:1008:CLA:H18	2.07	0.83
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.13	0.82
3:C:318:LEU:CD2	3:C:328:VAL:HG11	2.08	0.82
23:C:1025:CLA:HMB2	23:C:1025:CLA:H42	0.86	0.82
3:C:429:SER:O	3:C:432:VAL:HG12	1.80	0.82
4:D:58:TRP:HE1	5:E:64:PRO:HD2	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:1049:BCR:H392	26:H:1049:BCR:H23C	0.83	0.82
27:A:1063:LHG:H291	23:C:1032:CLA:H71	1.60	0.82
1:A:58:VAL:HG12	1:A:60:ILE:H	1.42	0.82
23:D:1008:CLA:H141	23:D:1008:CLA:H193	1.60	0.82
3:C:49:LEU:CD2	23:C:1035:CLA:HMA1	2.07	0.82
23:D:1008:CLA:HBC2	23:D:1008:CLA:HMC1	1.60	0.82
4:D:148:ALA:HB1	4:D:279:LEU:HD13	1.60	0.82
10:K:28:ILE:HD13	10:K:31:LEU:HD12	1.60	0.82
14:T:21:ILE:HD12	26:T:6046:BCR:HC42	1.61	0.82
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.58	0.82
23:B:1011:CLA:CAD	23:B:1013:CLA:C1	2.57	0.82
23:C:1033:CLA:C7	23:C:1033:CLA:C2	2.54	0.82
31:F:1040:HEM:HMB2	31:F:1040:HEM:HBB2	1.58	0.82
29:C:1056:DGD:C6D	29:C:1056:DGD:C5E	2.50	0.82
3:C:49:LEU:H	3:C:49:LEU:CD1	1.91	0.82
3:C:89:ILE:HG12	3:C:111:PHE:HD2	1.45	0.82
24:A:1038:PHO:CHD	24:A:1038:PHO:HBC3	2.10	0.82
2:B:224:ARG:HG2	7:H:25:TRP:NE1	1.95	0.82
2:B:301:ALA:O	2:B:304:ALA:HB3	1.80	0.82
1:A:279:ARG:HB3	4:D:212:ALA:HB2	1.60	0.82
1:A:317:TRP:N	4:D:63:LEU:HD21	1.94	0.82
2:B:80:ILE:HD11	2:B:93:PHE:HZ	1.45	0.82
13:O:45:CYS:HB2	13:O:46:PRO:HD2	1.62	0.82
23:A:1003:CLA:C14	24:A:1038:PHO:C8	2.58	0.82
2:B:12:LEU:HD22	2:B:19:LEU:HD13	1.61	0.82
23:A:1007:CLA:H42	23:C:1029:CLA:H191	1.60	0.82
3:C:117:VAL:CG1	3:C:118:HIS:N	2.43	0.82
4:D:201:VAL:HG23	23:D:1004:CLA:HMB3	1.60	0.82
23:A:1006:CLA:H172	26:D:1050:BCR:H272	1.62	0.81
23:B:1009:CLA:C2A	23:B:1009:CLA:CED	2.53	0.81
1:A:120:LEU:HD21	1:A:155:PHE:HA	1.62	0.81
3:C:263:ALA:CB	3:C:264:PHE:HE2	1.93	0.81
3:C:92:ILE:H	3:C:92:ILE:HD12	1.44	0.81
4:D:36:LEU:HD23	4:D:37:LEU:N	1.95	0.81
23:B:1023:CLA:H152	23:B:1024:CLA:CHB	2.10	0.81
3:C:48:LYS:HG3	3:C:49:LEU:HD12	1.62	0.81
1:A:325:ASN:HD22	1:A:328:MET:HE3	1.43	0.81
30:B:1060:MGE:C7B	30:B:1060:MGE:C3B	2.57	0.81
2:B:488:PRO:O	2:B:489:GLU:HB3	1.78	0.81
3:C:128:GLY:HA3	23:C:1037:CLA:HAC2	1.61	0.81
2:B:359:MET:O	2:B:359:MET:HG3	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:1034:CLA:C10	23:K:1034:CLA:H143	2.06	0.81
13:O:141:ARG:HH11	13:O:141:ARG:HG2	1.44	0.81
4:D:147:SER:HG	4:D:280:TRP:HE1	1.29	0.81
4:D:198:MET:CB	23:D:1005:CLA:HED2	2.10	0.81
11:L:8:GLN:H	11:L:8:GLN:NE2	1.78	0.81
1:A:259:ILE:N	4:D:128:ARG:HH22	1.79	0.81
23:B:1012:CLA:HHD	23:B:1012:CLA:HBC3	1.60	0.81
2:B:174:LEU:HD23	2:B:266:GLU:CG	2.10	0.81
2:B:298:LEU:O	2:B:301:ALA:HB3	1.80	0.81
3:C:293:ASN:HD21	3:C:295:THR:HB	1.44	0.81
25:D:1042:PQ9:C30	25:D:1042:PQ9:H342	2.10	0.81
13:O:172:PHE:CD1	13:O:221:GLY:HA3	2.14	0.81
23:B:1011:CLA:C2D	23:B:1013:CLA:C4	2.59	0.81
3:C:49:LEU:HD22	3:C:52:ALA:CB	2.10	0.81
23:D:1008:CLA:C14	23:D:1008:CLA:C17	2.59	0.81
23:A:1006:CLA:CBC	4:D:182:LEU:HD21	2.11	0.81
23:A:1003:CLA:HMB2	23:D:1004:CLA:HMB2	1.63	0.81
23:B:1009:CLA:C10	23:B:1009:CLA:C14	2.55	0.81
23:B:1010:CLA:H12	23:B:1010:CLA:CBD	2.11	0.81
23:C:1029:CLA:HMD3	23:C:1031:CLA:CAB	2.11	0.81
26:C:1054:BCR:C23	26:C:1054:BCR:C40	2.30	0.81
10:K:31:LEU:HB3	26:K:1051:BCR:H14C	1.63	0.81
13:O:223:ILE:HG22	13:O:243:SER:HB3	1.62	0.81
20:Z:28:ALA:O	20:Z:30:PRO:HD3	1.79	0.81
1:A:278:TRP:HE3	1:A:278:TRP:HA	1.46	0.81
23:C:1033:CLA:H91	23:C:1036:CLA:HAA1	1.62	0.81
29:C:1056:DGD:C9B	29:C:1056:DGD:HBF1	2.11	0.81
3:C:333:GLY:N	3:C:338:GLY:HA2	1.96	0.81
1:A:196:PRO:HA	1:A:199:GLN:HG3	1.62	0.80
23:B:1010:CLA:HMD3	23:B:1011:CLA:H92	1.63	0.80
2:B:103:LEU:CB	23:B:1014:CLA:H92	2.12	0.80
2:B:115:TRP:O	2:B:118:TRP:HB3	1.81	0.80
2:B:264:PRO:HG2	2:B:267:LEU:HB2	1.63	0.80
2:B:362:PHE:CZ	28:D:1068:IOD:I	3.04	0.80
3:C:185:LEU:HG	3:C:199:ILE:HD11	1.63	0.80
3:C:428:THR:HG23	3:C:429:SER:H	1.46	0.80
3:C:428:THR:HG23	3:C:429:SER:N	1.94	0.80
23:A:1006:CLA:C16	26:D:1050:BCR:H272	2.11	0.80
26:A:1044:BCR:H403	26:A:1044:BCR:H371	1.31	0.80
1:A:16:ARG:HA	1:A:19:ASN:HD21	1.46	0.80
1:A:129:ARG:CZ	4:D:256:ILE:HD12	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LEU:N	23:B:1020:CLA:HMD3	1.96	0.80
3:C:397:THR:OG1	3:C:398:HIS:N	2.13	0.80
2:B:98:LEU:O	2:B:98:LEU:HD13	1.81	0.80
29:C:1055:DGD:HA21	29:C:1055:DGD:HB21	1.62	0.80
24:A:1038:PHO:HBC3	24:A:1038:PHO:HHD	1.62	0.80
2:B:332:LYS:HB3	2:B:444:ARG:NH1	1.96	0.80
29:C:1056:DGD:HAV1	29:C:1057:DGD:HA82	1.64	0.80
3:C:107:ASP:HB3	3:C:110:PRO:CD	2.10	0.80
3:C:141:GLU:O	3:C:144:SER:HB2	1.81	0.80
7:H:38:PHE:HB2	26:H:1049:BCR:H10C	1.64	0.80
23:B:1009:CLA:C1A	23:B:1009:CLA:O1A	2.30	0.80
26:B:1045:BCR:H23C	26:B:1045:BCR:C38	2.06	0.80
23:C:1029:CLA:O1A	23:C:1029:CLA:CHA	2.30	0.80
3:C:49:LEU:HD11	23:C:1035:CLA:CMA	2.11	0.80
23:A:1003:CLA:H2A	23:A:1003:CLA:CED	2.11	0.80
29:B:1058:DGD:CAB	29:B:1058:DGD:C6B	2.55	0.80
23:C:1025:CLA:C1	23:C:1025:CLA:HHB	2.06	0.80
23:C:1029:CLA:H43	26:C:1054:BCR:H321	1.63	0.80
23:C:1033:CLA:CMA	23:K:1034:CLA:CAC	2.60	0.80
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.17	0.80
23:C:1031:CLA:H141	26:C:1054:BCR:C36	2.10	0.80
26:C:1052:BCR:C27	26:C:1052:BCR:H371	2.09	0.80
23:C:1027:CLA:H121	23:C:1027:CLA:C18	2.11	0.80
29:C:1057:DGD:HB82	30:D:1059:MGE:H8B2	1.60	0.80
23:B:1022:CLA:C4	23:B:1022:CLA:CGA	2.59	0.80
3:C:443:TRP:HD1	23:C:1032:CLA:HMD3	1.45	0.80
4:D:88:SER:HA	7:H:50:ASN:ND2	1.93	0.80
13:O:141:ARG:HG2	13:O:141:ARG:NH1	1.96	0.80
23:B:1016:CLA:CHA	23:B:1016:CLA:O1A	2.30	0.79
3:C:128:GLY:CA	23:C:1037:CLA:HAC2	2.12	0.79
4:D:120:PHE:HA	4:D:123:ILE:HD12	1.62	0.79
5:E:13:ILE:HA	5:E:16:SER:HB2	1.64	0.79
7:H:43:LEU:HD21	17:X:19:PHE:CZ	2.16	0.79
15:U:28:ASN:HD22	15:U:54:PRO:HB2	1.46	0.79
16:V:45:ILE:N	16:V:45:ILE:HD12	1.96	0.79
23:B:1011:CLA:C4	23:B:1011:CLA:O1A	2.30	0.79
23:B:1022:CLA:C4D	23:B:1022:CLA:C1	2.60	0.79
26:B:1045:BCR:C23	26:B:1045:BCR:H383	2.09	0.79
2:B:5:TRP:CA	2:B:8:VAL:HG13	2.11	0.79
15:U:68:THR:HG23	15:U:70:ARG:H	1.45	0.79
26:H:1049:BCR:H292	17:X:16:LEU:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:1055:DGD:CEB	29:C:1055:DGD:CIB	2.58	0.79
3:C:56:HIS:C	3:C:58:GLY:N	2.31	0.79
18:Y:43:ARG:CD	18:Y:44:GLY:H	1.95	0.79
1:A:325:ASN:HA	1:A:328:MET:HE3	1.61	0.79
23:B:1022:CLA:C4	23:B:1022:CLA:O1A	2.30	0.79
23:B:1022:CLA:O1D	23:B:1022:CLA:CGA	2.30	0.79
23:C:1030:CLA:H122	23:C:1030:CLA:H172	1.62	0.79
26:C:1052:BCR:H383	26:C:1052:BCR:H372	1.61	0.79
1:A:314:ILE:HD12	4:D:58:TRP:CZ3	2.17	0.79
7:H:30:LEU:HD12	7:H:33:VAL:HG21	1.64	0.79
20:Z:55:GLY:HA2	26:Z:1053:BCR:H311	1.65	0.79
3:C:292:PHE:CD1	29:C:1055:DGD:HD1	2.18	0.79
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.62	0.79
3:C:50:LEU:HD21	3:C:54:VAL:HG21	1.65	0.79
4:D:146:PHE:O	4:D:149:PRO:HD2	1.82	0.79
1:A:223:LEU:HD21	4:D:265:ARG:HG2	1.62	0.79
11:L:36:PHE:CE1	12:M:7:GLY:HA3	2.18	0.79
13:O:31:LEU:HD13	13:O:36:ILE:HD11	1.64	0.79
15:U:83:THR:HG22	15:U:84:VAL:H	1.47	0.79
1:A:270:SER:HA	4:D:232:PHE:CZ	2.17	0.79
1:A:224:ILE:HA	2:B:482:ILE:HG12	1.64	0.79
23:C:1025:CLA:H43	23:C:1025:CLA:C2B	2.11	0.79
3:C:161:LEU:HD23	3:C:162:GLY:N	1.96	0.79
2:B:464:PHE:CZ	30:B:1060:MGE:H4B1	2.18	0.79
2:B:125:ASP:OD2	7:H:18:TYR:HB2	1.81	0.79
23:C:1029:CLA:CMA	23:C:1029:CLA:CBA	2.57	0.79
23:D:1005:CLA:HMA2	25:D:1042:PQ9:H443	1.65	0.79
23:C:1025:CLA:C15	23:C:1031:CLA:C9	2.49	0.79
3:C:307:PRO:HA	3:C:358:PHE:CD1	2.17	0.79
4:D:57:SER:CB	4:D:79:SER:HB3	2.13	0.79
23:K:1034:CLA:H41	23:K:1034:CLA:H71	1.60	0.79
23:A:1003:CLA:HBB1	23:A:1006:CLA:HMD2	1.65	0.79
2:B:468:TRP:HE1	23:B:1019:CLA:HED2	1.47	0.79
26:C:1054:BCR:H403	26:C:1054:BCR:H23C	0.82	0.79
3:C:167:VAL:O	23:C:1036:CLA:H41	1.83	0.79
16:V:70:GLY:HA3	16:V:156:TRP:O	1.83	0.79
17:X:43:ILE:O	17:X:43:ILE:HG22	1.80	0.79
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.64	0.79
23:B:1009:CLA:CBF	23:B:1010:CLA:HBB1	1.94	0.79
23:C:1026:CLA:O1A	23:C:1026:CLA:C2	2.30	0.79
3:C:172:ALA:N	23:C:1025:CLA:CBC	2.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1038:PHO:C9	23:D:1005:CLA:H18	2.11	0.79
4:D:153:PHE:HB2	23:D:1004:CLA:H41	1.64	0.79
4:D:317:LYS:NZ	28:D:1064:IOD:I	2.85	0.79
1:A:116:ILE:HG23	1:A:117:PHE:H	1.47	0.78
1:A:196:PRO:HG3	3:C:404:LEU:HD12	1.63	0.78
1:A:215:HIS:NE2	1:A:271:LEU:HD11	1.97	0.78
23:B:1012:CLA:C1D	23:B:1020:CLA:H202	2.12	0.78
23:B:1013:CLA:C3B	23:B:1014:CLA:H51	2.13	0.78
23:B:1012:CLA:CMD	23:B:1020:CLA:H201	2.13	0.78
1:A:224:ILE:HA	2:B:482:ILE:CG1	2.13	0.78
2:B:99:ALA:HB1	23:B:1014:CLA:H42	1.64	0.78
3:C:107:ASP:HB3	3:C:110:PRO:HD2	1.65	0.78
23:B:1021:CLA:O2A	23:B:1021:CLA:HMA2	1.83	0.78
26:B:1047:BCR:H341	26:B:1047:BCR:C12	2.12	0.78
23:C:1025:CLA:H151	23:C:1031:CLA:H91	1.64	0.78
23:C:1028:CLA:H91	29:C:1056:DGD:HBT1	1.65	0.78
23:C:1031:CLA:OBD	23:C:1033:CLA:C12	2.28	0.78
3:C:220:GLY:O	3:C:221:GLU:HG3	1.81	0.78
6:F:45:ARG:NE	6:F:45:ARG:HA	1.97	0.78
23:B:1012:CLA:C2B	23:B:1015:CLA:CBB	2.62	0.78
3:C:397:THR:OG1	3:C:398:HIS:ND1	2.17	0.78
30:L:1061:MGE:C1G	30:L:1061:MGE:O1B	2.31	0.78
23:B:1022:CLA:CBC	23:B:1022:CLA:HHD	2.09	0.78
2:B:105:GLY:HA2	26:B:1047:BCR:H402	1.64	0.78
2:B:108:PHE:O	2:B:111:ALA:HB3	1.83	0.78
23:B:1012:CLA:C2B	23:B:1015:CLA:HBB2	2.14	0.78
23:C:1029:CLA:H42	23:C:1029:CLA:CHD	2.13	0.78
4:D:328:TRP:HZ3	16:V:161:VAL:HA	1.49	0.78
23:B:1023:CLA:C9	23:B:1024:CLA:H151	2.13	0.78
23:A:1007:CLA:H43	23:C:1029:CLA:C19	2.14	0.78
1:A:143:ILE:HB	4:D:220:ASN:ND2	1.99	0.78
6:F:19:ARG:O	6:F:23:VAL:HG23	1.84	0.78
11:L:21:LEU:HB2	14:T:16:LEU:HD21	1.64	0.78
23:B:1010:CLA:H151	29:B:1058:DGD:HA82	1.64	0.78
3:C:420:VAL:HB	3:C:425:TRP:HE1	1.49	0.78
13:O:243:SER:OG	13:O:261:ILE:HB	1.82	0.78
10:K:28:ILE:HD11	18:Y:28:ILE:HD12	1.65	0.78
3:C:121:SER:O	3:C:124:VAL:HG22	1.84	0.78
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.64	0.78
23:B:1022:CLA:H11	23:B:1022:CLA:C3D	2.14	0.78
23:C:1030:CLA:CED	23:C:1030:CLA:C3D	2.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:42:ARG:O	18:Y:43:ARG:HB3	1.83	0.78
1:A:91:LEU:HG	1:A:166:GLY:O	1.83	0.78
23:B:1012:CLA:CMB	23:B:1015:CLA:HBB1	2.12	0.78
23:C:1030:CLA:HBC2	23:C:1030:CLA:CHD	2.13	0.78
23:C:1037:CLA:HBC2	23:C:1037:CLA:CHD	2.12	0.78
3:C:42:LEU:HD11	3:C:49:LEU:HD12	1.66	0.78
3:C:92:ILE:N	3:C:92:ILE:HD12	1.99	0.78
23:K:1034:CLA:CGA	23:K:1034:CLA:H42	2.14	0.78
2:B:260:SER:OG	2:B:262:THR:HG23	1.83	0.77
3:C:171:GLY:CA	3:C:174:LEU:HB2	2.11	0.77
23:D:1004:CLA:H102	23:D:1004:CLA:H142	1.66	0.77
10:K:37:PHE:HB3	26:K:1051:BCR:H401	1.66	0.77
20:Z:46:LEU:O	20:Z:50:LEU:HB2	1.83	0.77
23:C:1025:CLA:H43	23:C:1025:CLA:C1B	2.14	0.77
10:K:18:PHE:O	10:K:22:VAL:HG23	1.85	0.77
16:V:64:ALA:O	16:V:68:VAL:CG1	2.26	0.77
23:A:1003:CLA:CAA	23:A:1003:CLA:CED	2.30	0.77
23:B:1021:CLA:OBD	23:B:1022:CLA:CHC	2.32	0.77
23:C:1030:CLA:HED3	23:C:1030:CLA:C4D	2.15	0.77
3:C:343:ARG:HH12	3:C:348:GLU:HG3	0.74	0.77
4:D:148:ALA:O	4:D:152:VAL:HG23	1.84	0.77
5:E:34:GLY:HA2	6:F:32:PHE:CE1	2.19	0.77
13:O:172:PHE:HB2	13:O:221:GLY:H	1.49	0.77
13:O:82:PRO:CG	13:O:89:ALA:HB1	2.15	0.77
15:U:51:LYS:HG3	15:U:52:ASN:H	1.48	0.77
17:X:25:SER:O	17:X:29:VAL:HG23	1.84	0.77
23:A:1007:CLA:HBD	23:A:1007:CLA:HBA2	1.64	0.77
2:B:249:ALA:HB2	23:B:1012:CLA:CBC	2.15	0.77
29:C:1057:DGD:HBG2	29:C:1057:DGD:CEB	2.10	0.77
10:K:21:LEU:HD11	18:Y:24:MET:HG3	1.66	0.77
23:A:1007:CLA:CAD	23:A:1007:CLA:HED2	2.15	0.77
3:C:56:HIS:HE1	23:C:1033:CLA:HMA1	1.49	0.77
4:D:246:MET:HE3	4:D:264:LYS:CG	2.15	0.77
1:A:279:ARG:CZ	24:A:1038:PHO:HMC1	2.14	0.77
4:D:36:LEU:HD21	4:D:124:GLY:HA2	1.66	0.77
13:O:52:ALA:HB1	13:O:230:VAL:N	1.99	0.77
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.50	0.77
23:C:1025:CLA:C4A	23:C:1025:CLA:O2A	2.32	0.77
25:A:1043:PQ9:C45	30:D:1059:MGE:CAA	2.57	0.77
23:C:1029:CLA:HBB1	23:C:1029:CLA:HHC	1.65	0.77
23:A:1006:CLA:H161	26:D:1050:BCR:H272	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:184:PHE:HE2	4:D:188:PHE:CD1	2.03	0.77
23:B:1024:CLA:H2A	23:B:1024:CLA:O2A	1.83	0.77
3:C:81:MET:HG3	3:C:86:LEU:CD1	2.13	0.77
26:D:1050:BCR:C20	30:D:1059:MGE:H5A1	2.15	0.77
1:A:147:TYR:HA	24:A:1038:PHO:HMD2	1.67	0.77
23:B:1012:CLA:CGA	23:B:1020:CLA:C14	2.63	0.77
23:B:1021:CLA:H101	23:B:1021:CLA:H142	1.65	0.77
23:B:1023:CLA:H13	23:B:1024:CLA:HMA3	0.82	0.77
2:B:5:TRP:O	2:B:8:VAL:HG13	1.85	0.77
23:C:1035:CLA:C9	26:C:1052:BCR:C40	2.63	0.77
3:C:199:ILE:HG21	3:C:234:VAL:CG1	2.15	0.77
4:D:188:PHE:HE2	4:D:326:ARG:HG2	1.47	0.77
23:B:1009:CLA:HAA1	26:H:1049:BCR:H363	1.66	0.77
23:B:1011:CLA:O1A	23:B:1011:CLA:C3A	2.30	0.76
2:B:190:PHE:CE1	23:B:1010:CLA:HMB2	2.20	0.76
29:C:1055:DGD:HA72	29:C:1055:DGD:HAW2	1.65	0.76
3:C:224:ILE:HG23	26:C:1054:BCR:C38	2.15	0.76
3:C:351:PHE:CE2	3:C:375:LEU:HD11	2.18	0.76
23:B:1009:CLA:H3A	26:H:1049:BCR:H372	1.67	0.76
18:Y:25:ILE:HG13	18:Y:26:ALA:N	2.00	0.76
2:B:249:ALA:O	2:B:252:VAL:HG12	1.85	0.76
23:C:1037:CLA:H2A	23:C:1037:CLA:O2D	1.85	0.76
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.20	0.76
4:D:261:PHE:CE2	4:D:267:LEU:HA	2.20	0.76
4:D:89:LEU:HD12	7:H:50:ASN:OD1	1.85	0.76
23:A:1003:CLA:H43	23:A:1003:CLA:H71	1.67	0.76
24:A:1038:PHO:H201	23:D:1005:CLA:CMB	2.13	0.76
1:A:197:PHE:HE1	1:A:285:PHE:HD2	1.33	0.76
23:B:1011:CLA:HMD3	23:B:1014:CLA:CAB	2.14	0.76
2:B:392:PHE:HA	2:B:397:VAL:HG23	1.68	0.76
1:A:246:TYR:H	1:A:246:TYR:HD1	1.34	0.76
23:B:1011:CLA:C1	23:B:1013:CLA:C9	2.63	0.76
23:C:1033:CLA:H141	23:C:1036:CLA:C2D	2.14	0.76
3:C:164:HIS:O	3:C:168:LEU:HD13	1.85	0.76
23:B:1016:CLA:H52	23:H:1017:CLA:H112	1.63	0.76
23:B:1009:CLA:H121	23:B:1009:CLA:H91	0.83	0.76
3:C:403:SER:OG	3:C:407:VAL:HG12	1.85	0.76
4:D:185:PHE:CD1	23:D:1004:CLA:HMD3	2.21	0.76
4:D:55:VAL:HG21	4:D:110:LEU:HD21	1.67	0.76
26:T:6048:BCR:H331	26:T:6048:BCR:C8	2.15	0.76
16:V:98:LEU:H	16:V:98:LEU:CD2	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1009:CLA:C8	23:B:1009:CLA:H142	2.09	0.76
23:B:1011:CLA:H43	23:B:1011:CLA:O1A	1.85	0.76
27:A:1063:LHG:C32	23:K:1034:CLA:H151	2.16	0.76
16:V:92:ARG:HG3	16:V:92:ARG:HH11	1.48	0.76
20:Z:15:LEU:HD12	20:Z:50:LEU:HD12	1.66	0.76
23:B:1011:CLA:C3D	23:B:1013:CLA:C1	2.63	0.76
23:B:1019:CLA:HHC	23:B:1019:CLA:HBB1	1.67	0.76
23:C:1026:CLA:C3	23:C:1026:CLA:O1A	2.33	0.76
23:C:1031:CLA:C14	26:C:1054:BCR:C36	2.64	0.76
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.15	0.76
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.21	0.76
26:B:1048:BCR:H331	26:B:1048:BCR:C8	2.15	0.76
2:B:460:LEU:HA	29:B:1058:DGD:CIA	2.15	0.76
29:C:1056:DGD:C4A	29:C:1056:DGD:O1A	2.34	0.76
3:C:202:PRO:HB3	3:C:235:GLY:HA2	1.67	0.76
16:V:151:ILE:HD13	16:V:151:ILE:H	1.51	0.76
23:B:1009:CLA:O2D	23:B:1009:CLA:CAA	2.30	0.76
23:B:1009:CLA:H142	23:B:1009:CLA:H8	1.62	0.76
23:B:1022:CLA:H122	23:B:1022:CLA:H93	1.63	0.76
2:B:174:LEU:CD2	2:B:312:TYR:OH	2.31	0.76
23:B:1022:CLA:C8	23:B:1022:CLA:C14	2.61	0.76
23:B:1022:CLA:HBC3	23:B:1022:CLA:H91	1.66	0.76
23:B:1022:CLA:C1A	23:B:1022:CLA:O2A	2.34	0.76
23:C:1033:CLA:CED	23:C:1033:CLA:CAD	2.64	0.76
3:C:167:VAL:HG11	23:C:1036:CLA:HBA2	1.67	0.76
3:C:266:TRP:HE3	3:C:271:TYR:HH	1.31	0.76
3:C:56:HIS:HD2	3:C:57:ALA:N	1.84	0.76
4:D:139:ARG:NH1	4:D:265:ARG:NH2	2.28	0.76
7:H:7:LEU:HD23	7:H:10:ILE:HD12	1.68	0.76
15:U:43:PRO:HG3	16:V:109:ASP:N	2.01	0.76
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.67	0.75
3:C:249:ILE:O	3:C:252:ILE:HG22	1.86	0.75
3:C:75:PHE:HZ	3:C:105:VAL:HG11	1.51	0.75
4:D:226:GLY:HA3	4:D:234:ALA:CB	2.16	0.75
14:T:14:ILE:O	14:T:17:PHE:HB2	1.85	0.75
23:A:1006:CLA:CHD	23:A:1006:CLA:HBC3	2.11	0.75
23:B:1022:CLA:O1D	23:B:1022:CLA:CAA	2.30	0.75
2:B:246:PHE:O	2:B:249:ALA:HB3	1.85	0.75
2:B:298:LEU:HD11	2:B:302:TRP:HE1	1.51	0.75
23:C:1029:CLA:HBC3	23:C:1029:CLA:HMC1	1.68	0.75
24:D:1039:PHO:HHD	24:D:1039:PHO:HBC2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:240:ALA:O	4:D:241:GLU:HG3	1.87	0.75
5:E:13:ILE:HA	5:E:16:SER:CB	2.16	0.75
1:A:94:TYR:HE1	1:A:105:TRP:HA	1.49	0.75
2:B:52:LEU:HD22	2:B:311:PHE:CD1	2.21	0.75
23:A:1006:CLA:C17	26:D:1050:BCR:H272	2.16	0.75
4:D:51:GLY:HA2	4:D:55:VAL:HB	1.69	0.75
1:A:224:ILE:N	2:B:482:ILE:HG23	2.01	0.75
3:C:117:VAL:HG11	23:C:1027:CLA:C4	2.15	0.75
1:A:225:ARG:O	1:A:226:GLU:HB2	1.87	0.75
2:B:12:LEU:H	2:B:12:LEU:HD12	1.52	0.75
2:B:384:ARG:HD3	15:U:102:LEU:HD21	1.69	0.75
2:B:429:ILE:HD12	2:B:429:ILE:H	1.52	0.75
3:C:165:LEU:HD22	23:C:1030:CLA:HMC3	1.68	0.75
23:C:1031:CLA:HAA1	23:C:1033:CLA:HED2	1.68	0.75
23:A:1006:CLA:HBC1	4:D:182:LEU:HD21	1.68	0.75
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.22	0.75
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.69	0.75
1:A:126:TYR:O	1:A:126:TYR:HD2	1.69	0.75
2:B:149:LEU:HB2	23:B:1012:CLA:C20	2.17	0.75
3:C:46:SER:CB	3:C:141:GLU:CB	2.59	0.75
3:C:86:LEU:HD22	3:C:89:ILE:HB	1.69	0.75
26:T:6046:BCR:H23C	26:T:6046:BCR:H403	1.69	0.75
23:B:1013:CLA:CMB	23:B:1014:CLA:H11	2.16	0.75
23:B:1021:CLA:H112	30:B:1060:MGE:CDA	2.17	0.75
23:B:1021:CLA:O1A	23:B:1021:CLA:CED	2.34	0.75
4:D:126:MET:HE3	4:D:146:PHE:HD2	1.50	0.75
5:E:42:LEU:O	5:E:46:VAL:HG23	1.86	0.75
13:O:80:GLU:O	13:O:82:PRO:CD	2.33	0.75
23:A:1007:CLA:CBD	23:A:1007:CLA:HBA2	2.17	0.75
23:A:1007:CLA:C4	23:C:1029:CLA:C19	2.64	0.75
2:B:191:ASN:ND2	7:H:60:VAL:HA	2.02	0.75
23:K:1034:CLA:H12	23:K:1034:CLA:C4D	2.17	0.75
13:O:82:PRO:HG3	13:O:89:ALA:HB1	1.68	0.75
15:U:31:ASN:HD22	15:U:32:ILE:H	1.35	0.75
23:B:1009:CLA:CBD	23:B:1009:CLA:HBA1	2.15	0.74
2:B:103:LEU:HD21	23:B:1013:CLA:HMC3	1.68	0.74
2:B:463:PHE:CG	29:B:1058:DGD:HAV1	2.22	0.74
1:A:293:MET:HG2	1:A:298:ASN:HA	1.68	0.74
23:B:1013:CLA:CAB	23:B:1014:CLA:H51	2.17	0.74
23:C:1031:CLA:CHD	23:C:1031:CLA:HBC2	2.11	0.74
4:D:118:GLY:CA	24:D:1039:PHO:H8	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:14:PHE:HE1	8:I:18:LEU:HD12	1.52	0.74
23:B:1009:CLA:CHA	23:B:1009:CLA:HBA1	2.15	0.74
3:C:284:PHE:HB3	29:C:1055:DGD:HB71	1.69	0.74
1:A:339:PHE:HB3	3:C:313:GLN:OE1	1.87	0.74
3:C:52:ALA:HB1	23:C:1035:CLA:HMB3	1.69	0.74
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.55	0.74
7:H:17:GLU:HB2	7:H:20:LYS:HB2	1.67	0.74
23:K:1034:CLA:O2A	23:K:1034:CLA:C4	2.33	0.74
1:A:13:LEU:H	1:A:13:LEU:HD12	1.51	0.74
1:A:16:ARG:HA	1:A:19:ASN:ND2	2.02	0.74
23:B:1018:CLA:CHC	23:B:1018:CLA:HBB1	2.14	0.74
23:B:1023:CLA:C9	23:B:1024:CLA:C15	2.65	0.74
2:B:12:LEU:N	2:B:12:LEU:HD12	2.02	0.74
3:C:32:GLY:HA3	3:C:41:ARG:CD	2.17	0.74
1:A:180:PHE:CE1	4:D:192:THR:HB	2.22	0.74
23:B:1020:CLA:H11	23:B:1023:CLA:O1A	1.87	0.74
7:H:33:VAL:O	7:H:37:LEU:HB2	1.87	0.74
10:K:33:PHE:HB2	23:K:1034:CLA:H3A	1.68	0.74
1:A:156:ALA:CA	1:A:160:ILE:HD12	2.17	0.74
23:B:1022:CLA:H202	23:B:1022:CLA:CMD	2.18	0.74
4:D:118:GLY:HA3	24:D:1039:PHO:H8	1.69	0.74
25:A:1043:PQ9:H352	4:D:45:LEU:HD22	1.69	0.74
1:A:156:ALA:HA	1:A:160:ILE:CD1	2.16	0.74
3:C:437:PHE:HA	23:C:1032:CLA:CMC	2.18	0.74
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.70	0.74
23:C:1033:CLA:CED	23:C:1033:CLA:OBD	2.35	0.74
4:D:74:LEU:HD23	4:D:175:VAL:HG11	1.70	0.74
23:C:1028:CLA:H93	29:C:1056:DGD:HB61	1.70	0.74
3:C:472:LEU:O	3:C:473:ASP:HB2	1.85	0.74
7:H:53:LEU:HD12	7:H:55:LEU:HD21	1.67	0.74
2:B:12:LEU:O	2:B:14:ASN:N	2.21	0.74
2:B:53:ASN:N	2:B:54:PRO:HD3	2.02	0.74
3:C:349:ILE:HG22	3:C:375:LEU:HB2	1.68	0.74
13:O:129:PHE:O	13:O:129:PHE:HD2	1.71	0.74
3:C:417:VAL:CG1	16:V:68:VAL:CG1	2.65	0.74
23:B:1023:CLA:O1D	23:B:1024:CLA:HBB2	1.88	0.73
2:B:135:LEU:HD12	2:B:135:LEU:H	1.53	0.73
2:B:156:PHE:O	2:B:162:PHE:HB3	1.88	0.73
15:U:43:PRO:HG3	16:V:109:ASP:CA	2.17	0.73
23:B:1011:CLA:HED2	23:B:1012:CLA:HED2	1.61	0.73
2:B:475:PHE:HD1	4:D:140:PRO:HD3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:428:THR:CG2	3:C:429:SER:H	2.01	0.73
3:C:89:ILE:HG12	3:C:111:PHE:CD2	2.23	0.73
4:D:36:LEU:HD21	4:D:124:GLY:CA	2.18	0.73
13:O:231:ASP:HB3	13:O:234:THR:OG1	1.88	0.73
27:A:1063:LHG:H322	23:K:1034:CLA:H13	1.70	0.73
1:A:116:ILE:HG23	1:A:117:PHE:N	2.04	0.73
23:C:1031:CLA:HMD1	23:C:1033:CLA:C16	2.19	0.73
23:C:1031:CLA:HMD1	23:C:1033:CLA:H162	1.70	0.73
29:C:1055:DGD:HBG3	29:C:1055:DGD:HBF1	1.69	0.73
3:C:112:PHE:O	3:C:116:VAL:HG23	1.87	0.73
5:E:37:PHE:CE1	5:E:46:VAL:HG21	2.23	0.73
13:O:198:ILE:HG23	13:O:199:ALA:H	1.53	0.73
23:B:1021:CLA:CHA	23:B:1021:CLA:CED	2.61	0.73
23:B:1023:CLA:C4C	23:B:1024:CLA:CBC	2.66	0.73
30:B:1060:MGE:H251	30:B:1060:MGE:H212	0.79	0.73
2:B:249:ALA:CB	2:B:459:ALA:HB2	2.19	0.73
3:C:237:HIS:O	3:C:240:ILE:HG22	1.88	0.73
16:V:46:THR:O	16:V:47:LEU:HB2	1.88	0.73
23:A:1007:CLA:H51	23:A:1007:CLA:H112	1.68	0.73
3:C:46:SER:OG	3:C:141:GLU:HB2	1.89	0.73
3:C:146:PHE:O	3:C:146:PHE:CG	2.40	0.73
3:C:164:HIS:HA	3:C:167:VAL:HB	1.71	0.73
2:B:385:ARG:HD3	15:U:14:ASP:OD2	1.87	0.73
23:A:1007:CLA:CHA	23:A:1007:CLA:HBA2	2.18	0.73
24:A:1038:PHO:H202	23:D:1005:CLA:HMB1	1.69	0.73
1:A:40:THR:HG21	1:A:122:GLY:H	1.53	0.73
1:A:215:HIS:CE1	1:A:271:LEU:HD11	2.24	0.73
2:B:27:THR:HG23	23:B:1013:CLA:CBC	2.18	0.73
23:B:1022:CLA:CHD	23:B:1022:CLA:HBC2	2.13	0.73
2:B:475:PHE:CD1	4:D:140:PRO:HD3	2.24	0.73
3:C:56:HIS:C	3:C:56:HIS:CD2	2.62	0.73
23:A:1006:CLA:H93	23:D:1004:CLA:H152	1.71	0.73
2:B:121:GLU:HB2	7:H:4:ARG:HB3	1.69	0.73
7:H:48:ILE:HA	7:H:53:LEU:HB3	1.71	0.73
1:A:202:VAL:HG11	23:A:1006:CLA:OBD	1.89	0.73
23:B:1019:CLA:C9	30:L:1061:MGE:H9A2	2.18	0.73
2:B:159:THR:HA	2:B:181:VAL:O	1.89	0.73
2:B:27:THR:HG23	23:B:1013:CLA:HBC1	1.69	0.73
3:C:167:VAL:HG13	23:C:1036:CLA:H42	1.69	0.73
23:D:1005:CLA:CBC	23:D:1004:CLA:CBB	2.64	0.73
7:H:31:MET:SD	23:H:1017:CLA:HAA1	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:1044:BCR:H331	26:A:1044:BCR:C8	2.19	0.73
1:A:205:VAL:HB	1:A:279:ARG:NH2	2.04	0.73
23:B:1016:CLA:C17	23:D:1008:CLA:HMA3	2.19	0.73
23:C:1030:CLA:HBB2	23:C:1031:CLA:CED	2.16	0.73
3:C:179:ALA:CB	3:C:199:ILE:HD13	2.19	0.73
3:C:287:THR:HG21	3:C:431:PHE:HB2	1.71	0.73
4:D:32:TRP:HA	4:D:32:TRP:CE3	2.23	0.73
16:V:38:LEU:HB2	16:V:45:ILE:HD11	1.70	0.73
2:B:139:PHE:CZ	23:H:1017:CLA:HMB3	2.23	0.73
23:K:1034:CLA:H102	23:K:1034:CLA:C14	2.13	0.73
3:C:396:MET:HE1	16:V:74:THR:HA	1.69	0.73
23:C:1030:CLA:HHD	23:C:1030:CLA:HBC3	1.69	0.73
3:C:187:ASP:HB2	3:C:230:LEU:HD11	1.70	0.73
3:C:369:LEU:HD13	3:C:380:ILE:HD12	1.70	0.73
14:T:3:THR:HA	14:T:6:TYR:HD2	1.53	0.73
15:U:42:TYR:CD2	15:U:43:PRO:N	2.57	0.73
15:U:64:ILE:HB	15:U:67:LEU:HD11	1.70	0.73
23:B:1009:CLA:HAA2	26:H:1049:BCR:H372	1.69	0.72
2:B:172:TYR:O	2:B:174:LEU:CA	2.29	0.72
2:B:357:ARG:HH11	2:B:357:ARG:HG2	1.53	0.72
3:C:140:LEU:HD23	3:C:140:LEU:O	1.88	0.72
23:D:1005:CLA:C4A	23:D:1005:CLA:O1A	2.37	0.72
23:B:1011:CLA:HBB1	23:B:1011:CLA:C9	2.19	0.72
7:H:29:PRO:O	7:H:33:VAL:HG13	1.89	0.72
7:H:56:ASP:O	7:H:58:VAL:HG23	1.89	0.72
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.69	0.72
16:V:92:ARG:HH11	16:V:92:ARG:CG	2.02	0.72
27:A:1063:LHG:O9	27:A:1063:LHG:HC62	1.77	0.72
23:B:1011:CLA:H92	23:B:1011:CLA:HBB1	1.71	0.72
2:B:220:ARG:CD	2:B:221:PRO:HD2	2.20	0.72
23:C:1033:CLA:HMA1	23:K:1034:CLA:C3C	2.18	0.72
3:C:116:VAL:HG11	26:Z:1053:BCR:HC31	1.70	0.72
23:D:1005:CLA:HBC2	23:D:1005:CLA:HHD	1.71	0.72
4:D:191:TRP:NE1	4:D:197:HIS:HD2	1.85	0.72
4:D:65:SER:HB2	4:D:77:ALA:O	1.88	0.72
6:F:24:HIS:HE1	31:F:1040:HEM:NC	1.88	0.72
26:T:6046:BCR:C23	26:T:6046:BCR:H392	2.17	0.72
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.24	0.72
27:A:1063:LHG:C29	23:C:1032:CLA:H71	2.16	0.72
4:D:201:VAL:HG23	23:D:1004:CLA:CMB	2.19	0.72
6:F:40:MET:O	6:F:42:PHE:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH1	24:A:1038:PHO:HMC3	1.99	0.72
23:B:1021:CLA:O1A	23:B:1021:CLA:CGD	2.37	0.72
3:C:348:GLU:CG	3:C:349:ILE:HG13	2.18	0.72
3:C:29:GLU:HA	3:C:41:ARG:NH1	2.04	0.72
5:E:20:TRP:CZ2	9:J:13:VAL:HG23	2.24	0.72
7:H:12:ARG:NH1	7:H:15:ASN:HB3	2.03	0.72
25:D:1042:PQ9:H242	30:L:1061:MGE:H263	1.70	0.72
3:C:334:PRO:HA	13:O:179:THR:OG1	1.89	0.72
1:A:159:LEU:HD12	1:A:159:LEU:O	1.90	0.72
23:B:1012:CLA:HMD2	23:B:1020:CLA:H201	1.72	0.72
2:B:213:GLY:O	2:B:217:ILE:HG13	1.89	0.72
3:C:287:THR:HG23	3:C:427:ALA:O	1.88	0.72
2:B:121:GLU:HG3	7:H:12:ARG:HD3	1.71	0.72
23:B:1019:CLA:H193	23:B:1021:CLA:H72	1.70	0.72
23:A:1007:CLA:H43	23:C:1029:CLA:H191	1.68	0.72
7:H:30:LEU:C	23:H:1017:CLA:HMD2	2.10	0.72
23:K:1034:CLA:O2A	23:K:1034:CLA:H42	1.89	0.72
18:Y:26:ALA:O	18:Y:30:ILE:HG22	1.90	0.72
1:A:272:HIS:NE2	4:D:214:HIS:CE1	2.58	0.72
23:B:1009:CLA:OBD	23:B:1010:CLA:HBB2	1.87	0.72
2:B:27:THR:OG1	23:B:1020:CLA:H43	1.90	0.72
23:B:1021:CLA:C4	30:B:1060:MGE:H242	2.20	0.72
2:B:12:LEU:HD22	2:B:19:LEU:CD1	2.20	0.72
23:C:1031:CLA:HMA2	23:C:1031:CLA:C1	2.19	0.72
3:C:171:GLY:C	23:C:1025:CLA:CBC	2.58	0.72
4:D:68:LEU:HD23	5:E:49:THR:HG21	1.72	0.72
6:F:36:ALA:O	6:F:39:ALA:HB3	1.89	0.72
10:K:37:PHE:CB	26:K:1051:BCR:H401	2.19	0.72
23:A:1006:CLA:HBB1	23:A:1006:CLA:CHC	2.19	0.72
23:B:1012:CLA:O1A	23:B:1020:CLA:H141	1.90	0.72
23:B:1012:CLA:CMB	23:B:1015:CLA:CBB	2.68	0.72
2:B:176:GLY:HA3	2:B:266:GLU:OE2	1.90	0.72
2:B:247:PHE:O	2:B:251:VAL:HG23	1.90	0.72
23:C:1029:CLA:CBD	23:C:1029:CLA:O1A	2.38	0.72
23:C:1030:CLA:C17	23:C:1030:CLA:C12	2.30	0.72
3:C:461:ARG:HG3	4:D:225:ASP:OD2	1.90	0.72
3:C:464:GLU:OE1	3:C:467:LEU:HD12	1.90	0.72
4:D:53:THR:HA	4:D:67:TYR:CD2	2.25	0.72
13:O:190:LEU:O	13:O:190:LEU:HD23	1.90	0.72
16:V:159:GLY:O	16:V:161:VAL:N	2.23	0.72
3:C:283:GLY:HA3	23:C:1026:CLA:HBC3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1016:CLA:C5	23:H:1017:CLA:C9	2.34	0.72
23:B:1023:CLA:C10	23:B:1023:CLA:H161	2.20	0.71
2:B:222:PRO:HD2	23:H:1017:CLA:O1D	1.90	0.71
4:D:299:ILE:O	4:D:301:GLN:N	2.23	0.71
7:H:4:ARG:O	7:H:5:THR:HG23	1.90	0.71
12:M:32:GLN:HA	12:M:32:GLN:HE21	1.55	0.71
17:X:34:PHE:O	17:X:38:ILE:HG12	1.90	0.71
27:A:1063:LHG:H321	23:K:1034:CLA:C15	2.21	0.71
1:A:135:TYR:CE1	3:C:449:ARG:HG3	2.25	0.71
2:B:103:LEU:HD11	2:B:107:LEU:HD11	1.69	0.71
2:B:222:PRO:HB2	2:B:225:LEU:CD1	2.20	0.71
2:B:482:ILE:O	2:B:483:ASP:HB3	1.90	0.71
4:D:18:LEU:O	4:D:22:LEU:HG	1.90	0.71
15:U:45:LEU:HD21	15:U:75:LEU:CD1	2.19	0.71
1:A:124:SER:O	1:A:127:MET:HB3	1.89	0.71
1:A:45:THR:HG23	1:A:46:ILE:N	2.05	0.71
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.25	0.71
3:C:52:ALA:O	3:C:55:ALA:HB3	1.91	0.71
2:B:119:ASP:HB3	7:H:3:ARG:HH21	1.54	0.71
14:T:3:THR:HA	14:T:6:TYR:CD2	2.25	0.71
16:V:39:ASN:ND2	16:V:40:SER:H	1.88	0.71
23:B:1010:CLA:H172	29:B:1058:DGD:HA82	1.72	0.71
1:A:301:ASN:ND2	3:C:407:VAL:HG11	2.05	0.71
30:D:1062:MGE:H3B2	30:D:1062:MGE:O1A	1.89	0.71
23:B:1016:CLA:C3	23:H:1017:CLA:H91	2.21	0.71
7:H:43:LEU:HD23	7:H:44:ILE:N	2.05	0.71
30:B:1060:MGE:CBB	30:B:1060:MGE:CGB	2.68	0.71
23:C:1032:CLA:CHB	23:K:1034:CLA:HBB2	2.21	0.71
3:C:56:HIS:O	3:C:58:GLY:N	2.23	0.71
13:O:45:CYS:H	13:O:72:GLN:NE2	1.88	0.71
16:V:98:LEU:HD22	16:V:98:LEU:N	2.03	0.71
3:C:48:LYS:NZ	3:C:133:ALA:O	2.23	0.71
24:D:1039:PHO:HMA1	23:D:1004:CLA:H142	1.70	0.71
4:D:297:ASP:CG	4:D:298:PHE:H	1.89	0.71
18:Y:43:ARG:HH21	18:Y:44:GLY:HA3	1.56	0.71
23:A:1003:CLA:H43	24:A:1038:PHO:C2B	2.21	0.71
29:C:1056:DGD:HAV1	29:C:1057:DGD:C8A	2.20	0.71
4:D:191:TRP:HE1	4:D:197:HIS:HD2	1.36	0.71
15:U:29:ASN:HD21	15:U:87:VAL:HA	1.55	0.71
30:B:1060:MGE:C7B	30:B:1060:MGE:H3B2	2.17	0.71
3:C:92:ILE:H	3:C:92:ILE:CD1	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:PRO:O	4:D:142:ASN:N	2.24	0.71
4:D:315:TYR:CE2	4:D:319:LEU:HD12	2.25	0.71
7:H:41:PHE:O	7:H:45:ILE:HG13	1.91	0.71
2:B:125:ASP:HB3	2:B:128:THR:OG1	1.89	0.71
23:C:1030:CLA:H43	26:C:1054:BCR:HC8	1.71	0.71
23:C:1031:CLA:O1A	23:C:1033:CLA:H51	1.90	0.71
3:C:117:VAL:HG12	3:C:118:HIS:H	1.56	0.71
4:D:103:ARG:HD3	4:D:106:GLN:NE2	2.05	0.71
4:D:305:ALA:HB1	13:O:186:LYS:HD2	1.71	0.71
27:A:1063:LHG:H383	27:A:1063:LHG:H341	0.79	0.71
2:B:9:HIS:HB2	23:B:1019:CLA:O1A	1.90	0.71
25:D:1042:PQ9:C39	30:L:1061:MGE:H241	2.21	0.71
23:K:1034:CLA:HBC3	23:K:1034:CLA:CHD	2.16	0.71
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.73	0.70
23:C:1025:CLA:OBD	23:C:1025:CLA:CED	2.32	0.70
3:C:275:SER:HB3	23:C:1033:CLA:HED3	1.72	0.70
25:A:1043:PQ9:C45	30:D:1059:MGE:H8A2	2.20	0.70
23:B:1022:CLA:HED2	23:B:1022:CLA:OBD	1.90	0.70
23:B:1019:CLA:CHA	23:B:1019:CLA:CBA	2.69	0.70
2:B:249:ALA:HB1	2:B:459:ALA:HB2	1.73	0.70
24:D:1039:PHO:CMA	23:D:1004:CLA:H142	2.18	0.70
7:H:44:ILE:O	7:H:48:ILE:HG13	1.90	0.70
13:O:214:LYS:HB3	13:O:251:MET:HB3	1.73	0.70
13:O:78:VAL:HG21	13:O:142:ILE:HG21	1.73	0.70
25:A:1043:PQ9:H212	24:D:1039:PHO:HED1	1.73	0.70
1:A:269:ARG:HD3	4:D:222:LEU:CD1	2.20	0.70
2:B:249:ALA:HB2	23:B:1012:CLA:HBC1	1.73	0.70
1:A:131:TRP:CZ3	23:C:1029:CLA:HMA3	2.25	0.70
3:C:188:THR:HG22	3:C:300:GLU:OE2	1.91	0.70
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.26	0.70
3:C:346:THR:HB	13:O:38:GLY:HA2	1.73	0.70
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.06	0.70
1:A:324:ALA:HB2	4:D:329:MET:SD	2.32	0.70
1:A:39:PRO:HA	1:A:42:LEU:HB2	1.73	0.70
23:B:1020:CLA:C16	23:B:1020:CLA:C11	2.69	0.70
3:C:348:GLU:OE2	3:C:349:ILE:HG13	1.92	0.70
4:D:253:TRP:CA	4:D:256:ILE:HG22	2.15	0.70
4:D:265:ARG:NH1	4:D:265:ARG:HG3	2.04	0.70
6:F:22:ALA:O	6:F:24:HIS:N	2.25	0.70
13:O:266:TYR:CD1	13:O:267:ALA:N	2.60	0.70
1:A:84:PRO:HA	1:A:112:TYR:CD1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:C3D	23:B:1013:CLA:C2	2.70	0.70
26:B:1045:BCR:C37	26:B:1045:BCR:H361	2.19	0.70
23:C:1025:CLA:C1	23:C:1025:CLA:H3A	2.22	0.70
24:D:1039:PHO:CMA	24:D:1039:PHO:CBA	2.30	0.70
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.73	0.70
4:D:50:THR:HG21	26:D:1050:BCR:H333	1.74	0.70
8:I:14:PHE:HD1	8:I:14:PHE:C	1.95	0.70
23:C:1025:CLA:HMB1	23:C:1025:CLA:HBB1	1.73	0.70
3:C:284:PHE:HB3	29:C:1055:DGD:C7B	2.22	0.70
30:D:1062:MGE:H2A2	14:T:20:ALA:HB1	1.73	0.70
7:H:50:ASN:O	7:H:51:SER:HB2	1.90	0.70
10:K:11:LEU:CD1	10:K:22:VAL:HG21	2.21	0.70
16:V:105:PRO:CG	16:V:115:ALA:HA	2.21	0.70
27:A:1063:LHG:C34	27:A:1063:LHG:C38	2.40	0.70
23:B:1014:CLA:HBC2	23:B:1014:CLA:CHD	2.11	0.70
2:B:40:TYR:CE1	23:B:1015:CLA:HED1	2.26	0.70
2:B:92:SER:O	2:B:94:GLU:N	2.24	0.70
23:C:1029:CLA:H43	26:C:1054:BCR:C32	2.22	0.70
3:C:187:ASP:HB3	3:C:190:ALA:HB2	1.73	0.70
3:C:282:MET:HA	3:C:285:ILE:HD12	1.74	0.70
4:D:209:LEU:HD22	25:D:1042:PQ9:H192	1.73	0.70
2:B:172:TYR:HD2	2:B:287:ARG:HH22	1.40	0.70
2:B:329:PRO:O	2:B:331:ASN:N	2.24	0.70
23:C:1030:CLA:CED	23:C:1030:CLA:C4D	2.69	0.70
23:D:1005:CLA:HBC2	23:D:1004:CLA:CBB	2.18	0.70
1:A:212:CYS:O	4:D:271:MET:HB3	1.92	0.70
4:D:148:ALA:HB1	4:D:279:LEU:CD1	2.22	0.70
4:D:32:TRP:HA	4:D:32:TRP:HE3	1.55	0.70
5:E:37:PHE:HE1	5:E:46:VAL:HG21	1.56	0.70
7:H:35:MET:HA	26:H:1049:BCR:H331	1.73	0.70
1:A:39:PRO:HD2	23:A:1007:CLA:HBB2	1.74	0.70
23:B:1011:CLA:O1D	23:B:1013:CLA:C1	2.35	0.70
2:B:323:GLY:HA3	2:B:326:ARG:HG3	1.74	0.70
2:B:399:VAL:HG23	2:B:417:VAL:HG13	1.72	0.70
30:D:1062:MGE:O6D	11:L:15:THR:HG21	1.92	0.70
13:O:215:ARG:HH11	13:O:215:ARG:HG2	1.57	0.70
1:A:272:HIS:CD2	4:D:214:HIS:CE1	2.80	0.69
29:C:1057:DGD:HD4	9:J:38:SER:O	1.91	0.69
3:C:263:ALA:C	3:C:264:PHE:HD2	1.95	0.69
3:C:393:ALA:O	3:C:397:THR:HG23	1.91	0.69
7:H:14:LEU:HD12	7:H:14:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:210:LEU:C	2.11	0.69
2:B:28:ALA:O	2:B:104:SER:HB2	1.92	0.69
3:C:199:ILE:H	3:C:199:ILE:HD12	1.58	0.69
3:C:450:ALA:CB	3:C:456:GLU:HB3	2.22	0.69
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.73	0.69
7:H:17:GLU:HG3	7:H:20:LYS:HE2	1.73	0.69
1:A:124:SER:OG	1:A:151:LEU:HD11	1.92	0.69
23:B:1009:CLA:CHA	23:B:1009:CLA:CBA	2.70	0.69
2:B:363:PHE:CD2	2:B:363:PHE:N	2.59	0.69
2:B:475:PHE:CD1	4:D:140:PRO:CD	2.75	0.69
4:D:26:ARG:O	4:D:26:ARG:HG2	1.92	0.69
13:O:76:PHE:HE2	13:O:132:VAL:HG21	1.56	0.69
1:A:228:THR:HG22	1:A:229:GLU:N	2.07	0.69
23:B:1018:CLA:H102	23:B:1023:CLA:CBA	2.23	0.69
2:B:10:THR:O	2:B:13:ILE:HG22	1.91	0.69
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.55	0.69
2:B:13:ILE:HG13	2:B:14:ASN:N	2.06	0.69
23:C:1025:CLA:HED3	23:C:1025:CLA:CAD	2.21	0.69
3:C:327:ASN:HD22	3:C:330:SER:H	1.41	0.69
3:C:438:LEU:HD13	3:C:438:LEU:O	1.92	0.69
4:D:101:PHE:O	4:D:105:CYS:HB2	1.92	0.69
4:D:57:SER:OG	4:D:65:SER:HB3	1.92	0.69
1:A:344:ALA:HB1	3:C:357:ARG:NH2	2.08	0.69
4:D:91:LEU:HD23	4:D:93:TRP:NE1	2.07	0.69
8:I:21:PHE:HD1	8:I:24:LEU:HD12	1.58	0.69
10:K:24:VAL:CG2	18:Y:25:ILE:HG22	2.18	0.69
16:V:38:LEU:HB2	16:V:45:ILE:CD1	2.23	0.69
1:A:140:ARG:CB	1:A:140:ARG:HH11	2.06	0.69
23:B:1021:CLA:H112	30:B:1060:MGE:H132	1.72	0.69
23:C:1025:CLA:HMB3	26:C:1054:BCR:C25	2.23	0.69
3:C:100:GLY:HA2	3:C:196:VAL:CG1	2.23	0.69
1:A:183:MET:SD	23:D:1005:CLA:HAC2	2.31	0.69
4:D:126:MET:HE2	4:D:143:ALA:O	1.93	0.69
13:O:190:LEU:C	13:O:190:LEU:HD23	2.12	0.69
17:X:12:ILE:HA	17:X:16:LEU:HD22	1.74	0.69
23:A:1003:CLA:C4	24:A:1038:PHO:C3B	2.70	0.69
3:C:453:ALA:HB2	8:I:31:ASN:HD22	1.57	0.69
23:D:1008:CLA:CMA	23:D:1008:CLA:CBA	2.30	0.69
4:D:184:PHE:CE2	4:D:188:PHE:CD1	2.81	0.69
1:A:244:GLU:HG3	4:D:242:GLU:HA	1.75	0.69
2:B:30:VAL:HG12	23:B:1013:CLA:HHD	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:LEU:HD13	3:C:139:THR:OG1	1.93	0.69
9:J:25:VAL:HA	9:J:28:PHE:HD2	1.58	0.69
26:K:1051:BCR:C8	26:K:1051:BCR:H321	2.23	0.69
15:U:45:LEU:HD21	15:U:75:LEU:HD12	1.73	0.69
16:V:50:LYS:HE2	16:V:50:LYS:HA	1.73	0.69
25:A:1043:PQ9:H37	25:A:1043:PQ9:C28	2.22	0.69
2:B:25:MET:C	2:B:27:THR:N	2.44	0.69
3:C:167:VAL:HG12	3:C:168:LEU:CD1	2.20	0.69
4:D:198:MET:SD	23:D:1005:CLA:HED3	2.33	0.69
9:J:21:VAL:O	9:J:25:VAL:HB	1.92	0.69
2:B:69:LEU:HD11	23:B:1011:CLA:OBD	1.93	0.69
23:B:1011:CLA:CMD	23:B:1014:CLA:HMB1	2.23	0.69
2:B:152:GLY:O	2:B:156:PHE:HB2	1.91	0.69
2:B:284:ILE:HG23	2:B:305:ILE:HD13	1.73	0.69
2:B:475:PHE:HD2	2:B:475:PHE:N	1.90	0.69
23:C:1031:CLA:CMA	23:C:1031:CLA:O2A	2.32	0.69
23:C:1035:CLA:HBB1	23:C:1035:CLA:CHC	2.14	0.69
3:C:81:MET:HG3	3:C:86:LEU:HD13	1.73	0.69
23:D:1008:CLA:HBB1	23:D:1008:CLA:CHC	2.13	0.69
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.23	0.69
4:D:265:ARG:CG	4:D:265:ARG:HH11	2.03	0.69
4:D:279:LEU:HD21	24:D:1039:PHO:HMC1	1.74	0.69
16:V:66:CYS:SG	31:V:1041:HEM:HAC	2.33	0.69
16:V:151:ILE:HG12	16:V:152:LEU:H	1.56	0.69
3:C:417:VAL:CG1	16:V:68:VAL:CB	2.70	0.69
23:B:1013:CLA:HAB	23:B:1014:CLA:H52	1.72	0.69
3:C:91:HIS:NE2	23:C:1026:CLA:HED1	2.07	0.69
23:C:1032:CLA:O2D	23:C:1032:CLA:H2A	1.92	0.69
29:C:1057:DGD:HAS2	30:D:1059:MGE:H232	1.74	0.69
4:D:210:LEU:CD2	4:D:274:VAL:HG21	2.23	0.69
11:L:4:ASN:OD1	11:L:5:PRO:HD2	1.93	0.69
2:B:13:ILE:HD12	2:B:234:ILE:CG2	2.23	0.68
23:C:1035:CLA:C8	26:C:1052:BCR:H403	2.10	0.68
4:D:207:GLY:CA	4:D:274:VAL:HG11	2.23	0.68
3:C:457:LYS:NZ	4:D:228:GLY:HA2	2.08	0.68
23:K:1034:CLA:CGD	23:K:1034:CLA:CAA	2.65	0.68
16:V:64:ALA:HB1	16:V:68:VAL:HA	1.74	0.68
16:V:66:CYS:O	16:V:73:LYS:HG3	1.93	0.68
1:A:254:TYR:CD1	1:A:255:PHE:N	2.61	0.68
2:B:277:SER:O	2:B:279:TYR:N	2.23	0.68
23:C:1030:CLA:CED	23:C:1030:CLA:CAD	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:LEU:O	4:D:99:GLY:N	2.26	0.68
5:E:34:GLY:HA2	6:F:32:PHE:HE1	1.56	0.68
26:B:1045:BCR:C8	26:B:1045:BCR:C33	2.66	0.68
30:B:1060:MGE:H211	30:B:1060:MGE:H263	1.75	0.68
2:B:363:PHE:HD2	2:B:363:PHE:N	1.91	0.68
23:C:1035:CLA:HMB2	26:C:1052:BCR:H272	1.75	0.68
23:A:1003:CLA:H203	23:D:1005:CLA:H92	1.75	0.68
4:D:23:LYS:HE3	4:D:135:LEU:HD11	1.75	0.68
4:D:221:THR:O	4:D:244:TYR:HA	1.93	0.68
23:A:1006:CLA:C16	25:A:1043:PQ9:H443	2.22	0.68
23:B:1009:CLA:CHC	23:B:1009:CLA:HBB1	2.15	0.68
2:B:394:GLN:HB3	15:U:17:LEU:CD2	2.23	0.68
23:C:1036:CLA:CBC	23:C:1036:CLA:HMC1	2.22	0.68
3:C:88:LEU:HD11	23:C:1027:CLA:HBC2	1.74	0.68
10:K:43:VAL:HG12	10:K:43:VAL:O	1.94	0.68
15:U:45:LEU:HD11	15:U:75:LEU:HD11	1.75	0.68
1:A:279:ARG:CZ	1:A:283:VAL:CG2	2.71	0.68
26:B:1047:BCR:C8	26:B:1047:BCR:H331	2.14	0.68
2:B:25:MET:HG3	26:B:1045:BCR:H391	1.74	0.68
3:C:117:VAL:HA	26:Z:1053:BCR:H343	1.76	0.68
4:D:109:GLY:O	4:D:111:TRP:N	2.27	0.68
4:D:59:TYR:O	5:E:66:VAL:HG23	1.94	0.68
11:L:14:ARG:CA	12:M:26:TYR:HE1	2.05	0.68
2:B:119:ASP:OD2	7:H:2:ALA:HA	1.94	0.68
3:C:49:LEU:HB3	3:C:133:ALA:CA	2.18	0.68
4:D:254:SER:OG	4:D:260:ALA:HB2	1.93	0.68
2:B:327:THR:HG21	12:M:4:ASN:ND2	2.09	0.68
13:O:101:THR:O	13:O:130:GLN:HG3	1.93	0.68
1:A:47:CYS:SG	26:A:1044:BCR:H373	2.34	0.68
2:B:32:GLY:HA3	26:B:1047:BCR:C36	2.24	0.68
1:A:196:PRO:HG3	3:C:404:LEU:CD1	2.23	0.68
4:D:15:PHE:CE1	4:D:32:TRP:HZ2	2.12	0.68
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.24	0.68
4:D:352:LEU:H	4:D:352:LEU:HD23	1.59	0.68
7:H:13:PRO:HG2	7:H:14:LEU:H	1.59	0.68
23:B:1009:CLA:HAA2	26:H:1049:BCR:H363	1.74	0.68
23:B:1019:CLA:H193	23:B:1021:CLA:C7	2.24	0.68
2:B:105:GLY:CA	26:B:1047:BCR:H402	2.19	0.68
3:C:295:THR:HG22	3:C:296:VAL:HG13	1.74	0.68
4:D:267:LEU:HD22	4:D:268:HIS:CE1	2.28	0.68
23:B:1019:CLA:C19	23:B:1021:CLA:C7	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:LEU:HD21	3:C:328:VAL:HG11	1.75	0.68
3:C:89:ILE:HG23	3:C:111:PHE:CE2	2.28	0.68
4:D:171:PRO:HA	4:D:181:PHE:CD2	2.28	0.68
4:D:43:LEU:N	4:D:43:LEU:HD23	2.08	0.68
13:O:82:PRO:CG	13:O:89:ALA:CB	2.71	0.68
18:Y:21:GLN:O	18:Y:25:ILE:HG23	1.94	0.68
1:A:149:ALA:HB1	1:A:283:VAL:CG1	2.24	0.68
1:A:78:ILE:N	1:A:78:ILE:HD12	2.09	0.68
2:B:12:LEU:O	2:B:13:ILE:HG23	1.94	0.68
23:C:1029:CLA:CMD	23:C:1031:CLA:CAB	2.68	0.68
3:C:451:ALA:HA	3:C:456:GLU:HG2	1.75	0.68
3:C:56:HIS:HA	3:C:59:LEU:CD1	2.23	0.68
4:D:218:VAL:HG12	4:D:219:GLU:N	2.08	0.68
13:O:82:PRO:HG2	13:O:89:ALA:CB	2.24	0.68
16:V:103:LYS:HD2	16:V:121:LEU:HD13	1.75	0.68
16:V:101:TYR:HE1	16:V:118:HIS:HD1	1.42	0.68
26:C:1052:BCR:H312	20:Z:9:LEU:HD11	1.75	0.68
1:A:337:HIS:O	4:D:351:ALA:CB	2.36	0.67
3:C:343:ARG:HG2	3:C:348:GLU:O	1.94	0.67
3:C:417:VAL:HG12	16:V:68:VAL:CB	2.21	0.67
4:D:281:MET:HA	4:D:281:MET:HE2	1.74	0.67
4:D:61:HIS:CE1	4:D:80:THR:HG23	2.30	0.67
26:H:1049:BCR:H321	26:H:1049:BCR:HC8	1.76	0.67
12:M:35:SER:O	12:M:36:SER:HB2	1.94	0.67
15:U:29:ASN:O	15:U:97:ARG:NE	2.24	0.67
23:A:1007:CLA:CHA	23:A:1007:CLA:CBA	2.72	0.67
1:A:174:LEU:HD22	24:A:1038:PHO:H152	1.76	0.67
23:B:1012:CLA:CAB	23:B:1015:CLA:HBB2	2.24	0.67
23:K:1034:CLA:O2A	23:K:1034:CLA:CHA	2.41	0.67
16:V:54:GLU:O	16:V:58:LEU:HD23	1.94	0.67
1:A:212:CYS:SG	4:D:210:LEU:HB3	2.34	0.67
1:A:224:ILE:HG23	1:A:225:ARG:N	2.08	0.67
23:B:1009:CLA:HMB2	26:H:1049:BCR:C27	2.23	0.67
23:B:1023:CLA:H2A	23:B:1023:CLA:O1D	1.95	0.67
2:B:221:PRO:O	7:H:21:VAL:HG23	1.94	0.67
2:B:271:THR:HG22	2:B:274:GLN:NE2	2.10	0.67
2:B:429:ILE:HD12	2:B:429:ILE:N	2.10	0.67
3:C:400:PRO:C	3:C:401:LEU:HD22	2.15	0.67
26:D:1050:BCR:C21	30:D:1059:MGE:C3A	2.72	0.67
3:C:199:ILE:HG12	3:C:234:VAL:HG11	1.76	0.67
25:D:1042:PQ9:C34	25:D:1042:PQ9:H301	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:LEU:HG	4:D:49:LEU:HD12	1.75	0.67
4:D:95:PRO:CG	17:X:15:SER:HB2	2.23	0.67
5:E:8:ARG:HE	6:F:13:TYR:CB	2.02	0.67
26:T:6046:BCR:H323	26:T:6046:BCR:HC41	1.77	0.67
15:U:59:GLU:O	15:U:61:VAL:N	2.27	0.67
2:B:31:ALA:HB2	23:B:1013:CLA:HAC1	1.74	0.67
23:B:1019:CLA:HBD	23:B:1019:CLA:HBA2	1.76	0.67
2:B:354:LEU:C	2:B:355:PHE:HD2	1.97	0.67
3:C:42:LEU:CD1	3:C:48:LYS:HG2	2.24	0.67
24:D:1039:PHO:H42	24:D:1039:PHO:O2A	1.95	0.67
4:D:110:LEU:O	4:D:114:ILE:HG13	1.95	0.67
4:D:250:ASN:HB2	4:D:260:ALA:CB	2.20	0.67
13:O:141:ARG:HH11	13:O:141:ARG:CG	2.07	0.67
16:V:35:THR:HA	16:V:46:THR:HA	1.77	0.67
1:A:224:ILE:HD13	1:A:225:ARG:H	1.59	0.67
2:B:25:MET:HG3	26:B:1045:BCR:C40	2.25	0.67
23:C:1025:CLA:O1D	23:C:1025:CLA:H2A	1.94	0.67
3:C:49:LEU:N	3:C:49:LEU:CD1	2.51	0.67
23:D:1004:CLA:CHC	23:D:1004:CLA:HBB1	2.15	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.27	0.67
4:D:188:PHE:CD2	4:D:326:ARG:HG2	2.29	0.67
4:D:45:LEU:HG	4:D:49:LEU:CD1	2.24	0.67
11:L:21:LEU:CB	14:T:16:LEU:HD21	2.24	0.67
20:Z:43:GLY:O	20:Z:47:TRP:N	2.27	0.67
2:B:69:LEU:HB3	23:B:1014:CLA:HMA3	1.76	0.67
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.30	0.67
3:C:59:LEU:HD22	23:K:1034:CLA:HBD	1.77	0.67
4:D:221:THR:HG23	4:D:248:THR:HB	1.75	0.67
5:E:79:PHE:O	5:E:83:LEU:HD13	1.94	0.67
3:C:334:PRO:HA	13:O:179:THR:CB	2.23	0.67
1:A:94:TYR:CE1	1:A:105:TRP:HA	2.29	0.67
23:B:1019:CLA:O1D	23:B:1019:CLA:H2A	1.95	0.67
24:A:1038:PHO:C20	23:D:1005:CLA:HMB3	2.23	0.67
24:D:1039:PHO:HHD	24:D:1039:PHO:CBC	2.23	0.67
25:D:1042:PQ9:C30	25:D:1042:PQ9:C34	2.67	0.67
4:D:50:THR:CG2	26:D:1050:BCR:H333	2.24	0.67
26:K:1051:BCR:C23	26:K:1051:BCR:C40	2.64	0.67
1:A:160:ILE:HG21	3:C:431:PHE:CE1	2.30	0.67
23:B:1009:CLA:O1A	23:B:1009:CLA:CHA	2.43	0.67
2:B:468:TRP:NE1	23:B:1019:CLA:HED2	2.09	0.67
3:C:166:ILE:HD12	3:C:249:ILE:CD1	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:274:VAL:HG22	25:D:1042:PQ9:H293	1.76	0.67
12:M:9:ILE:HD12	12:M:9:ILE:H	1.58	0.67
13:O:188:ARG:HB2	13:O:188:ARG:NH1	2.09	0.67
13:O:202:GLN:HA	13:O:202:GLN:OE1	1.93	0.67
1:A:218:LEU:HA	1:A:221:SER:OG	1.95	0.67
23:B:1013:CLA:CAB	23:B:1014:CLA:C5	2.73	0.67
2:B:373:LYS:C	2:B:374:ASN:HD22	1.99	0.67
2:B:75:TRP:CD1	2:B:94:GLU:HB2	2.30	0.67
8:I:12:VAL:O	8:I:16:VAL:HG23	1.95	0.67
3:C:453:ALA:HB2	8:I:31:ASN:ND2	2.10	0.67
3:C:60:ILE:HG22	23:K:1034:CLA:HMD2	1.76	0.67
15:U:83:THR:HG22	15:U:84:VAL:N	2.10	0.67
7:H:44:ILE:HD11	17:X:19:PHE:CD2	2.30	0.67
1:A:64:ARG:HE	13:O:98:THR:HG21	1.59	0.66
3:C:187:ASP:HB2	3:C:230:LEU:CD1	2.25	0.66
3:C:49:LEU:HD23	3:C:52:ALA:N	2.08	0.66
5:E:38:VAL:HG21	6:F:36:ALA:O	1.95	0.66
2:B:24:LEU:CD2	2:B:111:ALA:HA	2.25	0.66
23:C:1029:CLA:HBD	23:C:1029:CLA:O1A	1.96	0.66
3:C:266:TRP:HB3	3:C:271:TYR:OH	1.94	0.66
23:D:1005:CLA:H122	30:D:1062:MGE:H263	1.78	0.66
8:I:18:LEU:O	8:I:18:LEU:HD23	1.95	0.66
23:K:1034:CLA:O1A	23:K:1034:CLA:H43	1.95	0.66
23:A:1003:CLA:H142	24:A:1038:PHO:C8	2.11	0.66
2:B:238:LEU:CA	23:B:1020:CLA:HMD3	2.25	0.66
2:B:451:PHE:CZ	23:B:1012:CLA:O1D	2.47	0.66
2:B:5:TRP:C	2:B:8:VAL:HG13	2.15	0.66
4:D:198:MET:SD	23:D:1005:CLA:CED	2.83	0.66
4:D:44:ALA:HB1	24:D:1039:PHO:H102	1.77	0.66
4:D:350:ASN:O	4:D:351:ALA:HB2	1.95	0.66
11:L:8:GLN:H	11:L:8:GLN:HE21	1.41	0.66
13:O:172:PHE:HB2	13:O:221:GLY:N	2.08	0.66
15:U:59:GLU:C	15:U:61:VAL:H	1.98	0.66
16:V:105:PRO:HB2	16:V:114:ILE:HG23	1.77	0.66
24:A:1038:PHO:H201	23:D:1005:CLA:C3B	2.26	0.66
1:A:156:ALA:HB1	1:A:290:ILE:CG2	2.25	0.66
23:B:1020:CLA:H2A	23:B:1020:CLA:O2D	1.95	0.66
2:B:98:LEU:C	2:B:98:LEU:HD13	2.16	0.66
4:D:100:ASP:O	4:D:102:THR:N	2.28	0.66
1:A:210:LEU:HA	24:D:1039:PHO:HAC2	1.75	0.66
4:D:68:LEU:HA	6:F:40:MET:SD	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:53:LEU:HD12	7:H:55:LEU:CD2	2.25	0.66
15:U:25:ILE:HG21	15:U:35:PHE:HE2	1.59	0.66
17:X:11:THR:O	17:X:11:THR:HG23	1.96	0.66
2:B:122:LEU:HD21	7:H:11:LEU:C	2.16	0.66
3:C:224:ILE:CD1	26:C:1054:BCR:H383	2.25	0.66
3:C:298:PRO:O	3:C:299:SER:HB2	1.95	0.66
18:Y:42:ARG:HB3	18:Y:43:ARG:NH1	2.10	0.66
24:A:1038:PHO:C20	23:D:1005:CLA:C3B	2.74	0.66
23:B:1022:CLA:CHA	23:B:1022:CLA:H11	2.25	0.66
23:B:1023:CLA:HMB1	23:B:1023:CLA:HBB1	1.75	0.66
2:B:475:PHE:CZ	4:D:134:ARG:HB2	2.31	0.66
23:C:1030:CLA:HHC	23:C:1030:CLA:CBB	2.20	0.66
11:L:30:LEU:HD22	11:L:31:PHE:CD1	2.30	0.66
13:O:266:TYR:OH	13:O:268:SER:HB3	1.96	0.66
15:U:46:ALA:HA	15:U:49:ILE:HD12	1.77	0.66
18:Y:43:ARG:HD2	18:Y:44:GLY:H	1.60	0.66
23:A:1003:CLA:CHD	23:A:1003:CLA:HBC2	2.25	0.66
23:A:1006:CLA:CBB	23:D:1004:CLA:C5	2.72	0.66
1:A:90:GLY:HA2	1:A:167:SER:OG	1.95	0.66
2:B:174:LEU:HD22	2:B:312:TYR:CZ	2.31	0.66
3:C:274:TYR:CE2	23:C:1031:CLA:HMC2	2.31	0.66
3:C:63:TRP:NE1	23:C:1028:CLA:C2C	2.59	0.66
25:D:1042:PQ9:H242	30:L:1061:MGE:CBB	2.25	0.66
23:D:1005:CLA:HAA2	25:D:1042:PQ9:H412	0.75	0.66
8:I:14:PHE:C	8:I:14:PHE:CD1	2.67	0.66
13:O:86:ARG:HG3	13:O:86:ARG:HH11	1.60	0.66
1:A:62:GLY:HA2	1:A:87:ASN:HB2	1.76	0.66
2:B:237:VAL:HG12	23:B:1020:CLA:HMD1	1.78	0.66
3:C:405:ASN:O	3:C:406:SER:HB2	1.94	0.66
4:D:45:LEU:O	4:D:49:LEU:HD12	1.95	0.66
13:O:196:SER:OG	13:O:197:ALA:N	2.26	0.66
1:A:104:GLU:OE2	13:O:99:ARG:HB3	1.96	0.66
23:B:1009:CLA:HHC	23:B:1009:CLA:CBB	2.19	0.66
29:B:1058:DGD:O2D	29:B:1058:DGD:HG31	1.94	0.66
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.09	0.66
5:E:20:TRP:O	5:E:24:SER:HB3	1.95	0.66
5:E:26:THR:O	5:E:29:ALA:HB3	1.96	0.66
1:A:37:MET:SD	1:A:126:TYR:HB2	2.36	0.66
2:B:414:PRO:O	2:B:418:LYS:HG3	1.96	0.66
23:C:1030:CLA:H121	23:C:1030:CLA:H171	1.72	0.66
3:C:295:THR:HG22	3:C:296:VAL:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:HIS:CD2	3:C:57:ALA:N	2.64	0.66
4:D:276:VAL:O	4:D:280:TRP:HD1	1.79	0.66
13:O:206:GLU:CD	13:O:206:GLU:H	1.99	0.66
14:T:11:ALA:CB	26:T:6046:BCR:H362	2.25	0.66
1:A:147:TYR:CA	24:A:1038:PHO:HMD2	2.26	0.65
1:A:195:HIS:O	1:A:199:GLN:HG2	1.96	0.65
1:A:60:ILE:HG22	1:A:61:ASP:N	2.10	0.65
23:B:1009:CLA:CAA	23:B:1009:CLA:CGD	2.74	0.65
23:C:1029:CLA:H52	23:C:1029:CLA:C1C	2.27	0.65
1:A:93:PHE:HB2	3:C:218:PHE:HD2	1.62	0.65
3:C:84:GLN:O	3:C:86:LEU:HG	1.95	0.65
4:D:43:LEU:H	4:D:43:LEU:HD23	1.59	0.65
15:U:42:TYR:HB3	15:U:43:PRO:CD	2.26	0.65
2:B:168:VAL:HG12	2:B:169:SER:N	2.10	0.65
2:B:475:PHE:N	2:B:475:PHE:CD2	2.62	0.65
23:C:1028:CLA:O1D	23:C:1028:CLA:H2A	1.96	0.65
3:C:89:ILE:N	3:C:90:PRO:HD2	2.11	0.65
15:U:73:GLN:OE1	15:U:77:GLU:HG3	1.97	0.65
16:V:61:TYR:O	16:V:129:LYS:HD3	1.96	0.65
1:A:205:VAL:HB	1:A:279:ARG:HH22	1.60	0.65
23:B:1011:CLA:HMD2	23:B:1013:CLA:C4	2.20	0.65
2:B:419:SER:HA	2:B:422:ARG:NH1	2.10	0.65
3:C:418:ASN:ND2	29:C:1057:DGD:HE61	2.11	0.65
3:C:257:PHE:H	3:C:257:PHE:HD1	1.44	0.65
3:C:63:TRP:NE1	23:C:1028:CLA:CMC	2.59	0.65
3:C:459:ILE:H	4:D:224:GLN:H	1.44	0.65
15:U:43:PRO:HD3	16:V:108:TYR:HB3	1.78	0.65
1:A:207:GLY:O	1:A:210:LEU:N	2.27	0.65
1:A:247:ASN:HD21	2:B:486:LEU:HB3	1.59	0.65
29:C:1055:DGD:HBG3	29:C:1055:DGD:CEB	2.25	0.65
3:C:166:ILE:HD13	3:C:248:GLY:HA3	1.77	0.65
5:E:79:PHE:O	5:E:83:LEU:HB2	1.95	0.65
23:C:1029:CLA:HBA1	8:I:23:PHE:CE1	2.32	0.65
13:O:59:ASP:OD1	13:O:61:SER:HB2	1.96	0.65
1:A:64:ARG:NE	13:O:98:THR:HG21	2.10	0.65
15:U:28:ASN:HD21	15:U:55:TYR:N	1.95	0.65
1:A:252:HIS:NE2	1:A:264:SER:HB3	2.12	0.65
2:B:40:TYR:CD1	2:B:40:TYR:C	2.67	0.65
23:C:1033:CLA:C7	23:C:1033:CLA:H2	2.27	0.65
3:C:348:GLU:HB3	13:O:42:ALA:HB3	1.79	0.65
4:D:350:ASN:O	4:D:351:ALA:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:107:ILE:CG2	13:O:123:GLU:HG3	2.26	0.65
13:O:250:ASP:HB3	13:O:253:ALA:HB3	1.78	0.65
14:T:17:PHE:O	14:T:21:ILE:HG13	1.96	0.65
1:A:36:ILE:HD13	23:C:1029:CLA:C14	2.27	0.65
23:B:1020:CLA:HED1	23:B:1021:CLA:CMB	2.24	0.65
23:B:1023:CLA:C4C	23:B:1024:CLA:HBC2	2.26	0.65
2:B:464:PHE:CE1	30:B:1060:MGE:H4B1	2.30	0.65
3:C:428:THR:CG2	3:C:429:SER:N	2.57	0.65
4:D:329:MET:C	4:D:331:PRO:HD2	2.17	0.65
2:B:334:ASP:HB3	13:O:202:GLN:HG3	1.78	0.65
1:A:187:GLN:HG3	1:A:325:ASN:ND2	2.10	0.65
4:D:29:PHE:CE2	4:D:31:GLY:HA3	2.31	0.65
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.79	0.65
16:V:66:CYS:SG	31:V:1041:HEM:CAC	2.85	0.65
1:A:279:ARG:HE	24:A:1038:PHO:C2C	2.10	0.65
2:B:165:GLY:HA3	2:B:179:GLN:O	1.96	0.65
2:B:226:TYR:HD2	2:B:226:TYR:O	1.79	0.65
3:C:275:SER:CB	23:C:1033:CLA:HED1	2.20	0.65
26:C:1052:BCR:H361	10:K:32:PHE:CE2	2.31	0.65
3:C:263:ALA:CB	3:C:264:PHE:HD2	2.10	0.65
23:D:1004:CLA:O1D	23:D:1004:CLA:H2A	1.96	0.65
15:U:68:THR:HG22	15:U:71:GLN:N	2.10	0.65
1:A:13:LEU:HD12	1:A:13:LEU:N	2.12	0.65
1:A:210:LEU:O	1:A:210:LEU:HD23	1.96	0.65
1:A:267:ASN:HB3	1:A:270:SER:OG	1.96	0.65
23:B:1009:CLA:O1A	23:B:1009:CLA:NA	2.30	0.65
23:C:1030:CLA:HED3	23:C:1030:CLA:CHA	2.27	0.65
29:C:1056:DGD:HBG2	29:C:1056:DGD:HBG2	0.81	0.65
3:C:334:PRO:HD3	3:C:339:LYS:HE3	1.79	0.65
3:C:50:LEU:HD22	3:C:51:GLY:N	2.12	0.65
23:D:1004:CLA:C20	30:D:1059:MGE:H8A1	2.26	0.65
23:K:1034:CLA:HHD	23:K:1034:CLA:CBC	2.17	0.65
25:D:1042:PQ9:H241	30:L:1061:MGE:H263	1.79	0.65
14:T:24:ARG:HD2	14:T:24:ARG:O	1.97	0.65
27:A:1063:LHG:HC41	3:C:36:TRP:CH2	2.31	0.65
2:B:317:ASN:HA	2:B:330:MET:HE1	1.78	0.65
2:B:235:GLU:HG2	2:B:473:THR:HA	1.77	0.65
3:C:282:MET:SD	23:C:1025:CLA:H71	2.37	0.65
29:C:1056:DGD:HB92	29:C:1056:DGD:HBG1	1.77	0.65
3:C:281:MET:O	3:C:285:ILE:HG13	1.97	0.65
3:C:333:GLY:H	3:C:338:GLY:CA	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:184:PHE:CE2	4:D:188:PHE:HD1	2.11	0.65
7:H:41:PHE:HD1	26:H:1049:BCR:H362	1.61	0.65
1:A:89:ILE:HG21	1:A:94:TYR:HB2	1.77	0.64
23:C:1025:CLA:O2A	23:C:1025:CLA:C3A	2.44	0.64
3:C:171:GLY:CA	23:C:1025:CLA:HBC1	2.27	0.64
1:A:259:ILE:H	4:D:128:ARG:HH22	1.43	0.64
4:D:132:ILE:O	4:D:136:VAL:HG23	1.96	0.64
4:D:222:LEU:HD23	4:D:243:THR:O	1.98	0.64
14:T:20:ALA:O	14:T:24:ARG:HB3	1.96	0.64
1:A:310:LYS:HG2	16:V:151:ILE:HG22	1.77	0.64
1:A:150:PRO:CA	23:A:1003:CLA:H52	2.25	0.64
23:B:1011:CLA:HMD3	23:B:1014:CLA:HAB	1.79	0.64
23:D:1005:CLA:H202	23:D:1005:CLA:H152	1.79	0.64
24:D:1039:PHO:CBC	24:D:1039:PHO:CHD	2.74	0.64
4:D:217:THR:HG21	25:D:1042:PQ9:O4	1.96	0.64
5:E:13:ILE:HG13	5:E:19:TYR:HB2	1.79	0.64
13:O:75:THR:HB	13:O:262:GLN:HB2	1.77	0.64
1:A:36:ILE:HD13	23:C:1029:CLA:H142	1.78	0.64
2:B:174:LEU:HD21	2:B:312:TYR:CE1	2.31	0.64
3:C:240:ILE:HG13	23:C:1025:CLA:HAB	1.78	0.64
23:C:1029:CLA:HBC2	23:C:1029:CLA:HMC1	1.79	0.64
3:C:223:TRP:HE1	3:C:224:ILE:HG12	1.62	0.64
3:C:50:LEU:CD2	3:C:54:VAL:HG23	2.26	0.64
3:C:70:PHE:O	3:C:73:ALA:HB3	1.96	0.64
4:D:312:GLU:OE1	13:O:185:PRO:HB3	1.96	0.64
14:T:18:PHE:CA	26:T:6046:BCR:C33	2.74	0.64
16:V:81:ARG:HG3	16:V:157:GLY:HA3	1.78	0.64
18:Y:45:ASN:HD22	18:Y:45:ASN:C	2.00	0.64
3:C:450:ALA:HB3	3:C:456:GLU:HB3	1.79	0.64
4:D:158:LEU:O	4:D:162:LEU:HG	1.96	0.64
23:H:1017:CLA:HBB1	26:H:1049:BCR:H322	1.79	0.64
26:K:1051:BCR:H351	26:K:1051:BCR:C16	2.26	0.64
26:T:6046:BCR:C23	26:T:6046:BCR:H403	2.27	0.64
3:C:396:MET:CE	16:V:74:THR:HA	2.26	0.64
23:B:1011:CLA:H42	23:B:1011:CLA:CGA	2.28	0.64
23:C:1025:CLA:H143	26:C:1054:BCR:H353	1.80	0.64
1:A:159:LEU:HD21	29:C:1055:DGD:C7A	2.26	0.64
30:B:1060:MGE:CBB	30:B:1060:MGE:H263	2.28	0.64
2:B:372:ASP:HB3	2:B:376:VAL:HB	1.79	0.64
2:B:69:LEU:HD21	23:B:1013:CLA:O1A	1.97	0.64
3:C:81:MET:HG3	3:C:86:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:1005:CLA:H121	23:D:1005:CLA:C9	2.26	0.64
23:D:1005:CLA:H92	23:D:1005:CLA:H121	1.79	0.64
18:Y:43:ARG:HD3	20:Z:31:GLN:HE21	1.63	0.64
23:B:1016:CLA:CHD	23:B:1016:CLA:HBC3	2.26	0.64
23:C:1033:CLA:HMA1	23:K:1034:CLA:C2C	2.27	0.64
23:C:1033:CLA:H91	23:C:1036:CLA:CAA	2.27	0.64
3:C:172:ALA:O	3:C:176:VAL:HG23	1.97	0.64
3:C:229:ASN:ND2	3:C:229:ASN:H	1.85	0.64
4:D:207:GLY:HA2	4:D:274:VAL:HG11	1.79	0.64
1:A:223:LEU:HD11	4:D:265:ARG:HG2	1.78	0.64
7:H:13:PRO:HG2	7:H:14:LEU:CD1	2.22	0.64
8:I:24:LEU:C	8:I:26:GLY:H	2.01	0.64
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.27	0.64
15:U:42:TYR:HB3	15:U:43:PRO:HD2	1.78	0.64
15:U:53:ALA:HB1	15:U:54:PRO:HD2	1.79	0.64
1:A:39:PRO:HB2	23:A:1007:CLA:CBB	2.27	0.64
23:B:1010:CLA:HED3	23:B:1011:CLA:HMA1	1.80	0.64
23:B:1012:CLA:H43	23:B:1013:CLA:H41	1.79	0.64
3:C:374:GLY:HA2	13:O:33:TYR:CD1	2.33	0.64
3:C:49:LEU:CD2	3:C:52:ALA:CA	2.76	0.64
4:D:91:LEU:HG	23:D:1008:CLA:HED2	1.79	0.64
23:B:1015:CLA:H122	23:B:1015:CLA:H91	1.80	0.64
23:B:1021:CLA:H2	23:B:1021:CLA:HED1	1.79	0.64
2:B:280:PHE:O	2:B:284:ILE:HG13	1.96	0.64
23:C:1033:CLA:C2	23:C:1033:CLA:O1A	2.45	0.64
29:C:1055:DGD:HA61	29:C:1055:DGD:HAT1	1.78	0.64
15:U:68:THR:HG22	15:U:71:GLN:CB	2.28	0.64
23:A:1007:CLA:O1D	23:A:1007:CLA:H2A	1.98	0.64
23:B:1011:CLA:H42	23:B:1011:CLA:O1A	1.98	0.64
2:B:178:VAL:O	2:B:178:VAL:HG13	1.99	0.64
2:B:249:ALA:O	2:B:252:VAL:N	2.31	0.64
23:C:1029:CLA:C4	23:C:1029:CLA:C1C	2.75	0.64
4:D:145:ALA:HB2	4:D:272:LEU:CD1	2.28	0.64
10:K:21:LEU:HD11	18:Y:24:MET:CG	2.27	0.64
13:O:148:VAL:HG23	13:O:172:PHE:CE2	2.33	0.64
1:A:150:PRO:HA	23:A:1003:CLA:H52	1.81	0.63
23:B:1019:CLA:HBC3	23:B:1019:CLA:HMC1	1.80	0.63
2:B:40:TYR:C	2:B:40:TYR:HD1	2.01	0.63
23:C:1025:CLA:C4A	23:C:1025:CLA:C1	2.76	0.63
3:C:274:TYR:HE1	23:C:1029:CLA:O1D	1.81	0.63
23:K:1034:CLA:H91	23:K:1034:CLA:H121	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:32:GLU:HA	16:V:35:THR:OG1	1.97	0.63
1:A:192:ILE:HG12	1:A:293:MET:SD	2.37	0.63
1:A:52:PHE:O	1:A:71:LEU:HD12	1.98	0.63
2:B:10:THR:O	2:B:11:VAL:C	2.36	0.63
2:B:451:PHE:HZ	23:B:1012:CLA:O1D	1.81	0.63
2:B:75:TRP:HE1	2:B:94:GLU:HB2	1.63	0.63
23:C:1033:CLA:CBB	23:C:1033:CLA:HHC	2.27	0.63
4:D:201:VAL:O	4:D:205:LEU:HB3	1.97	0.63
5:E:17:VAL:O	5:E:21:VAL:HG23	1.98	0.63
8:I:4:LEU:O	8:I:8:VAL:HG22	1.97	0.63
13:O:129:PHE:O	13:O:129:PHE:CD2	2.50	0.63
13:O:152:VAL:HG13	13:O:152:VAL:O	1.98	0.63
23:A:1006:CLA:O2D	23:A:1006:CLA:H2A	1.99	0.63
4:D:155:SER:HA	4:D:159:ILE:HB	1.78	0.63
11:L:29:LEU:O	11:L:29:LEU:HD13	1.98	0.63
23:B:1022:CLA:H121	12:M:24:ILE:HD12	1.80	0.63
13:O:190:LEU:C	13:O:190:LEU:CD2	2.67	0.63
4:D:328:TRP:CZ3	16:V:161:VAL:HA	2.33	0.63
23:B:1014:CLA:C9	26:B:1048:BCR:H342	2.28	0.63
3:C:425:TRP:CH2	23:C:1028:CLA:O1A	2.52	0.63
23:C:1036:CLA:HBB1	23:C:1036:CLA:CHC	2.28	0.63
4:D:123:ILE:O	4:D:127:LEU:HG	1.97	0.63
4:D:87:HIS:NE2	4:D:162:LEU:HA	2.13	0.63
13:O:104:LEU:O	13:O:104:LEU:HD12	1.98	0.63
18:Y:39:LEU:HD21	20:Z:28:ALA:CB	2.27	0.63
1:A:323:ARG:NE	4:D:332:GLN:NE2	2.46	0.63
30:B:1060:MGE:H211	30:B:1060:MGE:CGB	2.29	0.63
2:B:103:LEU:HD12	2:B:107:LEU:HG	1.79	0.63
2:B:357:ARG:NH1	2:B:357:ARG:HG2	2.08	0.63
3:C:362:ARG:HD2	3:C:367:GLU:OE2	1.98	0.63
4:D:194:ASN:O	4:D:198:MET:HG3	1.97	0.63
23:K:1034:CLA:H12	23:K:1034:CLA:ND	2.12	0.63
3:C:417:VAL:CG1	16:V:68:VAL:HG11	2.25	0.63
20:Z:5:PHE:HE1	20:Z:54:VAL:HG13	1.63	0.63
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.34	0.63
1:A:256:GLY:C	1:A:261:GLN:HA	2.18	0.63
23:B:1013:CLA:HMB3	23:B:1014:CLA:C1	2.27	0.63
23:C:1031:CLA:O2D	23:C:1031:CLA:H2A	1.98	0.63
23:C:1032:CLA:HHD	23:C:1032:CLA:HBC2	1.79	0.63
26:C:1054:BCR:C8	26:C:1054:BCR:H311	2.29	0.63
23:C:1032:CLA:H161	29:C:1056:DGD:CDB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:418:ASN:OD1	29:C:1056:DGD:HE2	1.99	0.63
3:C:230:LEU:O	3:C:234:VAL:HG12	1.98	0.63
3:C:443:TRP:CE3	3:C:443:TRP:HA	2.33	0.63
2:B:220:ARG:HG3	7:H:21:VAL:HA	1.80	0.63
23:K:1034:CLA:CGA	23:K:1034:CLA:CGD	2.76	0.63
13:O:148:VAL:O	13:O:148:VAL:HG22	1.98	0.63
18:Y:42:ARG:HB3	18:Y:43:ARG:HE	1.64	0.63
1:A:93:PHE:O	1:A:95:PRO:HD3	1.99	0.63
3:C:240:ILE:HG13	23:C:1025:CLA:CAB	2.29	0.63
3:C:155:ASN:CA	3:C:158:THR:HG22	2.26	0.63
3:C:170:ILE:HG22	3:C:171:GLY:N	2.13	0.63
3:C:223:TRP:CD1	3:C:224:ILE:CG1	2.81	0.63
3:C:229:ASN:ND2	3:C:229:ASN:N	2.44	0.63
3:C:49:LEU:CD1	23:C:1035:CLA:HMA2	2.27	0.63
23:D:1004:CLA:H142	23:D:1004:CLA:C10	2.28	0.63
4:D:182:LEU:O	4:D:185:PHE:N	2.29	0.63
4:D:189:HIS:CG	4:D:289:LEU:HD22	2.34	0.63
7:H:11:LEU:C	7:H:13:PRO:HD2	2.19	0.63
23:K:1034:CLA:C4D	23:K:1034:CLA:C1	2.77	0.63
1:A:116:ILE:CD1	1:A:158:PHE:HB3	2.27	0.63
2:B:288:VAL:O	2:B:292:LEU:HB2	1.99	0.63
3:C:280:SER:OG	3:C:438:LEU:HB2	1.98	0.63
3:C:443:TRP:HE3	3:C:443:TRP:HA	1.64	0.63
4:D:19:ASP:OD2	4:D:23:LYS:HD3	1.99	0.63
26:H:1049:BCR:H401	17:X:20:PHE:HZ	1.64	0.63
13:O:144:LEU:HD23	13:O:144:LEU:H	1.64	0.63
15:U:70:ARG:O	15:U:73:GLN:HB3	1.99	0.63
15:U:78:ASN:HB3	15:U:82:PHE:HE2	1.64	0.63
16:V:62:ALA:HB1	31:V:1041:HEM:HBB1	1.80	0.63
16:V:38:LEU:O	16:V:94:ASN:HB3	1.99	0.63
23:A:1007:CLA:H41	23:A:1007:CLA:H71	1.80	0.63
25:A:1043:PQ9:H293	24:D:1039:PHO:CBA	2.29	0.63
1:A:105:TRP:HZ3	26:A:1044:BCR:H393	1.62	0.63
2:B:25:MET:HE2	26:B:1045:BCR:H403	1.81	0.63
2:B:63:LEU:N	2:B:64:PRO:CD	2.61	0.63
3:C:146:PHE:O	3:C:146:PHE:CD1	2.52	0.63
3:C:159:THR:HA	3:C:252:ILE:HA	1.81	0.63
24:D:1039:PHO:CMA	23:D:1004:CLA:H102	2.28	0.63
23:A:1006:CLA:C17	26:D:1050:BCR:C27	2.66	0.63
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.24	0.63
8:I:9:TYR:O	8:I:12:VAL:HG12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:N	2:B:16:PRO:HD3	2.14	0.62
3:C:184:GLY:O	3:C:185:LEU:HD23	1.99	0.62
3:C:265:ILE:CD1	3:C:452:ALA:CB	2.61	0.62
27:A:1063:LHG:HC82	3:C:36:TRP:CE2	2.33	0.62
3:C:51:GLY:O	3:C:55:ALA:N	2.24	0.62
11:L:26:VAL:HG12	11:L:27:LEU:N	2.14	0.62
1:A:335:ASN:ND2	13:O:182:PHE:CE1	2.67	0.62
18:Y:43:ARG:HH21	18:Y:44:GLY:CA	2.12	0.62
24:A:1038:PHO:CBC	24:A:1038:PHO:HHD	2.28	0.62
2:B:433:ASP:OD1	2:B:433:ASP:C	2.37	0.62
3:C:42:LEU:HD22	23:C:1035:CLA:HMA3	1.82	0.62
23:C:1035:CLA:O2D	23:C:1035:CLA:H2A	1.99	0.62
26:D:1050:BCR:C22	30:D:1059:MGE:C3A	2.75	0.62
4:D:150:ILE:O	4:D:154:VAL:HG23	1.99	0.62
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.35	0.62
1:A:87:ASN:ND2	3:C:357:ARG:HE	1.97	0.62
23:B:1011:CLA:CAA	23:B:1011:CLA:CGD	2.77	0.62
23:B:1011:CLA:H11	23:B:1011:CLA:CHB	2.29	0.62
6:F:21:VAL:O	6:F:25:THR:HG23	1.98	0.62
23:C:1033:CLA:HMA3	23:K:1034:CLA:HMC1	1.77	0.62
13:O:242:GLU:CD	13:O:260:LYS:HD3	2.19	0.62
1:A:309:ALA:HB3	16:V:28:GLU:HB2	1.79	0.62
25:A:1043:PQ9:C29	25:A:1043:PQ9:H37	2.29	0.62
1:A:105:TRP:CZ2	1:A:111:PRO:HA	2.34	0.62
2:B:103:LEU:HD13	23:B:1014:CLA:C9	2.28	0.62
26:B:1048:BCR:H392	26:B:1048:BCR:H371	1.32	0.62
2:B:452:THR:O	2:B:456:ALA:HB2	1.99	0.62
2:B:45:PHE:HA	2:B:58:GLN:HE22	1.64	0.62
3:C:318:LEU:HD23	3:C:318:LEU:O	1.98	0.62
3:C:58:GLY:HA2	3:C:61:VAL:HG12	1.82	0.62
4:D:174:GLY:HA3	4:D:177:ALA:HB3	1.81	0.62
1:A:223:LEU:HD21	4:D:265:ARG:CG	2.29	0.62
8:I:5:LYS:O	8:I:8:VAL:HG23	2.00	0.62
23:C:1035:CLA:H141	26:K:1051:BCR:C34	2.30	0.62
11:L:20:GLY:HA3	12:M:22:LEU:HD13	1.82	0.62
1:A:109:GLY:C	1:A:111:PRO:HD2	2.20	0.62
1:A:199:GLN:O	1:A:202:VAL:HG12	1.98	0.62
1:A:41:LEU:HD22	1:A:41:LEU:N	2.15	0.62
23:B:1018:CLA:H2A	23:B:1018:CLA:O2D	1.99	0.62
2:B:119:ASP:C	2:B:120:LEU:HD23	2.20	0.62
2:B:138:MET:SD	23:B:1023:CLA:HAC2	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LEU:HB2	3:C:248:GLY:CA	2.30	0.62
3:C:348:GLU:CD	3:C:373:ASN:HB3	2.19	0.62
3:C:48:LYS:CD	23:C:1035:CLA:HED1	2.27	0.62
4:D:170:ALA:O	4:D:171:PRO:O	2.18	0.62
10:K:20:PRO:HA	18:Y:21:GLN:HG2	1.81	0.62
30:B:1060:MGE:H5B2	4:D:276:VAL:HB	1.81	0.62
2:B:24:LEU:HD21	2:B:110:ALA:O	1.99	0.62
2:B:24:LEU:HD23	2:B:111:ALA:HA	1.81	0.62
3:C:75:PHE:CD1	3:C:86:LEU:HD11	2.34	0.62
30:D:1059:MGE:O5D	6:F:40:MET:HB2	2.00	0.62
30:D:1062:MGE:H4B1	30:D:1062:MGE:O1A	2.00	0.62
4:D:275:PRO:O	4:D:277:THR:N	2.33	0.62
26:H:1049:BCR:C8	26:H:1049:BCR:H321	2.29	0.62
8:I:16:VAL:O	8:I:20:VAL:HG23	2.00	0.62
11:L:30:LEU:C	11:L:30:LEU:HD23	2.19	0.62
13:O:181:ASN:O	13:O:182:PHE:HB2	1.99	0.62
15:U:16:LYS:HG2	15:U:21:TYR:CD1	2.34	0.62
16:V:105:PRO:HG2	16:V:115:ALA:N	2.14	0.62
23:B:1014:CLA:CBC	23:B:1014:CLA:CHD	2.72	0.62
2:B:297:THR:OG1	2:B:300:GLU:HG3	1.99	0.62
2:B:91:TRP:CD1	23:B:1014:CLA:HBA2	2.35	0.62
3:C:384:ILE:O	3:C:384:ILE:HG23	2.00	0.62
3:C:407:VAL:O	3:C:407:VAL:HG13	1.99	0.62
4:D:274:VAL:HG22	25:D:1042:PQ9:H261	1.81	0.62
3:C:386:PRO:HB2	16:V:116:GLU:OE1	2.00	0.62
16:V:54:GLU:OE2	16:V:57:ARG:HD3	1.99	0.62
1:A:160:ILE:HD13	3:C:431:PHE:CE1	2.35	0.62
1:A:215:HIS:CD2	1:A:275:LEU:HD11	2.35	0.62
1:A:290:ILE:HG22	1:A:291:SER:N	2.14	0.62
23:B:1023:CLA:C9	23:B:1024:CLA:H152	2.30	0.62
2:B:181:VAL:CG1	2:B:196:GLY:HA2	2.29	0.62
2:B:23:HIS:O	2:B:27:THR:HB	1.98	0.62
2:B:315:ILE:HG22	2:B:426:PHE:O	1.99	0.62
23:C:1035:CLA:HBB2	23:K:1034:CLA:CHB	2.29	0.62
6:F:34:LEU:HD12	9:J:24:ILE:CD1	2.28	0.62
11:L:29:LEU:C	11:L:29:LEU:HD13	2.20	0.62
1:A:270:SER:O	1:A:273:PHE:HB3	2.00	0.62
23:C:1035:CLA:C3B	26:C:1052:BCR:H271	2.29	0.62
23:C:1025:CLA:C9	26:C:1054:BCR:H373	2.29	0.62
3:C:135:ARG:HG2	20:Z:27:TYR:HB3	1.82	0.62
4:D:223:PHE:CE1	4:D:245:SER:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:HIS:HE1	4:D:80:THR:HG23	1.63	0.62
5:E:77:GLU:O	5:E:81:GLU:N	2.33	0.62
15:U:45:LEU:HD13	15:U:71:GLN:HG2	1.80	0.62
1:A:330:VAL:HG11	4:D:348:ARG:HG2	1.82	0.62
2:B:121:GLU:CB	7:H:4:ARG:HB3	2.29	0.62
2:B:419:SER:HA	2:B:422:ARG:HH12	1.65	0.62
3:C:451:ALA:CA	3:C:456:GLU:HG2	2.30	0.62
2:B:225:LEU:HD11	7:H:28:THR:OG1	2.00	0.62
11:L:22:LEU:HG	30:L:1061:MGE:H221	1.82	0.62
13:O:59:ASP:H	13:O:64:TYR:HE1	1.47	0.62
14:T:8:PHE:CE1	28:T:1066:IOD:I	3.23	0.62
23:A:1007:CLA:C5	23:A:1007:CLA:H112	2.30	0.61
23:B:1021:CLA:C1	23:B:1021:CLA:HMA2	2.30	0.61
23:B:1023:CLA:H41	26:B:1048:BCR:C34	2.29	0.61
2:B:222:PRO:HB2	2:B:225:LEU:HD13	1.82	0.61
2:B:271:THR:HG23	2:B:274:GLN:HB2	1.81	0.61
2:B:285:ASN:HA	2:B:288:VAL:HG12	1.82	0.61
2:B:429:ILE:CD1	2:B:429:ILE:H	2.13	0.61
3:C:321:ASP:O	3:C:324:LEU:N	2.33	0.61
3:C:42:LEU:HD13	3:C:49:LEU:HD11	1.80	0.61
23:D:1008:CLA:C19	23:D:1008:CLA:H141	2.18	0.61
7:H:30:LEU:HB3	23:H:1017:CLA:CMD	2.30	0.61
1:A:64:ARG:NH2	13:O:131:PRO:O	2.33	0.61
16:V:66:CYS:SG	31:V:1041:HEM:C3C	2.93	0.61
23:A:1006:CLA:HHC	23:A:1006:CLA:CBB	2.23	0.61
1:A:322:ASN:HA	1:A:325:ASN:HB2	1.82	0.61
2:B:90:PHE:HZ	2:B:98:LEU:HD12	1.65	0.61
3:C:160:ILE:HG22	3:C:161:LEU:N	2.14	0.61
3:C:264:PHE:O	3:C:266:TRP:CD1	2.54	0.61
3:C:39:ASN:HB2	23:C:1032:CLA:CBA	2.28	0.61
1:A:297:LEU:CD2	3:C:404:LEU:HD23	2.30	0.61
5:E:75:GLN:O	5:E:76:VAL:C	2.36	0.61
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.83	0.61
1:A:273:PHE:CE1	27:A:1063:LHG:HC61	2.35	0.61
23:B:1023:CLA:H152	23:B:1024:CLA:C4A	2.29	0.61
2:B:374:ASN:HD22	2:B:374:ASN:N	1.98	0.61
23:C:1028:CLA:C6	29:C:1057:DGD:HA42	2.31	0.61
3:C:351:PHE:CD2	3:C:375:LEU:HD11	2.35	0.61
3:C:49:LEU:HD22	3:C:52:ALA:CA	2.29	0.61
4:D:136:VAL:O	4:D:136:VAL:HG12	2.00	0.61
5:E:11:SER:O	5:E:15:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:PHE:HB3	5:E:47:PHE:HD1	1.65	0.61
1:A:197:PHE:HD1	1:A:285:PHE:HB3	1.65	0.61
1:A:258:LEU:C	1:A:259:ILE:HG13	2.21	0.61
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.36	0.61
23:B:1023:CLA:C15	23:B:1024:CLA:C4A	2.78	0.61
2:B:135:LEU:HD12	2:B:135:LEU:N	2.15	0.61
3:C:117:VAL:HG11	23:C:1027:CLA:C1	2.31	0.61
26:C:1052:BCR:H361	10:K:32:PHE:HE2	1.63	0.61
12:M:3:VAL:HG23	12:M:4:ASN:O	2.01	0.61
15:U:27:LEU:HD21	15:U:82:PHE:HD1	1.65	0.61
23:A:1003:CLA:C2A	23:A:1003:CLA:CED	2.64	0.61
25:A:1043:PQ9:H37	25:A:1043:PQ9:C30	2.29	0.61
2:B:463:PHE:HE1	23:B:1016:CLA:CBB	2.12	0.61
2:B:17:GLY:HA2	2:B:123:PHE:CE1	2.35	0.61
2:B:99:ALA:HB1	23:B:1014:CLA:H43	1.82	0.61
29:C:1056:DGD:HBV2	29:C:1056:DGD:HB81	1.81	0.61
3:C:240:ILE:O	3:C:240:ILE:HD13	2.00	0.61
3:C:363:GLY:O	3:C:367:GLU:HG2	2.00	0.61
26:C:1052:BCR:H352	26:K:1051:BCR:H322	1.82	0.61
13:O:132:VAL:CG2	13:O:144:LEU:HD21	2.30	0.61
13:O:188:ARG:HH11	13:O:188:ARG:CB	2.14	0.61
1:A:340:PRO:HD3	15:U:103:TYR:CE2	2.36	0.61
16:V:151:ILE:HG12	16:V:152:LEU:N	2.15	0.61
1:A:126:TYR:C	1:A:126:TYR:HD2	2.03	0.61
1:A:185:VAL:O	1:A:188:ALA:HB3	2.00	0.61
1:A:290:ILE:CG2	1:A:291:SER:N	2.63	0.61
2:B:61:PHE:HB2	23:B:1015:CLA:HMA3	1.82	0.61
23:C:1031:CLA:CHD	23:C:1031:CLA:CBC	2.71	0.61
3:C:418:ASN:OD1	3:C:418:ASN:C	2.38	0.61
3:C:56:HIS:CE1	23:C:1033:CLA:HMA1	2.35	0.61
23:D:1005:CLA:H93	30:D:1062:MGE:H211	1.83	0.61
4:D:126:MET:HE3	4:D:146:PHE:CD2	2.34	0.61
4:D:219:GLU:O	4:D:222:LEU:HB2	2.00	0.61
7:H:12:ARG:N	7:H:13:PRO:HD2	2.15	0.61
6:F:41:GLN:NE2	9:J:31:GLY:HA3	2.16	0.61
13:O:68:ARG:O	13:O:68:ARG:HG3	2.00	0.61
16:V:38:LEU:HA	16:V:95:ILE:CG2	2.26	0.61
20:Z:20:VAL:O	20:Z:24:PRO:CD	2.45	0.61
29:C:1056:DGD:HB51	9:J:29:PHE:HE1	1.66	0.61
4:D:267:LEU:HD23	4:D:267:LEU:C	2.21	0.61
23:A:1007:CLA:C6	23:A:1007:CLA:H112	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1043:PQ9:C45	30:D:1059:MGE:C9A	2.79	0.61
1:A:12:ASN:O	1:A:15:GLU:HG3	1.99	0.61
2:B:174:LEU:HD21	2:B:312:TYR:HE1	1.66	0.61
2:B:462:PHE:CE1	23:B:1021:CLA:HMB3	2.36	0.61
3:C:293:ASN:ND2	3:C:295:THR:HB	2.15	0.61
4:D:190:ASN:HD22	4:D:296:TYR:HA	1.66	0.61
4:D:313:THR:O	4:D:316:THR:HG23	2.00	0.61
26:K:1051:BCR:H353	18:Y:32:GLY:CA	2.20	0.61
23:A:1007:CLA:C7	23:A:1007:CLA:H41	2.30	0.61
23:B:1011:CLA:CGD	23:B:1011:CLA:HAA1	2.30	0.61
23:B:1011:CLA:C1D	23:B:1013:CLA:C3	2.78	0.61
23:C:1030:CLA:CBC	23:C:1030:CLA:CHD	2.58	0.61
23:C:1031:CLA:HMA2	23:C:1031:CLA:C2	2.30	0.61
3:C:276:LEU:C	3:C:276:LEU:HD23	2.22	0.61
4:D:210:LEU:HD11	25:D:1042:PQ9:H152	1.82	0.61
4:D:37:LEU:HD13	4:D:125:PHE:HA	1.81	0.61
4:D:182:LEU:O	4:D:183:LEU:C	2.37	0.61
8:I:29:ALA:O	8:I:30:ARG:HB2	2.01	0.61
13:O:223:ILE:HD13	13:O:225:LEU:HD13	1.83	0.61
23:B:1018:CLA:H141	23:B:1018:CLA:H172	1.82	0.61
2:B:113:TRP:CD1	2:B:114:HIS:N	2.69	0.61
23:C:1025:CLA:O2A	23:C:1025:CLA:H3A	1.99	0.61
3:C:171:GLY:HA3	23:C:1025:CLA:HBC1	1.81	0.61
23:C:1026:CLA:C7	23:C:1026:CLA:C12	2.76	0.61
3:C:117:VAL:HG21	23:C:1027:CLA:H162	1.81	0.61
6:F:20:TRP:HE1	6:F:24:HIS:CE1	2.18	0.61
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.65	0.61
9:J:15:THR:HG21	10:K:38:VAL:HG22	1.82	0.61
13:O:55:ALA:CB	13:O:161:SER:HB3	2.30	0.61
1:A:129:ARG:HG2	1:A:129:ARG:O	2.01	0.60
23:C:1028:CLA:C9	29:C:1056:DGD:HB91	2.30	0.60
24:D:1039:PHO:O2D	24:D:1039:PHO:H2A	2.01	0.60
4:D:78:VAL:HG12	4:D:173:PHE:HB3	1.82	0.60
26:H:1049:BCR:H393	26:H:1049:BCR:C23	2.30	0.60
1:A:142:TRP:HB3	3:C:443:TRP:CZ2	2.36	0.60
1:A:151:LEU:HG	1:A:155:PHE:HD2	1.65	0.60
1:A:197:PHE:CE2	29:C:1056:DGD:HAN2	2.37	0.60
2:B:49:ASP:OD1	2:B:53:ASN:N	2.34	0.60
29:C:1057:DGD:HG31	9:J:33:TYR:CE2	2.35	0.60
3:C:223:TRP:CD1	3:C:224:ILE:N	2.69	0.60
3:C:318:LEU:HD23	3:C:328:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:221:THR:HG21	4:D:245:SER:O	2.01	0.60
13:O:62:GLN:HE21	13:O:62:GLN:HA	1.66	0.60
23:A:1006:CLA:HBC2	4:D:182:LEU:HD21	1.81	0.60
3:C:263:ALA:HB1	3:C:264:PHE:CE2	2.34	0.60
4:D:39:PRO:O	4:D:43:LEU:HG	2.01	0.60
8:I:4:LEU:HA	8:I:7:THR:OG1	2.00	0.60
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.36	0.60
13:O:82:PRO:HG3	13:O:89:ALA:CB	2.31	0.60
1:A:140:ARG:CB	1:A:140:ARG:NH1	2.64	0.60
1:A:217:SER:O	1:A:220:THR:HG22	2.01	0.60
1:A:222:SER:C	2:B:482:ILE:HG21	2.21	0.60
23:B:1011:CLA:CMD	23:B:1014:CLA:CMB	2.79	0.60
23:B:1011:CLA:O2D	23:B:1012:CLA:HED1	2.00	0.60
2:B:62:VAL:CG1	23:B:1013:CLA:HED2	2.31	0.60
29:B:1058:DGD:HB62	29:B:1058:DGD:CAB	2.31	0.60
23:C:1028:CLA:O2A	29:C:1056:DGD:HG11	2.00	0.60
23:C:1029:CLA:C1A	23:C:1029:CLA:CGA	2.78	0.60
3:C:216:SER:HB2	3:C:221:GLU:HB2	1.82	0.60
3:C:63:TRP:NE1	23:C:1028:CLA:HMC3	2.15	0.60
4:D:325:ILE:O	4:D:329:MET:HG2	2.02	0.60
6:F:41:GLN:HE21	9:J:28:PHE:HA	1.65	0.60
23:C:1035:CLA:HMC3	23:K:1034:CLA:CMB	2.31	0.60
16:V:66:CYS:O	16:V:73:LYS:CG	2.49	0.60
1:A:186:PHE:O	1:A:187:GLN:C	2.40	0.60
1:A:256:GLY:HA2	1:A:264:SER:HB2	1.84	0.60
1:A:336:ALA:O	1:A:338:ASN:ND2	2.34	0.60
2:B:111:ALA:O	2:B:113:TRP:N	2.34	0.60
23:C:1033:CLA:CHC	23:C:1033:CLA:HBB1	2.25	0.60
23:C:1035:CLA:HBB2	23:K:1034:CLA:CMA	2.31	0.60
2:B:468:TRP:CE3	4:D:144:ILE:HD13	2.36	0.60
3:C:457:LYS:HZ1	4:D:228:GLY:HA2	1.64	0.60
4:D:313:THR:OG1	4:D:316:THR:HG22	2.01	0.60
1:A:315:ASN:O	4:D:63:LEU:HD23	2.01	0.60
14:T:18:PHE:HD1	26:T:6046:BCR:H332	1.66	0.60
16:V:94:ASN:HB2	16:V:97:GLY:H	1.66	0.60
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.36	0.60
1:A:317:TRP:HA	4:D:63:LEU:HD11	1.83	0.60
23:B:1022:CLA:H93	23:B:1022:CLA:C12	2.09	0.60
2:B:124:ARG:HE	2:B:131:PRO:HB3	1.66	0.60
3:C:271:TYR:HE1	23:C:1031:CLA:HAC1	1.64	0.60
4:D:352:LEU:H	4:D:352:LEU:CD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:LEU:HD23	4:D:37:LEU:H	1.65	0.60
4:D:103:ARG:HD2	5:E:76:VAL:HG21	1.84	0.60
16:V:38:LEU:CA	16:V:45:ILE:HD11	2.31	0.60
1:A:193:LEU:HD22	4:D:179:PHE:CD2	2.36	0.60
2:B:90:PHE:CD2	2:B:90:PHE:C	2.75	0.60
3:C:264:PHE:O	3:C:266:TRP:NE1	2.34	0.60
3:C:436:PHE:O	3:C:439:VAL:HB	2.00	0.60
4:D:22:LEU:O	4:D:30:VAL:O	2.20	0.60
4:D:148:ALA:HB2	4:D:276:VAL:HG12	1.84	0.60
10:K:28:ILE:O	10:K:29:PRO:C	2.36	0.60
13:O:107:ILE:HG23	13:O:123:GLU:HG3	1.84	0.60
13:O:206:GLU:O	13:O:207:GLU:CB	2.48	0.60
13:O:90:GLU:HA	13:O:90:GLU:OE1	2.00	0.60
15:U:31:ASN:ND2	15:U:32:ILE:N	2.48	0.60
15:U:52:ASN:OD1	15:U:64:ILE:HD13	2.02	0.60
20:Z:55:GLY:HA2	26:Z:1053:BCR:H313	1.82	0.60
1:A:119:PHE:CD2	1:A:123:ALA:HB2	2.37	0.60
1:A:258:LEU:O	1:A:259:ILE:HD12	2.01	0.60
2:B:91:TRP:CG	23:B:1014:CLA:HBA2	2.37	0.60
23:C:1029:CLA:C5	23:C:1029:CLA:C1C	2.79	0.60
23:C:1037:CLA:CHC	23:C:1037:CLA:HBB1	2.14	0.60
3:C:146:PHE:O	3:C:148:GLY:N	2.34	0.60
3:C:274:TYR:O	3:C:276:LEU:N	2.34	0.60
6:F:40:MET:HB3	6:F:43:ILE:HD11	1.82	0.60
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.01	0.60
23:A:1007:CLA:CAD	23:A:1007:CLA:CED	2.80	0.60
24:A:1038:PHO:C9	23:D:1005:CLA:C18	2.80	0.60
1:A:136:ARG:HH12	8:I:27:ASP:HB3	1.67	0.60
1:A:201:GLY:O	1:A:205:VAL:HG12	2.01	0.60
1:A:63:ILE:HG12	1:A:64:ARG:N	2.15	0.60
23:B:1018:CLA:C14	23:B:1018:CLA:OBD	2.49	0.60
2:B:406:LEU:O	2:B:407:ASN:O	2.20	0.60
2:B:454:ALA:C	2:B:456:ALA:H	2.05	0.60
2:B:46:ASP:HB3	2:B:58:GLN:OE1	2.01	0.60
3:C:276:LEU:O	3:C:276:LEU:HD23	2.02	0.60
25:D:1042:PQ9:H243	25:D:1042:PQ9:H292	1.84	0.60
16:V:94:ASN:C	16:V:96:GLU:N	2.52	0.60
20:Z:27:TYR:HD2	20:Z:27:TYR:N	1.99	0.60
1:A:196:PRO:CA	1:A:199:GLN:HG3	2.31	0.60
1:A:213:ALA:HB3	24:D:1039:PHO:HBC1	1.84	0.60
23:B:1020:CLA:H8	23:B:1020:CLA:H41	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1029:CLA:CBB	23:C:1029:CLA:HHC	2.32	0.60
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.01	0.60
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.31	0.60
1:A:244:GLU:HG2	4:D:264:LYS:NZ	2.17	0.59
1:A:334:ARG:HB2	1:A:335:ASN:OD1	2.02	0.59
23:B:1009:CLA:CGA	23:B:1009:CLA:NA	2.64	0.59
2:B:188:ASP:OD1	2:B:191:ASN:HB2	2.02	0.59
23:C:1026:CLA:C2B	23:C:1028:CLA:HBB2	2.32	0.59
3:C:52:ALA:CB	23:C:1035:CLA:HMB3	2.31	0.59
29:C:1055:DGD:C2A	29:C:1055:DGD:HB21	2.30	0.59
3:C:89:ILE:HA	3:C:92:ILE:HD13	1.83	0.59
23:A:1006:CLA:HAB	24:D:1039:PHO:C14	2.32	0.59
4:D:304:ARG:NH1	4:D:311:PHE:CD2	2.70	0.59
7:H:30:LEU:O	7:H:33:VAL:HG22	2.02	0.59
14:T:11:ALA:HB3	26:T:6046:BCR:H362	1.82	0.59
26:K:1051:BCR:C35	18:Y:32:GLY:HA3	2.21	0.59
1:A:141:PRO:C	1:A:143:ILE:H	2.05	0.59
23:B:1018:CLA:H8	23:B:1023:CLA:CBA	2.32	0.59
2:B:264:PRO:HG3	2:B:267:LEU:HB2	1.83	0.59
2:B:392:PHE:HA	2:B:397:VAL:CG2	2.32	0.59
23:C:1030:CLA:CHC	23:C:1030:CLA:HBB1	2.14	0.59
23:C:1035:CLA:C2B	26:C:1052:BCR:C27	2.77	0.59
3:C:118:HIS:O	3:C:121:SER:HB3	2.02	0.59
3:C:72:LEU:HD13	3:C:112:PHE:HB2	1.84	0.59
23:D:1008:CLA:HBC3	23:D:1008:CLA:HMC1	1.82	0.59
4:D:199:MET:HA	4:D:202:ALA:HB3	1.83	0.59
9:J:10:LEU:HD22	9:J:11:TRP:H	1.67	0.59
23:K:1034:CLA:CBA	23:K:1034:CLA:C4	2.81	0.59
13:O:70:CYS:HB2	13:O:105:ASP:HB2	1.84	0.59
13:O:83:LYS:HD2	13:O:85:LYS:HE3	1.83	0.59
15:U:35:PHE:HD1	15:U:46:ALA:CB	2.15	0.59
16:V:109:ASP:HB3	16:V:111:GLU:H	1.67	0.59
2:B:465:GLY:N	23:B:1019:CLA:HAC1	2.17	0.59
2:B:26:HIS:HB2	23:B:1020:CLA:HMB2	1.84	0.59
23:B:1021:CLA:HBC3	26:B:1047:BCR:H343	1.83	0.59
3:C:403:SER:O	3:C:406:SER:N	2.34	0.59
4:D:173:PHE:CD1	24:D:1039:PHO:H13	2.36	0.59
4:D:122:LEU:HD22	4:D:122:LEU:H	1.66	0.59
4:D:156:VAL:HG12	4:D:156:VAL:O	2.02	0.59
1:A:320:ILE:HG21	4:D:180:ARG:HG3	1.84	0.59
30:B:1060:MGE:H6D1	4:D:269:PHE:CE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1006:CLA:H91	23:D:1004:CLA:H171	1.84	0.59
23:B:1009:CLA:C3D	23:B:1010:CLA:HBB2	2.26	0.59
2:B:222:PRO:HB2	2:B:225:LEU:HD12	1.84	0.59
23:C:1030:CLA:CHA	23:C:1030:CLA:CED	2.81	0.59
3:C:140:LEU:HD21	3:C:146:PHE:CE1	2.29	0.59
3:C:269:GLU:OE1	3:C:447:ARG:HD2	2.02	0.59
3:C:97:TRP:O	3:C:99:VAL:HG23	2.02	0.59
4:D:39:PRO:HB2	23:D:1008:CLA:CBB	2.32	0.59
26:D:1050:BCR:C21	30:D:1059:MGE:H3A1	2.32	0.59
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.84	0.59
16:V:62:ALA:O	16:V:63:CYS:CB	2.48	0.59
20:Z:32:ASP:HB3	20:Z:35:ARG:HG2	1.84	0.59
1:A:120:LEU:HD13	1:A:120:LEU:O	2.02	0.59
1:A:196:PRO:HB2	29:C:1057:DGD:C8A	2.26	0.59
1:A:338:ASN:O	1:A:339:PHE:CD1	2.56	0.59
23:B:1023:CLA:H112	23:B:1024:CLA:H8	1.84	0.59
2:B:450:TRP:CH2	23:B:1015:CLA:H2	2.37	0.59
23:C:1026:CLA:H42	23:C:1026:CLA:CGA	2.31	0.59
23:C:1029:CLA:H51	23:C:1029:CLA:NB	2.15	0.59
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.67	0.59
4:D:55:VAL:HG21	4:D:110:LEU:CD2	2.33	0.59
4:D:18:LEU:HD11	17:X:37:LEU:HD13	1.83	0.59
7:H:54:ILE:C	7:H:55:LEU:HD22	2.23	0.59
7:H:55:LEU:HB2	7:H:58:VAL:HB	1.84	0.59
18:Y:22:LEU:O	18:Y:25:ILE:HG12	2.02	0.59
2:B:18:ARG:HB3	2:B:115:TRP:CZ3	2.37	0.59
2:B:353:GLU:O	2:B:373:LYS:HE3	2.03	0.59
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.83	0.59
3:C:176:VAL:HG21	3:C:238:ILE:HG12	1.85	0.59
3:C:315:MET:O	3:C:315:MET:HE2	2.02	0.59
4:D:108:GLY:O	4:D:110:LEU:N	2.36	0.59
4:D:299:ILE:HG22	4:D:300:SER:N	2.17	0.59
23:K:1034:CLA:O2A	23:K:1034:CLA:C1A	2.50	0.59
11:L:32:SER:HA	12:M:11:THR:OG1	2.03	0.59
13:O:148:VAL:HG23	13:O:172:PHE:HE2	1.66	0.59
26:T:6046:BCR:H323	26:T:6046:BCR:C4	2.33	0.59
1:A:126:TYR:CD2	1:A:126:TYR:C	2.76	0.59
1:A:325:ASN:ND2	1:A:328:MET:HE3	2.17	0.59
23:B:1009:CLA:O1D	23:B:1009:CLA:HBA1	1.99	0.59
23:B:1012:CLA:HMD2	23:B:1020:CLA:C20	2.33	0.59
23:B:1022:CLA:CHA	23:B:1022:CLA:C1	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:O	2:B:138:MET:C	2.41	0.59
2:B:173:GLY:HA3	2:B:174:LEU:C	2.23	0.59
3:C:155:ASN:O	3:C:158:THR:HG22	2.02	0.59
3:C:348:GLU:OE1	3:C:373:ASN:HB3	2.02	0.59
3:C:353:GLY:HA3	3:C:355:THR:HG23	1.84	0.59
2:B:320:ALA:HB1	4:D:292:ASN:HD22	1.67	0.59
4:D:29:PHE:CE2	4:D:31:GLY:N	2.71	0.59
1:A:337:HIS:O	4:D:350:ASN:O	2.20	0.59
4:D:35:ILE:O	4:D:39:PRO:HG3	2.01	0.59
6:F:41:GLN:OE1	6:F:41:GLN:HA	2.03	0.59
13:O:227:VAL:HG11	13:O:230:VAL:HG22	1.85	0.59
16:V:28:GLU:OE2	16:V:28:GLU:HA	2.02	0.59
20:Z:27:TYR:CD2	20:Z:27:TYR:N	2.70	0.59
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.33	0.59
23:B:1018:CLA:HHD	23:B:1018:CLA:HBC3	1.85	0.59
2:B:18:ARG:NH2	2:B:115:TRP:NE1	2.51	0.59
2:B:6:TYR:OH	30:L:1061:MGE:H2D	2.01	0.59
23:C:1025:CLA:H171	23:C:1031:CLA:H102	1.83	0.59
26:C:1052:BCR:HC8	26:C:1052:BCR:C33	2.31	0.59
3:C:65:GLY:HA3	3:C:119:LEU:HB2	1.85	0.59
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.83	0.59
29:B:1058:DGD:O2D	4:D:87:HIS:HB2	2.02	0.59
8:I:31:ASN:HB2	8:I:32:PRO:CD	2.31	0.59
16:V:58:LEU:O	16:V:61:TYR:N	2.36	0.59
18:Y:43:ARG:CD	18:Y:44:GLY:N	2.63	0.59
23:A:1003:CLA:HAB	23:D:1004:CLA:NB	2.18	0.59
23:B:1011:CLA:C4D	23:B:1013:CLA:C2	2.80	0.59
23:B:1011:CLA:C2	23:B:1013:CLA:H92	2.21	0.59
23:C:1035:CLA:H91	26:C:1052:BCR:H402	1.81	0.59
23:C:1028:CLA:H61	29:C:1057:DGD:HA42	1.84	0.59
3:C:43:ILE:HG23	3:C:43:ILE:O	2.03	0.59
24:D:1039:PHO:HMA1	23:D:1004:CLA:H102	1.84	0.59
25:A:1043:PQ9:H452	30:D:1059:MGE:C9A	2.33	0.59
6:F:15:ILE:HG13	6:F:16:PHE:CD1	2.30	0.59
10:K:28:ILE:HG13	26:K:1051:BCR:C31	2.33	0.59
13:O:72:GLN:HA	13:O:103:SER:OG	2.02	0.59
14:T:4:ILE:CD1	14:T:5:THR:N	2.61	0.59
20:Z:27:TYR:HD2	20:Z:27:TYR:H	1.49	0.59
1:A:133:LEU:O	1:A:137:LEU:HB2	2.03	0.59
23:B:1015:CLA:C12	23:B:1015:CLA:H91	2.33	0.59
23:B:1021:CLA:CMD	23:B:1022:CLA:HBB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:CD	2:B:128:THR:HG23	2.32	0.59
2:B:97:ALA:C	2:B:99:ALA:N	2.54	0.59
23:C:1027:CLA:O2A	23:C:1027:CLA:H3A	2.03	0.59
26:C:1052:BCR:H341	26:K:1051:BCR:HC21	1.84	0.59
3:C:266:TRP:HE3	3:C:271:TYR:OH	1.85	0.59
3:C:430:HIS:HD1	3:C:430:HIS:H	1.51	0.59
4:D:198:MET:HA	23:D:1005:CLA:OBD	2.03	0.59
1:A:243:GLU:HB3	4:D:240:ALA:HB1	1.85	0.59
4:D:72:ASN:O	4:D:76:VAL:HG22	2.03	0.59
7:H:30:LEU:C	7:H:33:VAL:HG22	2.24	0.59
7:H:63:LYS:O	7:H:64:ALA:HB2	2.03	0.59
16:V:105:PRO:HG3	16:V:115:ALA:HA	1.83	0.59
16:V:149:PRO:HB3	16:V:156:TRP:HD1	1.67	0.59
1:A:119:PHE:CD2	1:A:119:PHE:C	2.76	0.58
1:A:190:HIS:HE1	1:A:296:ASN:HD22	1.50	0.58
23:B:1021:CLA:HED3	23:B:1021:CLA:CGA	2.32	0.58
23:C:1025:CLA:C1	23:C:1025:CLA:C3A	2.81	0.58
3:C:60:ILE:HG13	23:C:1027:CLA:HMD1	1.84	0.58
23:C:1029:CLA:H51	23:C:1029:CLA:CHC	2.18	0.58
1:A:151:LEU:HD21	29:C:1055:DGD:HBS2	1.83	0.58
3:C:131:TYR:O	3:C:133:ALA:N	2.36	0.58
3:C:225:VAL:HG23	3:C:226:SER:N	2.19	0.58
3:C:371:GLY:O	13:O:33:TYR:HB2	2.03	0.58
3:C:458:GLY:HA3	4:D:224:GLN:HB2	1.84	0.58
3:C:458:GLY:CA	4:D:224:GLN:HB2	2.33	0.58
4:D:251:ARG:HH22	4:D:255:GLN:HE22	1.49	0.58
13:O:105:ASP:OD1	13:O:106:GLN:N	2.36	0.58
13:O:196:SER:O	13:O:198:ILE:HG22	2.03	0.58
1:A:142:TRP:HB3	3:C:443:TRP:CZ3	2.38	0.58
1:A:142:TRP:HZ2	4:D:219:GLU:HG3	1.67	0.58
1:A:149:ALA:HB1	1:A:283:VAL:HG12	1.85	0.58
2:B:65:PHE:HE2	23:B:1012:CLA:CMA	1.97	0.58
2:B:113:TRP:O	2:B:115:TRP:N	2.36	0.58
2:B:59:GLY:CA	2:B:329:PRO:HB3	2.29	0.58
23:C:1027:CLA:HMB2	23:C:1027:CLA:C5	2.33	0.58
23:H:1017:CLA:H3A	23:H:1017:CLA:O1A	2.02	0.58
8:I:21:PHE:CD1	8:I:24:LEU:HD12	2.37	0.58
14:T:18:PHE:HD1	26:T:6046:BCR:C33	2.16	0.58
23:B:1018:CLA:H102	23:B:1023:CLA:HBA2	1.85	0.58
23:B:1023:CLA:C3C	23:B:1024:CLA:HBC1	2.33	0.58
2:B:3:LEU:HD22	11:L:8:GLN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:GLY:O	3:C:174:LEU:N	2.36	0.58
23:B:1016:CLA:C2	23:H:1017:CLA:H91	2.31	0.58
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.34	0.58
13:O:77:LEU:CD2	13:O:93:PRO:HA	2.33	0.58
18:Y:43:ARG:O	18:Y:44:GLY:O	2.21	0.58
23:A:1003:CLA:HMC2	23:D:1004:CLA:CMC	2.33	0.58
1:A:275:LEU:HB2	4:D:215:GLY:HA3	1.85	0.58
1:A:30:VAL:O	1:A:30:VAL:HG22	2.02	0.58
2:B:92:SER:O	2:B:95:GLY:N	2.36	0.58
29:C:1057:DGD:HBG3	29:C:1057:DGD:CEB	2.21	0.58
3:C:322:GLN:NE2	3:C:381:LYS:HA	2.18	0.58
3:C:87:ILE:HG22	3:C:426:LEU:HD11	1.83	0.58
4:D:152:VAL:HG21	4:D:279:LEU:HD22	1.86	0.58
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.38	0.58
1:A:183:MET:HB3	23:A:1003:CLA:CB	2.27	0.58
2:B:111:ALA:C	2:B:113:TRP:H	2.07	0.58
2:B:150:CYS:HB2	23:B:1011:CLA:HMC3	1.85	0.58
2:B:311:PHE:CE2	2:B:317:ASN:ND2	2.64	0.58
2:B:442:ILE:HD11	13:O:200:LEU:CD2	2.33	0.58
2:B:55:MET:HE3	2:B:80:ILE:CG2	2.30	0.58
23:C:1036:CLA:HED2	23:C:1037:CLA:HBB2	1.84	0.58
3:C:128:GLY:HA3	23:C:1037:CLA:CAC	2.33	0.58
3:C:289:PHE:HD2	3:C:289:PHE:O	1.87	0.58
4:D:110:LEU:O	4:D:113:PHE:HB3	2.04	0.58
4:D:33:SER:O	4:D:35:ILE:N	2.36	0.58
4:D:53:THR:HA	4:D:67:TYR:HD2	1.69	0.58
2:B:191:ASN:HD22	7:H:60:VAL:HG12	1.67	0.58
10:K:24:VAL:O	10:K:27:VAL:HG23	2.03	0.58
13:O:172:PHE:HB2	13:O:221:GLY:CA	2.33	0.58
13:O:79:LYS:HE2	13:O:89:ALA:CB	2.33	0.58
18:Y:39:LEU:HD21	20:Z:28:ALA:HB3	1.86	0.58
3:C:121:SER:O	3:C:125:LEU:HD12	2.04	0.58
3:C:193:GLY:O	3:C:194:GLY:C	2.40	0.58
23:D:1004:CLA:C14	23:D:1004:CLA:H102	2.34	0.58
24:D:1039:PHO:HBA2	24:D:1039:PHO:HMA3	0.68	0.58
1:A:213:ALA:HB2	4:D:275:PRO:HG2	1.85	0.58
5:E:57:ALA:HB3	5:E:60:GLN:CG	2.33	0.58
7:H:28:THR:HB	7:H:29:PRO:HD3	1.85	0.58
5:E:22:ILE:HG23	19:N:18:UNK:HA	1.86	0.58
1:A:121:LEU:O	1:A:123:ALA:N	2.36	0.58
23:B:1010:CLA:C2D	23:B:1011:CLA:HMB1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1025:CLA:C4	23:C:1025:CLA:C1B	2.77	0.58
23:C:1025:CLA:H143	26:C:1054:BCR:C35	2.33	0.58
26:C:1054:BCR:C31	26:C:1054:BCR:C8	2.80	0.58
3:C:143:TYR:O	3:C:143:TYR:CD1	2.57	0.58
3:C:42:LEU:HD12	3:C:48:LYS:HG2	1.85	0.58
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.85	0.58
4:D:330:ALA:N	4:D:331:PRO:HD2	2.19	0.58
13:O:155:THR:HG22	13:O:167:ASP:O	2.03	0.58
26:T:6048:BCR:C33	26:T:6048:BCR:C8	2.81	0.58
16:V:62:ALA:O	31:V:1041:HEM:HBB1	2.04	0.58
23:B:1022:CLA:CHA	23:B:1022:CLA:O2A	2.52	0.58
3:C:33:PHE:N	3:C:33:PHE:CD1	2.71	0.58
23:D:1004:CLA:H201	30:D:1059:MGE:C8A	2.32	0.58
5:E:28:PRO:O	5:E:32:ILE:HB	2.04	0.58
5:E:47:PHE:C	5:E:49:THR:H	2.07	0.58
20:Z:36:SER:HA	20:Z:39:LEU:HG	1.85	0.58
24:A:1038:PHO:CBC	24:A:1038:PHO:CHD	2.81	0.58
1:A:289:GLY:O	1:A:293:MET:HE2	2.03	0.58
2:B:153:PHE:CD1	2:B:157:HIS:HB3	2.39	0.58
2:B:193:TYR:O	2:B:261:ALA:HB2	2.03	0.58
23:C:1036:CLA:CBB	23:C:1036:CLA:HHC	2.29	0.58
3:C:239:TRP:O	3:C:243:ILE:HG13	2.04	0.58
3:C:33:PHE:CE2	3:C:40:ALA:HB1	2.39	0.58
4:D:106:GLN:C	4:D:108:GLY:H	2.07	0.58
4:D:18:LEU:HD23	4:D:32:TRP:HH2	1.68	0.58
4:D:72:ASN:H	4:D:75:THR:HB	1.68	0.58
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.72	0.58
13:O:120:THR:HG23	13:O:154:SER:OG	2.03	0.58
15:U:68:THR:HG22	15:U:71:GLN:HB2	1.85	0.58
1:A:309:ALA:CB	16:V:28:GLU:HB2	2.34	0.58
24:A:1038:PHO:HED2	4:D:213:ILE:HD13	1.86	0.58
1:A:202:VAL:HG11	23:A:1006:CLA:CAD	2.33	0.58
1:A:325:ASN:HD22	1:A:328:MET:CE	2.14	0.58
23:C:1027:CLA:H121	23:C:1027:CLA:H18	1.84	0.58
3:C:143:TYR:O	3:C:143:TYR:HD1	1.86	0.58
3:C:223:TRP:CD1	3:C:224:ILE:CD1	2.87	0.58
3:C:287:THR:OG1	3:C:430:HIS:HB2	2.04	0.58
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.85	0.58
4:D:222:LEU:HD21	4:D:243:THR:OG1	2.04	0.58
10:K:28:ILE:O	10:K:31:LEU:HB2	2.04	0.58
10:K:28:ILE:HA	10:K:31:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:194:TYR:O	13:O:195:ASP:HB3	2.03	0.58
13:O:172:PHE:HB2	13:O:221:GLY:HA3	1.85	0.58
15:U:52:ASN:O	15:U:53:ALA:O	2.22	0.58
15:U:75:LEU:HD12	15:U:75:LEU:H	1.69	0.58
16:V:81:ARG:HG3	16:V:157:GLY:CA	2.33	0.58
1:A:197:PHE:CE1	1:A:285:PHE:HD2	2.18	0.57
1:A:94:TYR:OH	1:A:104:GLU:HG2	2.04	0.57
23:B:1012:CLA:CMD	23:B:1020:CLA:C20	2.78	0.57
2:B:179:GLN:HB3	2:B:180:PRO:HD2	1.86	0.57
2:B:284:ILE:CG2	2:B:305:ILE:HD13	2.34	0.57
23:C:1028:CLA:C2	29:C:1056:DGD:O1A	2.46	0.57
23:D:1004:CLA:HAA2	23:D:1004:CLA:HBD	1.86	0.57
9:J:7:ARG:HG2	9:J:7:ARG:HH11	1.69	0.57
1:A:78:ILE:HA	1:A:176:ILE:HD12	1.86	0.57
1:A:259:ILE:HG23	4:D:128:ARG:NH1	2.18	0.57
1:A:45:THR:HG23	1:A:46:ILE:H	1.68	0.57
23:B:1016:CLA:H193	23:H:1017:CLA:C19	2.15	0.57
2:B:25:MET:C	2:B:27:THR:H	2.06	0.57
23:C:1029:CLA:C3	23:C:1029:CLA:C1C	2.82	0.57
3:C:167:VAL:HG12	3:C:168:LEU:N	2.17	0.57
3:C:369:LEU:HD11	3:C:384:ILE:HG13	1.86	0.57
24:D:1039:PHO:HMC3	23:D:1004:CLA:O1A	2.04	0.57
8:I:13:THR:O	8:I:14:PHE:C	2.43	0.57
2:B:2:GLY:C	11:L:11:GLU:HB2	2.25	0.57
15:U:58:VAL:O	15:U:61:VAL:HG23	2.03	0.57
17:X:43:ILE:CG2	17:X:43:ILE:O	2.52	0.57
1:A:256:GLY:O	1:A:261:GLN:N	2.36	0.57
23:B:1009:CLA:O1A	23:B:1009:CLA:C4D	2.53	0.57
2:B:229:LEU:O	2:B:231:MET:N	2.37	0.57
2:B:226:TYR:HA	2:B:231:MET:SD	2.45	0.57
23:C:1031:CLA:CAD	23:C:1033:CLA:H161	2.34	0.57
1:A:279:ARG:HG2	4:D:212:ALA:HB2	1.86	0.57
4:D:266:TRP:CD1	30:D:1062:MGE:H2D	2.39	0.57
12:M:19:SER:O	12:M:23:ILE:HG12	2.04	0.57
15:U:69:GLU:HA	15:U:72:LYS:HE3	1.86	0.57
15:U:61:VAL:CG1	15:U:75:LEU:HD23	2.32	0.57
16:V:38:LEU:CA	16:V:95:ILE:HG22	2.28	0.57
26:Z:1053:BCR:C38	26:Z:1053:BCR:C23	2.59	0.57
1:A:114:LEU:HD22	23:A:1007:CLA:HED3	1.86	0.57
1:A:192:ILE:CD1	1:A:198:HIS:HB2	2.34	0.57
1:A:32:TRP:O	1:A:35:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1010:CLA:H11	23:B:1010:CLA:HBD	1.81	0.57
23:B:1012:CLA:HAA1	23:B:1012:CLA:HBD	1.86	0.57
2:B:24:LEU:HD21	2:B:110:ALA:C	2.25	0.57
2:B:52:LEU:HD11	2:B:339:ALA:HA	1.85	0.57
4:D:193:LEU:HD23	4:D:193:LEU:O	2.04	0.57
4:D:89:LEU:HB2	4:D:91:LEU:CD1	2.35	0.57
31:F:1040:HEM:HMB2	31:F:1040:HEM:CBB	2.32	0.57
16:V:109:ASP:HB3	16:V:111:GLU:HB2	1.85	0.57
2:B:20:ILE:O	2:B:24:LEU:HB2	2.05	0.57
2:B:9:HIS:CG	23:B:1020:CLA:HBB2	2.40	0.57
23:C:1029:CLA:CGA	23:C:1029:CLA:CHA	2.83	0.57
3:C:278:ALA:O	3:C:282:MET:HB2	2.03	0.57
4:D:110:LEU:HD12	4:D:110:LEU:H	1.70	0.57
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.86	0.57
1:A:184:ILE:CG1	4:D:186:GLN:NE2	2.66	0.57
3:C:465:PRO:HG2	8:I:32:PRO:HB3	1.87	0.57
23:C:1032:CLA:H2	23:K:1034:CLA:CMB	2.35	0.57
15:U:59:GLU:C	15:U:61:VAL:N	2.58	0.57
23:B:1012:CLA:HMB3	23:B:1015:CLA:HBB1	1.85	0.57
23:B:1023:CLA:CED	23:B:1024:CLA:HBB2	2.32	0.57
5:E:20:TRP:HZ2	9:J:13:VAL:CG2	2.14	0.57
16:V:38:LEU:CB	16:V:45:ILE:HD11	2.33	0.57
1:A:288:LEU:HD22	3:C:432:VAL:HG23	1.87	0.57
26:B:1047:BCR:H403	26:B:1047:BCR:C22	2.34	0.57
2:B:144:PHE:O	2:B:148:LEU:HB2	2.04	0.57
2:B:402:TYR:N	2:B:402:TYR:CD1	2.73	0.57
23:C:1026:CLA:C1B	23:C:1028:CLA:HBB2	2.35	0.57
3:C:160:ILE:HG21	23:C:1033:CLA:H202	1.85	0.57
3:C:299:SER:O	3:C:302:TYR:O	2.23	0.57
3:C:438:LEU:HD13	3:C:438:LEU:C	2.24	0.57
24:D:1039:PHO:O2A	24:D:1039:PHO:C4	2.53	0.57
18:Y:39:LEU:CD2	20:Z:28:ALA:CB	2.83	0.57
1:A:259:ILE:HG23	4:D:128:ARG:HH12	1.70	0.57
3:C:146:PHE:CZ	23:C:1037:CLA:HMA1	2.40	0.57
3:C:327:ASN:HD21	3:C:330:SER:C	2.08	0.57
3:C:377:LEU:C	3:C:377:LEU:HD13	2.24	0.57
4:D:188:PHE:HE2	4:D:326:ARG:HA	1.70	0.57
9:J:10:LEU:O	9:J:13:VAL:HG12	2.05	0.57
11:L:29:LEU:HB2	14:T:9:ILE:CG2	2.29	0.57
16:V:117:VAL:O	16:V:117:VAL:HG12	2.05	0.57
16:V:38:LEU:HD12	16:V:95:ILE:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASP:CB	2:B:171:PRO:HD2	2.32	0.57
2:B:208:VAL:HG21	23:B:1010:CLA:HMC1	1.86	0.57
29:C:1056:DGD:HBF1	29:C:1056:DGD:CAB	2.30	0.57
4:D:17:ILE:HD12	17:X:41:SER:OG	2.04	0.57
4:D:66:SER:HB3	4:D:69:GLU:HG3	1.87	0.57
8:I:24:LEU:O	8:I:26:GLY:N	2.37	0.57
15:U:43:PRO:HG3	16:V:108:TYR:C	2.25	0.57
1:A:320:ILE:O	1:A:321:ILE:C	2.43	0.57
1:A:59:ASP:O	1:A:60:ILE:C	2.43	0.57
2:B:3:LEU:HD22	11:L:8:GLN:CB	2.34	0.57
23:C:1032:CLA:HAB	23:K:1034:CLA:HMC1	1.76	0.57
3:C:307:PRO:HB3	3:C:358:PHE:HB3	1.87	0.57
3:C:75:PHE:CZ	3:C:105:VAL:HG11	2.37	0.57
1:A:279:ARG:CB	4:D:212:ALA:HB2	2.31	0.57
1:A:63:ILE:HD13	1:A:63:ILE:H	1.69	0.56
2:B:251:VAL:HG13	23:B:1010:CLA:H2	1.86	0.56
2:B:258:TYR:CE2	29:B:1058:DGD:HG32	2.40	0.56
2:B:390:TYR:CD1	2:B:390:TYR:N	2.73	0.56
3:C:155:ASN:HA	3:C:158:THR:CG2	2.29	0.56
25:D:1042:PQ9:H241	25:D:1042:PQ9:C28	2.35	0.56
6:F:45:ARG:HE	6:F:45:ARG:CA	1.97	0.56
13:O:172:PHE:CZ	13:O:223:ILE:HG23	2.40	0.56
1:A:104:GLU:OE1	13:O:99:ARG:HD2	2.04	0.56
15:U:78:ASN:HB3	15:U:82:PHE:CE2	2.40	0.56
16:V:38:LEU:HB2	16:V:45:ILE:CG1	2.34	0.56
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.40	0.56
23:B:1023:CLA:ND	23:B:1024:CLA:CMC	2.69	0.56
23:B:1019:CLA:H91	30:B:1060:MGE:H112	1.86	0.56
1:A:200:LEU:HD23	29:C:1057:DGD:HBW2	1.86	0.56
3:C:40:ALA:O	3:C:43:ILE:HG22	2.05	0.56
4:D:326:ARG:HH11	4:D:326:ARG:HG3	1.70	0.56
23:C:1035:CLA:HBB2	23:K:1034:CLA:HMA2	1.86	0.56
2:B:327:THR:HG23	11:L:37:ASN:HD22	1.69	0.56
11:L:4:ASN:HD21	11:L:6:ASN:HD22	1.53	0.56
18:Y:45:ASN:ND2	18:Y:45:ASN:C	2.59	0.56
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.05	0.56
20:Z:44:SER:O	20:Z:48:ILE:HD13	2.05	0.56
1:A:119:PHE:CE2	1:A:123:ALA:HB2	2.40	0.56
1:A:123:ALA:O	1:A:126:TYR:HB3	2.06	0.56
2:B:389:LYS:HB3	2:B:390:TYR:CD1	2.40	0.56
23:C:1029:CLA:HBB1	23:C:1029:CLA:CHC	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ARG:HB2	20:Z:27:TYR:CD1	2.41	0.56
3:C:33:PHE:N	3:C:33:PHE:HD1	2.04	0.56
4:D:185:PHE:CE1	4:D:289:LEU:HD13	2.40	0.56
4:D:186:GLN:N	23:D:1004:CLA:HBC1	2.21	0.56
4:D:251:ARG:HB3	4:D:251:ARG:NH1	2.20	0.56
6:F:37:ILE:HA	6:F:40:MET:CE	2.36	0.56
7:H:30:LEU:HD12	7:H:33:VAL:CG2	2.35	0.56
7:H:50:ASN:O	7:H:50:ASN:ND2	2.39	0.56
23:K:1034:CLA:O1D	23:K:1034:CLA:CAA	2.30	0.56
13:O:82:PRO:HG2	13:O:89:ALA:HB2	1.86	0.56
23:B:1016:CLA:O1D	23:B:1016:CLA:H2A	2.06	0.56
2:B:30:VAL:HG13	23:B:1013:CLA:HMD3	1.86	0.56
23:C:1031:CLA:HBD	23:C:1031:CLA:HAA2	1.88	0.56
3:C:156:LYS:O	3:C:160:ILE:HD13	2.06	0.56
5:E:27:ILE:CB	5:E:28:PRO:HD3	2.35	0.56
26:H:1049:BCR:H401	17:X:20:PHE:CZ	2.41	0.56
8:I:10:ILE:HD13	8:I:10:ILE:H	1.70	0.56
13:O:73:PRO:HA	13:O:263:GLY:HA3	1.87	0.56
13:O:39:THR:OG1	13:O:41:LEU:HB2	2.05	0.56
1:A:171:GLY:O	1:A:172:MET:C	2.44	0.56
2:B:190:PHE:CE1	23:B:1009:CLA:HMA3	2.40	0.56
23:C:1026:CLA:HAA1	23:C:1026:CLA:HBD	1.87	0.56
3:C:437:PHE:HA	23:C:1032:CLA:HMC3	1.85	0.56
23:C:1031:CLA:HMD1	23:C:1033:CLA:H161	1.87	0.56
3:C:266:TRP:CD1	3:C:266:TRP:N	2.73	0.56
23:D:1004:CLA:CBB	23:D:1004:CLA:HHC	2.21	0.56
4:D:261:PHE:CE1	4:D:267:LEU:HG	2.41	0.56
4:D:29:PHE:HE2	4:D:31:GLY:HA3	1.69	0.56
23:C:1035:CLA:HMC3	23:K:1034:CLA:HMB2	1.86	0.56
2:B:5:TRP:CE2	30:L:1061:MGE:H2A2	2.40	0.56
13:O:69:LEU:HG	13:O:107:ILE:HD12	1.87	0.56
13:O:231:ASP:OD1	13:O:234:THR:HG23	2.06	0.56
1:A:94:TYR:HE2	13:O:99:ARG:NE	2.04	0.56
16:V:45:ILE:H	16:V:45:ILE:CD1	2.06	0.56
10:K:20:PRO:HB3	18:Y:21:GLN:HA	1.87	0.56
20:Z:5:PHE:CD1	20:Z:57:LEU:HB3	2.41	0.56
1:A:140:ARG:HH21	27:A:1063:LHG:C3	2.19	0.56
23:B:1016:CLA:HMA1	4:D:130:PHE:CE1	2.40	0.56
2:B:317:ASN:HA	2:B:330:MET:CE	2.36	0.56
2:B:96:VAL:O	2:B:99:ALA:HB3	2.04	0.56
23:C:1029:CLA:H12	26:C:1054:BCR:H323	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:ILE:O	3:C:249:ILE:HD13	2.05	0.56
3:C:350:ILE:HG21	3:C:359:TRP:CB	2.28	0.56
3:C:377:LEU:O	3:C:377:LEU:HD13	2.05	0.56
3:C:48:LYS:HD2	23:C:1035:CLA:CED	2.33	0.56
23:D:1005:CLA:H92	23:D:1005:CLA:C12	2.28	0.56
23:B:1011:CLA:H202	7:H:38:PHE:CE2	2.41	0.56
7:H:38:PHE:HB2	26:H:1049:BCR:C10	2.34	0.56
16:V:102:MET:SD	16:V:138:LEU:HD22	2.45	0.56
1:A:199:GLN:NE2	23:A:1006:CLA:O1D	2.39	0.56
1:A:142:TRP:HH2	27:A:1063:LHG:HC5	1.71	0.56
23:B:1021:CLA:HMA3	23:B:1021:CLA:H2	1.87	0.56
23:C:1025:CLA:CGA	23:C:1025:CLA:H3A	2.28	0.56
23:C:1026:CLA:HBB2	23:K:1034:CLA:C1	2.36	0.56
23:C:1031:CLA:OBD	23:C:1033:CLA:C16	2.48	0.56
3:C:286:ALA:O	3:C:289:PHE:N	2.34	0.56
3:C:334:PRO:CA	13:O:179:THR:OG1	2.53	0.56
7:H:43:LEU:HD23	7:H:43:LEU:C	2.26	0.56
15:U:16:LYS:HA	15:U:19:THR:HG23	1.88	0.56
16:V:87:LEU:HB2	16:V:108:TYR:OH	2.06	0.56
10:K:21:LEU:HD21	18:Y:24:MET:HG2	1.86	0.56
18:Y:43:ARG:NH2	18:Y:44:GLY:N	2.53	0.56
23:A:1007:CLA:H142	8:I:13:THR:CG2	2.36	0.56
1:A:64:ARG:NH2	13:O:98:THR:HG21	2.21	0.56
23:B:1011:CLA:CMD	23:B:1014:CLA:CAB	2.83	0.56
29:B:1058:DGD:HE5	29:B:1058:DGD:C6D	2.35	0.56
4:D:282:SER:C	23:D:1004:CLA:CED	2.74	0.56
4:D:55:VAL:HG22	4:D:105:CYS:SG	2.45	0.56
6:F:29:PRO:O	6:F:32:PHE:N	2.39	0.56
13:O:221:GLY:O	13:O:222:GLN:HB2	2.05	0.56
13:O:59:ASP:O	13:O:60:SER:CB	2.54	0.56
13:O:70:CYS:SG	13:O:105:ASP:HB3	2.46	0.56
13:O:69:LEU:HD11	13:O:71:LEU:HD21	1.88	0.56
16:V:39:ASN:C	16:V:41:GLU:H	2.09	0.56
1:A:110:GLY:N	1:A:111:PRO:HD2	2.20	0.56
23:B:1023:CLA:HMC1	23:B:1023:CLA:CBC	2.30	0.56
23:B:1023:CLA:H41	26:B:1048:BCR:H343	1.87	0.56
2:B:74:SER:HB3	2:B:78:TRP:CE2	2.41	0.56
3:C:147:PHE:O	3:C:156:LYS:HD2	2.06	0.56
4:D:58:TRP:CZ3	5:E:55:TYR:HB3	2.41	0.56
15:U:21:TYR:HE2	15:U:30:THR:HG1	1.51	0.56
16:V:134:THR:H	16:V:137:ASP:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:159:GLY:HA2	16:V:163:TYR:CE1	2.41	0.56
18:Y:43:ARG:HD2	18:Y:44:GLY:N	2.19	0.56
1:A:258:LEU:O	1:A:259:ILE:CD1	2.54	0.56
23:B:1016:CLA:HAA1	23:B:1016:CLA:HBD	1.86	0.56
23:C:1033:CLA:C17	23:C:1033:CLA:C14	2.68	0.56
3:C:248:GLY:O	3:C:252:ILE:HB	2.06	0.56
3:C:271:TYR:CE1	23:C:1031:CLA:CAC	2.83	0.56
3:C:276:LEU:HG	23:C:1032:CLA:HBB1	1.88	0.56
1:A:323:ARG:HG3	4:D:329:MET:HA	1.88	0.56
2:B:380:ASP:OD1	4:D:344:GLU:HG3	2.06	0.56
13:O:168:PHE:N	13:O:225:LEU:O	2.37	0.56
16:V:38:LEU:HD12	16:V:95:ILE:HG21	1.87	0.56
1:A:143:ILE:HG23	1:A:144:CYS:N	2.21	0.56
2:B:250:PHE:HB3	29:B:1058:DGD:C8B	2.36	0.56
2:B:446:SER:O	2:B:449:GLY:N	2.38	0.56
3:C:36:TRP:CE3	3:C:37:ALA:HB2	2.41	0.56
1:A:110:GLY:N	1:A:111:PRO:CD	2.69	0.55
1:A:111:PRO:HG2	1:A:112:TYR:H	1.71	0.55
1:A:151:LEU:HD11	1:A:155:PHE:HE2	1.71	0.55
2:B:6:TYR:HA	23:B:1019:CLA:O2A	2.06	0.55
2:B:97:ALA:O	2:B:101:ILE:HG12	2.07	0.55
2:B:107:LEU:O	2:B:111:ALA:HB2	2.06	0.55
2:B:332:LYS:HG2	2:B:439:SER:HA	1.87	0.55
3:C:199:ILE:CG2	3:C:234:VAL:HG11	2.33	0.55
4:D:261:PHE:CE2	4:D:267:LEU:CA	2.89	0.55
4:D:274:VAL:CB	4:D:275:PRO:HD3	2.30	0.55
18:Y:25:ILE:CG1	18:Y:26:ALA:N	2.69	0.55
20:Z:50:LEU:O	20:Z:54:VAL:HG23	2.05	0.55
27:A:1063:LHG:H321	23:K:1034:CLA:H172	1.88	0.55
2:B:103:LEU:HD21	23:B:1013:CLA:CMC	2.35	0.55
4:D:301:GLN:NE2	4:D:313:THR:HG21	2.20	0.55
4:D:342:PRO:O	4:D:345:VAL:HG23	2.06	0.55
5:E:78:THR:O	5:E:82:GLN:HG2	2.05	0.55
7:H:31:MET:HB2	23:H:1017:CLA:CAD	2.35	0.55
29:B:1058:DGD:HA31	7:H:46:LEU:HD21	1.88	0.55
13:O:41:LEU:HD22	13:O:44:LYS:HD2	1.86	0.55
23:A:1006:CLA:HBD	23:A:1006:CLA:HAA1	1.88	0.55
1:A:202:VAL:HA	1:A:205:VAL:CG1	2.36	0.55
2:B:122:LEU:HD23	7:H:8:GLY:HA2	1.86	0.55
2:B:267:LEU:C	2:B:268:PHE:HD1	2.10	0.55
4:D:33:SER:OG	4:D:128:ARG:CG	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:273:PHE:O	4:D:274:VAL:C	2.42	0.55
2:B:221:PRO:HA	23:H:1017:CLA:HED3	1.88	0.55
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.40	0.55
8:I:30:ARG:HH11	8:I:30:ARG:HG3	1.72	0.55
26:K:1051:BCR:H331	18:Y:28:ILE:HB	1.87	0.55
12:M:15:VAL:O	12:M:19:SER:HB2	2.07	0.55
13:O:91:PHE:CE1	13:O:260:LYS:HE3	2.41	0.55
23:A:1003:CLA:HMC2	23:D:1004:CLA:HMC2	1.87	0.55
1:A:116:ILE:HD11	1:A:158:PHE:O	2.06	0.55
23:B:1020:CLA:H42	23:B:1020:CLA:O2A	2.06	0.55
23:B:1021:CLA:HMD2	23:B:1022:CLA:HBB2	1.89	0.55
2:B:278:SER:CB	2:B:281:GLN:HG2	2.26	0.55
2:B:83:GLU:CG	2:B:86:ILE:HD11	2.31	0.55
3:C:107:ASP:O	3:C:110:PRO:HD2	2.06	0.55
3:C:171:GLY:HA2	3:C:174:LEU:CB	2.22	0.55
3:C:291:TRP:HD1	3:C:292:PHE:CE2	2.25	0.55
3:C:425:TRP:O	3:C:428:THR:HG22	2.06	0.55
1:A:214:MET:HE3	24:D:1039:PHO:O1D	2.07	0.55
26:D:1050:BCR:C17	30:D:1059:MGE:H102	2.35	0.55
4:D:53:THR:HG23	4:D:67:TYR:CE2	2.41	0.55
18:Y:43:ARG:CG	18:Y:44:GLY:N	2.66	0.55
1:A:102:LEU:HD12	1:A:102:LEU:O	2.07	0.55
1:A:14:TRP:C	1:A:14:TRP:CD1	2.80	0.55
1:A:254:TYR:HD1	1:A:255:PHE:N	2.05	0.55
1:A:303:ASN:HD22	1:A:303:ASN:N	2.04	0.55
23:B:1016:CLA:HAB	4:D:123:ILE:HG23	1.86	0.55
23:C:1031:CLA:CAD	23:C:1033:CLA:H122	2.32	0.55
23:C:1037:CLA:C1B	26:Z:1053:BCR:H272	2.37	0.55
3:C:279:LEU:O	3:C:280:SER:C	2.44	0.55
3:C:431:PHE:C	3:C:431:PHE:CD2	2.79	0.55
3:C:431:PHE:O	3:C:431:PHE:HD2	1.90	0.55
4:D:188:PHE:HE2	4:D:326:ARG:CG	2.17	0.55
6:F:19:ARG:NH2	6:F:20:TRP:HD1	2.05	0.55
15:U:43:PRO:CB	16:V:109:ASP:HB2	2.35	0.55
23:A:1007:CLA:OBD	23:A:1007:CLA:CED	2.39	0.55
1:A:147:TYR:C	1:A:150:PRO:HD2	2.27	0.55
1:A:192:ILE:HG12	1:A:293:MET:CE	2.36	0.55
1:A:80:GLY:O	1:A:81:ALA:HB2	2.07	0.55
2:B:208:VAL:HG21	23:B:1010:CLA:CMC	2.37	0.55
23:B:1023:CLA:C13	23:B:1024:CLA:CMA	2.56	0.55
2:B:15:ASP:CG	2:B:15:ASP:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1031:CLA:H2	23:C:1031:CLA:CMA	2.36	0.55
3:C:127:PHE:O	3:C:130:VAL:HG12	2.07	0.55
3:C:287:THR:CG2	3:C:427:ALA:O	2.55	0.55
2:B:464:PHE:HB2	4:D:280:TRP:CH2	2.41	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.41	0.55
4:D:296:TYR:O	4:D:297:ASP:O	2.25	0.55
4:D:48:TRP:CE3	4:D:49:LEU:HG	2.42	0.55
4:D:58:TRP:C	4:D:58:TRP:CD1	2.79	0.55
13:O:167:ASP:HA	13:O:225:LEU:O	2.07	0.55
15:U:42:TYR:CB	15:U:43:PRO:CD	2.84	0.55
16:V:123:SER:HB2	16:V:126:ILE:HD11	1.89	0.55
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.42	0.55
23:B:1022:CLA:C20	23:B:1022:CLA:C1	2.85	0.55
23:B:1024:CLA:HAA2	23:B:1024:CLA:HBD	1.88	0.55
2:B:384:ARG:HD3	15:U:102:LEU:CD2	2.36	0.55
2:B:465:GLY:CA	23:B:1019:CLA:HAC1	2.37	0.55
2:B:68:ARG:HD3	23:B:1011:CLA:HED1	1.89	0.55
27:A:1063:LHG:H292	23:C:1032:CLA:C7	2.37	0.55
3:C:127:PHE:O	3:C:127:PHE:HD2	1.88	0.55
3:C:453:ALA:HB3	3:C:455:PHE:CE2	2.42	0.55
25:D:1042:PQ9:H241	25:D:1042:PQ9:C27	2.37	0.55
25:A:1043:PQ9:C45	30:D:1059:MGE:C8A	2.80	0.55
30:D:1059:MGE:CGB	30:D:1059:MGE:H211	2.37	0.55
4:D:37:LEU:HD13	4:D:125:PHE:CA	2.37	0.55
1:A:258:LEU:HA	4:D:128:ARG:NH2	2.21	0.55
4:D:74:LEU:CD2	4:D:175:VAL:HG11	2.35	0.55
26:H:1049:BCR:H23C	26:H:1049:BCR:H393	1.71	0.55
9:J:18:GLY:O	9:J:21:VAL:HG12	2.06	0.55
3:C:334:PRO:HA	13:O:179:THR:HB	1.88	0.55
17:X:29:VAL:O	17:X:33:THR:HB	2.07	0.55
23:B:1010:CLA:H112	23:B:1010:CLA:C17	2.36	0.55
2:B:149:LEU:HD13	23:B:1012:CLA:C20	2.37	0.55
23:B:1020:CLA:C1	23:B:1023:CLA:O1A	2.55	0.55
26:B:1045:BCR:C34	26:B:1047:BCR:H10C	2.36	0.55
2:B:23:HIS:HD2	23:B:1020:CLA:C4A	2.19	0.55
2:B:33:TRP:CH2	2:B:62:VAL:HG21	2.41	0.55
23:C:1025:CLA:H3A	23:C:1025:CLA:H11	1.88	0.55
23:C:1025:CLA:HMB3	26:C:1054:BCR:C26	2.37	0.55
3:C:414:ILE:HG22	3:C:415:ASN:O	2.07	0.55
4:D:210:LEU:HD23	4:D:274:VAL:HG21	1.89	0.55
10:K:40:GLN:HA	10:K:40:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:GLY:HA2	13:O:33:TYR:HD1	1.72	0.55
11:L:25:LEU:HB3	14:T:13:ILE:CG1	2.37	0.55
15:U:84:VAL:HG12	15:U:85:THR:N	2.21	0.55
1:A:40:THR:N	23:A:1007:CLA:HBB1	2.21	0.55
26:B:1048:BCR:C22	26:B:1048:BCR:H392	2.35	0.55
2:B:181:VAL:HB	2:B:199:VAL:HG21	1.88	0.55
2:B:5:TRP:HE3	23:B:1019:CLA:H42	1.72	0.55
3:C:56:HIS:HB2	3:C:59:LEU:HD13	1.89	0.55
1:A:332:HIS:HA	28:D:1064:IOD:I	2.76	0.55
13:O:241:PHE:HD2	13:O:265:PHE:HB3	1.72	0.55
23:B:1014:CLA:C4	23:B:1014:CLA:H71	2.34	0.55
23:B:1020:CLA:H111	23:B:1021:CLA:HAB	1.89	0.55
23:B:1022:CLA:HMD2	23:B:1022:CLA:H202	1.89	0.55
2:B:153:PHE:HB2	23:B:1014:CLA:HMC3	1.88	0.55
2:B:400:SER:CB	2:B:410:THR:HG22	2.38	0.55
23:C:1033:CLA:HMA3	23:K:1034:CLA:HMC2	1.87	0.55
3:C:285:ILE:O	3:C:289:PHE:HB2	2.07	0.55
3:C:343:ARG:CG	3:C:348:GLU:O	2.55	0.55
3:C:346:THR:HB	13:O:38:GLY:CA	2.37	0.55
1:A:322:ASN:HD21	3:C:412:THR:HA	1.72	0.55
4:D:250:ASN:ND2	14:T:27:PRO:HG3	2.22	0.55
4:D:352:LEU:N	4:D:352:LEU:CD2	2.69	0.55
7:H:17:GLU:HB2	7:H:20:LYS:HD3	1.89	0.55
23:C:1032:CLA:CAB	23:K:1034:CLA:CMC	2.53	0.55
10:K:29:PRO:C	23:K:1034:CLA:O1D	2.45	0.55
10:K:24:VAL:HG21	18:Y:25:ILE:CG2	2.26	0.55
11:L:15:THR:O	11:L:18:TYR:N	2.40	0.55
24:A:1038:PHO:H93	23:D:1005:CLA:C18	2.28	0.54
1:A:130:GLN:HG2	1:A:144:CYS:HA	1.89	0.54
1:A:193:LEU:HD11	4:D:182:LEU:HD12	1.89	0.54
1:A:197:PHE:CD1	1:A:285:PHE:HB3	2.41	0.54
1:A:331:MET:O	1:A:332:HIS:C	2.44	0.54
23:B:1012:CLA:CHD	23:B:1012:CLA:HBC3	2.33	0.54
23:B:1019:CLA:HHC	23:B:1019:CLA:CBB	2.34	0.54
2:B:248:ALA:HA	23:B:1011:CLA:H51	1.90	0.54
3:C:199:ILE:N	3:C:199:ILE:HD12	2.21	0.54
3:C:257:PHE:N	3:C:257:PHE:CD1	2.73	0.54
3:C:451:ALA:N	3:C:456:GLU:HG2	2.22	0.54
23:D:1008:CLA:HAA1	23:D:1008:CLA:HBD	1.88	0.54
4:D:43:LEU:HD12	4:D:117:HIS:CE1	2.43	0.54
4:D:14:TRP:CD1	4:D:15:PHE:N	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:HIS:HA	4:D:217:THR:HG22	1.88	0.54
13:O:242:GLU:HA	13:O:261:ILE:O	2.08	0.54
15:U:28:ASN:HD22	15:U:54:PRO:CB	2.18	0.54
16:V:56:LYS:HA	16:V:144:HIS:CE1	2.41	0.54
1:A:272:HIS:CD2	4:D:218:VAL:CG2	2.86	0.54
1:A:93:PHE:O	1:A:95:PRO:CD	2.55	0.54
2:B:220:ARG:HD3	2:B:221:PRO:CD	2.29	0.54
2:B:346:PHE:CE1	2:B:421:ALA:HB2	2.43	0.54
23:C:1031:CLA:H142	26:C:1054:BCR:C36	2.37	0.54
3:C:332:GLN:HE22	13:O:175:PRO:HG3	1.71	0.54
1:A:172:MET:SD	23:D:1005:CLA:HMC3	2.47	0.54
6:F:42:PHE:O	6:F:44:GLN:N	2.40	0.54
7:H:6:TRP:NE1	7:H:10:ILE:HD11	2.21	0.54
8:I:27:ASP:N	8:I:28:PRO:HD3	2.23	0.54
13:O:86:ARG:HG3	13:O:86:ARG:NH1	2.22	0.54
15:U:16:LYS:O	15:U:21:TYR:HB3	2.06	0.54
15:U:36:ILE:HG22	15:U:42:TYR:CG	2.41	0.54
16:V:38:LEU:HB2	16:V:45:ILE:HG13	1.88	0.54
18:Y:32:GLY:O	18:Y:35:ILE:CG2	2.53	0.54
18:Y:43:ARG:HD3	20:Z:31:GLN:NE2	2.22	0.54
1:A:103:ASP:O	1:A:106:LEU:HB2	2.07	0.54
1:A:112:TYR:O	1:A:116:ILE:HG22	2.07	0.54
1:A:187:GLN:O	1:A:191:ASN:N	2.37	0.54
1:A:218:LEU:HD11	1:A:255:PHE:HB2	1.90	0.54
23:B:1011:CLA:C4A	23:B:1011:CLA:CGA	2.84	0.54
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.90	0.54
2:B:247:PHE:CD1	2:B:247:PHE:C	2.81	0.54
2:B:384:ARG:NH1	15:U:102:LEU:HD23	2.23	0.54
2:B:97:ALA:C	2:B:99:ALA:H	2.10	0.54
1:A:160:ILE:HD13	3:C:431:PHE:CZ	2.42	0.54
4:D:246:MET:O	4:D:249:ALA:HB3	2.07	0.54
4:D:263:ASN:OD1	4:D:265:ARG:N	2.40	0.54
8:I:33:LYS:O	8:I:35:LYS:N	2.40	0.54
23:K:1034:CLA:H12	23:K:1034:CLA:C1D	2.37	0.54
30:D:1062:MGE:H222	11:L:22:LEU:HD11	1.89	0.54
1:A:335:ASN:ND2	13:O:182:PHE:CZ	2.76	0.54
10:K:14:ALA:HB2	20:Z:61:VAL:HG22	1.90	0.54
1:A:22:THR:O	1:A:22:THR:HG22	2.07	0.54
23:B:1015:CLA:HAA1	23:B:1015:CLA:HBD	1.90	0.54
23:B:1022:CLA:C20	23:B:1022:CLA:C2D	2.82	0.54
23:B:1018:CLA:C10	23:B:1023:CLA:CBA	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1023:CLA:HBD	23:B:1023:CLA:HAA2	1.88	0.54
2:B:21:ALA:HA	2:B:24:LEU:HB3	1.89	0.54
2:B:47:PRO:O	2:B:49:ASP:N	2.40	0.54
1:A:269:ARG:CZ	4:D:222:LEU:HD22	2.37	0.54
30:B:1060:MGE:C5B	4:D:276:VAL:HB	2.37	0.54
5:E:52:PRO:HG2	9:J:36:LEU:HD11	1.88	0.54
23:B:1016:CLA:C3	23:H:1017:CLA:C9	2.83	0.54
8:I:12:VAL:CG1	8:I:13:THR:N	2.70	0.54
10:K:39:VAL:HG12	10:K:40:GLN:N	2.21	0.54
13:O:63:THR:HG23	13:O:271:PRO:O	2.08	0.54
20:Z:35:ARG:HG3	20:Z:36:SER:N	2.22	0.54
20:Z:53:VAL:C	20:Z:55:GLY:N	2.57	0.54
1:A:138:GLY:HA2	3:C:455:PHE:CE2	2.43	0.54
2:B:233:ASN:O	2:B:236:THR:HG22	2.08	0.54
2:B:275:TRP:CD1	2:B:318:ASN:ND2	2.75	0.54
3:C:369:LEU:HD13	3:C:380:ILE:CD1	2.37	0.54
1:A:217:SER:OG	4:D:142:ASN:HA	2.06	0.54
7:H:28:THR:O	7:H:31:MET:HB3	2.08	0.54
15:U:76:ARG:O	15:U:79:LEU:HB2	2.08	0.54
23:A:1006:CLA:CBC	23:A:1006:CLA:CHD	2.74	0.54
1:A:113:GLN:HA	1:A:116:ILE:CG2	2.37	0.54
2:B:12:LEU:H	2:B:12:LEU:CD1	2.15	0.54
23:C:1031:CLA:O1A	23:C:1033:CLA:C5	2.54	0.54
3:C:348:GLU:CD	3:C:349:ILE:HG13	2.28	0.54
3:C:450:ALA:HB1	3:C:456:GLU:HB3	1.90	0.54
23:A:1006:CLA:C17	26:D:1050:BCR:C28	2.70	0.54
4:D:140:PRO:O	4:D:143:ALA:N	2.39	0.54
2:B:468:TRP:HE3	4:D:144:ILE:HD13	1.73	0.54
4:D:257:PHE:CD2	4:D:257:PHE:O	2.60	0.54
4:D:139:ARG:NH1	4:D:265:ARG:HH21	1.94	0.54
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.41	0.54
15:U:64:ILE:HG22	15:U:67:LEU:HG	1.89	0.54
18:Y:42:ARG:HB2	18:Y:43:ARG:HH11	1.70	0.54
23:B:1019:CLA:HBB1	23:B:1019:CLA:CHC	2.37	0.54
2:B:390:TYR:HD1	2:B:390:TYR:N	2.04	0.54
3:C:415:ASN:HB3	29:C:1057:DGD:O2E	2.08	0.54
25:D:1042:PQ9:C24	25:D:1042:PQ9:H292	2.37	0.54
4:D:276:VAL:HG23	4:D:277:THR:N	2.23	0.54
2:B:257:TRP:CE3	4:D:291:LEU:HD22	2.43	0.54
1:A:223:LEU:O	1:A:224:ILE:CB	2.41	0.54
1:A:58:VAL:HB	1:A:83:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:PHE:CZ	23:B:1021:CLA:HMB3	2.43	0.54
23:B:1023:CLA:H152	23:B:1024:CLA:C1B	2.37	0.54
3:C:190:ALA:O	3:C:191:PRO:O	2.25	0.54
4:D:249:ALA:HB1	25:D:1042:PQ9:H62	1.90	0.54
2:B:137:LYS:NZ	7:H:14:LEU:O	2.41	0.54
9:J:20:GLY:HA2	9:J:23:VAL:HG12	1.89	0.54
12:M:9:ILE:HG23	12:M:13:LEU:HD23	1.89	0.54
13:O:105:ASP:OD1	13:O:106:GLN:HG2	2.07	0.54
16:V:68:VAL:HG13	16:V:73:LYS:HE3	1.90	0.54
23:A:1003:CLA:CBA	23:A:1003:CLA:HED2	2.33	0.54
1:A:116:ILE:CG2	1:A:117:PHE:H	2.19	0.54
1:A:180:PHE:CE1	4:D:192:THR:O	2.61	0.54
1:A:267:ASN:HB3	1:A:270:SER:HG	1.71	0.54
1:A:307:ILE:HG22	1:A:308:ASP:N	2.23	0.54
23:B:1015:CLA:O1D	23:B:1015:CLA:H2A	2.07	0.54
26:B:1048:BCR:H403	26:B:1048:BCR:C22	2.34	0.54
3:C:322:GLN:HE22	3:C:381:LYS:HA	1.73	0.54
1:A:296:ASN:HB2	3:C:400:PRO:O	2.07	0.54
3:C:59:LEU:HD23	10:K:29:PRO:HA	1.89	0.54
4:D:259:ILE:HG22	4:D:260:ALA:N	2.23	0.54
1:A:315:ASN:O	4:D:63:LEU:CD2	2.56	0.54
9:J:10:LEU:HD13	9:J:10:LEU:N	2.14	0.54
13:O:132:VAL:HG23	13:O:144:LEU:HD23	1.86	0.54
2:B:383:PHE:O	13:O:192:SER:HA	2.08	0.54
1:A:107:TYR:C	1:A:109:GLY:H	2.12	0.54
2:B:237:VAL:HG13	23:B:1018:CLA:C1D	2.38	0.54
3:C:135:ARG:NH1	20:Z:33:TRP:CE3	2.76	0.54
1:A:131:TRP:HZ2	3:C:449:ARG:HG2	1.71	0.54
4:D:221:THR:O	4:D:221:THR:HG22	2.08	0.54
4:D:251:ARG:HB3	4:D:251:ARG:HH11	1.73	0.54
4:D:55:VAL:O	4:D:66:SER:HB2	2.08	0.54
4:D:97:ALA:O	5:E:73:LYS:HE2	2.08	0.54
5:E:34:GLY:HA3	6:F:32:PHE:O	2.08	0.54
23:A:1007:CLA:HAB	8:I:15:PHE:CD2	2.43	0.54
1:A:64:ARG:CZ	13:O:98:THR:HG21	2.38	0.54
15:U:82:PHE:CD2	15:U:82:PHE:N	2.76	0.54
26:A:1044:BCR:C22	26:A:1044:BCR:H403	2.36	0.53
1:A:267:ASN:O	1:A:270:SER:N	2.41	0.53
1:A:336:ALA:O	1:A:338:ASN:N	2.41	0.53
1:A:339:PHE:HB2	28:A:1065:IOD:I	2.78	0.53
23:B:1011:CLA:C2D	23:B:1013:CLA:C3	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1023:CLA:O1D	23:B:1024:CLA:CBB	2.56	0.53
2:B:19:LEU:HG	2:B:23:HIS:CE1	2.43	0.53
2:B:394:GLN:OE1	15:U:17:LEU:HD21	2.08	0.53
29:C:1056:DGD:C6D	29:C:1056:DGD:C4E	2.86	0.53
3:C:117:VAL:HG21	23:C:1027:CLA:H43	1.90	0.53
3:C:429:SER:HB3	29:C:1056:DGD:C9A	2.34	0.53
3:C:435:PHE:O	3:C:438:LEU:N	2.41	0.53
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.90	0.53
4:D:58:TRP:CH2	5:E:55:TYR:HB3	2.43	0.53
9:J:30:TYR:CD2	9:J:31:GLY:N	2.77	0.53
25:D:1042:PQ9:C23	30:L:1061:MGE:H263	2.37	0.53
13:O:188:ARG:HB2	13:O:188:ARG:HH11	1.68	0.53
1:A:270:SER:HB2	27:A:1063:LHG:H142	1.90	0.53
1:A:236:GLY:O	1:A:237:TYR:HB2	2.08	0.53
1:A:90:GLY:HA2	1:A:167:SER:CB	2.38	0.53
23:B:1018:CLA:H8	23:B:1023:CLA:HBA1	1.91	0.53
2:B:103:LEU:HD11	2:B:107:LEU:CD1	2.37	0.53
2:B:460:LEU:O	4:D:280:TRP:HZ3	1.90	0.53
2:B:69:LEU:HB3	23:B:1014:CLA:CMA	2.37	0.53
3:C:203:THR:H	3:C:235:GLY:HA3	1.74	0.53
3:C:451:ALA:O	3:C:453:ALA:N	2.40	0.53
11:L:14:ARG:O	11:L:18:TYR:CD2	2.61	0.53
12:M:35:SER:O	12:M:36:SER:CB	2.56	0.53
13:O:146:PHE:CE2	13:O:261:ILE:HG21	2.44	0.53
13:O:79:LYS:HE2	13:O:89:ALA:HB1	1.90	0.53
16:V:114:ILE:O	16:V:114:ILE:HG12	2.07	0.53
23:B:1019:CLA:HBD	23:B:1019:CLA:CBA	2.38	0.53
2:B:283:GLU:CG	2:B:286:ARG:HH12	2.21	0.53
2:B:461:LEU:O	2:B:464:PHE:N	2.37	0.53
2:B:95:GLY:O	2:B:99:ALA:N	2.41	0.53
3:C:119:LEU:HD11	26:C:1052:BCR:H343	1.89	0.53
3:C:216:SER:O	3:C:221:GLU:O	2.27	0.53
1:A:258:LEU:HA	4:D:128:ARG:HH21	1.72	0.53
4:D:18:LEU:HD23	4:D:32:TRP:CH2	2.44	0.53
4:D:29:PHE:CE2	4:D:31:GLY:CA	2.91	0.53
4:D:78:VAL:HG13	4:D:78:VAL:O	2.09	0.53
5:E:77:GLU:O	5:E:79:PHE:N	2.41	0.53
6:F:40:MET:CB	6:F:43:ILE:HD11	2.38	0.53
7:H:12:ARG:HA	7:H:12:ARG:HH11	1.74	0.53
8:I:10:ILE:CD1	8:I:10:ILE:H	2.20	0.53
3:C:465:PRO:CG	8:I:32:PRO:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1018:CLA:H2	23:B:1018:CLA:H71	1.89	0.53
2:B:103:LEU:HG	2:B:104:SER:N	2.24	0.53
23:B:1014:CLA:H93	26:B:1048:BCR:H342	1.89	0.53
2:B:280:PHE:CZ	2:B:312:TYR:HD1	2.26	0.53
2:B:453:PHE:O	2:B:456:ALA:HB3	2.08	0.53
23:C:1026:CLA:C12	23:C:1026:CLA:H93	2.38	0.53
23:C:1030:CLA:HMC2	23:C:1031:CLA:H72	1.91	0.53
3:C:56:HIS:CE1	23:C:1033:CLA:HHB	2.44	0.53
3:C:265:ILE:CG2	3:C:270:ALA:HB1	2.39	0.53
3:C:56:HIS:O	3:C:60:ILE:HG23	2.08	0.53
1:A:244:GLU:CG	4:D:242:GLU:HA	2.38	0.53
1:A:140:ARG:NH2	27:A:1063:LHG:O4	2.41	0.53
1:A:172:MET:SD	1:A:179:THR:HG22	2.47	0.53
23:B:1024:CLA:H2	23:B:1024:CLA:HMA2	1.91	0.53
2:B:113:TRP:C	2:B:115:TRP:H	2.11	0.53
2:B:246:PHE:C	2:B:246:PHE:CD1	2.81	0.53
2:B:92:SER:O	2:B:93:PHE:C	2.46	0.53
3:C:65:GLY:CA	3:C:119:LEU:HB2	2.39	0.53
1:A:258:LEU:HA	4:D:132:ILE:HD12	1.90	0.53
4:D:299:ILE:O	4:D:300:SER:C	2.46	0.53
6:F:34:LEU:HD12	9:J:24:ILE:HD13	1.90	0.53
7:H:40:VAL:O	7:H:44:ILE:HB	2.08	0.53
3:C:59:LEU:CD2	23:K:1034:CLA:HBD	2.38	0.53
10:K:19:ASP:N	10:K:20:PRO:CD	2.72	0.53
16:V:159:GLY:HA2	16:V:163:TYR:HE1	1.72	0.53
18:Y:37:PHE:O	18:Y:41:VAL:HG22	2.08	0.53
18:Y:39:LEU:HD22	20:Z:28:ALA:HB1	1.91	0.53
20:Z:1:MET:SD	20:Z:4:LEU:HD23	2.48	0.53
23:B:1022:CLA:H203	23:B:1022:CLA:C1	2.38	0.53
2:B:25:MET:HG3	26:B:1045:BCR:C39	2.38	0.53
2:B:158:LEU:HB2	2:B:199:VAL:HG13	1.90	0.53
23:C:1025:CLA:CAD	23:C:1025:CLA:CED	2.86	0.53
23:C:1026:CLA:H121	23:C:1026:CLA:H93	1.90	0.53
3:C:315:MET:HE3	3:C:315:MET:HA	1.90	0.53
5:E:10:PHE:CZ	6:F:19:ARG:HD2	2.43	0.53
31:F:1040:HEM:CMA	31:F:1040:HEM:CBA	2.60	0.53
6:F:24:HIS:O	6:F:28:VAL:HG23	2.09	0.53
16:V:149:PRO:HB3	16:V:156:TRP:CD1	2.44	0.53
16:V:148:GLU:CA	16:V:151:ILE:HD11	2.29	0.53
1:A:130:GLN:CG	1:A:144:CYS:HA	2.38	0.53
23:B:1010:CLA:O2D	23:B:1010:CLA:CGA	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CBB	23:B:1011:CLA:C9	2.86	0.53
23:B:1019:CLA:HMD2	30:B:1060:MGE:H1G1	1.90	0.53
2:B:306:PRO:HG2	2:B:309:LEU:HB3	1.90	0.53
2:B:452:THR:HB	4:D:291:LEU:HD13	1.89	0.53
3:C:290:VAL:HG21	3:C:426:LEU:HD23	1.91	0.53
3:C:84:GLN:O	3:C:86:LEU:N	2.41	0.53
23:B:1016:CLA:H171	23:D:1008:CLA:HMA3	1.89	0.53
30:D:1059:MGE:H2B1	30:D:1059:MGE:O1G	2.09	0.53
4:D:209:LEU:O	4:D:213:ILE:HG22	2.09	0.53
4:D:58:TRP:NE1	5:E:64:PRO:HD2	2.21	0.53
11:L:15:THR:HG22	11:L:16:SER:N	2.23	0.53
26:T:6048:BCR:H403	26:T:6048:BCR:C22	2.34	0.53
23:A:1007:CLA:HAC1	26:A:1044:BCR:C15	2.38	0.53
25:A:1043:PQ9:H453	25:A:1043:PQ9:C40	2.39	0.53
1:A:47:CYS:SG	1:A:115:ILE:HD11	2.49	0.53
2:B:61:PHE:CE1	23:B:1015:CLA:HMB3	2.44	0.53
2:B:460:LEU:HG	29:B:1058:DGD:HAG3	1.91	0.53
2:B:237:VAL:HB	23:B:1020:CLA:HMD2	1.91	0.53
2:B:246:PHE:CD1	2:B:247:PHE:N	2.77	0.53
2:B:278:SER:HB3	2:B:281:GLN:CG	2.28	0.53
2:B:425:ILE:HG23	2:B:425:ILE:O	2.09	0.53
3:C:117:VAL:CG1	23:C:1027:CLA:H42	2.32	0.53
3:C:340:TYR:N	3:C:340:TYR:CD2	2.70	0.53
1:A:305:SER:HB3	3:C:415:ASN:ND2	2.24	0.53
4:D:249:ALA:HB1	25:D:1042:PQ9:C6	2.39	0.53
4:D:21:TRP:HZ3	17:X:37:LEU:HD21	1.73	0.53
4:D:297:ASP:CG	4:D:298:PHE:N	2.59	0.53
10:K:38:VAL:HG12	10:K:39:VAL:N	2.23	0.53
11:L:23:LEU:O	11:L:27:LEU:HG	2.09	0.53
16:V:39:ASN:ND2	16:V:40:SER:N	2.54	0.53
25:A:1043:PQ9:H293	24:D:1039:PHO:HBA1	1.91	0.53
2:B:203:ILE:HG23	2:B:204:ALA:N	2.24	0.53
2:B:26:HIS:NE2	23:B:1021:CLA:NB	2.57	0.53
3:C:188:THR:HA	3:C:194:GLY:HA2	1.90	0.53
3:C:49:LEU:HD21	23:C:1035:CLA:CMA	2.15	0.53
4:D:152:VAL:HG11	23:D:1004:CLA:H11	1.90	0.53
24:D:1039:PHO:CGA	24:D:1039:PHO:C4	2.87	0.53
1:A:216:GLY:O	4:D:268:HIS:O	2.27	0.53
4:D:272:LEU:O	4:D:276:VAL:HG22	2.08	0.53
7:H:31:MET:HB2	23:H:1017:CLA:C3D	2.38	0.53
13:O:214:LYS:HE3	13:O:251:MET:CG	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:35:ILE:HD13	18:Y:36:ILE:N	2.24	0.53
18:Y:43:ARG:NH2	18:Y:44:GLY:CA	2.72	0.53
27:A:1063:LHG:H242	23:C:1032:CLA:OBD	2.09	0.53
1:A:225:ARG:HB2	2:B:484:PRO:HD3	1.91	0.53
1:A:146:ALA:HA	1:A:280:VAL:HG11	1.91	0.53
1:A:51:ALA:HA	1:A:55:ALA:HB2	1.91	0.53
2:B:62:VAL:HG13	23:B:1013:CLA:O1D	2.09	0.53
2:B:331:ASN:C	2:B:333:GLY:H	2.12	0.53
2:B:79:SER:OG	2:B:80:ILE:N	2.41	0.53
3:C:50:LEU:HD23	3:C:51:GLY:CA	2.39	0.53
25:D:1042:PQ9:C23	30:L:1061:MGE:CGB	2.87	0.53
4:D:36:LEU:HD21	4:D:124:GLY:HA3	1.91	0.53
4:D:172:SER:O	4:D:173:PHE:HB2	2.08	0.53
4:D:182:LEU:HD23	4:D:182:LEU:N	2.24	0.53
4:D:43:LEU:HD13	26:D:1050:BCR:H322	1.91	0.53
5:E:43:ALA:O	5:E:46:VAL:HB	2.08	0.53
11:L:32:SER:OG	11:L:33:SER:N	2.42	0.53
12:M:9:ILE:HG23	12:M:13:LEU:CD2	2.39	0.53
3:C:330:SER:C	13:O:129:PHE:HE1	2.11	0.53
13:O:63:THR:CG2	13:O:271:PRO:O	2.57	0.53
23:A:1007:CLA:H142	8:I:13:THR:HG21	1.91	0.52
23:A:1007:CLA:H43	23:C:1029:CLA:H192	1.89	0.52
1:A:215:HIS:CE1	25:A:1043:PQ9:H93	2.44	0.52
1:A:134:SER:OG	1:A:141:PRO:HB3	2.09	0.52
1:A:279:ARG:O	1:A:283:VAL:HG23	2.09	0.52
1:A:40:THR:H	23:A:1007:CLA:HBB1	1.75	0.52
23:B:1012:CLA:CHD	23:B:1020:CLA:H201	2.37	0.52
23:B:1022:CLA:H43	23:B:1022:CLA:O2A	2.10	0.52
2:B:45:PHE:HA	2:B:58:GLN:NE2	2.23	0.52
23:C:1032:CLA:H112	23:C:1032:CLA:H62	1.91	0.52
3:C:405:ASN:OD1	29:C:1057:DGD:HD61	2.09	0.52
3:C:417:VAL:HG11	16:V:68:VAL:HG12	1.86	0.52
4:D:67:TYR:CE1	30:D:1059:MGE:H1G1	2.44	0.52
1:A:17:PHE:CZ	8:I:18:LEU:HD11	2.44	0.52
4:D:302:GLU:OE1	13:O:186:LYS:CD	2.57	0.52
14:T:11:ALA:O	14:T:12:CYS:C	2.46	0.52
26:T:6046:BCR:C39	26:T:6046:BCR:H23C	2.26	0.52
20:Z:5:PHE:CE1	20:Z:54:VAL:HG13	2.42	0.52
27:A:1063:LHG:H292	23:C:1032:CLA:C5	2.27	0.52
1:A:224:ILE:HA	2:B:482:ILE:HG13	1.91	0.52
1:A:285:PHE:HA	1:A:288:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1009:CLA:CGA	23:B:1009:CLA:CHA	2.87	0.52
26:B:1047:BCR:C37	26:B:1047:BCR:C30	2.61	0.52
2:B:106:LEU:HD12	26:B:1048:BCR:H352	1.91	0.52
2:B:275:TRP:HB3	2:B:318:ASN:HD22	1.75	0.52
2:B:74:SER:C	2:B:76:SER:H	2.12	0.52
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.91	0.52
1:A:223:LEU:CD2	4:D:265:ARG:HG2	2.35	0.52
4:D:210:LEU:HD22	4:D:274:VAL:HG21	1.90	0.52
4:D:32:TRP:HE3	4:D:35:ILE:HD11	1.72	0.52
1:A:316:THR:HG22	4:D:75:THR:HG23	1.91	0.52
5:E:13:ILE:CD1	5:E:19:TYR:HB2	2.40	0.52
5:E:17:VAL:HG13	9:J:8:ILE:HD11	1.91	0.52
7:H:35:MET:HA	26:H:1049:BCR:C33	2.39	0.52
26:H:1049:BCR:C31	26:H:1049:BCR:HC8	2.26	0.52
9:J:20:GLY:O	9:J:23:VAL:HG12	2.09	0.52
13:O:184:ASP:O	13:O:185:PRO:C	2.47	0.52
16:V:40:SER:HB3	16:V:94:ASN:HD21	1.74	0.52
18:Y:35:ILE:HD13	18:Y:36:ILE:HD12	1.91	0.52
1:A:140:ARG:HB2	1:A:140:ARG:HH11	1.74	0.52
23:C:1033:CLA:C14	23:C:1036:CLA:C2D	2.87	0.52
3:C:176:VAL:O	3:C:180:MET:HG3	2.08	0.52
3:C:185:LEU:HG	3:C:199:ILE:CD1	2.37	0.52
3:C:165:LEU:HB2	3:C:248:GLY:HA3	1.90	0.52
3:C:314:ALA:HB1	3:C:351:PHE:CD1	2.45	0.52
3:C:315:MET:O	3:C:319:ILE:HG13	2.10	0.52
23:D:1008:CLA:HMA2	23:D:1008:CLA:HBA1	0.65	0.52
4:D:118:GLY:O	4:D:122:LEU:HD22	2.09	0.52
1:A:269:ARG:CD	4:D:222:LEU:HD11	2.28	0.52
2:B:486:LEU:HD11	4:D:239:GLN:HE22	1.74	0.52
4:D:265:ARG:HD3	4:D:265:ARG:O	2.10	0.52
6:F:37:ILE:HA	6:F:40:MET:HE2	1.89	0.52
1:A:335:ASN:ND2	13:O:182:PHE:CD1	2.77	0.52
13:O:92:VAL:HG11	13:O:137:ALA:HB2	1.90	0.52
20:Z:58:ASN:C	20:Z:60:PHE:H	2.13	0.52
1:A:172:MET:HE1	1:A:179:THR:HB	1.92	0.52
1:A:296:ASN:HB3	3:C:401:LEU:HD13	1.91	0.52
2:B:25:MET:CG	26:B:1045:BCR:H401	2.35	0.52
2:B:169:SER:CB	2:B:176:GLY:HA2	2.17	0.52
2:B:25:MET:CG	26:B:1045:BCR:H391	2.37	0.52
2:B:374:ASN:ND2	2:B:374:ASN:N	2.58	0.52
23:C:1029:CLA:H11	23:C:1029:CLA:CHA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:TRP:HE1	3:C:224:ILE:CG1	2.22	0.52
3:C:223:TRP:NE1	3:C:224:ILE:CG1	2.69	0.52
3:C:50:LEU:CD2	3:C:51:GLY:CA	2.87	0.52
25:D:1042:PQ9:H252	30:L:1061:MGE:H261	1.92	0.52
29:C:1057:DGD:CGA	30:D:1059:MGE:H232	2.39	0.52
10:K:14:ALA:H	20:Z:62:VAL:HG11	1.73	0.52
11:L:29:LEU:CB	14:T:9:ILE:HG21	2.32	0.52
15:U:16:LYS:HG2	15:U:21:TYR:HD1	1.74	0.52
16:V:144:HIS:CD2	16:V:148:GLU:HG3	2.44	0.52
17:X:36:VAL:O	17:X:39:ALA:HB3	2.10	0.52
26:A:1044:BCR:H331	26:A:1044:BCR:C34	2.39	0.52
2:B:354:LEU:CD2	2:B:378:LYS:HB2	2.40	0.52
2:B:372:ASP:OD2	2:B:376:VAL:HG23	2.10	0.52
2:B:235:GLU:HG3	2:B:473:THR:OG1	2.09	0.52
26:C:1052:BCR:C38	26:C:1052:BCR:H372	2.23	0.52
29:C:1056:DGD:C8B	29:C:1056:DGD:HBF1	2.39	0.52
3:C:209:ILE:HD13	3:C:236:GLY:HA2	1.90	0.52
4:D:214:HIS:HA	4:D:217:THR:CG2	2.40	0.52
4:D:246:MET:HE2	4:D:264:LYS:HD3	1.92	0.52
4:D:284:ILE:O	4:D:287:VAL:HB	2.09	0.52
7:H:30:LEU:HA	7:H:33:VAL:HG22	1.91	0.52
10:K:21:LEU:CD2	18:Y:24:MET:HG2	2.39	0.52
13:O:44:LYS:HA	13:O:72:GLN:CD	2.30	0.52
16:V:106:THR:CA	16:V:114:ILE:HG22	2.38	0.52
16:V:108:TYR:HD2	16:V:108:TYR:O	1.93	0.52
16:V:118:HIS:CD2	16:V:119:PRO:CD	2.85	0.52
1:A:328:MET:CE	4:D:183:LEU:HD13	2.39	0.52
1:A:76:ASN:CB	1:A:79:THR:HG23	2.39	0.52
23:B:1011:CLA:C4	23:B:1011:CLA:CGA	2.87	0.52
26:B:1045:BCR:C23	26:B:1045:BCR:C38	2.71	0.52
2:B:134:ASP:O	2:B:138:MET:HB2	2.09	0.52
2:B:15:ASP:OD2	2:B:18:ARG:HG3	2.09	0.52
2:B:483:ASP:O	2:B:485:GLU:N	2.43	0.52
23:D:1005:CLA:NA	23:D:1005:CLA:O1A	2.43	0.52
24:D:1039:PHO:CGA	24:D:1039:PHO:H42	2.39	0.52
1:A:181:ASN:HA	4:D:318:ASN:OD1	2.09	0.52
5:E:23:HIS:O	5:E:24:SER:C	2.47	0.52
6:F:38:ALA:HA	9:J:27:LEU:HD21	1.91	0.52
13:O:250:ASP:O	13:O:252:GLY:N	2.35	0.52
15:U:16:LYS:NZ	15:U:85:THR:HB	2.25	0.52
1:A:156:ALA:CB	1:A:160:ILE:HD12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:O	1:A:261:GLN:HA	2.10	0.52
1:A:336:ALA:O	1:A:337:HIS:C	2.48	0.52
23:B:1014:CLA:CBA	23:B:1014:CLA:CHA	2.78	0.52
23:B:1022:CLA:C13	23:B:1022:CLA:C9	2.78	0.52
23:B:1022:CLA:CED	23:B:1022:CLA:OBD	2.55	0.52
2:B:249:ALA:O	2:B:251:VAL:N	2.42	0.52
3:C:87:ILE:HG22	3:C:426:LEU:CD1	2.40	0.52
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.45	0.52
23:A:1006:CLA:CAB	23:D:1004:CLA:H51	2.37	0.52
16:V:160:LYS:N	16:V:163:TYR:CD1	2.78	0.52
16:V:34:LEU:CD2	16:V:47:LEU:HB3	2.30	0.52
26:A:1044:BCR:H392	26:A:1044:BCR:C22	2.35	0.52
1:A:272:HIS:O	4:D:215:GLY:CA	2.58	0.52
1:A:279:ARG:NH2	1:A:283:VAL:CG2	2.73	0.52
1:A:288:LEU:O	1:A:292:THR:N	2.42	0.52
2:B:5:TRP:CZ2	30:L:1061:MGE:C2A	2.80	0.52
3:C:414:ILE:HG22	3:C:415:ASN:N	2.25	0.52
26:D:1050:BCR:C8	26:D:1050:BCR:H331	2.28	0.52
6:F:40:MET:C	6:F:42:PHE:H	2.13	0.52
7:H:47:GLU:O	7:H:53:LEU:N	2.40	0.52
15:U:43:PRO:HB2	16:V:109:ASP:HB2	1.91	0.52
1:A:167:SER:C	1:A:169:SER:H	2.13	0.52
26:C:1052:BCR:C34	26:K:1051:BCR:HC21	2.39	0.52
4:D:281:MET:HE2	4:D:281:MET:CA	2.39	0.52
5:E:59:GLU:OE1	5:E:59:GLU:HA	2.09	0.52
6:F:32:PHE:HD1	6:F:32:PHE:O	1.93	0.52
7:H:56:ASP:C	7:H:58:VAL:N	2.63	0.52
23:K:1034:CLA:H42	23:K:1034:CLA:HBA1	1.92	0.52
11:L:31:PHE:O	11:L:32:SER:C	2.47	0.52
13:O:82:PRO:HG2	13:O:89:ALA:HB1	1.87	0.52
1:A:167:SER:C	1:A:169:SER:N	2.60	0.52
1:A:156:ALA:HB1	1:A:290:ILE:HG21	1.90	0.52
1:A:58:VAL:HG21	1:A:83:VAL:HG23	1.91	0.52
23:B:1016:CLA:C1A	23:B:1016:CLA:O1A	2.58	0.52
23:B:1020:CLA:H111	23:B:1020:CLA:C16	2.39	0.52
30:B:1060:MGE:H261	30:B:1060:MGE:H5A2	1.91	0.52
2:B:19:LEU:O	2:B:22:ALA:HB3	2.10	0.52
2:B:67:ALA:HB3	2:B:267:LEU:CD1	2.40	0.52
2:B:365:SER:O	2:B:366:PHE:HB2	2.10	0.52
2:B:413:ASP:O	2:B:413:ASP:OD1	2.28	0.52
23:C:1035:CLA:HMB2	26:C:1052:BCR:C27	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:GLY:O	3:C:195:ASP:HB2	2.09	0.52
3:C:200:THR:O	3:C:202:PRO:HD3	2.10	0.52
4:D:55:VAL:HG12	4:D:56:THR:O	2.10	0.52
4:D:78:VAL:HG12	4:D:173:PHE:CB	2.40	0.52
7:H:27:THR:HB	23:H:1017:CLA:OBD	2.10	0.52
13:O:215:ARG:NH1	13:O:215:ARG:HG2	2.24	0.52
1:A:50:ILE:HG21	26:A:1044:BCR:H402	1.93	0.51
1:A:92:HIS:CD2	3:C:219:GLY:O	2.64	0.51
2:B:142:HIS:HA	2:B:145:LEU:HD12	1.92	0.51
23:C:1027:CLA:HBD	23:C:1027:CLA:HAA1	1.92	0.51
3:C:142:GLU:C	3:C:144:SER:N	2.63	0.51
3:C:79:LYS:HD3	3:C:84:GLN:HG2	1.92	0.51
4:D:23:LYS:NZ	4:D:135:LEU:HD21	2.25	0.51
4:D:251:ARG:NH2	4:D:255:GLN:NE2	2.58	0.51
5:E:13:ILE:HA	5:E:16:SER:HB3	1.92	0.51
5:E:28:PRO:HA	5:E:31:PHE:HB3	1.92	0.51
23:K:1034:CLA:CBC	23:K:1034:CLA:CHD	2.84	0.51
10:K:31:LEU:HD13	26:K:1051:BCR:H14C	1.91	0.51
13:O:241:PHE:CD1	13:O:241:PHE:C	2.84	0.51
13:O:55:ALA:HA	13:O:162:ILE:O	2.10	0.51
1:A:180:PHE:O	1:A:184:ILE:HD12	2.09	0.51
23:B:1019:CLA:H93	30:L:1061:MGE:C8A	2.41	0.51
23:B:1022:CLA:C20	23:B:1022:CLA:C3D	2.88	0.51
23:B:1015:CLA:CBC	26:B:1047:BCR:H10C	2.40	0.51
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.92	0.51
2:B:310:ALA:O	2:B:313:ASP:N	2.41	0.51
23:C:1035:CLA:HAA1	23:C:1035:CLA:HBD	1.92	0.51
26:C:1054:BCR:H402	26:C:1054:BCR:H23C	1.73	0.51
3:C:171:GLY:C	3:C:173:LEU:N	2.59	0.51
3:C:33:PHE:CZ	3:C:40:ALA:HB1	2.45	0.51
3:C:53:HIS:HB3	23:C:1036:CLA:HMD1	1.92	0.51
2:B:362:PHE:HZ	28:D:1068:IOD:I	2.63	0.51
4:D:274:VAL:HG12	4:D:275:PRO:N	2.24	0.51
5:E:56:TYR:C	5:E:57:ALA:O	2.48	0.51
8:I:27:ASP:N	8:I:28:PRO:CD	2.74	0.51
13:O:148:VAL:HG23	13:O:151:LEU:HD13	1.92	0.51
15:U:45:LEU:HD21	15:U:75:LEU:HD11	1.92	0.51
16:V:94:ASN:C	16:V:96:GLU:H	2.12	0.51
23:A:1006:CLA:HAA2	29:C:1057:DGD:CFB	2.40	0.51
1:A:107:TYR:CD2	13:O:97:VAL:HG11	2.44	0.51
1:A:180:PHE:CZ	4:D:192:THR:O	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:CZ	1:A:283:VAL:HG22	2.40	0.51
1:A:26:ASN:O	1:A:27:ARG:C	2.48	0.51
1:A:335:ASN:OD1	1:A:335:ASN:N	2.43	0.51
1:A:75:ASN:HD22	1:A:80:GLY:HA2	1.76	0.51
2:B:30:VAL:CG1	23:B:1013:CLA:HHD	2.40	0.51
2:B:125:ASP:HA	7:H:12:ARG:HH21	1.75	0.51
2:B:14:ASN:O	2:B:15:ASP:HB3	2.09	0.51
3:C:137:PRO:C	3:C:139:THR:H	2.12	0.51
4:D:126:MET:CE	4:D:146:PHE:HB3	2.40	0.51
4:D:214:HIS:CE1	4:D:268:HIS:CE1	2.98	0.51
5:E:72:ALA:O	5:E:76:VAL:HG22	2.11	0.51
3:C:72:LEU:HD22	10:K:11:LEU:HD23	1.91	0.51
11:L:26:VAL:O	11:L:29:LEU:N	2.43	0.51
1:A:151:LEU:HG	1:A:155:PHE:CD2	2.44	0.51
2:B:152:GLY:O	2:B:156:PHE:CB	2.57	0.51
2:B:99:ALA:O	2:B:102:VAL:CG2	2.59	0.51
23:C:1026:CLA:C2B	23:C:1028:CLA:CBB	2.88	0.51
27:A:1063:LHG:C31	23:C:1032:CLA:H71	2.41	0.51
4:D:186:GLN:H	23:D:1004:CLA:HBC1	1.75	0.51
4:D:118:GLY:HA2	24:D:1039:PHO:H71	1.93	0.51
4:D:154:VAL:HA	4:D:158:LEU:HD13	1.92	0.51
4:D:167:TRP:O	4:D:170:ALA:HB3	2.10	0.51
4:D:188:PHE:CE2	4:D:326:ARG:HA	2.46	0.51
30:B:1060:MGE:H6B1	4:D:280:TRP:CD1	2.46	0.51
2:B:121:GLU:CG	7:H:12:ARG:HD3	2.40	0.51
1:A:310:LYS:H	16:V:28:GLU:HB2	1.76	0.51
1:A:17:PHE:O	1:A:21:VAL:HG23	2.10	0.51
1:A:81:ALA:HA	1:A:175:GLY:HA3	1.92	0.51
23:B:1022:CLA:HBC1	12:M:21:PHE:CG	2.46	0.51
2:B:368:VAL:HG22	2:B:381:ILE:HG13	1.93	0.51
23:C:1028:CLA:H91	29:C:1056:DGD:CAB	2.36	0.51
23:C:1030:CLA:C14	23:C:1030:CLA:H171	2.21	0.51
3:C:268:GLY:C	23:C:1033:CLA:HBC1	2.30	0.51
23:C:1028:CLA:C10	29:C:1056:DGD:HAS2	2.36	0.51
3:C:109:PHE:HB3	3:C:110:PRO:CD	2.40	0.51
3:C:206:PRO:HG2	3:C:207:ARG:NH1	2.26	0.51
3:C:290:VAL:HG13	3:C:427:ALA:HB2	1.93	0.51
30:D:1062:MGE:C3G	30:D:1062:MGE:O1B	2.34	0.51
4:D:198:MET:SD	23:D:1005:CLA:HED2	2.50	0.51
1:A:181:ASN:HD22	4:D:314:PHE:HD2	1.56	0.51
23:K:1034:CLA:CBA	23:K:1034:CLA:H42	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:ILE:CG2	23:K:1034:CLA:HMD2	2.40	0.51
30:L:1061:MGE:H7B1	30:L:1061:MGE:H3B2	1.92	0.51
13:O:63:THR:HG23	13:O:64:TYR:N	2.25	0.51
14:T:19:PHE:N	14:T:19:PHE:CD2	2.77	0.51
26:T:6048:BCR:H392	26:T:6048:BCR:C22	2.35	0.51
20:Z:20:VAL:HG12	20:Z:21:ILE:N	2.26	0.51
20:Z:23:VAL:HB	20:Z:24:PRO:HD3	1.91	0.51
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.36	0.51
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.46	0.51
1:A:45:THR:CG2	1:A:46:ILE:N	2.71	0.51
29:B:1058:DGD:HE5	29:B:1058:DGD:HD61	1.93	0.51
2:B:325:PHE:O	2:B:327:THR:N	2.37	0.51
3:C:158:THR:HG23	3:C:159:THR:N	2.25	0.51
3:C:171:GLY:CA	3:C:174:LEU:CB	2.86	0.51
3:C:202:PRO:HB3	3:C:235:GLY:CA	2.40	0.51
3:C:56:HIS:C	3:C:56:HIS:HD2	2.07	0.51
23:D:1008:CLA:H141	23:D:1008:CLA:C18	2.19	0.51
4:D:67:TYR:CD1	4:D:76:VAL:HG11	2.46	0.51
2:B:267:LEU:C	2:B:268:PHE:CD1	2.84	0.51
2:B:283:GLU:HG2	2:B:286:ARG:HH12	1.76	0.51
2:B:99:ALA:O	2:B:102:VAL:HG22	2.11	0.51
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.46	0.51
7:H:38:PHE:O	7:H:39:LEU:C	2.49	0.51
8:I:7:THR:O	8:I:11:VAL:HG23	2.11	0.51
25:A:1043:PQ9:H293	24:D:1039:PHO:HBA2	1.91	0.51
1:A:148:SER:OG	1:A:149:ALA:N	2.43	0.51
1:A:269:ARG:CZ	4:D:222:LEU:CD2	2.89	0.51
1:A:26:ASN:O	1:A:28:LEU:N	2.44	0.51
1:A:310:LYS:H	16:V:28:GLU:CB	2.24	0.51
1:A:325:ASN:ND2	1:A:328:MET:CE	2.73	0.51
23:B:1011:CLA:OBD	23:B:1013:CLA:H12	2.10	0.51
2:B:271:THR:O	2:B:274:GLN:HB2	2.11	0.51
2:B:27:THR:HG23	23:B:1013:CLA:HBC3	1.93	0.51
2:B:418:LYS:O	2:B:419:SER:C	2.48	0.51
3:C:274:TYR:CE1	23:C:1029:CLA:O1D	2.62	0.51
23:C:1035:CLA:H93	26:C:1052:BCR:H402	1.87	0.51
23:C:1028:CLA:NB	29:C:1056:DGD:HA42	2.26	0.51
4:D:274:VAL:HG13	25:D:1042:PQ9:H262	1.93	0.51
14:T:22:PHE:C	14:T:23:PHE:HD2	2.14	0.51
15:U:31:ASN:HD22	15:U:31:ASN:C	2.14	0.51
20:Z:12:LEU:HA	20:Z:50:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HG21	1:A:174:LEU:HD13	1.93	0.51
23:B:1016:CLA:CGA	23:B:1016:CLA:C1A	2.88	0.51
2:B:24:LEU:HD22	2:B:114:HIS:HD2	1.75	0.51
2:B:24:LEU:HB2	23:B:1023:CLA:HED1	1.92	0.51
2:B:338:GLN:HA	2:B:338:GLN:NE2	2.16	0.51
1:A:333:GLU:OE1	3:C:354:GLU:OE1	2.28	0.51
5:E:23:HIS:HB3	5:E:27:ILE:CD1	2.40	0.51
7:H:38:PHE:O	7:H:41:PHE:N	2.41	0.51
8:I:11:VAL:O	8:I:15:PHE:CD1	2.64	0.51
23:K:1034:CLA:C4D	23:K:1034:CLA:O2A	2.59	0.51
10:K:20:PRO:O	10:K:23:ASP:HB2	2.11	0.51
14:T:11:ALA:O	14:T:13:ILE:N	2.44	0.51
16:V:58:LEU:O	16:V:60:GLN:N	2.44	0.51
1:A:216:GLY:HA2	4:D:268:HIS:O	2.11	0.51
1:A:338:ASN:O	1:A:339:PHE:CD2	2.64	0.51
1:A:41:LEU:O	1:A:45:THR:HG22	2.11	0.51
23:B:1010:CLA:O2D	23:B:1010:CLA:H2A	2.11	0.51
23:B:1016:CLA:C9	23:D:1008:CLA:H201	2.40	0.51
23:B:1018:CLA:CBB	23:B:1018:CLA:HHC	2.20	0.51
2:B:302:TRP:CE3	2:B:305:ILE:HD12	2.45	0.51
2:B:74:SER:O	2:B:76:SER:N	2.44	0.51
3:C:185:LEU:CG	3:C:199:ILE:HD11	2.38	0.51
3:C:318:LEU:HD11	3:C:380:ILE:HG12	1.92	0.51
3:C:48:LYS:CG	3:C:49:LEU:HD12	2.38	0.51
3:C:72:LEU:C	3:C:72:LEU:HD23	2.31	0.51
1:A:143:ILE:HD11	4:D:253:TRP:CZ2	2.46	0.51
1:A:76:ASN:HB2	4:D:298:PHE:HE1	1.76	0.51
5:E:73:LYS:O	5:E:76:VAL:CG2	2.54	0.51
12:M:18:PRO:HG2	12:M:19:SER:N	2.26	0.51
12:M:18:PRO:O	12:M:21:PHE:HB3	2.11	0.51
19:N:2:UNK:O	19:N:3:UNK:O	2.28	0.51
13:O:80:GLU:HB2	13:O:92:VAL:HG23	1.93	0.51
5:E:84:LYS:NZ	16:V:27:ALA:O	2.43	0.51
16:V:90:PRO:HD2	16:V:92:ARG:CZ	2.40	0.51
20:Z:4:LEU:C	20:Z:4:LEU:HD12	2.32	0.51
1:A:29:TYR:H	4:D:255:GLN:HB3	1.75	0.50
1:A:76:ASN:HB2	1:A:79:THR:HG23	1.91	0.50
2:B:21:ALA:HA	2:B:24:LEU:HD23	1.94	0.50
2:B:340:TRP:HE1	2:B:428:GLU:HB3	1.76	0.50
2:B:454:ALA:C	2:B:456:ALA:N	2.65	0.50
3:C:251:HIS:HE1	23:C:1030:CLA:NA	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:1005:CLA:CHD	23:D:1005:CLA:HBC2	2.41	0.50
2:B:467:ILE:HD13	4:D:126:MET:SD	2.52	0.50
13:O:137:ALA:O	13:O:138:GLY:O	2.28	0.50
1:A:64:ARG:HH21	13:O:98:THR:HG21	1.76	0.50
13:O:97:VAL:HG12	13:O:98:THR:N	2.25	0.50
14:T:22:PHE:N	14:T:22:PHE:CD1	2.79	0.50
7:H:43:LEU:CD2	17:X:19:PHE:CZ	2.92	0.50
18:Y:43:ARG:CZ	18:Y:43:ARG:N	2.74	0.50
23:A:1003:CLA:HMB2	23:D:1004:CLA:CMB	2.38	0.50
1:A:269:ARG:HG3	4:D:235:PHE:HB2	1.94	0.50
23:B:1010:CLA:HAA2	23:B:1010:CLA:HBD	1.92	0.50
23:B:1019:CLA:HMD1	30:B:1060:MGE:H2G	1.94	0.50
23:B:1023:CLA:ND	23:B:1024:CLA:HMC1	2.25	0.50
2:B:106:LEU:HD12	26:B:1048:BCR:C35	2.42	0.50
23:C:1025:CLA:O1A	23:C:1026:CLA:OBD	2.29	0.50
1:A:325:ASN:HB3	3:C:412:THR:HG21	1.93	0.50
4:D:331:PRO:HA	4:D:339:PHE:HB2	1.92	0.50
4:D:37:LEU:CD1	4:D:125:PHE:HB2	2.41	0.50
15:U:37:GLN:O	15:U:38:TYR:CG	2.64	0.50
15:U:39:ARG:HH11	15:U:39:ARG:HG3	1.76	0.50
15:U:50:VAL:C	15:U:51:LYS:O	2.46	0.50
20:Z:52:LEU:O	20:Z:55:GLY:HA3	2.11	0.50
23:B:1021:CLA:H112	30:B:1060:MGE:H131	1.94	0.50
3:C:274:TYR:CE1	23:C:1029:CLA:OBD	2.64	0.50
3:C:297:TYR:HA	3:C:302:TYR:CE2	2.46	0.50
3:C:328:VAL:HG12	3:C:340:TYR:HB2	1.91	0.50
3:C:62:PHE:CZ	10:K:28:ILE:HB	2.46	0.50
3:C:84:GLN:O	3:C:85:GLY:C	2.50	0.50
26:D:1050:BCR:C38	26:D:1050:BCR:C23	2.59	0.50
9:J:8:ILE:H	9:J:8:ILE:HD12	1.76	0.50
10:K:21:LEU:O	10:K:24:VAL:N	2.44	0.50
10:K:28:ILE:HD13	10:K:31:LEU:CD1	2.38	0.50
12:M:11:THR:O	12:M:14:PHE:HB3	2.10	0.50
13:O:105:ASP:O	13:O:106:GLN:HB2	2.12	0.50
13:O:242:GLU:HG3	13:O:262:GLN:HG2	1.93	0.50
1:A:116:ILE:CG2	1:A:117:PHE:N	2.74	0.50
1:A:53:ILE:HA	1:A:71:LEU:CD1	2.41	0.50
2:B:153:PHE:HD1	2:B:157:HIS:HB3	1.76	0.50
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.46	0.50
2:B:38:ALA:O	2:B:42:LEU:HB2	2.10	0.50
23:C:1031:CLA:C14	26:C:1054:BCR:H361	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LEU:CD1	23:C:1035:CLA:CMA	2.88	0.50
25:D:1042:PQ9:H252	30:L:1061:MGE:CGB	2.41	0.50
4:D:213:ILE:HG23	4:D:214:HIS:N	2.26	0.50
4:D:214:HIS:O	4:D:217:THR:HG22	2.11	0.50
1:A:239:PHE:CZ	4:D:247:VAL:HA	2.47	0.50
9:J:23:VAL:CG1	9:J:24:ILE:N	2.75	0.50
2:B:327:THR:HG21	12:M:4:ASN:HD22	1.75	0.50
15:U:58:VAL:HB	15:U:59:GLU:OE2	2.11	0.50
1:A:128:GLY:C	1:A:130:GLN:H	2.13	0.50
1:A:147:TYR:O	1:A:150:PRO:HD2	2.11	0.50
1:A:244:GLU:HG2	4:D:264:LYS:HZ1	1.76	0.50
23:B:1018:CLA:HAA2	23:B:1018:CLA:HBD	1.94	0.50
2:B:28:ALA:HB2	2:B:107:LEU:HB2	1.93	0.50
3:C:177:ALA:O	3:C:181:PHE:N	2.24	0.50
3:C:222:GLY:HA3	3:C:225:VAL:CG2	2.41	0.50
4:D:173:PHE:HD1	24:D:1039:PHO:H13	1.76	0.50
4:D:317:LYS:HG2	28:D:1064:IOD:I	2.82	0.50
5:E:74:GLN:O	5:E:75:GLN:C	2.48	0.50
13:O:62:GLN:NE2	13:O:62:GLN:HA	2.26	0.50
16:V:38:LEU:HB3	16:V:43:LYS:O	2.11	0.50
18:Y:43:ARG:HG2	18:Y:44:GLY:H	1.73	0.50
1:A:111:PRO:O	1:A:112:TYR:C	2.48	0.50
1:A:205:VAL:HG13	1:A:206:PHE:H	1.77	0.50
23:B:1019:CLA:HBB2	23:B:1021:CLA:CMB	2.41	0.50
23:B:1021:CLA:CMA	23:B:1021:CLA:H2	2.41	0.50
2:B:153:PHE:CA	23:B:1014:CLA:HMC3	2.42	0.50
2:B:292:LEU:C	2:B:294:SER:H	2.15	0.50
23:C:1033:CLA:H2	23:C:1033:CLA:H72	1.92	0.50
23:C:1037:CLA:CBC	23:C:1037:CLA:CHD	2.76	0.50
26:C:1054:BCR:C23	26:C:1054:BCR:H402	2.31	0.50
3:C:309:ALA:O	3:C:312:ALA:N	2.44	0.50
4:D:15:PHE:O	4:D:18:LEU:N	2.45	0.50
4:D:29:PHE:CD2	4:D:30:VAL:N	2.79	0.50
5:E:32:ILE:HG22	5:E:33:ALA:N	2.26	0.50
12:M:18:PRO:HG2	12:M:19:SER:H	1.77	0.50
13:O:154:SER:O	13:O:168:PHE:HA	2.11	0.50
13:O:182:PHE:C	13:O:182:PHE:CD2	2.85	0.50
13:O:206:GLU:O	13:O:207:GLU:HB3	2.11	0.50
14:T:8:PHE:HE1	28:T:1066:IOD:I	2.63	0.50
16:V:151:ILE:HD13	16:V:151:ILE:N	2.23	0.50
1:A:202:VAL:HG22	1:A:206:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:O	1:A:217:SER:N	2.43	0.50
1:A:33:PHE:HB2	1:A:129:ARG:HB2	1.94	0.50
1:A:71:LEU:O	14:T:3:THR:HG21	2.11	0.50
23:B:1011:CLA:C1D	23:B:1013:CLA:C4	2.89	0.50
23:B:1023:CLA:C4C	23:B:1024:CLA:HBC1	2.41	0.50
2:B:256:MET:HE1	2:B:268:PHE:CE2	2.47	0.50
2:B:308:LYS:O	2:B:312:TYR:HD2	1.94	0.50
2:B:57:ARG:HD2	2:B:311:PHE:CZ	2.46	0.50
3:C:348:GLU:H	13:O:42:ALA:HB3	1.76	0.50
3:C:438:LEU:O	3:C:442:LEU:HD12	2.11	0.50
1:A:221:SER:HA	4:D:139:ARG:HB2	1.93	0.50
4:D:194:ASN:O	4:D:195:PRO:C	2.50	0.50
4:D:196:PHE:HB3	4:D:281:MET:O	2.12	0.50
8:I:30:ARG:NH1	8:I:30:ARG:HG3	2.25	0.50
13:O:55:ALA:HB2	13:O:163:THR:HB	1.94	0.50
2:B:434:THR:OG1	13:O:204:LYS:HD3	2.11	0.50
3:C:359:TRP:HZ3	13:O:33:TYR:HH	1.58	0.50
13:O:52:ALA:HA	13:O:230:VAL:O	2.11	0.50
30:D:1062:MGE:H7A2	14:T:21:ILE:HD11	1.94	0.50
15:U:64:ILE:HB	15:U:67:LEU:CD1	2.38	0.50
18:Y:43:ARG:CD	20:Z:31:GLN:NE2	2.75	0.50
1:A:120:LEU:HD11	1:A:155:PHE:CE1	2.46	0.50
1:A:139:MET:O	1:A:140:ARG:C	2.48	0.50
1:A:55:ALA:H	1:A:70:SER:HB2	1.77	0.50
2:B:456:ALA:CA	29:B:1058:DGD:HBV1	2.42	0.50
3:C:274:TYR:HE2	23:C:1031:CLA:HMC2	1.74	0.50
23:C:1031:CLA:H142	26:C:1054:BCR:H362	1.91	0.50
3:C:222:GLY:HA3	29:C:1055:DGD:O1B	2.12	0.50
29:C:1057:DGD:HB81	30:D:1059:MGE:C8B	2.24	0.50
3:C:307:PRO:HA	3:C:358:PHE:CE1	2.47	0.50
4:D:218:VAL:CG1	4:D:219:GLU:N	2.74	0.50
4:D:269:PHE:O	4:D:272:LEU:N	2.38	0.50
7:H:35:MET:SD	26:H:1049:BCR:H333	2.51	0.50
10:K:31:LEU:O	10:K:34:ALA:HB3	2.12	0.50
11:L:5:PRO:O	11:L:7:ARG:N	2.44	0.50
13:O:150:ASN:HD22	13:O:173:ASN:CB	2.24	0.50
13:O:200:LEU:HB3	13:O:203:ALA:HB2	1.94	0.50
13:O:221:GLY:O	13:O:222:GLN:CB	2.59	0.50
15:U:32:ILE:HG12	15:U:32:ILE:O	2.12	0.50
15:U:42:TYR:O	15:U:43:PRO:C	2.50	0.50
16:V:36:VAL:HG12	16:V:150:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:46:THR:O	16:V:47:LEU:CB	2.58	0.50
16:V:58:LEU:O	16:V:59:PHE:C	2.49	0.50
1:A:126:TYR:CD2	1:A:126:TYR:O	2.58	0.50
1:A:189:GLU:O	3:C:411:ALA:HB2	2.11	0.50
23:B:1012:CLA:HMB1	23:B:1015:CLA:HBB1	1.90	0.50
23:B:1021:CLA:O1A	23:B:1021:CLA:C2	2.60	0.50
1:A:322:ASN:OD1	3:C:412:THR:HB	2.12	0.50
3:C:63:TRP:HE1	23:C:1028:CLA:C3C	2.24	0.50
4:D:191:TRP:HH2	4:D:285:GLY:HA3	1.77	0.50
8:I:29:ALA:O	8:I:30:ARG:CB	2.59	0.50
9:J:19:MET:O	9:J:23:VAL:N	2.45	0.50
3:C:73:ALA:O	10:K:10:LYS:N	2.45	0.50
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.42	0.50
1:A:279:ARG:NE	24:A:1038:PHO:HMC1	2.27	0.49
1:A:205:VAL:HG13	1:A:206:PHE:N	2.27	0.49
1:A:224:ILE:CD1	1:A:225:ARG:H	2.24	0.49
23:C:1027:CLA:C15	26:Z:1053:BCR:C33	2.87	0.49
1:A:200:LEU:HD11	29:C:1057:DGD:HA92	1.93	0.49
3:C:146:PHE:O	3:C:147:PHE:CB	2.59	0.49
3:C:152:LYS:O	3:C:154:LYS:N	2.45	0.49
3:C:175:LEU:HD23	3:C:176:VAL:N	2.27	0.49
3:C:324:LEU:CD2	15:U:32:ILE:HD13	2.43	0.49
3:C:79:LYS:HB3	3:C:84:GLN:HE21	1.75	0.49
4:D:300:SER:HA	12:M:2:GLU:O	2.12	0.49
5:E:51:ARG:O	5:E:53:ASP:N	2.45	0.49
5:E:27:ILE:HG13	31:F:1040:HEM:HMB1	1.94	0.49
13:O:181:ASN:O	13:O:182:PHE:CB	2.60	0.49
13:O:59:ASP:HB2	13:O:62:GLN:HB2	1.94	0.49
15:U:84:VAL:CG1	15:U:85:THR:N	2.75	0.49
16:V:35:THR:HG23	16:V:46:THR:HA	1.94	0.49
1:A:227:THR:OG1	1:A:228:THR:N	2.45	0.49
1:A:302:PHE:HB3	1:A:305:SER:OG	2.12	0.49
1:A:53:ILE:HA	1:A:71:LEU:HD13	1.93	0.49
23:B:1015:CLA:HBB1	23:B:1015:CLA:HHC	1.95	0.49
23:B:1020:CLA:O2A	23:B:1020:CLA:C4	2.59	0.49
2:B:308:LYS:HG2	2:B:312:TYR:CE2	2.47	0.49
2:B:363:PHE:H	2:B:363:PHE:HD2	1.57	0.49
4:D:103:ARG:HD3	4:D:106:GLN:HE21	1.74	0.49
4:D:261:PHE:HB2	25:D:1042:PQ9:C10	2.42	0.49
4:D:33:SER:OG	4:D:128:ARG:HG3	2.11	0.49
4:D:246:MET:CE	4:D:264:LYS:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:ARG:HH11	4:D:26:ARG:HG3	1.76	0.49
4:D:32:TRP:CE3	4:D:35:ILE:HD11	2.47	0.49
4:D:48:TRP:CZ2	4:D:52:THR:HG21	2.47	0.49
5:E:34:GLY:HA2	6:F:32:PHE:CD1	2.46	0.49
7:H:38:PHE:CZ	7:H:42:LEU:HD21	2.47	0.49
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.94	0.49
16:V:67:HIS:CE1	16:V:80:LEU:HD11	2.47	0.49
26:A:1044:BCR:C33	26:A:1044:BCR:C8	2.86	0.49
23:B:1021:CLA:O1A	23:B:1021:CLA:O2D	2.30	0.49
29:B:1058:DGD:C6D	29:B:1058:DGD:C5E	2.90	0.49
2:B:277:SER:C	2:B:279:TYR:H	2.13	0.49
2:B:325:PHE:O	2:B:327:THR:HG23	2.12	0.49
23:C:1027:CLA:H141	26:Z:1053:BCR:H333	1.94	0.49
3:C:39:ASN:CB	23:C:1032:CLA:HBA1	2.35	0.49
3:C:62:PHE:HB2	3:C:122:SER:CB	2.42	0.49
3:C:146:PHE:C	3:C:147:PHE:CG	2.85	0.49
3:C:344:SER:OG	3:C:345:PRO:HD2	2.12	0.49
3:C:71:GLU:OE1	3:C:89:ILE:HB	2.12	0.49
4:D:109:GLY:C	4:D:111:TRP:N	2.62	0.49
1:A:321:ILE:CD1	4:D:176:ALA:HB1	2.17	0.49
4:D:195:PRO:HA	4:D:198:MET:SD	2.53	0.49
4:D:249:ALA:O	4:D:252:PHE:HB3	2.11	0.49
5:E:65:LEU:HD13	5:E:66:VAL:N	2.27	0.49
6:F:29:PRO:O	6:F:32:PHE:HB3	2.11	0.49
7:H:34:PHE:CD2	23:H:1017:CLA:HAC1	2.47	0.49
7:H:19:GLY:O	7:H:21:VAL:HG12	2.11	0.49
7:H:54:ILE:HG22	7:H:55:LEU:N	2.27	0.49
9:J:38:SER:O	9:J:39:SER:CB	2.59	0.49
13:O:125:ASP:CG	13:O:126:GLY:N	2.66	0.49
13:O:223:ILE:HG22	13:O:243:SER:CB	2.36	0.49
15:U:94:GLY:O	15:U:95:GLY:C	2.51	0.49
20:Z:25:VAL:O	20:Z:28:ALA:HB3	2.12	0.49
23:A:1006:CLA:H143	25:A:1043:PQ9:H443	1.94	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.33	0.49
1:A:215:HIS:O	1:A:219:VAL:HG23	2.11	0.49
1:A:218:LEU:CD2	1:A:218:LEU:N	2.75	0.49
1:A:279:ARG:CZ	1:A:283:VAL:HG21	2.42	0.49
23:B:1021:CLA:HBD	23:B:1021:CLA:HAA2	1.94	0.49
2:B:16:PRO:O	2:B:20:ILE:HG12	2.12	0.49
2:B:53:ASN:N	2:B:54:PRO:CD	2.74	0.49
3:C:45:LEU:CD2	3:C:141:GLU:OE1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:MET:HE2	3:C:319:ILE:HG13	1.94	0.49
1:A:135:TYR:CD1	3:C:449:ARG:HG3	2.48	0.49
23:D:1005:CLA:HMA2	25:D:1042:PQ9:C44	2.40	0.49
4:D:230:SER:C	4:D:232:PHE:H	2.15	0.49
10:K:37:PHE:HB2	26:K:1051:BCR:H401	1.94	0.49
18:Y:28:ILE:HG12	18:Y:29:GLY:N	2.27	0.49
23:C:1027:CLA:H141	26:Z:1053:BCR:C33	2.42	0.49
23:B:1011:CLA:C4A	23:B:1011:CLA:H11	2.42	0.49
23:B:1019:CLA:HMA1	23:B:1020:CLA:C2C	2.43	0.49
2:B:168:VAL:CG1	2:B:169:SER:N	2.76	0.49
2:B:308:LYS:HG2	2:B:312:TYR:HE2	1.78	0.49
23:C:1030:CLA:HBC3	23:C:1030:CLA:CHD	2.37	0.49
3:C:179:ALA:CA	3:C:199:ILE:HD13	2.42	0.49
3:C:265:ILE:CG2	3:C:270:ALA:CB	2.90	0.49
5:E:10:PHE:O	5:E:11:SER:C	2.51	0.49
5:E:31:PHE:O	6:F:35:GLY:HA3	2.13	0.49
6:F:19:ARG:HH22	31:F:1040:HEM:CAC	2.17	0.49
13:O:100:GLU:C	13:O:102:THR:H	2.16	0.49
16:V:138:LEU:O	16:V:139:VAL:C	2.50	0.49
1:A:265:PHE:CE1	25:A:1043:PQ9:H143	2.48	0.49
1:A:113:GLN:HA	1:A:116:ILE:HG22	1.95	0.49
1:A:183:MET:C	23:A:1003:CLA:HBC1	2.32	0.49
1:A:224:ILE:HB	1:A:245:THR:O	2.12	0.49
1:A:303:ASN:ND2	1:A:303:ASN:N	2.60	0.49
1:A:71:LEU:HD12	1:A:71:LEU:H	1.77	0.49
2:B:97:ALA:O	2:B:99:ALA:N	2.45	0.49
23:C:1027:CLA:HMB2	23:C:1027:CLA:H52	1.93	0.49
3:C:187:ASP:CG	3:C:190:ALA:H	2.15	0.49
3:C:209:ILE:HD12	3:C:239:TRP:CD1	2.48	0.49
3:C:270:ALA:O	3:C:273:SER:HB3	2.12	0.49
3:C:286:ALA:HB2	23:C:1026:CLA:HMD3	1.94	0.49
3:C:296:VAL:HG23	3:C:297:TYR:HD1	1.70	0.49
3:C:342:MET:HG2	3:C:343:ARG:H	1.77	0.49
3:C:400:PRO:O	3:C:401:LEU:HD22	2.12	0.49
4:D:152:VAL:HB	23:D:1004:CLA:H43	1.94	0.49
25:D:1042:PQ9:H391	25:D:1042:PQ9:H42	0.62	0.49
4:D:73:PHE:HB2	30:D:1059:MGE:H2B2	1.95	0.49
1:A:219:VAL:HB	4:D:268:HIS:HB3	1.95	0.49
4:D:32:TRP:HB2	4:D:131:GLU:OE1	2.11	0.49
4:D:61:HIS:CE1	4:D:80:THR:CG2	2.96	0.49
7:H:34:PHE:CE2	23:H:1017:CLA:HAC1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:40:VAL:O	7:H:44:ILE:HG12	2.13	0.49
13:O:116:ASP:OD2	13:O:157:PRO:HB3	2.12	0.49
13:O:239:GLY:O	13:O:265:PHE:N	2.44	0.49
16:V:96:GLU:O	16:V:99:VAL:N	2.39	0.49
18:Y:43:ARG:NE	18:Y:43:ARG:N	2.61	0.49
24:A:1038:PHO:C2A	24:A:1038:PHO:O1D	2.57	0.49
1:A:161:TYR:CE2	1:A:186:PHE:HE2	2.30	0.49
1:A:187:GLN:NE2	1:A:193:LEU:HB2	2.27	0.49
1:A:271:LEU:O	1:A:272:HIS:C	2.49	0.49
2:B:115:TRP:HB3	28:B:1067:IOD:I	2.82	0.49
2:B:463:PHE:CE1	23:B:1016:CLA:CBB	2.89	0.49
1:A:225:ARG:CB	2:B:484:PRO:HD3	2.43	0.49
2:B:69:LEU:CD1	23:B:1011:CLA:OBD	2.59	0.49
2:B:6:TYR:CD2	2:B:6:TYR:N	2.76	0.49
3:C:105:VAL:O	3:C:105:VAL:CG2	2.61	0.49
3:C:72:LEU:CD1	3:C:112:PHE:HB2	2.43	0.49
3:C:29:GLU:HA	3:C:41:ARG:HH11	1.74	0.49
3:C:438:LEU:CD1	3:C:442:LEU:HD11	2.42	0.49
4:D:101:PHE:CG	4:D:101:PHE:O	2.65	0.49
4:D:279:LEU:CD2	24:D:1039:PHO:HMC1	2.43	0.49
1:A:142:TRP:HE1	4:D:219:GLU:CB	2.25	0.49
1:A:139:MET:HE1	4:D:248:THR:HG22	1.93	0.49
4:D:273:PHE:CE2	30:L:1061:MGE:H5B1	2.47	0.49
9:J:10:LEU:O	9:J:13:VAL:CG1	2.60	0.49
13:O:128:ASP:OD1	13:O:149:LYS:CG	2.61	0.49
16:V:114:ILE:CD1	31:V:1041:HEM:HBD2	2.43	0.49
16:V:138:LEU:O	16:V:141:ILE:HG22	2.12	0.49
16:V:38:LEU:HA	16:V:45:ILE:HD11	1.94	0.49
16:V:64:ALA:O	16:V:68:VAL:N	2.46	0.49
1:A:201:GLY:C	1:A:203:ALA:N	2.65	0.49
2:B:120:LEU:HD23	2:B:120:LEU:N	2.28	0.49
2:B:201:HIS:HD2	2:B:202:HIS:CD2	2.30	0.49
2:B:354:LEU:C	2:B:355:PHE:CD2	2.84	0.49
2:B:401:PHE:CZ	2:B:406:LEU:HD23	2.47	0.49
2:B:80:ILE:O	2:B:80:ILE:HG22	2.11	0.49
3:C:137:PRO:C	3:C:139:THR:N	2.66	0.49
3:C:149:TYR:O	3:C:150:ASP:HB2	2.13	0.49
3:C:39:ASN:HB3	23:C:1033:CLA:CBB	2.43	0.49
3:C:438:LEU:HD13	3:C:442:LEU:HD11	1.94	0.49
23:D:1004:CLA:HHD	23:D:1004:CLA:HBC3	1.95	0.49
2:B:460:LEU:HD12	4:D:159:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:THR:HA	4:D:111:TRP:CD1	2.47	0.49
4:D:91:LEU:HD23	4:D:93:TRP:CE2	2.47	0.49
6:F:28:VAL:HB	6:F:29:PRO:CD	2.38	0.49
7:H:12:ARG:O	7:H:12:ARG:NH1	2.45	0.49
4:D:88:SER:CA	7:H:50:ASN:HD21	2.03	0.49
9:J:39:SER:O	9:J:40:LEU:HD23	2.13	0.49
16:V:62:ALA:CB	31:V:1041:HEM:HBB1	2.42	0.49
18:Y:30:ILE:O	18:Y:30:ILE:HD13	2.12	0.49
18:Y:43:ARG:H	18:Y:43:ARG:NH1	2.09	0.49
1:A:257:ARG:O	1:A:259:ILE:N	2.46	0.49
1:A:52:PHE:C	1:A:71:LEU:HD12	2.33	0.49
23:B:1014:CLA:CB	23:B:1014:CLA:HBA1	2.43	0.49
2:B:462:PHE:HA	23:B:1019:CLA:HMC1	1.95	0.49
2:B:302:TRP:C	2:B:304:ALA:N	2.66	0.49
2:B:52:LEU:CD2	2:B:311:PHE:HD1	2.20	0.49
2:B:338:GLN:O	2:B:339:ALA:HB2	2.13	0.49
2:B:418:LYS:O	2:B:421:ALA:N	2.43	0.49
2:B:457:VAL:CG1	4:D:284:ILE:HG23	2.43	0.49
3:C:88:LEU:CD1	23:C:1027:CLA:HBC2	2.42	0.49
4:D:148:ALA:CB	4:D:149:PRO:HD3	2.29	0.49
4:D:193:LEU:HA	4:D:198:MET:CE	2.43	0.49
23:B:1016:CLA:H51	23:H:1017:CLA:H91	1.76	0.49
23:K:1034:CLA:O2D	23:K:1034:CLA:O1A	2.30	0.49
12:M:21:PHE:CE1	12:M:25:LEU:HG	2.47	0.49
14:T:19:PHE:HD2	14:T:19:PHE:N	2.10	0.49
16:V:103:LYS:CE	16:V:138:LEU:HD12	2.43	0.49
16:V:95:ILE:HA	16:V:146:LEU:HD11	1.95	0.49
1:A:181:ASN:HD21	4:D:317:LYS:HZ2	1.60	0.49
1:A:258:LEU:O	1:A:259:ILE:HG13	2.12	0.49
1:A:290:ILE:HA	1:A:290:ILE:HD12	1.65	0.49
1:A:48:PHE:O	1:A:50:ILE:N	2.46	0.49
1:A:76:ASN:HD21	11:L:33:SER:C	2.15	0.49
23:B:1010:CLA:HED3	23:B:1011:CLA:CMA	2.43	0.49
23:B:1020:CLA:H111	23:B:1020:CLA:H162	1.95	0.49
26:B:1047:BCR:C22	26:B:1047:BCR:H392	2.35	0.49
2:B:297:THR:HB	2:B:300:GLU:H	1.78	0.49
2:B:30:VAL:HG13	23:B:1013:CLA:CMD	2.43	0.49
2:B:486:LEU:O	2:B:488:PRO:HD3	2.12	0.49
2:B:95:GLY:O	2:B:99:ALA:HB2	2.13	0.49
23:C:1030:CLA:HBD	23:C:1030:CLA:HAA1	1.95	0.49
23:C:1031:CLA:H2	23:C:1031:CLA:HMA2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:PHE:O	3:C:182:PHE:HD2	1.96	0.49
3:C:314:ALA:HB1	3:C:351:PHE:HD1	1.78	0.49
3:C:316:THR:HG21	16:V:74:THR:HG23	1.94	0.49
3:C:437:PHE:O	3:C:440:GLY:N	2.46	0.49
23:D:1005:CLA:C15	23:D:1005:CLA:H202	2.42	0.49
4:D:16:ASP:O	4:D:20:ASP:N	2.45	0.49
4:D:302:GLU:O	4:D:305:ALA:HB3	2.13	0.49
4:D:33:SER:OG	4:D:128:ARG:HG2	2.12	0.49
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.28	0.49
7:H:4:ARG:O	7:H:5:THR:CG2	2.60	0.49
8:I:10:ILE:N	8:I:10:ILE:HD13	2.28	0.49
3:C:70:PHE:CD1	10:K:26:PRO:HG3	2.48	0.49
13:O:148:VAL:HA	13:O:172:PHE:CE2	2.47	0.49
15:U:25:ILE:HD11	15:U:34:ALA:O	2.13	0.49
16:V:109:ASP:OD1	16:V:111:GLU:HG3	2.12	0.49
16:V:70:GLY:O	16:V:157:GLY:O	2.30	0.49
20:Z:53:VAL:HG12	20:Z:57:LEU:HD12	1.95	0.49
1:A:148:SER:O	1:A:149:ALA:C	2.50	0.48
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.48	0.48
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.46	0.48
1:A:316:THR:C	1:A:318:ALA:H	2.15	0.48
1:A:76:ASN:ND2	11:L:33:SER:CB	2.67	0.48
1:A:78:ILE:N	1:A:78:ILE:CD1	2.76	0.48
23:B:1009:CLA:CMB	26:H:1049:BCR:C27	2.69	0.48
2:B:149:LEU:CD2	23:B:1011:CLA:HBC1	2.43	0.48
23:B:1019:CLA:CBA	23:B:1019:CLA:CBD	2.92	0.48
2:B:174:LEU:CD2	2:B:312:TYR:CE1	2.95	0.48
2:B:327:THR:HG23	11:L:37:ASN:ND2	2.28	0.48
23:C:1035:CLA:CMB	26:C:1052:BCR:C27	2.90	0.48
23:C:1028:CLA:H18	29:C:1056:DGD:HA51	1.94	0.48
3:C:189:TRP:O	3:C:190:ALA:C	2.51	0.48
3:C:311:GLN:O	3:C:314:ALA:HB3	2.13	0.48
3:C:315:MET:CE	3:C:315:MET:HA	2.43	0.48
3:C:284:PHE:HE1	3:C:431:PHE:CD2	2.31	0.48
23:D:1005:CLA:CBA	25:D:1042:PQ9:H412	2.38	0.48
4:D:54:PHE:CB	5:E:47:PHE:CD1	2.96	0.48
15:U:16:LYS:HZ1	15:U:85:THR:HB	1.78	0.48
20:Z:14:ILE:O	20:Z:18:VAL:HG23	2.13	0.48
20:Z:15:LEU:HD11	20:Z:46:LEU:HG	1.95	0.48
26:A:1044:BCR:HC7	8:I:15:PHE:HZ	1.78	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1010:CLA:O2D	23:B:1010:CLA:O1A	2.30	0.48
2:B:18:ARG:NH1	11:L:4:ASN:HB3	2.28	0.48
2:B:355:PHE:CD2	2:B:355:PHE:N	2.81	0.48
23:C:1035:CLA:H93	26:C:1052:BCR:C40	2.42	0.48
3:C:459:ILE:N	4:D:224:GLN:H	2.08	0.48
3:C:50:LEU:CD2	3:C:51:GLY:HA2	2.43	0.48
25:D:1042:PQ9:C24	30:L:1061:MGE:CGB	2.81	0.48
4:D:319:LEU:O	4:D:323:GLU:HG3	2.13	0.48
4:D:53:THR:CG2	4:D:67:TYR:HD2	2.26	0.48
7:H:38:PHE:O	7:H:41:PHE:HB3	2.14	0.48
11:L:5:PRO:HG2	11:L:6:ASN:H	1.78	0.48
13:O:172:PHE:CG	13:O:221:GLY:HA3	2.48	0.48
2:B:384:ARG:CD	15:U:102:LEU:HD21	2.42	0.48
15:U:44:THR:O	15:U:45:LEU:C	2.51	0.48
16:V:148:GLU:N	16:V:149:PRO:HD2	2.29	0.48
20:Z:37:LYS:HG3	20:Z:38:GLN:N	2.28	0.48
24:A:1038:PHO:C4C	4:D:209:LEU:HG	2.43	0.48
1:A:308:ASP:OD1	1:A:312:ASN:O	2.31	0.48
1:A:323:ARG:NE	4:D:332:GLN:HE22	2.11	0.48
1:A:37:MET:O	1:A:38:ILE:C	2.51	0.48
23:B:1015:CLA:OBD	23:B:1015:CLA:CED	2.38	0.48
2:B:137:LYS:HG3	2:B:217:ILE:HA	1.95	0.48
2:B:271:THR:HG23	2:B:274:GLN:CB	2.42	0.48
2:B:324:LEU:HA	4:D:293:LEU:CD2	2.31	0.48
3:C:406:SER:CB	29:C:1056:DGD:HE1	2.39	0.48
24:D:1039:PHO:HMA3	23:D:1004:CLA:C14	2.39	0.48
23:D:1008:CLA:H61	23:D:1008:CLA:H101	1.69	0.48
4:D:24:ARG:HA	4:D:24:ARG:HE	1.77	0.48
2:B:257:TRP:CD2	4:D:291:LEU:HD22	2.48	0.48
4:D:302:GLU:HA	4:D:305:ALA:HB2	1.96	0.48
4:D:342:PRO:HD2	4:D:345:VAL:HG21	1.94	0.48
5:E:13:ILE:CG1	5:E:19:TYR:HB2	2.43	0.48
6:F:19:ARG:NH2	6:F:20:TRP:CD1	2.81	0.48
13:O:69:LEU:HD11	13:O:71:LEU:CD2	2.43	0.48
16:V:160:LYS:O	16:V:163:TYR:HB2	2.13	0.48
16:V:39:ASN:HD22	16:V:40:SER:H	1.59	0.48
16:V:35:THR:CA	16:V:46:THR:HA	2.43	0.48
1:A:129:ARG:O	4:D:256:ILE:HD13	2.13	0.48
1:A:200:LEU:CD2	29:C:1057:DGD:HBW2	2.43	0.48
23:B:1022:CLA:H141	23:B:1022:CLA:H62	1.75	0.48
2:B:373:LYS:HG2	2:B:373:LYS:H	1.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:TRP:N	2:B:5:TRP:CD1	2.76	0.48
3:C:155:ASN:O	3:C:158:THR:CG2	2.61	0.48
3:C:414:ILE:CG2	3:C:415:ASN:N	2.76	0.48
3:C:449:ARG:HB2	23:C:1029:CLA:CED	2.43	0.48
3:C:46:SER:OG	3:C:141:GLU:CB	2.60	0.48
3:C:87:ILE:O	3:C:90:PRO:CG	2.61	0.48
26:D:1050:BCR:C20	30:D:1059:MGE:C5A	2.88	0.48
6:F:22:ALA:C	6:F:24:HIS:N	2.62	0.48
26:K:1051:BCR:C8	26:K:1051:BCR:H311	2.44	0.48
11:L:36:PHE:CZ	14:T:2:GLU:HB3	2.48	0.48
13:O:162:ILE:CD1	13:O:269:ILE:HD12	2.43	0.48
16:V:160:LYS:N	16:V:163:TYR:CE1	2.78	0.48
4:D:17:ILE:HD12	17:X:41:SER:HG	1.79	0.48
18:Y:19:ILE:HG22	18:Y:20:ALA:N	2.28	0.48
1:A:118:HIS:O	1:A:121:LEU:HB3	2.13	0.48
1:A:184:ILE:CD1	4:D:186:GLN:HE22	2.26	0.48
2:B:62:VAL:HG13	23:B:1013:CLA:HED2	1.95	0.48
2:B:196:GLY:C	2:B:198:VAL:H	2.17	0.48
2:B:326:ARG:HH11	4:D:297:ASP:CA	2.11	0.48
23:C:1026:CLA:H122	23:C:1026:CLA:C6	2.44	0.48
3:C:46:SER:CB	3:C:141:GLU:N	2.77	0.48
3:C:171:GLY:O	3:C:172:ALA:C	2.52	0.48
3:C:212:TYR:HB3	3:C:223:TRP:O	2.13	0.48
24:D:1039:PHO:HMA2	23:D:1004:CLA:H102	1.94	0.48
4:D:209:LEU:HD23	4:D:209:LEU:C	2.33	0.48
5:E:7:GLU:OE2	6:F:19:ARG:HB2	2.13	0.48
8:I:16:VAL:O	8:I:20:VAL:CG2	2.61	0.48
1:A:96:ILE:HD12	23:A:1007:CLA:CMD	2.43	0.48
1:A:142:TRP:CH2	27:A:1063:LHG:HC5	2.47	0.48
1:A:279:ARG:CG	4:D:212:ALA:HB2	2.43	0.48
23:B:1018:CLA:H18	23:B:1023:CLA:HMD2	1.95	0.48
2:B:135:LEU:HA	2:B:138:MET:HB3	1.95	0.48
2:B:25:MET:O	2:B:28:ALA:N	2.47	0.48
2:B:83:GLU:HG2	2:B:86:ILE:CD1	2.32	0.48
23:C:1032:CLA:HBA2	23:C:1032:CLA:H3A	1.40	0.48
3:C:176:VAL:HA	3:C:234:VAL:HG23	1.95	0.48
3:C:272:LEU:HD12	3:C:272:LEU:O	2.13	0.48
3:C:370:ARG:HG3	3:C:371:GLY:N	2.28	0.48
3:C:465:PRO:O	3:C:469:MET:HG3	2.13	0.48
5:E:47:PHE:O	5:E:49:THR:N	2.41	0.48
26:D:1050:BCR:H363	6:F:30:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7:LEU:HA	7:H:10:ILE:HD12	1.94	0.48
8:I:1:MET:O	8:I:3:THR:N	2.47	0.48
2:B:18:ARG:HH11	11:L:4:ASN:HD22	1.60	0.48
11:L:8:GLN:HE21	11:L:8:GLN:N	2.07	0.48
13:O:147:THR:OG1	13:O:149:LYS:HG3	2.13	0.48
15:U:100:ASN:OD1	15:U:100:ASN:O	2.32	0.48
18:Y:35:ILE:C	18:Y:35:ILE:HD13	2.34	0.48
1:A:161:TYR:CZ	1:A:186:PHE:HE2	2.31	0.48
1:A:302:PHE:CD1	1:A:302:PHE:N	2.82	0.48
2:B:162:PHE:CD2	23:B:1014:CLA:HBC1	2.48	0.48
2:B:12:LEU:CD1	23:B:1020:CLA:HMC2	2.39	0.48
2:B:8:VAL:HG21	23:B:1022:CLA:C3D	2.44	0.48
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.96	0.48
2:B:61:PHE:C	2:B:64:PRO:HD2	2.34	0.48
23:C:1037:CLA:H8	23:C:1037:CLA:H142	1.96	0.48
3:C:263:ALA:HB1	3:C:264:PHE:CD2	2.45	0.48
1:A:340:PRO:HG3	3:C:317:PHE:CZ	2.48	0.48
4:D:127:LEU:O	4:D:130:PHE:N	2.45	0.48
4:D:155:SER:HA	4:D:159:ILE:CB	2.44	0.48
23:A:1006:CLA:HED3	4:D:175:VAL:HG13	1.96	0.48
4:D:183:LEU:HD23	4:D:183:LEU:N	2.14	0.48
4:D:19:ASP:O	4:D:20:ASP:C	2.51	0.48
1:A:272:HIS:NE2	4:D:214:HIS:NE2	2.61	0.48
9:J:25:VAL:HA	9:J:28:PHE:CD2	2.43	0.48
19:N:1:UNK:O	19:N:2:UNK:CB	2.62	0.48
13:O:128:ASP:OD1	13:O:149:LYS:HG2	2.13	0.48
13:O:163:THR:O	13:O:165:SER:N	2.46	0.48
13:O:224:SER:C	13:O:225:LEU:HD12	2.33	0.48
14:T:1:MET:HG2	14:T:2:GLU:N	2.27	0.48
15:U:78:ASN:O	15:U:80:GLU:N	2.46	0.48
16:V:36:VAL:HG21	16:V:146:LEU:HD12	1.95	0.48
16:V:154:ASP:O	16:V:156:TRP:N	2.47	0.48
18:Y:39:LEU:CD2	20:Z:28:ALA:HB1	2.42	0.48
1:A:124:SER:OG	1:A:155:PHE:HE2	1.97	0.48
1:A:202:VAL:HG22	1:A:206:PHE:HD1	1.78	0.48
23:B:1022:CLA:H201	23:B:1022:CLA:C3D	2.44	0.48
23:B:1022:CLA:C2	23:B:1022:CLA:H203	2.44	0.48
26:B:1048:BCR:C8	26:B:1048:BCR:C33	2.81	0.48
29:C:1056:DGD:HB81	29:C:1056:DGD:HBF1	1.95	0.48
3:C:305:THR:HG23	3:C:308:GLU:H	1.79	0.48
3:C:87:ILE:O	3:C:91:HIS:CE1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:LEU:C	3:C:90:PRO:HD2	2.34	0.48
4:D:49:LEU:HD13	26:D:1050:BCR:C15	2.44	0.48
2:B:460:LEU:HD23	4:D:280:TRP:CZ3	2.49	0.48
6:F:20:TRP:HE1	31:F:1040:HEM:CHD	2.27	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HD3	2.14	0.48
13:O:69:LEU:HD12	13:O:70:CYS:N	2.28	0.48
14:T:18:PHE:CD1	26:T:6046:BCR:H332	2.48	0.48
15:U:17:LEU:HD23	15:U:17:LEU:O	2.13	0.48
23:A:1003:CLA:CGA	23:A:1003:CLA:CED	2.92	0.48
25:A:1043:PQ9:H453	25:A:1043:PQ9:H401	1.96	0.48
1:A:111:PRO:HG2	1:A:112:TYR:N	2.28	0.48
23:B:1023:CLA:H93	23:B:1024:CLA:H152	1.95	0.48
2:B:30:VAL:O	2:B:31:ALA:C	2.50	0.48
2:B:334:ASP:N	2:B:334:ASP:OD2	2.32	0.48
2:B:40:TYR:O	2:B:43:ALA:N	2.46	0.48
2:B:55:MET:CE	2:B:80:ILE:HG21	2.33	0.48
3:C:117:VAL:HG11	23:C:1027:CLA:H12	1.94	0.48
23:C:1035:CLA:CBB	23:K:1034:CLA:CMA	2.91	0.48
23:C:1037:CLA:HBA2	23:C:1037:CLA:H3A	1.44	0.48
3:C:157:MET:HB3	23:C:1031:CLA:HBC1	1.95	0.48
3:C:351:PHE:CZ	3:C:366:LEU:HD11	2.48	0.48
5:E:13:ILE:HD12	5:E:16:SER:CB	2.44	0.48
26:K:1051:BCR:H392	26:K:1051:BCR:H23C	1.96	0.48
3:C:324:LEU:HD11	15:U:42:TYR:OH	2.13	0.48
23:A:1006:CLA:HBC1	4:D:182:LEU:CD2	2.41	0.48
1:A:283:VAL:HG21	24:A:1038:PHO:HMC1	1.95	0.48
1:A:199:GLN:C	1:A:201:GLY:N	2.67	0.48
1:A:228:THR:CG2	1:A:229:GLU:H	2.10	0.48
1:A:288:LEU:HD21	3:C:435:PHE:CD2	2.49	0.48
23:B:1010:CLA:H151	29:B:1058:DGD:C8A	2.38	0.48
23:B:1022:CLA:C20	23:B:1022:CLA:H11	2.43	0.48
23:B:1022:CLA:O1D	23:B:1022:CLA:C1	2.62	0.48
3:C:212:TYR:O	3:C:215:LYS:HB2	2.13	0.48
3:C:342:MET:HB2	3:C:352:GLY:HA3	1.96	0.48
4:D:189:HIS:O	4:D:190:ASN:C	2.52	0.48
4:D:251:ARG:HH22	4:D:255:GLN:NE2	2.10	0.48
4:D:82:ALA:C	4:D:84:SER:H	2.16	0.48
5:E:23:HIS:HB3	5:E:27:ILE:HD13	1.95	0.48
1:A:119:PHE:CD1	24:A:1038:PHO:H122	2.50	0.47
25:A:1043:PQ9:H241	25:A:1043:PQ9:H27	1.95	0.47
1:A:131:TRP:HD1	1:A:141:PRO:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:HE2	4:D:183:LEU:HD13	1.94	0.47
2:B:302:TRP:C	2:B:304:ALA:H	2.16	0.47
2:B:174:LEU:CD2	2:B:312:TYR:CZ	2.94	0.47
23:C:1033:CLA:H141	23:C:1036:CLA:CMD	2.44	0.47
3:C:117:VAL:HG11	23:C:1027:CLA:H11	1.95	0.47
3:C:164:HIS:H	3:C:164:HIS:HD1	1.61	0.47
3:C:466:VAL:C	3:C:468:SER:H	2.16	0.47
3:C:60:ILE:HG22	23:K:1034:CLA:CMD	2.42	0.47
4:D:275:PRO:O	4:D:276:VAL:C	2.52	0.47
2:B:457:VAL:CG2	4:D:284:ILE:HG23	2.44	0.47
1:A:65:GLU:OE1	4:D:312:GLU:OE2	2.31	0.47
6:F:22:ALA:C	6:F:24:HIS:H	2.17	0.47
7:H:10:ILE:HG22	7:H:10:ILE:O	2.14	0.47
10:K:28:ILE:HA	10:K:31:LEU:CD1	2.43	0.47
12:M:8:PHE:O	12:M:12:ALA:HB3	2.13	0.47
13:O:151:LEU:HD12	13:O:171:GLU:O	2.13	0.47
16:V:114:ILE:O	16:V:114:ILE:CG1	2.62	0.47
16:V:39:ASN:C	16:V:41:GLU:N	2.67	0.47
16:V:61:TYR:C	16:V:63:CYS:N	2.68	0.47
1:A:214:MET:O	1:A:217:SER:HB3	2.15	0.47
1:A:215:HIS:NE2	1:A:272:HIS:CE1	2.82	0.47
1:A:40:THR:HG21	1:A:122:GLY:N	2.25	0.47
23:B:1019:CLA:HMB2	23:B:1020:CLA:NB	2.29	0.47
23:B:1021:CLA:C11	30:B:1060:MGE:H132	2.42	0.47
2:B:355:PHE:HD2	2:B:355:PHE:N	2.11	0.47
2:B:461:LEU:O	2:B:464:PHE:HB3	2.14	0.47
2:B:49:ASP:O	2:B:49:ASP:OD1	2.32	0.47
4:D:37:LEU:CD2	4:D:128:ARG:HD3	2.27	0.47
4:D:223:PHE:CZ	4:D:245:SER:HB2	2.48	0.47
2:B:452:THR:HG22	4:D:291:LEU:HD11	1.95	0.47
4:D:33:SER:O	4:D:34:GLY:C	2.52	0.47
4:D:84:SER:O	5:E:69:ARG:HB3	2.14	0.47
2:B:122:LEU:HD21	7:H:12:ARG:N	2.29	0.47
30:D:1062:MGE:H231	11:L:26:VAL:CG2	2.44	0.47
12:M:9:ILE:O	12:M:13:LEU:HB2	2.15	0.47
16:V:101:TYR:HA	16:V:104:ASN:O	2.14	0.47
20:Z:53:VAL:C	20:Z:55:GLY:H	2.17	0.47
24:A:1038:PHO:H93	24:A:1038:PHO:H62	1.68	0.47
1:A:172:MET:HB2	1:A:182:PHE:CD2	2.50	0.47
1:A:61:ASP:HB2	1:A:63:ILE:CD1	2.44	0.47
2:B:147:GLY:HA2	2:B:150:CYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:PHE:C	2:B:215:PHE:CD2	2.88	0.47
1:A:224:ILE:O	2:B:481:GLY:HA2	2.15	0.47
2:B:90:PHE:CZ	2:B:98:LEU:HD12	2.48	0.47
23:C:1026:CLA:H62	23:C:1026:CLA:H2	1.63	0.47
29:C:1056:DGD:C5A	29:C:1056:DGD:O1A	2.62	0.47
13:O:163:THR:HG23	13:O:165:SER:H	1.78	0.47
13:O:52:ALA:O	13:O:53:ARG:CB	2.62	0.47
1:A:340:PRO:HB3	15:U:103:TYR:CD2	2.49	0.47
16:V:90:PRO:HB2	16:V:91:PRO:HD2	1.96	0.47
1:A:327:GLY:HA2	4:D:328:TRP:CD1	2.50	0.47
1:A:91:LEU:O	1:A:92:HIS:C	2.50	0.47
23:B:1018:CLA:H13	23:B:1018:CLA:OBD	2.14	0.47
2:B:171:PRO:HB3	2:B:279:TYR:OH	2.15	0.47
2:B:199:VAL:O	2:B:203:ILE:HG22	2.15	0.47
2:B:271:THR:H	2:B:274:GLN:NE2	2.13	0.47
2:B:271:THR:N	2:B:274:GLN:NE2	2.62	0.47
2:B:397:VAL:HG12	2:B:398:THR:N	2.29	0.47
2:B:400:SER:HA	2:B:410:THR:HG22	1.96	0.47
2:B:463:PHE:CD2	2:B:463:PHE:C	2.87	0.47
3:C:447:ARG:O	3:C:450:ALA:HB3	2.15	0.47
23:D:1008:CLA:HED3	23:D:1008:CLA:OBD	2.14	0.47
4:D:172:SER:OG	4:D:177:ALA:HB1	2.14	0.47
10:K:28:ILE:HA	10:K:31:LEU:CG	2.45	0.47
2:B:2:GLY:HA2	11:L:11:GLU:HB2	1.96	0.47
12:M:17:VAL:N	12:M:18:PRO:HD2	2.29	0.47
13:O:128:ASP:O	13:O:147:THR:HA	2.15	0.47
13:O:45:CYS:N	13:O:72:GLN:NE2	2.61	0.47
20:Z:27:TYR:HE2	20:Z:40:ILE:HD13	1.79	0.47
1:A:41:LEU:CD1	1:A:119:PHE:HA	2.44	0.47
1:A:259:ILE:HD12	1:A:259:ILE:O	2.15	0.47
23:B:1009:CLA:HMB2	26:H:1049:BCR:C26	2.44	0.47
2:B:122:LEU:HD21	7:H:11:LEU:HB2	1.95	0.47
2:B:346:PHE:CZ	2:B:421:ALA:HA	2.49	0.47
2:B:65:PHE:O	2:B:67:ALA:N	2.48	0.47
3:C:213:LEU:HD21	26:C:1054:BCR:H372	1.97	0.47
3:C:187:ASP:CB	3:C:190:ALA:HB2	2.44	0.47
23:D:1008:CLA:HBC2	23:D:1008:CLA:CMC	2.40	0.47
4:D:27:PHE:CD1	4:D:28:VAL:HG23	2.50	0.47
4:D:48:TRP:CE2	4:D:52:THR:HG21	2.49	0.47
6:F:32:PHE:C	6:F:32:PHE:CD1	2.87	0.47
18:Y:28:ILE:CG1	18:Y:29:GLY:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:HB2	23:B:1020:CLA:CMB	2.44	0.47
23:B:1018:CLA:H91	23:B:1023:CLA:H3A	1.96	0.47
2:B:196:GLY:O	2:B:198:VAL:N	2.47	0.47
2:B:446:SER:O	2:B:447:PRO:C	2.52	0.47
23:C:1028:CLA:O1D	29:C:1056:DGD:HE62	2.15	0.47
23:C:1029:CLA:HBD	23:C:1029:CLA:HAA1	1.97	0.47
3:C:292:PHE:CE1	29:C:1055:DGD:HD1	2.49	0.47
23:A:1006:CLA:HAA2	29:C:1057:DGD:HBN1	1.96	0.47
3:C:171:GLY:C	23:C:1025:CLA:HBC3	2.35	0.47
3:C:171:GLY:C	3:C:174:LEU:H	2.18	0.47
3:C:327:ASN:ND2	3:C:330:SER:H	2.09	0.47
30:D:1062:MGE:H251	30:D:1062:MGE:CBB	2.43	0.47
4:D:286:VAL:HG13	4:D:287:VAL:N	2.28	0.47
2:B:326:ARG:HE	4:D:297:ASP:HB2	1.78	0.47
9:J:31:GLY:O	9:J:35:GLY:CA	2.58	0.47
9:J:8:ILE:HD12	9:J:8:ILE:N	2.29	0.47
2:B:2:GLY:CA	11:L:11:GLU:HB2	2.44	0.47
15:U:35:PHE:HD1	15:U:46:ALA:HB2	1.78	0.47
20:Z:16:SER:HA	20:Z:19:MET:HB2	1.97	0.47
23:A:1006:CLA:HMB3	24:D:1039:PHO:H172	1.96	0.47
2:B:475:PHE:C	2:B:477:ASP:H	2.16	0.47
2:B:46:ASP:H	2:B:58:GLN:HE22	1.63	0.47
2:B:65:PHE:C	2:B:67:ALA:N	2.67	0.47
23:C:1030:CLA:HMB2	23:C:1031:CLA:CHC	2.45	0.47
3:C:165:LEU:O	3:C:244:CYS:SG	2.73	0.47
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.96	0.47
3:C:377:LEU:HD11	3:C:381:LYS:NZ	2.29	0.47
3:C:406:SER:O	3:C:418:ASN:HB2	2.15	0.47
1:A:258:LEU:HD21	4:D:129:GLN:HG2	1.95	0.47
4:D:185:PHE:O	4:D:189:HIS:N	2.48	0.47
4:D:214:HIS:CA	4:D:217:THR:HG22	2.45	0.47
4:D:250:ASN:C	4:D:252:PHE:H	2.17	0.47
4:D:38:PHE:N	4:D:39:PRO:HD2	2.29	0.47
4:D:64:ALA:O	4:D:71:CYS:SG	2.72	0.47
4:D:88:SER:C	4:D:90:LEU:H	2.17	0.47
23:B:1018:CLA:HBB2	23:H:1017:CLA:H2	1.96	0.47
23:B:1011:CLA:H202	7:H:38:PHE:HE2	1.78	0.47
19:N:4:UNK:C	19:N:6:UNK:N	2.74	0.47
13:O:241:PHE:HE1	13:O:261:ILE:HG22	1.79	0.47
13:O:266:TYR:O	13:O:267:ALA:HB2	2.15	0.47
15:U:27:LEU:HD21	15:U:82:PHE:CD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:O	1:A:158:PHE:HD2	1.98	0.47
1:A:290:ILE:HG22	1:A:291:SER:H	1.78	0.47
2:B:355:PHE:O	2:B:370:LEU:HA	2.15	0.47
26:C:1054:BCR:H371	26:C:1054:BCR:H24C	1.63	0.47
3:C:370:ARG:HD2	13:O:33:TYR:CD1	2.50	0.47
4:D:301:GLN:HE22	4:D:313:THR:HG21	1.79	0.47
26:A:1044:BCR:HC7	8:I:15:PHE:CZ	2.50	0.47
25:D:1042:PQ9:C40	11:L:30:LEU:HD12	2.38	0.47
13:O:148:VAL:CG2	13:O:151:LEU:HD22	2.45	0.47
13:O:215:ARG:HD3	13:O:215:ARG:H	1.78	0.47
13:O:170:GLY:O	13:O:222:GLN:HA	2.14	0.47
15:U:43:PRO:HG3	16:V:109:ASP:HA	1.97	0.47
15:U:51:LYS:O	15:U:52:ASN:HB2	2.15	0.47
16:V:35:THR:CB	16:V:46:THR:HA	2.44	0.47
16:V:83:GLU:O	16:V:87:LEU:HG	2.15	0.47
1:A:179:THR:O	1:A:180:PHE:C	2.52	0.47
1:A:189:GLU:C	3:C:411:ALA:HB2	2.35	0.47
1:A:244:GLU:OE2	4:D:243:THR:HG22	2.15	0.47
23:B:1020:CLA:C8	23:B:1020:CLA:H41	2.45	0.47
2:B:111:ALA:C	2:B:113:TRP:N	2.68	0.47
2:B:248:ALA:HA	23:B:1011:CLA:C5	2.45	0.47
29:C:1055:DGD:CAA	29:C:1055:DGD:C6A	2.85	0.47
3:C:403:SER:OG	3:C:405:ASN:HB3	2.15	0.47
3:C:75:PHE:HD1	3:C:86:LEU:HD11	1.78	0.47
3:C:461:ARG:HG2	4:D:223:PHE:CD2	2.50	0.47
4:D:269:PHE:O	4:D:272:LEU:HB3	2.15	0.47
4:D:308:ASP:C	4:D:310:GLU:H	2.17	0.47
5:E:13:ILE:HD12	5:E:16:SER:HB3	1.96	0.47
23:A:1007:CLA:C9	8:I:16:VAL:HG11	2.45	0.47
13:O:134:VAL:HG23	13:O:142:ILE:CG2	2.44	0.47
15:U:64:ILE:O	15:U:67:LEU:HG	2.14	0.47
1:A:86:SER:C	1:A:88:ALA:H	2.18	0.47
2:B:133:LEU:HD23	2:B:138:MET:HE3	1.97	0.47
3:C:273:SER:O	3:C:274:TYR:O	2.33	0.47
3:C:348:GLU:OE2	3:C:349:ILE:CG1	2.63	0.47
4:D:262:SER:O	4:D:263:ASN:CB	2.61	0.47
4:D:267:LEU:C	4:D:269:PHE:H	2.18	0.47
23:K:1034:CLA:O2D	23:K:1034:CLA:CGA	2.63	0.47
5:E:26:THR:HG22	19:N:14:UNK:O	2.15	0.47
4:D:309:PRO:O	13:O:185:PRO:HD2	2.15	0.47
1:A:209:ALA:HB2	4:D:204:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD21	4:D:265:ARG:CD	2.44	0.47
1:A:265:PHE:HD1	1:A:271:LEU:HA	1.79	0.47
1:A:205:VAL:CB	1:A:279:ARG:NH2	2.78	0.47
26:B:1047:BCR:C34	26:B:1047:BCR:C12	2.88	0.47
2:B:22:ALA:O	2:B:25:MET:N	2.41	0.47
2:B:347:ARG:HB2	2:B:398:THR:HG23	1.96	0.47
2:B:360:PRO:O	2:B:362:PHE:N	2.48	0.47
29:C:1055:DGD:CEB	29:C:1055:DGD:HBG2	2.27	0.47
3:C:312:ALA:HA	3:C:365:TRP:CH2	2.50	0.47
4:D:297:ASP:OD1	4:D:298:PHE:N	2.27	0.47
4:D:312:GLU:HG3	13:O:185:PRO:HB3	1.97	0.47
23:B:1018:CLA:CBB	23:H:1017:CLA:O1A	2.63	0.47
15:U:68:THR:HG23	15:U:70:ARG:N	2.22	0.47
16:V:98:LEU:HB3	16:V:102:MET:HE2	1.96	0.47
16:V:92:ARG:CG	16:V:92:ARG:NH1	2.67	0.47
1:A:290:ILE:HD11	23:A:1003:CLA:HMD1	1.95	0.46
1:A:197:PHE:HE1	1:A:285:PHE:CD2	2.23	0.46
2:B:149:LEU:HD13	23:B:1012:CLA:H201	1.97	0.46
2:B:115:TRP:CB	28:B:1067:IOD:I	3.33	0.46
2:B:33:TRP:O	2:B:36:SER:HB2	2.15	0.46
3:C:43:ILE:HG13	23:C:1033:CLA:HAC2	1.96	0.46
3:C:307:PRO:HB3	3:C:358:PHE:CG	2.50	0.46
3:C:443:TRP:CD1	23:C:1032:CLA:CMD	2.90	0.46
3:C:42:LEU:CD1	3:C:49:LEU:HD12	2.37	0.46
4:D:319:LEU:HD23	4:D:319:LEU:O	2.15	0.46
5:E:27:ILE:HG13	31:F:1040:HEM:CMB	2.46	0.46
11:L:26:VAL:HG12	11:L:27:LEU:HD23	1.96	0.46
1:A:76:ASN:HD22	11:L:33:SER:HB3	1.75	0.46
12:M:9:ILE:O	12:M:13:LEU:HD23	2.15	0.46
16:V:126:ILE:N	16:V:126:ILE:HD13	2.30	0.46
17:X:19:PHE:O	17:X:22:GLY:N	2.48	0.46
20:Z:37:LYS:CG	20:Z:38:GLN:N	2.77	0.46
1:A:193:LEU:HD23	1:A:193:LEU:O	2.15	0.46
1:A:224:ILE:CG2	1:A:225:ARG:N	2.77	0.46
1:A:279:ARG:NH2	1:A:283:VAL:HG22	2.30	0.46
1:A:63:ILE:HG21	3:C:335:THR:HB	1.98	0.46
2:B:190:PHE:CZ	23:B:1009:CLA:HMA3	2.50	0.46
23:B:1018:CLA:H2	23:B:1018:CLA:H111	1.97	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.96	0.46
2:B:360:PRO:HG2	2:B:363:PHE:CD2	2.50	0.46
2:B:354:LEU:HD21	2:B:378:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:GLY:CA	23:C:1025:CLA:CB	2.93	0.46
23:D:1005:CLA:H61	23:D:1005:CLA:H41	1.58	0.46
4:D:103:ARG:O	4:D:106:GLN:N	2.48	0.46
26:D:1050:BCR:H24C	26:D:1050:BCR:H371	1.64	0.46
4:D:226:GLY:CA	4:D:234:ALA:CB	2.92	0.46
1:A:219:VAL:HG11	4:D:268:HIS:CB	2.45	0.46
4:D:57:SER:HB3	4:D:65:SER:OG	2.15	0.46
8:I:8:VAL:O	8:I:9:TYR:C	2.52	0.46
13:O:76:PHE:CE2	13:O:132:VAL:HG21	2.45	0.46
16:V:88:ALA:HA	16:V:108:TYR:CD2	2.48	0.46
1:A:147:TYR:HE2	24:A:1038:PHO:HAA1	1.80	0.46
1:A:156:ALA:HB1	1:A:290:ILE:HG22	1.97	0.46
1:A:339:PHE:CB	1:A:340:PRO:HD2	2.41	0.46
23:B:1011:CLA:HMD3	23:B:1014:CLA:C3B	2.45	0.46
23:B:1021:CLA:OBD	23:B:1022:CLA:HMC3	2.14	0.46
2:B:188:ASP:HB2	7:H:58:VAL:HG22	1.96	0.46
2:B:265:ILE:H	2:B:265:ILE:CD1	2.05	0.46
2:B:37:MET:O	2:B:40:TYR:HB3	2.14	0.46
2:B:392:PHE:CE2	2:B:417:VAL:HG12	2.50	0.46
2:B:475:PHE:C	2:B:477:ASP:N	2.69	0.46
2:B:5:TRP:HA	2:B:8:VAL:HG11	1.88	0.46
2:B:75:TRP:H	2:B:75:TRP:HD1	1.63	0.46
3:C:42:LEU:O	3:C:42:LEU:HG	2.16	0.46
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.97	0.46
5:E:8:ARG:HB2	6:F:13:TYR:HB3	1.98	0.46
6:F:41:GLN:HG3	9:J:27:LEU:HD21	1.96	0.46
2:B:220:ARG:CD	7:H:20:LYS:O	2.58	0.46
10:K:19:ASP:O	10:K:23:ASP:OD1	2.33	0.46
11:L:13:ASN:O	11:L:15:THR:N	2.48	0.46
12:M:8:PHE:CE2	14:T:1:MET:HG3	2.50	0.46
1:A:104:GLU:HG3	13:O:97:VAL:O	2.16	0.46
16:V:162:TYR:O	16:V:163:TYR:C	2.53	0.46
16:V:54:GLU:O	16:V:58:LEU:HB2	2.15	0.46
1:A:193:LEU:HD22	4:D:179:PHE:CE2	2.50	0.46
1:A:210:LEU:HA	24:D:1039:PHO:CAC	2.43	0.46
23:B:1023:CLA:H151	23:B:1024:CLA:NA	2.31	0.46
3:C:165:LEU:HD21	23:C:1030:CLA:HBB1	1.96	0.46
1:A:278:TRP:CH2	29:C:1057:DGD:HAV2	2.51	0.46
4:D:53:THR:CG2	4:D:67:TYR:CD2	2.99	0.46
1:A:107:TYR:CD2	13:O:97:VAL:CG1	2.99	0.46
15:U:46:ALA:O	15:U:50:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1012:CLA:H12	23:B:1013:CLA:C4	2.37	0.46
23:B:1013:CLA:CMB	23:B:1014:CLA:C1	2.88	0.46
2:B:133:LEU:HD23	2:B:138:MET:CE	2.45	0.46
2:B:250:PHE:HB3	29:B:1058:DGD:HB82	1.98	0.46
23:C:1032:CLA:H12	23:C:1035:CLA:C3C	2.44	0.46
23:C:1036:CLA:H13	23:C:1036:CLA:H102	1.50	0.46
3:C:259:TRP:CE3	3:C:260:ALA:N	2.84	0.46
3:C:277:GLY:HA3	3:C:441:HIS:HD2	1.81	0.46
3:C:369:LEU:HD11	3:C:384:ILE:CG1	2.46	0.46
3:C:472:LEU:O	3:C:473:ASP:CB	2.58	0.46
4:D:122:LEU:O	4:D:123:ILE:C	2.54	0.46
4:D:287:VAL:O	4:D:290:ALA:HB3	2.16	0.46
23:H:1017:CLA:HBB1	26:H:1049:BCR:C32	2.42	0.46
9:J:25:VAL:HG12	9:J:26:GLY:N	2.29	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	0.46
2:B:432:PHE:CE2	13:O:202:GLN:NE2	2.83	0.46
16:V:105:PRO:HD3	16:V:120:SER:CB	2.46	0.46
17:X:13:THR:O	17:X:16:LEU:N	2.49	0.46
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.50	0.46
2:B:149:LEU:CB	23:B:1011:CLA:HBC1	2.46	0.46
23:B:1022:CLA:C4	23:B:1022:CLA:O2A	2.64	0.46
2:B:172:TYR:CG	2:B:173:GLY:N	2.84	0.46
2:B:224:ARG:HG2	7:H:25:TRP:CD1	2.51	0.46
29:C:1056:DGD:HA52	29:C:1056:DGD:O1A	2.16	0.46
3:C:376:ASP:OD1	3:C:378:ASN:HB2	2.15	0.46
3:C:87:ILE:O	3:C:90:PRO:HG2	2.15	0.46
4:D:210:LEU:HD12	4:D:210:LEU:HA	1.64	0.46
1:A:330:VAL:CG1	4:D:348:ARG:HG2	2.45	0.46
4:D:88:SER:C	4:D:90:LEU:N	2.69	0.46
5:E:18:ARG:O	5:E:22:ILE:HG13	2.16	0.46
13:O:176:SER:O	13:O:177:TYR:C	2.54	0.46
3:C:316:THR:CG2	16:V:74:THR:HG23	2.45	0.46
1:A:288:LEU:HD13	3:C:432:VAL:HG23	1.98	0.46
1:A:45:THR:CG2	1:A:46:ILE:H	2.27	0.46
2:B:109:LEU:O	2:B:110:ALA:C	2.54	0.46
2:B:171:PRO:CB	2:B:279:TYR:OH	2.64	0.46
29:C:1056:DGD:HAG1	29:C:1057:DGD:HA92	1.98	0.46
3:C:176:VAL:O	3:C:180:MET:N	2.45	0.46
3:C:275:SER:C	23:C:1033:CLA:HED1	2.35	0.46
6:F:37:ILE:HG22	9:J:28:PHE:HE1	1.81	0.46
12:M:32:GLN:NE2	12:M:32:GLN:HA	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:116:ASP:O	13:O:116:ASP:OD2	2.34	0.46
13:O:216:PHE:HD2	13:O:217:SER:N	2.14	0.46
15:U:28:ASN:ND2	15:U:55:TYR:N	2.62	0.46
20:Z:32:ASP:HB3	20:Z:35:ARG:CG	2.46	0.46
1:A:269:ARG:HD2	4:D:231:THR:O	2.16	0.46
1:A:61:ASP:HB2	1:A:63:ILE:HD13	1.96	0.46
23:B:1009:CLA:OBD	23:B:1010:CLA:CBB	2.55	0.46
3:C:36:TRP:O	23:C:1032:CLA:H42	2.16	0.46
23:C:1033:CLA:HAA2	23:C:1033:CLA:HBD	1.97	0.46
23:C:1036:CLA:CED	23:C:1037:CLA:HBB2	2.46	0.46
3:C:142:GLU:OE2	3:C:143:TYR:HB2	2.16	0.46
3:C:223:TRP:CD1	3:C:223:TRP:C	2.89	0.46
3:C:271:TYR:O	3:C:275:SER:HB2	2.16	0.46
3:C:374:GLY:HA2	13:O:33:TYR:CE1	2.51	0.46
3:C:437:PHE:HA	23:C:1032:CLA:HMC1	1.96	0.46
3:C:93:ALA:HB1	3:C:99:VAL:HG21	1.96	0.46
4:D:14:TRP:O	4:D:17:ILE:HG13	2.16	0.46
4:D:183:LEU:CD2	4:D:183:LEU:H	2.18	0.46
7:H:30:LEU:O	7:H:34:PHE:HD2	1.98	0.46
1:A:305:SER:HA	9:J:39:SER:HB3	1.97	0.46
1:A:31:GLY:HA3	1:A:132:GLU:OE2	2.16	0.46
23:B:1012:CLA:C2D	23:B:1020:CLA:H203	2.39	0.46
23:B:1011:CLA:O1D	23:B:1013:CLA:C2	2.64	0.46
23:B:1015:CLA:HBA2	23:B:1015:CLA:H3A	1.55	0.46
23:B:1016:CLA:H92	23:H:1017:CLA:H111	1.98	0.46
2:B:68:ARG:NH1	2:B:167:TRP:O	2.49	0.46
23:C:1031:CLA:H161	23:C:1031:CLA:H121	1.62	0.46
3:C:190:ALA:O	3:C:191:PRO:C	2.54	0.46
3:C:29:GLU:OE1	3:C:30:SER:N	2.49	0.46
3:C:362:ARG:NE	3:C:367:GLU:OE1	2.48	0.46
24:D:1039:PHO:HHB	23:D:1004:CLA:H121	1.98	0.46
23:D:1008:CLA:CMC	23:D:1008:CLA:CBC	2.81	0.46
2:B:364:GLU:HG3	4:D:296:TYR:CD2	2.51	0.46
4:D:302:GLU:HA	4:D:305:ALA:CB	2.46	0.46
5:E:37:PHE:CE1	5:E:43:ALA:HA	2.50	0.46
8:I:16:VAL:O	8:I:19:PHE:HB3	2.16	0.46
8:I:4:LEU:O	8:I:7:THR:OG1	2.26	0.46
9:J:10:LEU:H	9:J:10:LEU:CD1	2.10	0.46
15:U:35:PHE:HE1	15:U:49:ILE:HB	1.80	0.46
17:X:44:ASP:O	17:X:44:ASP:OD1	2.34	0.46
1:A:39:PRO:CD	23:A:1007:CLA:HBB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1043:PQ9:H91	25:A:1043:PQ9:H61	1.78	0.46
1:A:204:GLY:O	1:A:207:GLY:N	2.48	0.46
1:A:210:LEU:HA	24:D:1039:PHO:CBC	2.46	0.46
1:A:340:PRO:HD3	15:U:103:TYR:HE2	1.77	0.46
1:A:33:PHE:O	1:A:34:GLY:C	2.54	0.46
23:B:1018:CLA:C8	23:B:1023:CLA:CBA	2.94	0.46
23:B:1015:CLA:H18	30:B:1060:MGE:CCA	2.46	0.46
2:B:360:PRO:HG2	2:B:363:PHE:CE2	2.52	0.46
2:B:74:SER:C	2:B:76:SER:N	2.69	0.46
23:C:1033:CLA:H141	23:C:1036:CLA:HMD2	1.98	0.46
29:C:1056:DGD:C4E	29:C:1056:DGD:HD62	2.43	0.46
3:C:272:LEU:HD12	3:C:276:LEU:HB2	1.98	0.46
3:C:398:HIS:H	3:C:398:HIS:HD1	1.62	0.46
4:D:191:TRP:O	4:D:194:ASN:N	2.49	0.46
4:D:218:VAL:HG22	4:D:244:TYR:CD1	2.51	0.46
4:D:274:VAL:CB	4:D:275:PRO:CD	2.94	0.46
11:L:25:LEU:HD12	14:T:16:LEU:HD22	1.97	0.46
4:D:250:ASN:HD21	14:T:27:PRO:HG3	1.81	0.46
1:A:47:CYS:SG	1:A:115:ILE:CD1	3.04	0.45
1:A:143:ILE:HB	4:D:220:ASN:HD22	1.79	0.45
1:A:157:VAL:O	1:A:158:PHE:CD2	2.69	0.45
1:A:210:LEU:HD22	1:A:211:PHE:CD2	2.51	0.45
23:B:1011:CLA:C2D	23:B:1013:CLA:H12	2.45	0.45
23:B:1016:CLA:H93	23:B:1016:CLA:H61	1.64	0.45
2:B:231:MET:HG2	23:B:1018:CLA:HAC2	1.98	0.45
2:B:140:GLY:O	2:B:143:LEU:HB3	2.16	0.45
2:B:456:ALA:HB1	29:B:1058:DGD:CHB	2.28	0.45
3:C:60:ILE:HG13	23:C:1027:CLA:CMD	2.46	0.45
3:C:128:GLY:HA3	23:C:1037:CLA:C3C	2.46	0.45
3:C:131:TYR:CG	3:C:132:HIS:N	2.83	0.45
3:C:206:PRO:O	3:C:210:PHE:HB2	2.16	0.45
3:C:348:GLU:HG2	3:C:349:ILE:CG1	2.36	0.45
4:D:126:MET:O	4:D:129:GLN:HB2	2.16	0.45
4:D:140:PRO:O	4:D:141:TYR:C	2.53	0.45
4:D:87:HIS:HA	4:D:167:TRP:NE1	2.31	0.45
7:H:12:ARG:N	7:H:13:PRO:CD	2.79	0.45
7:H:17:GLU:CB	7:H:20:LYS:HD3	2.45	0.45
2:B:122:LEU:HD23	7:H:8:GLY:CA	2.46	0.45
9:J:23:VAL:HG13	9:J:24:ILE:N	2.30	0.45
9:J:38:SER:O	9:J:39:SER:OG	2.31	0.45
1:A:205:VAL:HA	1:A:279:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:CG	1:A:325:ASN:HD21	2.17	0.45
1:A:86:SER:C	1:A:88:ALA:N	2.68	0.45
23:B:1019:CLA:HBB2	23:B:1021:CLA:HMB2	1.98	0.45
23:B:1022:CLA:CAA	23:B:1022:CLA:CGD	2.65	0.45
23:B:1023:CLA:C1D	23:B:1024:CLA:HMC1	2.45	0.45
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.45	0.45
2:B:135:LEU:HB2	23:B:1018:CLA:HBC1	1.98	0.45
2:B:149:LEU:HD22	23:B:1012:CLA:H203	1.97	0.45
2:B:195:PRO:O	2:B:196:GLY:C	2.53	0.45
2:B:401:PHE:CE1	2:B:406:LEU:HD23	2.51	0.45
2:B:7:ARG:CG	2:B:7:ARG:NH1	2.58	0.45
2:B:90:PHE:HD2	2:B:90:PHE:C	2.18	0.45
23:C:1029:CLA:H62	23:C:1029:CLA:H92	1.80	0.45
23:C:1036:CLA:HBA1	23:C:1036:CLA:H3A	1.59	0.45
3:C:119:LEU:C	3:C:119:LEU:HD12	2.37	0.45
3:C:284:PHE:CE1	3:C:431:PHE:CD2	3.03	0.45
3:C:334:PRO:HG2	4:D:350:ASN:ND2	2.31	0.45
1:A:288:LEU:HD22	3:C:432:VAL:HA	1.98	0.45
3:C:456:GLU:HG3	3:C:456:GLU:H	1.42	0.45
4:D:189:HIS:ND1	4:D:294:ARG:HD3	2.31	0.45
4:D:267:LEU:CD2	4:D:268:HIS:ND1	2.62	0.45
5:E:24:SER:O	5:E:28:PRO:HD2	2.17	0.45
26:H:1049:BCR:H24C	26:H:1049:BCR:H371	1.63	0.45
9:J:30:TYR:O	9:J:32:ALA:N	2.49	0.45
13:O:48:LEU:O	13:O:229:LYS:HD3	2.15	0.45
13:O:71:LEU:HB3	13:O:241:PHE:CE2	2.51	0.45
13:O:210:ARG:NE	13:O:252:GLY:O	2.49	0.45
16:V:103:LYS:HE3	16:V:138:LEU:HD12	1.97	0.45
17:X:39:ALA:O	17:X:43:ILE:HD13	2.15	0.45
18:Y:39:LEU:HD21	20:Z:25:VAL:HA	1.98	0.45
1:A:259:ILE:CD1	25:A:1043:PQ9:H242	2.37	0.45
1:A:129:ARG:CZ	4:D:256:ILE:CD1	2.91	0.45
1:A:252:HIS:CD2	1:A:264:SER:HB3	2.51	0.45
23:B:1023:CLA:CHD	23:B:1024:CLA:HBC2	2.46	0.45
2:B:247:PHE:CE1	23:B:1010:CLA:H93	2.51	0.45
2:B:317:ASN:O	2:B:319:PRO:HD3	2.16	0.45
2:B:346:PHE:CD1	2:B:399:VAL:HG22	2.51	0.45
2:B:47:PRO:HB3	2:B:78:TRP:CE3	2.51	0.45
1:A:304:HIS:CD2	3:C:414:ILE:HD13	2.52	0.45
4:D:103:ARG:HG3	5:E:73:LYS:HD3	1.97	0.45
4:D:221:THR:O	4:D:244:TYR:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:315:TYR:O	4:D:319:LEU:HB2	2.16	0.45
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.81	0.45
13:O:227:VAL:HG11	13:O:230:VAL:CG2	2.45	0.45
13:O:79:LYS:CE	13:O:89:ALA:HB3	2.47	0.45
15:U:51:LYS:HG3	15:U:52:ASN:N	2.23	0.45
16:V:63:CYS:SG	16:V:129:LYS:NZ	2.72	0.45
17:X:13:THR:O	17:X:14:PRO:C	2.54	0.45
24:A:1038:PHO:H161	24:A:1038:PHO:H143	1.62	0.45
1:A:103:ASP:HA	1:A:106:LEU:CD1	2.39	0.45
2:B:69:LEU:CD2	23:B:1013:CLA:O1A	2.64	0.45
2:B:298:LEU:HD11	2:B:302:TRP:NE1	2.26	0.45
2:B:309:LEU:HD12	2:B:309:LEU:O	2.17	0.45
2:B:321:LYS:O	2:B:322:GLY:O	2.34	0.45
2:B:393:GLU:HG3	2:B:414:PRO:HB3	1.98	0.45
2:B:74:SER:HA	2:B:92:SER:OG	2.16	0.45
2:B:42:LEU:HD21	2:B:93:PHE:HB3	1.97	0.45
3:C:142:GLU:C	3:C:144:SER:H	2.19	0.45
3:C:207:ARG:O	3:C:211:GLY:HA3	2.17	0.45
1:A:93:PHE:CB	3:C:218:PHE:HD2	2.28	0.45
3:C:309:ALA:C	3:C:311:GLN:H	2.20	0.45
3:C:362:ARG:HH22	13:O:34:ASP:CG	2.20	0.45
3:C:429:SER:O	3:C:432:VAL:CG1	2.60	0.45
4:D:173:PHE:CE1	24:D:1039:PHO:H13	2.51	0.45
4:D:129:GLN:O	4:D:133:ALA:HB2	2.16	0.45
23:B:1009:CLA:HED1	7:H:41:PHE:CE1	2.51	0.45
6:F:41:GLN:HE22	9:J:28:PHE:HA	1.74	0.45
10:K:24:VAL:C	10:K:26:PRO:HD2	2.37	0.45
14:T:18:PHE:HD2	14:T:19:PHE:CE2	2.33	0.45
15:U:44:THR:O	15:U:47:LYS:N	2.49	0.45
2:B:24:LEU:HD13	23:B:1024:CLA:HBB1	1.97	0.45
2:B:109:LEU:C	2:B:111:ALA:N	2.66	0.45
2:B:191:ASN:O	2:B:192:PRO:C	2.54	0.45
2:B:174:LEU:CD2	2:B:265:ILE:HB	2.46	0.45
2:B:350:GLU:N	2:B:350:GLU:OE2	2.49	0.45
3:C:239:TRP:HE3	3:C:243:ILE:HD11	1.81	0.45
3:C:349:ILE:CG2	3:C:375:LEU:HB2	2.44	0.45
4:D:155:SER:HA	4:D:159:ILE:CG1	2.47	0.45
4:D:274:VAL:HB	4:D:275:PRO:CD	2.38	0.45
4:D:314:PHE:O	4:D:318:ASN:N	2.45	0.45
4:D:326:ARG:O	4:D:328:TRP:N	2.49	0.45
4:D:63:LEU:HD23	4:D:64:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:12:VAL:HG12	8:I:13:THR:N	2.31	0.45
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.97	0.45
4:D:312:GLU:CG	13:O:185:PRO:HB3	2.46	0.45
18:Y:42:ARG:HB3	18:Y:43:ARG:NE	2.28	0.45
18:Y:43:ARG:H	18:Y:43:ARG:CZ	2.30	0.45
23:A:1003:CLA:H141	24:A:1038:PHO:C8	2.45	0.45
25:A:1043:PQ9:H212	24:D:1039:PHO:CED	2.45	0.45
1:A:192:ILE:CG2	1:A:193:LEU:N	2.79	0.45
1:A:258:LEU:O	1:A:259:ILE:CG1	2.64	0.45
23:B:1023:CLA:C15	23:B:1024:CLA:HMA3	2.40	0.45
30:B:1060:MGE:H7A1	30:B:1060:MGE:H102	1.31	0.45
2:B:259:GLY:HA3	7:H:62:TRP:CZ2	2.52	0.45
2:B:297:THR:C	2:B:299:GLU:N	2.66	0.45
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.98	0.45
3:C:184:GLY:C	3:C:185:LEU:HD23	2.37	0.45
3:C:327:ASN:C	3:C:328:VAL:HG23	2.37	0.45
3:C:318:LEU:HA	3:C:340:TYR:HD1	1.80	0.45
3:C:46:SER:OG	3:C:141:GLU:CA	2.65	0.45
25:D:1042:PQ9:H211	25:D:1042:PQ9:H251	1.71	0.45
4:D:185:PHE:CD1	4:D:289:LEU:HD13	2.52	0.45
4:D:319:LEU:O	4:D:322:ASN:HB2	2.17	0.45
4:D:49:LEU:HD13	26:D:1050:BCR:C14	2.47	0.45
4:D:53:THR:HG23	4:D:67:TYR:CD2	2.51	0.45
5:E:35:TRP:HA	6:F:39:ALA:HB2	1.98	0.45
13:O:80:GLU:N	13:O:90:GLU:O	2.48	0.45
17:X:19:PHE:O	17:X:20:PHE:C	2.52	0.45
1:A:119:PHE:CZ	23:A:1003:CLA:H102	2.52	0.45
27:A:1063:LHG:H332	27:A:1063:LHG:H302	1.58	0.45
27:A:1063:LHG:O9	27:A:1063:LHG:C6	2.52	0.45
1:A:121:LEU:HD22	23:A:1007:CLA:HMA1	1.98	0.45
23:B:1013:CLA:C14	23:B:1013:CLA:C17	2.93	0.45
23:B:1022:CLA:C7	23:B:1022:CLA:C14	2.70	0.45
2:B:21:ALA:HB2	2:B:114:HIS:CB	2.47	0.45
2:B:25:MET:O	2:B:27:THR:N	2.50	0.45
3:C:46:SER:HG	3:C:141:GLU:HB2	1.80	0.45
3:C:206:PRO:HG2	3:C:207:ARG:HH11	1.82	0.45
23:D:1008:CLA:HHC	23:D:1008:CLA:CBB	2.19	0.45
30:D:1062:MGE:C3B	30:D:1062:MGE:O1A	2.60	0.45
4:D:147:SER:O	4:D:148:ALA:C	2.55	0.45
4:D:261:PHE:HE2	4:D:266:TRP:CD1	2.35	0.45
4:D:331:PRO:HD3	4:D:341:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASP:H	7:H:15:ASN:ND2	2.15	0.45
11:L:30:LEU:C	11:L:30:LEU:CD2	2.83	0.45
15:U:88:GLU:HB3	15:U:91:LEU:HB2	1.99	0.45
26:H:1049:BCR:C40	17:X:20:PHE:HZ	2.28	0.45
17:X:33:THR:HG22	17:X:34:PHE:N	2.31	0.45
23:C:1037:CLA:HMB2	26:Z:1053:BCR:H282	1.98	0.45
27:A:1063:LHG:C32	23:K:1034:CLA:C15	2.87	0.45
1:A:199:GLN:HB3	1:A:199:GLN:HE21	1.47	0.45
23:B:1015:CLA:H141	23:B:1015:CLA:H161	1.77	0.45
2:B:462:PHE:HE1	23:B:1021:CLA:HMB3	1.81	0.45
30:B:1060:MGE:H5B2	4:D:276:VAL:CB	2.46	0.45
2:B:271:THR:O	2:B:271:THR:HG23	2.16	0.45
2:B:55:MET:CE	2:B:80:ILE:CG2	2.93	0.45
23:C:1025:CLA:CGA	23:C:1025:CLA:C3A	2.90	0.45
23:C:1026:CLA:HMB3	23:C:1028:CLA:CBB	2.47	0.45
23:C:1027:CLA:HHC	23:C:1027:CLA:HBB1	1.98	0.45
23:C:1035:CLA:H61	26:C:1052:BCR:H401	1.99	0.45
3:C:167:VAL:CG1	3:C:168:LEU:HD12	2.30	0.45
3:C:320:ARG:O	3:C:324:LEU:HB2	2.17	0.45
3:C:371:GLY:N	3:C:374:GLY:O	2.49	0.45
23:D:1005:CLA:HBA2	23:D:1005:CLA:H3A	1.44	0.45
4:D:275:PRO:O	4:D:278:GLY:N	2.50	0.45
4:D:326:ARG:NH1	4:D:326:ARG:HG3	2.32	0.45
26:H:1049:BCR:C32	26:H:1049:BCR:HC8	2.40	0.45
23:K:1034:CLA:H91	23:K:1034:CLA:C12	2.44	0.45
13:O:52:ALA:O	13:O:53:ARG:HB3	2.15	0.45
13:O:59:ASP:HB3	13:O:61:SER:H	1.82	0.45
13:O:97:VAL:HB	13:O:133:THR:O	2.17	0.45
15:U:36:ILE:O	15:U:38:TYR:N	2.46	0.45
16:V:96:GLU:O	16:V:97:GLY:C	2.55	0.45
20:Z:26:ALA:CB	20:Z:40:ILE:HD11	2.47	0.45
1:A:151:LEU:CD2	29:C:1055:DGD:HBS2	2.46	0.45
1:A:265:PHE:HD1	1:A:271:LEU:CB	2.30	0.45
2:B:193:TYR:HE1	2:B:259:GLY:C	2.20	0.45
2:B:290:ALA:O	2:B:294:SER:HB2	2.16	0.45
2:B:88:PRO:HB2	2:B:92:SER:HB2	1.99	0.45
3:C:296:VAL:HG23	3:C:297:TYR:CE1	2.51	0.45
3:C:461:ARG:HE	4:D:223:PHE:HD2	1.64	0.45
25:D:1042:PQ9:C39	25:D:1042:PQ9:C42	2.36	0.45
4:D:109:GLY:O	4:D:110:LEU:C	2.55	0.45
4:D:15:PHE:CE1	4:D:32:TRP:CZ2	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:HB3	4:D:218:VAL:HG11	1.97	0.45
3:C:33:PHE:CD2	4:D:229:ALA:HB1	2.51	0.45
4:D:308:ASP:O	4:D:310:GLU:N	2.50	0.45
5:E:13:ILE:HG21	31:F:1040:HEM:CBC	2.47	0.45
1:A:112:TYR:O	1:A:113:GLN:C	2.55	0.45
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.98	0.45
2:B:340:TRP:CZ3	2:B:342:GLY:HA2	2.51	0.45
3:C:223:TRP:CD1	3:C:224:ILE:HD13	2.51	0.45
3:C:53:HIS:O	3:C:57:ALA:HB2	2.17	0.45
3:C:69:LEU:O	3:C:73:ALA:HB2	2.17	0.45
4:D:114:ILE:CG2	24:D:1039:PHO:H121	2.47	0.45
4:D:217:THR:HG23	4:D:218:VAL:N	2.32	0.45
7:H:30:LEU:HA	7:H:33:VAL:CG2	2.47	0.45
11:L:26:VAL:CG1	11:L:27:LEU:N	2.80	0.45
19:N:2:UNK:O	19:N:3:UNK:C	2.65	0.45
13:O:185:PRO:O	13:O:186:LYS:HB3	2.17	0.45
13:O:45:CYS:CB	13:O:46:PRO:HD2	2.32	0.45
15:U:32:ILE:HG13	15:U:50:VAL:HG21	1.98	0.45
15:U:37:GLN:O	15:U:38:TYR:CD2	2.70	0.45
1:A:119:PHE:O	1:A:121:LEU:N	2.50	0.44
23:B:1015:CLA:CBB	23:B:1015:CLA:HHC	2.46	0.44
26:B:1048:BCR:H372	26:B:1048:BCR:C40	2.29	0.44
2:B:460:LEU:HG	29:B:1058:DGD:CIA	2.47	0.44
2:B:46:ASP:N	2:B:58:GLN:HE22	2.15	0.44
23:C:1036:CLA:H122	23:C:1036:CLA:H162	1.60	0.44
23:C:1029:CLA:HMD2	26:C:1054:BCR:H331	1.99	0.44
3:C:250:TRP:CD1	3:C:250:TRP:C	2.90	0.44
23:D:1005:CLA:H203	23:D:1005:CLA:H161	1.75	0.44
26:D:1050:BCR:C21	30:D:1059:MGE:H3A2	2.47	0.44
4:D:265:ARG:CD	4:D:265:ARG:C	2.85	0.44
9:J:24:ILE:CG2	9:J:25:VAL:N	2.80	0.44
13:O:151:LEU:HG	13:O:152:VAL:N	2.31	0.44
13:O:163:THR:OG1	13:O:164:THR:N	2.50	0.44
13:O:47:THR:O	13:O:48:LEU:HD23	2.16	0.44
15:U:57:SER:OG	15:U:60:ASP:OD2	2.34	0.44
18:Y:21:GLN:O	18:Y:25:ILE:CG2	2.65	0.44
23:A:1007:CLA:C6	23:A:1007:CLA:C11	2.92	0.44
1:A:193:LEU:HD22	4:D:179:PHE:CG	2.52	0.44
1:A:27:ARG:NH1	1:A:27:ARG:HG3	2.33	0.44
1:A:38:ILE:HG22	1:A:39:PRO:CD	2.46	0.44
2:B:121:GLU:HB2	7:H:4:ARG:CB	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:HA	2:B:319:PRO:HD2	1.99	0.44
2:B:477:ASP:OD2	4:D:134:ARG:NH1	2.43	0.44
23:C:1028:CLA:H93	29:C:1056:DGD:HB91	1.97	0.44
23:C:1035:CLA:CMB	26:C:1052:BCR:H271	2.46	0.44
29:C:1057:DGD:HAS2	30:D:1059:MGE:CDB	2.47	0.44
3:C:139:THR:HG23	3:C:142:GLU:HG3	1.98	0.44
3:C:168:LEU:C	3:C:170:ILE:N	2.71	0.44
3:C:210:PHE:HE1	3:C:239:TRP:CE3	2.35	0.44
3:C:225:VAL:HG23	3:C:226:SER:H	1.80	0.44
3:C:53:HIS:CB	23:C:1036:CLA:HMD1	2.47	0.44
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.47	0.44
4:D:297:ASP:O	4:D:298:PHE:HB2	2.15	0.44
4:D:308:ASP:OD1	4:D:310:GLU:HG2	2.17	0.44
10:K:18:PHE:O	10:K:19:ASP:C	2.53	0.44
3:C:62:PHE:HE2	10:K:29:PRO:CD	2.30	0.44
12:M:27:VAL:O	12:M:27:VAL:HG12	2.18	0.44
13:O:48:LEU:HD12	13:O:229:LYS:O	2.17	0.44
14:T:4:ILE:O	14:T:8:PHE:N	2.48	0.44
15:U:24:LYS:HB3	15:U:81:HIS:O	2.17	0.44
16:V:90:PRO:HD2	16:V:92:ARG:NH1	2.32	0.44
18:Y:43:ARG:CD	20:Z:29:SER:HA	2.46	0.44
1:A:121:LEU:C	1:A:123:ALA:N	2.70	0.44
1:A:276:ALA:O	1:A:280:VAL:HG23	2.17	0.44
1:A:320:ILE:HD13	1:A:320:ILE:HA	1.91	0.44
2:B:15:ASP:N	2:B:16:PRO:CD	2.79	0.44
2:B:215:PHE:HD2	2:B:215:PHE:C	2.20	0.44
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.00	0.44
23:C:1035:CLA:CBB	23:C:1035:CLA:HHC	2.20	0.44
3:C:223:TRP:HD1	3:C:224:ILE:N	2.13	0.44
3:C:455:PHE:O	3:C:458:GLY:O	2.35	0.44
4:D:249:ALA:O	4:D:252:PHE:N	2.41	0.44
4:D:27:PHE:CD1	6:F:19:ARG:HG3	2.52	0.44
4:D:286:VAL:O	4:D:287:VAL:C	2.56	0.44
4:D:31:GLY:C	4:D:33:SER:N	2.66	0.44
5:E:37:PHE:CZ	5:E:46:VAL:HG21	2.52	0.44
7:H:18:TYR:CD2	7:H:18:TYR:C	2.90	0.44
13:O:59:ASP:CB	13:O:62:GLN:HB2	2.47	0.44
15:U:61:VAL:HG12	15:U:75:LEU:CD2	2.37	0.44
16:V:103:LYS:CD	16:V:121:LEU:HD12	2.28	0.44
16:V:154:ASP:C	16:V:156:TRP:H	2.21	0.44
16:V:154:ASP:C	16:V:156:TRP:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:16:LEU:HD23	17:X:16:LEU:C	2.38	0.44
1:A:104:GLU:OE1	13:O:99:ARG:CD	2.65	0.44
1:A:215:HIS:ND1	25:A:1043:PQ9:O1	2.51	0.44
1:A:286:ALA:O	1:A:289:GLY:N	2.51	0.44
1:A:55:ALA:H	1:A:70:SER:CB	2.30	0.44
23:B:1012:CLA:CHD	23:B:1020:CLA:C20	2.94	0.44
2:B:113:TRP:C	2:B:115:TRP:N	2.69	0.44
2:B:136:PRO:HB3	2:B:221:PRO:HG3	2.00	0.44
2:B:237:VAL:HB	23:B:1020:CLA:CMD	2.48	0.44
23:C:1028:CLA:H91	29:C:1056:DGD:C9B	2.47	0.44
23:C:1033:CLA:H3A	23:C:1033:CLA:HBA1	1.75	0.44
3:C:385:GLN:HB3	3:C:386:PRO:CD	2.48	0.44
3:C:89:ILE:O	3:C:111:PHE:HE2	2.00	0.44
4:D:262:SER:N	30:D:1062:MGE:O3D	2.51	0.44
8:I:25:SER:O	8:I:26:GLY:O	2.36	0.44
8:I:6:ILE:O	8:I:10:ILE:HD11	2.17	0.44
13:O:64:TYR:HA	13:O:271:PRO:HA	1.99	0.44
15:U:68:THR:HG22	15:U:71:GLN:CG	2.48	0.44
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.44
1:A:89:ILE:HD13	1:A:94:TYR:CG	2.53	0.44
2:B:153:PHE:HD1	2:B:157:HIS:CB	2.30	0.44
2:B:191:ASN:HD21	7:H:60:VAL:CA	2.19	0.44
2:B:35:GLY:O	2:B:39:LEU:HG	2.18	0.44
23:C:1025:CLA:CHB	23:C:1025:CLA:O2A	2.60	0.44
23:C:1029:CLA:CMC	23:C:1029:CLA:CBC	2.84	0.44
26:C:1052:BCR:H403	26:C:1052:BCR:H24C	1.76	0.44
3:C:70:PHE:O	3:C:74:HIS:ND1	2.47	0.44
8:I:1:MET:C	8:I:3:THR:N	2.71	0.44
3:C:330:SER:HB2	13:O:126:GLY:O	2.17	0.44
13:O:172:PHE:HD1	13:O:221:GLY:HA3	1.77	0.44
13:O:235:GLY:HA3	13:O:269:ILE:O	2.17	0.44
13:O:65:ARG:HG2	13:O:66:ILE:N	2.33	0.44
14:T:24:ARG:HD2	14:T:24:ARG:C	2.38	0.44
25:A:1043:PQ9:H393	25:A:1043:PQ9:H292	1.99	0.44
1:A:121:LEU:O	1:A:124:SER:N	2.51	0.44
1:A:309:ALA:HB3	16:V:28:GLU:CB	2.47	0.44
23:B:1019:CLA:H122	23:B:1019:CLA:H162	1.51	0.44
23:B:1022:CLA:H152	12:M:24:ILE:HG21	1.99	0.44
2:B:151:PHE:HB2	2:B:206:GLY:HA3	1.98	0.44
2:B:488:PRO:O	2:B:489:GLU:CB	2.59	0.44
23:C:1028:CLA:H91	29:C:1056:DGD:HB91	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C:1057:DGD:HB72	30:D:1059:MGE:H7B1	1.99	0.44
3:C:257:PHE:N	3:C:257:PHE:HD1	2.09	0.44
3:C:420:VAL:HG21	3:C:425:TRP:HZ2	1.83	0.44
3:C:87:ILE:HG13	3:C:88:LEU:H	1.82	0.44
23:D:1008:CLA:H151	23:D:1008:CLA:H18	1.58	0.44
23:B:1016:CLA:H202	23:D:1008:CLA:HAA2	2.00	0.44
23:D:1005:CLA:H91	30:D:1062:MGE:H263	1.99	0.44
4:D:14:TRP:CD1	4:D:14:TRP:C	2.91	0.44
4:D:194:ASN:C	4:D:194:ASN:OD1	2.55	0.44
4:D:217:THR:CG2	4:D:218:VAL:N	2.81	0.44
4:D:265:ARG:NH1	4:D:265:ARG:CG	2.70	0.44
4:D:145:ALA:HA	4:D:276:VAL:HG11	2.00	0.44
10:K:17:ILE:HB	10:K:18:PHE:CD1	2.53	0.44
13:O:52:ALA:HB1	13:O:229:LYS:HA	2.00	0.44
1:A:160:ILE:HD13	3:C:431:PHE:HE1	1.80	0.44
1:A:202:VAL:O	1:A:206:PHE:HB2	2.18	0.44
1:A:215:HIS:CD2	1:A:275:LEU:CD1	3.00	0.44
1:A:308:ASP:HB2	5:E:52:PRO:O	2.17	0.44
2:B:247:PHE:CE1	2:B:251:VAL:CG2	3.01	0.44
2:B:367:PRO:HG2	2:B:367:PRO:O	2.18	0.44
23:C:1029:CLA:CMA	23:C:1029:CLA:HBA2	2.03	0.44
1:A:131:TRP:CH2	23:C:1029:CLA:HMA3	2.52	0.44
3:C:244:CYS:HA	23:C:1030:CLA:HMC1	2.00	0.44
23:C:1035:CLA:H111	26:C:1052:BCR:H24C	1.98	0.44
3:C:143:TYR:CE2	23:C:1037:CLA:HED2	2.53	0.44
3:C:223:TRP:HD1	3:C:224:ILE:HD13	1.83	0.44
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.82	0.44
3:C:428:THR:O	3:C:429:SER:C	2.56	0.44
3:C:457:LYS:HD2	4:D:224:GLN:NE2	2.33	0.44
30:D:1062:MGE:H2G	30:D:1062:MGE:H1D	1.40	0.44
4:D:85:MET:HA	5:E:69:ARG:HB3	2.00	0.44
13:O:236:GLU:C	13:O:237:ILE:HG22	2.37	0.44
13:O:59:ASP:O	13:O:60:SER:HB2	2.16	0.44
13:O:92:VAL:HG12	13:O:93:PRO:HD2	2.00	0.44
15:U:51:LYS:O	15:U:52:ASN:O	2.36	0.44
31:V:1041:HEM:HBB2	31:V:1041:HEM:HHC	1.99	0.44
1:A:284:TRP:O	1:A:285:PHE:C	2.56	0.44
1:A:310:LYS:HD3	1:A:312:ASN:ND2	2.33	0.44
2:B:168:VAL:HG12	2:B:169:SER:H	1.79	0.44
2:B:264:PRO:HG3	2:B:267:LEU:HD12	1.99	0.44
2:B:272:ARG:NH2	2:B:276:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:HG22	23:B:1021:CLA:C2C	2.48	0.44
2:B:6:TYR:H	2:B:6:TYR:HD2	1.57	0.44
23:C:1031:CLA:H142	23:C:1031:CLA:H111	1.75	0.44
26:C:1052:BCR:C33	26:C:1052:BCR:C8	2.91	0.44
4:D:161:PRO:CG	4:D:170:ALA:CB	2.96	0.44
4:D:250:ASN:O	4:D:252:PHE:N	2.51	0.44
4:D:308:ASP:C	4:D:310:GLU:N	2.72	0.44
6:F:41:GLN:HG3	9:J:27:LEU:CD2	2.48	0.44
3:C:262:ARG:O	8:I:28:PRO:HG2	2.17	0.44
13:O:173:ASN:HD22	13:O:173:ASN:HA	1.54	0.44
15:U:41:LEU:HD11	15:U:74:ILE:HG22	2.00	0.44
10:K:38:VAL:CG1	18:Y:36:ILE:HG12	2.48	0.44
1:A:223:LEU:CD1	4:D:265:ARG:HG2	2.46	0.44
1:A:95:PRO:HD2	1:A:98:GLU:HB2	2.00	0.44
2:B:68:ARG:CD	23:B:1011:CLA:HED1	2.48	0.44
2:B:69:LEU:HD21	23:B:1014:CLA:HMB3	2.00	0.44
2:B:101:ILE:O	26:B:1047:BCR:H391	2.17	0.44
2:B:345:VAL:HG23	2:B:345:VAL:O	2.18	0.44
2:B:407:ASN:O	2:B:409:GLN:N	2.51	0.44
2:B:451:PHE:C	2:B:451:PHE:CD2	2.90	0.44
2:B:452:THR:HB	4:D:291:LEU:CD1	2.48	0.44
2:B:482:ILE:O	2:B:483:ASP:CB	2.62	0.44
29:C:1056:DGD:C2B	29:C:1056:DGD:HG12	2.40	0.44
3:C:155:ASN:C	3:C:158:THR:HG22	2.38	0.44
3:C:305:THR:O	3:C:308:GLU:N	2.50	0.44
4:D:180:ARG:NH1	4:D:184:PHE:CD1	2.85	0.44
4:D:221:THR:CG2	4:D:248:THR:HB	2.46	0.44
1:A:133:LEU:HB3	4:D:252:PHE:HE2	1.83	0.44
4:D:281:MET:HA	4:D:281:MET:CE	2.46	0.44
4:D:90:LEU:CD2	4:D:109:GLY:H	2.31	0.44
7:H:30:LEU:HB3	23:H:1017:CLA:HMD2	1.99	0.44
10:K:30:VAL:O	10:K:32:PHE:N	2.50	0.44
4:D:303:ILE:HG21	12:M:2:GLU:HB3	2.00	0.44
16:V:106:THR:HA	16:V:114:ILE:HG22	2.00	0.44
16:V:126:ILE:O	16:V:128:PRO:HD3	2.18	0.44
16:V:35:THR:HG23	16:V:46:THR:CA	2.47	0.44
1:A:119:PHE:C	1:A:121:LEU:N	2.71	0.43
1:A:255:PHE:O	1:A:256:GLY:C	2.57	0.43
1:A:341:LEU:O	1:A:343:LEU:N	2.48	0.43
23:B:1023:CLA:H61	23:B:1023:CLA:H2	1.47	0.43
23:B:1023:CLA:H91	23:B:1024:CLA:H152	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:HD3	2:B:124:ARG:HA	1.74	0.43
23:C:1029:CLA:H11	23:C:1029:CLA:C1A	2.47	0.43
23:C:1028:CLA:C1C	29:C:1056:DGD:HA31	2.47	0.43
3:C:281:MET:CG	3:C:285:ILE:HD11	2.48	0.43
3:C:87:ILE:HG13	3:C:88:LEU:N	2.32	0.43
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.98	0.43
1:A:213:ALA:CB	24:D:1039:PHO:HBC1	2.47	0.43
30:D:1062:MGE:C4B	30:D:1062:MGE:O1A	2.66	0.43
4:D:250:ASN:C	4:D:252:PHE:N	2.72	0.43
4:D:270:PHE:O	4:D:270:PHE:CD1	2.70	0.43
5:E:10:PHE:CE1	6:F:19:ARG:HD2	2.52	0.43
23:C:1026:CLA:HBB2	23:K:1034:CLA:H11	1.98	0.43
10:K:28:ILE:HA	10:K:31:LEU:HG	1.99	0.43
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.48	0.43
13:O:44:LYS:HB3	13:O:72:GLN:OE1	2.18	0.43
16:V:90:PRO:HD2	16:V:92:ARG:NH2	2.33	0.43
24:A:1038:PHO:CED	24:A:1038:PHO:OBD	2.66	0.43
1:A:177:SER:HA	1:A:180:PHE:HD2	1.83	0.43
1:A:192:ILE:CD1	1:A:293:MET:HE1	2.48	0.43
23:B:1013:CLA:HMC1	23:B:1013:CLA:CBC	2.37	0.43
2:B:28:ALA:HB2	2:B:107:LEU:CB	2.48	0.43
2:B:63:LEU:N	2:B:64:PRO:HD3	2.33	0.43
23:C:1032:CLA:HAA1	23:C:1032:CLA:HBD	2.01	0.43
23:C:1035:CLA:CMB	26:C:1052:BCR:H272	2.45	0.43
3:C:284:PHE:HB3	29:C:1055:DGD:HB81	2.00	0.43
3:C:293:ASN:OD1	3:C:294:ASN:N	2.51	0.43
3:C:460:ASP:OD1	3:C:462:GLU:HG2	2.18	0.43
3:C:45:LEU:HB3	3:C:46:SER:H	1.59	0.43
3:C:69:LEU:HD21	3:C:116:VAL:HG22	2.01	0.43
23:D:1005:CLA:HBC1	23:D:1004:CLA:CBB	2.34	0.43
5:E:8:ARG:HB2	6:F:13:TYR:CB	2.48	0.43
29:C:1057:DGD:O2D	9:J:32:ALA:HB1	2.18	0.43
13:O:70:CYS:HB2	13:O:105:ASP:CB	2.47	0.43
23:A:1007:CLA:HAC1	26:A:1044:BCR:C16	2.48	0.43
1:A:285:PHE:O	1:A:288:LEU:HB2	2.19	0.43
1:A:51:ALA:O	1:A:55:ALA:HB3	2.18	0.43
23:B:1015:CLA:H42	23:B:1015:CLA:H71	1.94	0.43
23:B:1023:CLA:H151	23:B:1024:CLA:C4A	2.48	0.43
2:B:54:PRO:O	2:B:55:MET:C	2.57	0.43
2:B:69:LEU:HA	2:B:69:LEU:HD12	1.84	0.43
3:C:265:ILE:HG23	3:C:270:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:337:LEU:HD22	3:C:342:MET:HG3	1.99	0.43
3:C:440:GLY:O	3:C:442:LEU:N	2.50	0.43
3:C:54:VAL:O	3:C:55:ALA:C	2.55	0.43
3:C:56:HIS:O	3:C:59:LEU:N	2.52	0.43
4:D:106:GLN:C	4:D:108:GLY:N	2.72	0.43
4:D:250:ASN:CG	4:D:251:ARG:N	2.70	0.43
4:D:48:TRP:CD1	24:D:1039:PHO:H162	2.53	0.43
4:D:57:SER:OG	4:D:65:SER:CB	2.64	0.43
4:D:96:GLU:HG2	4:D:97:ALA:H	1.82	0.43
23:H:1017:CLA:H93	23:H:1017:CLA:H62	1.59	0.43
23:A:1007:CLA:C14	8:I:13:THR:OG1	2.66	0.43
9:J:10:LEU:CD2	9:J:11:TRP:H	2.31	0.43
3:C:75:PHE:O	10:K:10:LYS:HE3	2.18	0.43
25:D:1042:PQ9:H393	11:L:26:VAL:CG1	2.48	0.43
13:O:129:PHE:C	13:O:129:PHE:CD2	2.92	0.43
13:O:184:ASP:OD2	13:O:188:ARG:NH1	2.50	0.43
15:U:36:ILE:HG22	15:U:42:TYR:CB	2.48	0.43
15:U:36:ILE:HA	15:U:42:TYR:HB2	2.01	0.43
15:U:85:THR:O	15:U:86:GLU:C	2.56	0.43
16:V:95:ILE:O	16:V:99:VAL:HG23	2.18	0.43
23:C:1035:CLA:H152	20:Z:20:VAL:HG13	1.98	0.43
24:A:1038:PHO:H3A	24:A:1038:PHO:HBA1	1.26	0.43
1:A:161:TYR:CZ	1:A:186:PHE:CE2	3.06	0.43
1:A:93:PHE:HB2	3:C:218:PHE:CD2	2.47	0.43
23:B:1009:CLA:HBC2	23:B:1009:CLA:HMC1	1.99	0.43
23:B:1013:CLA:H142	23:B:1013:CLA:H111	1.73	0.43
23:B:1022:CLA:CHD	23:B:1022:CLA:CBC	2.79	0.43
23:B:1024:CLA:H111	23:B:1024:CLA:H143	1.77	0.43
2:B:103:LEU:O	2:B:104:SER:C	2.56	0.43
2:B:113:TRP:HD1	2:B:114:HIS:N	2.16	0.43
2:B:185:TRP:HZ3	2:B:204:ALA:HB2	1.84	0.43
2:B:226:TYR:CD2	2:B:226:TYR:O	2.66	0.43
2:B:23:HIS:C	2:B:25:MET:H	2.21	0.43
23:C:1026:CLA:C3	23:C:1026:CLA:CGA	2.96	0.43
3:C:123:ALA:HA	26:C:1052:BCR:C14	2.48	0.43
3:C:305:THR:O	3:C:306:GLY:C	2.56	0.43
3:C:321:ASP:HB2	3:C:340:TYR:HE1	1.83	0.43
3:C:64:ALA:O	3:C:68:THR:HB	2.18	0.43
4:D:53:THR:HG23	4:D:67:TYR:HE2	1.83	0.43
4:D:90:LEU:O	23:D:1008:CLA:HED1	2.18	0.43
26:K:1051:BCR:H392	26:K:1051:BCR:C23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:27:VAL:O	10:K:31:LEU:HG	2.18	0.43
16:V:47:LEU:HD21	16:V:51:GLN:HB2	2.01	0.43
1:A:13:LEU:H	1:A:13:LEU:CD1	2.27	0.43
1:A:311:GLY:O	1:A:312:ASN:C	2.55	0.43
23:B:1021:CLA:H62	30:B:1060:MGE:H231	2.01	0.43
2:B:108:PHE:C	2:B:111:ALA:HB3	2.38	0.43
2:B:359:MET:HB3	2:B:425:ILE:HG23	2.00	0.43
2:B:33:TRP:HA	2:B:36:SER:HB2	1.99	0.43
2:B:460:LEU:O	4:D:280:TRP:CZ3	2.70	0.43
2:B:57:ARG:C	2:B:59:GLY:H	2.21	0.43
3:C:224:ILE:CG2	26:C:1054:BCR:H381	2.34	0.43
3:C:81:MET:SD	3:C:90:PRO:HA	2.57	0.43
4:D:103:ARG:HA	4:D:106:GLN:HE21	1.83	0.43
4:D:16:ASP:O	4:D:20:ASP:HB2	2.18	0.43
4:D:337:GLU:HG2	4:D:339:PHE:CZ	2.53	0.43
8:I:24:LEU:C	8:I:26:GLY:N	2.70	0.43
12:M:9:ILE:CG2	12:M:13:LEU:HD23	2.48	0.43
15:U:70:ARG:CZ	15:U:74:ILE:HD11	2.49	0.43
16:V:101:TYR:HE1	16:V:118:HIS:ND1	2.14	0.43
16:V:45:ILE:O	16:V:45:ILE:HG22	2.19	0.43
17:X:37:LEU:HD23	17:X:37:LEU:HA	1.74	0.43
24:A:1038:PHO:C4	24:A:1038:PHO:C7	2.93	0.43
24:A:1038:PHO:C9	23:D:1005:CLA:C17	2.97	0.43
25:A:1043:PQ9:C40	25:A:1043:PQ9:C45	2.96	0.43
1:A:141:PRO:C	1:A:143:ILE:N	2.71	0.43
1:A:143:ILE:CG2	1:A:144:CYS:N	2.81	0.43
1:A:271:LEU:O	1:A:274:PHE:N	2.52	0.43
1:A:281:VAL:CG1	1:A:285:PHE:HE1	2.32	0.43
1:A:320:ILE:O	1:A:323:ARG:N	2.50	0.43
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.72	0.43
1:A:59:ASP:OD2	1:A:59:ASP:N	2.51	0.43
2:B:468:TRP:CE2	23:B:1019:CLA:HED2	2.53	0.43
2:B:12:LEU:HD23	2:B:19:LEU:HA	1.99	0.43
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.19	0.43
2:B:347:ARG:HG2	2:B:347:ARG:HH11	1.83	0.43
2:B:328:GLY:O	2:B:444:ARG:HG2	2.18	0.43
2:B:6:TYR:CE1	30:B:1060:MGE:H2D	2.53	0.43
23:C:1027:CLA:HHC	23:C:1027:CLA:CBB	2.48	0.43
3:C:60:ILE:CG1	23:C:1027:CLA:HMD1	2.49	0.43
3:C:139:THR:O	3:C:139:THR:HG23	2.18	0.43
3:C:229:ASN:ND2	3:C:232:ASP:OD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:440:GLY:O	3:C:441:HIS:C	2.56	0.43
3:C:438:LEU:HD13	3:C:442:LEU:CD1	2.49	0.43
3:C:81:MET:SD	3:C:89:ILE:HG22	2.59	0.43
26:D:1050:BCR:C19	30:D:1059:MGE:H102	2.48	0.43
4:D:158:LEU:O	4:D:162:LEU:CG	2.66	0.43
4:D:46:GLY:CA	26:D:1050:BCR:H10C	2.48	0.43
4:D:67:TYR:O	4:D:70:GLY:N	2.47	0.43
23:C:1026:CLA:HBB1	23:K:1034:CLA:HMD3	1.99	0.43
10:K:21:LEU:O	10:K:22:VAL:C	2.57	0.43
13:O:58:ILE:HG23	13:O:160:THR:O	2.18	0.43
15:U:55:TYR:N	15:U:55:TYR:CD1	2.82	0.43
20:Z:44:SER:O	20:Z:48:ILE:CD1	2.66	0.43
20:Z:4:LEU:HD12	20:Z:4:LEU:O	2.17	0.43
25:A:1043:PQ9:H311	25:A:1043:PQ9:H291	1.68	0.43
1:A:128:GLY:C	1:A:130:GLN:N	2.72	0.43
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.54	0.43
1:A:259:ILE:HD13	25:A:1043:PQ9:C24	2.38	0.43
1:A:259:ILE:N	4:D:128:ARG:NH2	2.58	0.43
1:A:60:ILE:O	1:A:61:ASP:O	2.37	0.43
23:B:1011:CLA:H42	23:B:1011:CLA:O2A	2.19	0.43
23:B:1021:CLA:C2	23:B:1021:CLA:CED	2.89	0.43
30:B:1060:MGE:O1B	30:B:1060:MGE:C3G	2.63	0.43
2:B:389:LYS:HB3	2:B:390:TYR:CE1	2.54	0.43
2:B:486:LEU:O	2:B:487:SER:HB2	2.19	0.43
2:B:6:TYR:OH	30:B:1060:MGE:H3D	2.19	0.43
3:C:145:SER:O	3:C:147:PHE:N	2.52	0.43
3:C:298:PRO:O	3:C:300:GLU:OE1	2.36	0.43
3:C:343:ARG:NH1	3:C:348:GLU:CB	2.82	0.43
3:C:348:GLU:OE2	3:C:373:ASN:HB3	2.18	0.43
1:A:301:ASN:HB3	3:C:407:VAL:HG11	2.00	0.43
4:D:185:PHE:O	4:D:190:ASN:N	2.50	0.43
4:D:277:THR:HG22	4:D:278:GLY:N	2.34	0.43
1:A:330:VAL:HG11	4:D:347:PRO:O	2.19	0.43
5:E:68:ASP:H	5:E:75:GLN:HE21	1.65	0.43
6:F:41:GLN:HG3	9:J:27:LEU:HG	2.01	0.43
9:J:7:ARG:HG2	9:J:7:ARG:NH1	2.31	0.43
23:K:1034:CLA:C4	23:K:1034:CLA:HBA1	2.49	0.43
13:O:160:THR:O	13:O:160:THR:CG2	2.66	0.43
3:C:332:GLN:NE2	13:O:175:PRO:HG3	2.34	0.43
13:O:184:ASP:OD1	13:O:188:ARG:HB2	2.18	0.43
13:O:172:PHE:CB	13:O:221:GLY:HA3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:231:ASP:HB3	13:O:234:THR:HG1	1.83	0.43
13:O:92:VAL:HG12	13:O:93:PRO:N	2.33	0.43
14:T:14:ILE:HG21	26:T:6046:BCR:H352	2.00	0.43
1:A:295:PHE:HD2	3:C:291:TRP:CE2	2.37	0.43
1:A:38:ILE:O	1:A:42:LEU:HD23	2.18	0.43
1:A:63:ILE:HG12	1:A:65:GLU:N	2.34	0.43
23:B:1011:CLA:HAA2	23:B:1011:CLA:CGD	2.48	0.43
23:B:1023:CLA:H111	23:B:1023:CLA:H142	1.61	0.43
2:B:181:VAL:HG11	2:B:196:GLY:HA2	1.98	0.43
2:B:291:SER:O	2:B:296:ALA:HB3	2.18	0.43
23:C:1035:CLA:H143	23:C:1035:CLA:H112	1.79	0.43
23:A:1006:CLA:CAA	29:C:1057:DGD:HBN2	2.48	0.43
3:C:139:THR:HG23	3:C:142:GLU:CG	2.48	0.43
3:C:327:ASN:HD21	3:C:331:ALA:N	2.17	0.43
3:C:327:ASN:ND2	3:C:330:SER:N	2.67	0.43
2:B:3:LEU:O	11:L:10:VAL:HA	2.19	0.43
18:Y:43:ARG:HH21	18:Y:44:GLY:N	2.14	0.43
1:A:101:SER:O	1:A:102:LEU:C	2.56	0.43
1:A:147:TYR:CE2	24:A:1038:PHO:HAA1	2.53	0.43
1:A:329:GLU:O	1:A:332:HIS:ND1	2.47	0.43
23:B:1021:CLA:HBC3	26:B:1047:BCR:C34	2.49	0.43
23:C:1037:CLA:H142	23:C:1037:CLA:C10	2.48	0.43
23:C:1028:CLA:H62	29:C:1057:DGD:HA42	2.01	0.43
3:C:322:GLN:NE2	3:C:381:LYS:HG2	2.34	0.43
4:D:113:PHE:O	4:D:114:ILE:C	2.57	0.43
4:D:39:PRO:CB	23:D:1008:CLA:CBB	2.97	0.43
7:H:30:LEU:CA	7:H:33:VAL:HG22	2.48	0.43
23:K:1034:CLA:H41	23:K:1034:CLA:C8	2.48	0.43
10:K:18:PHE:N	10:K:18:PHE:CD1	2.86	0.43
16:V:125:ASP:CG	16:V:126:ILE:HD13	2.39	0.43
17:X:11:THR:O	17:X:11:THR:CG2	2.65	0.43
17:X:13:THR:HG22	17:X:14:PRO:HD2	2.00	0.43
20:Z:29:SER:HB2	20:Z:31:GLN:HE21	1.83	0.43
23:B:1009:CLA:O2D	23:B:1009:CLA:CBA	2.60	0.43
2:B:62:VAL:HG11	23:B:1013:CLA:HED2	2.00	0.43
2:B:153:PHE:CB	23:B:1014:CLA:HMC3	2.49	0.43
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.01	0.43
2:B:24:LEU:HA	23:B:1023:CLA:HED3	2.01	0.43
2:B:298:LEU:HG	2:B:402:TYR:CD2	2.53	0.43
2:B:338:GLN:CA	2:B:338:GLN:HE21	2.17	0.43
3:C:172:ALA:H	23:C:1025:CLA:HBC2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:GLY:O	3:C:102:GLY:O	2.36	0.43
3:C:163:PHE:O	3:C:166:ILE:HG12	2.19	0.43
3:C:82:TYR:CD2	3:C:302:TYR:O	2.72	0.43
3:C:397:THR:O	3:C:399:ALA:N	2.52	0.43
4:D:145:ALA:HB2	4:D:272:LEU:HD12	2.00	0.43
4:D:263:ASN:OD1	4:D:264:LYS:N	2.52	0.43
13:O:142:ILE:HA	13:O:143:PRO:HD3	1.78	0.43
13:O:74:THR:HG22	13:O:263:GLY:HA2	2.00	0.43
13:O:266:TYR:CG	13:O:267:ALA:N	2.86	0.43
13:O:36:ILE:O	13:O:36:ILE:CG2	2.66	0.43
16:V:101:TYR:CE2	31:V:1041:HEM:HAA1	2.54	0.43
23:B:1013:CLA:CMC	23:B:1013:CLA:HBC3	2.38	0.42
2:B:162:PHE:CD1	2:B:162:PHE:C	2.92	0.42
2:B:23:HIS:C	2:B:25:MET:N	2.73	0.42
2:B:309:LEU:O	2:B:310:ALA:C	2.57	0.42
2:B:359:MET:HA	2:B:360:PRO:HD2	1.85	0.42
2:B:98:LEU:O	2:B:98:LEU:HD22	2.19	0.42
23:C:1027:CLA:H41	23:C:1027:CLA:H62	1.60	0.42
23:C:1036:CLA:H42	23:C:1036:CLA:O2A	2.19	0.42
3:C:128:GLY:N	23:C:1037:CLA:HAC2	2.34	0.42
3:C:321:ASP:N	3:C:321:ASP:OD2	2.52	0.42
1:A:305:SER:HB3	3:C:415:ASN:HD21	1.84	0.42
3:C:441:HIS:C	3:C:441:HIS:ND1	2.72	0.42
3:C:83:GLU:CD	16:V:129:LYS:HZ1	2.23	0.42
1:A:133:LEU:HD23	4:D:252:PHE:CD2	2.53	0.42
4:D:269:PHE:CD1	4:D:269:PHE:C	2.92	0.42
4:D:276:VAL:HG23	4:D:277:THR:H	1.83	0.42
4:D:281:MET:CE	4:D:281:MET:CA	2.97	0.42
4:D:299:ILE:C	4:D:301:GLN:N	2.72	0.42
13:O:227:VAL:HG13	13:O:237:ILE:HG13	2.00	0.42
16:V:105:PRO:HD3	16:V:120:SER:HB3	2.01	0.42
18:Y:44:GLY:O	18:Y:45:ASN:CB	2.49	0.42
23:A:1006:CLA:H161	26:D:1050:BCR:C27	2.44	0.42
1:A:113:GLN:CA	1:A:116:ILE:HG22	2.48	0.42
1:A:316:THR:C	1:A:318:ALA:N	2.72	0.42
1:A:318:ALA:HA	1:A:321:ILE:HD12	2.00	0.42
1:A:323:ARG:C	1:A:325:ASN:N	2.73	0.42
1:A:58:VAL:CG2	1:A:83:VAL:HG23	2.49	0.42
2:B:13:ILE:HD12	2:B:234:ILE:HG23	2.01	0.42
2:B:284:ILE:HD11	2:B:309:LEU:HG	2.01	0.42
2:B:30:VAL:O	2:B:33:TRP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:HE	2:B:264:PRO:HD3	1.84	0.42
2:B:6:TYR:O	23:B:1019:CLA:CBA	2.66	0.42
23:C:1031:CLA:OBD	23:C:1033:CLA:C15	2.68	0.42
3:C:130:VAL:CG2	23:C:1035:CLA:H102	2.49	0.42
3:C:170:ILE:CG2	3:C:171:GLY:N	2.82	0.42
3:C:191:PRO:O	3:C:192:GLY:C	2.58	0.42
3:C:54:VAL:HG12	3:C:125:LEU:O	2.19	0.42
3:C:89:ILE:HG23	3:C:111:PHE:HE2	1.80	0.42
4:D:120:PHE:CD1	4:D:123:ILE:HD12	2.55	0.42
23:B:1016:CLA:HMB3	4:D:126:MET:SD	2.59	0.42
4:D:127:LEU:O	4:D:130:PHE:HB2	2.19	0.42
4:D:87:HIS:C	4:D:167:TRP:HE1	2.20	0.42
5:E:13:ILE:O	5:E:13:ILE:HG13	2.18	0.42
7:H:35:MET:SD	23:H:1017:CLA:H42	2.59	0.42
23:K:1034:CLA:CGA	23:K:1034:CLA:C1A	2.97	0.42
23:C:1035:CLA:CBB	23:K:1034:CLA:CHB	2.96	0.42
10:K:12:PRO:HB3	20:Z:62:VAL:HG21	2.00	0.42
23:B:1015:CLA:C20	11:L:27:LEU:HD13	2.49	0.42
12:M:31:SER:HA	12:M:35:SER:O	2.19	0.42
17:X:12:ILE:O	17:X:12:ILE:CG1	2.67	0.42
1:A:219:VAL:CB	4:D:268:HIS:HB3	2.49	0.42
1:A:280:VAL:CG2	4:D:212:ALA:HB1	2.49	0.42
1:A:290:ILE:HG12	23:A:1003:CLA:OBD	2.19	0.42
23:B:1020:CLA:H8	23:B:1020:CLA:H51	1.91	0.42
2:B:346:PHE:CD2	2:B:346:PHE:N	2.87	0.42
2:B:347:ARG:O	2:B:398:THR:HG22	2.20	0.42
23:C:1035:CLA:HBA1	23:C:1035:CLA:H3A	1.88	0.42
23:C:1033:CLA:C9	23:C:1036:CLA:CAA	2.97	0.42
23:C:1037:CLA:H111	23:C:1037:CLA:H72	1.60	0.42
29:C:1056:DGD:HB32	29:C:1057:DGD:HA31	2.01	0.42
3:C:164:HIS:CA	3:C:167:VAL:HB	2.47	0.42
25:D:1042:PQ9:H312	25:D:1042:PQ9:H27	1.57	0.42
4:D:191:TRP:CD1	4:D:197:HIS:CD2	3.07	0.42
29:B:1058:DGD:HBV2	4:D:287:VAL:HG22	2.01	0.42
6:F:15:ILE:HD12	31:F:1040:HEM:CMD	2.49	0.42
6:F:16:PHE:CZ	31:F:1040:HEM:HBD2	2.54	0.42
8:I:1:MET:C	8:I:3:THR:H	2.22	0.42
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.98	0.42
26:T:6046:BCR:C8	26:T:6046:BCR:C33	2.72	0.42
1:A:340:PRO:CD	15:U:103:TYR:HE2	2.32	0.42
16:V:138:LEU:HA	16:V:138:LEU:HD23	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1003:CLA:HMC2	23:D:1004:CLA:C2C	2.49	0.42
23:A:1006:CLA:H2	23:A:1006:CLA:H61	1.68	0.42
1:A:183:MET:O	1:A:186:PHE:N	2.52	0.42
1:A:254:TYR:CD1	1:A:254:TYR:C	2.93	0.42
1:A:281:VAL:O	1:A:284:TRP:HB2	2.19	0.42
1:A:310:LYS:HE2	16:V:151:ILE:HG22	2.00	0.42
1:A:309:ALA:O	1:A:311:GLY:N	2.51	0.42
1:A:62:GLY:CA	1:A:87:ASN:HB2	2.46	0.42
23:B:1018:CLA:H112	23:B:1018:CLA:H142	1.64	0.42
23:B:1022:CLA:CBC	23:B:1022:CLA:C9	2.62	0.42
2:B:159:THR:HG22	2:B:199:VAL:HG11	2.01	0.42
2:B:268:PHE:N	2:B:268:PHE:CD1	2.88	0.42
2:B:329:PRO:C	2:B:331:ASN:H	2.23	0.42
2:B:437:LEU:O	2:B:438:ASN:HB3	2.19	0.42
2:B:61:PHE:HB2	23:B:1015:CLA:CMA	2.48	0.42
2:B:95:GLY:O	2:B:99:ALA:CB	2.67	0.42
3:C:117:VAL:HG21	23:C:1027:CLA:C4	2.49	0.42
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.01	0.42
3:C:82:TYR:HD1	3:C:419:PHE:HE2	1.66	0.42
23:A:1003:CLA:CMC	23:D:1004:CLA:HMC2	2.49	0.42
23:D:1005:CLA:HBD	23:D:1005:CLA:HAA1	2.01	0.42
4:D:125:PHE:C	4:D:125:PHE:CD1	2.92	0.42
4:D:14:TRP:O	4:D:17:ILE:CG1	2.67	0.42
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.01	0.42
4:D:348:ARG:HH21	4:D:352:LEU:C	2.22	0.42
5:E:22:ILE:O	5:E:25:ILE:HG13	2.18	0.42
6:F:17:THR:O	6:F:18:VAL:C	2.58	0.42
29:B:1058:DGD:HG11	7:H:50:ASN:HD22	1.84	0.42
4:D:89:LEU:CD1	7:H:50:ASN:OD1	2.62	0.42
23:C:1035:CLA:CBB	23:K:1034:CLA:HMA2	2.50	0.42
13:O:52:ALA:CB	13:O:229:LYS:HA	2.50	0.42
13:O:260:LYS:O	13:O:261:ILE:HD13	2.19	0.42
16:V:108:TYR:CD2	16:V:108:TYR:O	2.72	0.42
20:Z:45:GLY:O	20:Z:49:ALA:CB	2.67	0.42
23:A:1003:CLA:C14	24:A:1038:PHO:C7	2.97	0.42
23:A:1007:CLA:H72	23:A:1007:CLA:H112	1.53	0.42
1:A:105:TRP:CD1	1:A:110:GLY:HA3	2.55	0.42
1:A:113:GLN:HB3	1:A:117:PHE:CE1	2.54	0.42
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.84	0.42
23:B:1021:CLA:C12	30:B:1060:MGE:H132	2.50	0.42
2:B:103:LEU:CG	2:B:104:SER:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:LEU:HB3	26:B:1048:BCR:H23C	2.01	0.42
2:B:247:PHE:O	2:B:247:PHE:CD1	2.72	0.42
2:B:332:LYS:O	2:B:444:ARG:NH1	2.53	0.42
3:C:305:THR:HG22	3:C:308:GLU:CB	2.41	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.19	0.42
3:C:89:ILE:N	3:C:90:PRO:CD	2.80	0.42
4:D:191:TRP:O	4:D:193:LEU:N	2.52	0.42
7:H:17:GLU:O	7:H:17:GLU:HG2	2.19	0.42
7:H:3:ARG:HB3	7:H:3:ARG:HE	1.54	0.42
13:O:254:HIS:H	13:O:254:HIS:CD2	2.38	0.42
13:O:79:LYS:HB2	13:O:91:PHE:CE2	2.53	0.42
26:T:6046:BCR:C23	26:T:6046:BCR:C40	2.92	0.42
15:U:36:ILE:HG22	15:U:42:TYR:HB2	2.02	0.42
18:Y:30:ILE:O	18:Y:30:ILE:CG1	2.67	0.42
1:A:180:PHE:O	1:A:184:ILE:CD1	2.68	0.42
1:A:199:GLN:C	1:A:201:GLY:H	2.22	0.42
1:A:27:ARG:NH1	1:A:28:LEU:HD12	2.34	0.42
1:A:41:LEU:HD22	1:A:41:LEU:H	1.83	0.42
23:B:1011:CLA:H2	23:B:1013:CLA:H91	1.93	0.42
23:B:1011:CLA:ND	23:B:1013:CLA:H51	2.35	0.42
2:B:65:PHE:CE1	23:B:1012:CLA:HED2	2.54	0.42
2:B:237:VAL:C	23:B:1020:CLA:HMD3	2.39	0.42
2:B:311:PHE:HD2	2:B:311:PHE:O	2.03	0.42
2:B:370:LEU:N	2:B:370:LEU:HD12	2.35	0.42
23:C:1035:CLA:CBB	23:K:1034:CLA:HMA1	2.50	0.42
3:C:166:ILE:CD1	3:C:248:GLY:HA3	2.44	0.42
3:C:440:GLY:C	3:C:442:LEU:N	2.72	0.42
4:D:120:PHE:O	4:D:121:GLY:C	2.55	0.42
4:D:93:TRP:HA	4:D:99:GLY:H	1.84	0.42
5:E:18:ARG:HG2	5:E:22:ILE:HD11	2.01	0.42
5:E:27:ILE:CD1	5:E:27:ILE:N	2.82	0.42
9:J:18:GLY:HA3	26:K:1051:BCR:H371	2.00	0.42
3:C:62:PHE:HZ	10:K:28:ILE:HB	1.83	0.42
13:O:134:VAL:HG23	13:O:142:ILE:HG22	2.02	0.42
13:O:37:VAL:O	13:O:37:VAL:HG13	2.19	0.42
13:O:80:GLU:O	13:O:82:PRO:N	2.53	0.42
15:U:64:ILE:H	15:U:67:LEU:HD12	1.84	0.42
15:U:78:ASN:C	15:U:82:PHE:HE2	2.23	0.42
1:A:105:TRP:CH2	1:A:111:PRO:HA	2.55	0.42
1:A:271:LEU:O	1:A:275:LEU:HG	2.19	0.42
1:A:285:PHE:O	1:A:289:GLY:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:CG	1:A:328:MET:HE1	2.49	0.42
2:B:248:ALA:CA	23:B:1011:CLA:H51	2.50	0.42
2:B:21:ALA:HB2	2:B:114:HIS:HB2	2.02	0.42
2:B:392:PHE:HE2	2:B:417:VAL:HG12	1.85	0.42
23:C:1037:CLA:H121	23:C:1037:CLA:H162	1.26	0.42
3:C:119:LEU:HD11	26:C:1052:BCR:C34	2.48	0.42
3:C:431:PHE:O	3:C:431:PHE:CD2	2.69	0.42
3:C:64:ALA:O	3:C:68:THR:CB	2.68	0.42
4:D:307:GLU:O	4:D:308:ASP:C	2.58	0.42
4:D:82:ALA:C	4:D:84:SER:N	2.73	0.42
7:H:28:THR:N	23:H:1017:CLA:OBD	2.52	0.42
8:I:14:PHE:CE1	8:I:18:LEU:HD12	2.43	0.42
11:L:24:ILE:HD11	12:M:18:PRO:HB2	2.01	0.42
12:M:32:GLN:CA	12:M:32:GLN:HE21	2.25	0.42
13:O:104:LEU:CD1	13:O:107:ILE:HD11	2.49	0.42
13:O:234:THR:HB	13:O:236:GLU:HG3	2.01	0.42
15:U:71:GLN:O	15:U:72:LYS:C	2.57	0.42
23:A:1006:CLA:HAA1	23:A:1006:CLA:CBD	2.49	0.42
24:A:1038:PHO:OBD	24:A:1038:PHO:O2D	2.38	0.42
27:A:1063:LHG:HC11	3:C:447:ARG:HH12	1.85	0.42
1:A:161:TYR:N	1:A:162:PRO:CD	2.83	0.42
1:A:37:MET:SD	1:A:126:TYR:CB	3.08	0.42
2:B:219:VAL:HG12	2:B:220:ARG:N	2.34	0.42
2:B:313:ASP:OD2	2:B:358:ARG:NH2	2.50	0.42
2:B:326:ARG:NH2	2:B:442:ILE:CG2	2.83	0.42
2:B:474:LEU:C	2:B:475:PHE:HD2	2.23	0.42
3:C:146:PHE:O	3:C:147:PHE:HB2	2.19	0.42
3:C:342:MET:HG2	3:C:343:ARG:N	2.34	0.42
3:C:45:LEU:HA	3:C:45:LEU:HD23	1.75	0.42
1:A:206:PHE:CE2	23:D:1004:CLA:O1A	2.73	0.42
5:E:74:GLN:O	5:E:77:GLU:HB2	2.20	0.42
5:E:79:PHE:C	5:E:81:GLU:N	2.72	0.42
5:E:79:PHE:C	5:E:83:LEU:HD13	2.38	0.42
7:H:28:THR:O	7:H:31:MET:N	2.44	0.42
2:B:188:ASP:CB	7:H:58:VAL:HG22	2.50	0.42
12:M:8:PHE:O	12:M:12:ALA:CB	2.67	0.42
13:O:104:LEU:HD12	13:O:104:LEU:C	2.40	0.42
14:T:28:ARG:HE	14:T:28:ARG:HA	1.83	0.42
15:U:26:ASP:HB3	15:U:30:THR:H	1.84	0.42
16:V:105:PRO:HG2	16:V:115:ALA:HA	2.00	0.42
1:A:304:HIS:HE1	16:V:163:TYR:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:47:LEU:CG	16:V:48:THR:H	2.33	0.42
18:Y:30:ILE:O	18:Y:30:ILE:HG12	2.20	0.42
18:Y:43:ARG:CD	20:Z:31:GLN:HE21	2.28	0.42
24:A:1038:PHO:H91	23:D:1005:CLA:C17	2.49	0.42
1:A:131:TRP:CE3	1:A:132:GLU:N	2.87	0.42
1:A:142:TRP:HE1	4:D:219:GLU:HB3	1.84	0.42
1:A:38:ILE:CB	1:A:39:PRO:HD3	2.50	0.42
23:B:1010:CLA:H61	23:B:1010:CLA:H41	1.84	0.42
2:B:150:CYS:N	23:B:1011:CLA:HBC2	2.34	0.42
2:B:135:LEU:HA	2:B:138:MET:HE2	2.01	0.42
23:C:1033:CLA:H162	23:C:1033:CLA:H202	1.78	0.42
23:C:1033:CLA:C14	23:C:1036:CLA:HMD2	2.50	0.42
3:C:130:VAL:O	3:C:134:ILE:CD1	2.68	0.42
3:C:362:ARG:HD2	3:C:367:GLU:CD	2.40	0.42
23:A:1003:CLA:HAB	23:D:1004:CLA:C4B	2.49	0.42
23:B:1016:CLA:H143	23:D:1008:CLA:HMB2	2.01	0.42
3:C:457:LYS:HZ2	4:D:228:GLY:HA2	1.80	0.42
1:A:129:ARG:NH1	4:D:256:ILE:HD12	2.32	0.42
10:K:35:LEU:O	10:K:37:PHE:N	2.53	0.42
12:M:18:PRO:CG	12:M:19:SER:N	2.83	0.42
13:O:145:LEU:O	13:O:146:PHE:C	2.59	0.42
15:U:28:ASN:ND2	15:U:54:PRO:HB2	2.24	0.42
17:X:13:THR:O	17:X:15:SER:N	2.53	0.42
20:Z:5:PHE:O	20:Z:8:ALA:HB3	2.19	0.42
1:A:37:MET:SD	1:A:126:TYR:HA	2.59	0.42
1:A:134:SER:HA	1:A:139:MET:HG2	2.01	0.42
1:A:81:ALA:CA	1:A:175:GLY:HA3	2.49	0.42
1:A:310:LYS:HG2	16:V:151:ILE:CG2	2.46	0.42
1:A:318:ALA:HA	1:A:321:ILE:CD1	2.50	0.42
1:A:330:VAL:HG21	4:D:328:TRP:CZ2	2.55	0.42
1:A:99:ALA:O	1:A:100:ALA:O	2.38	0.42
23:B:1011:CLA:CAD	23:B:1013:CLA:H11	2.48	0.42
23:B:1015:CLA:HAA1	23:B:1015:CLA:CBD	2.50	0.42
2:B:99:ALA:O	2:B:101:ILE:N	2.53	0.42
2:B:463:PHE:CD2	29:B:1058:DGD:HAV1	2.54	0.42
2:B:215:PHE:CE2	2:B:219:VAL:HG21	2.55	0.42
2:B:25:MET:O	2:B:26:HIS:C	2.56	0.42
2:B:329:PRO:C	2:B:331:ASN:N	2.73	0.42
2:B:49:ASP:HA	2:B:50:PRO:HD3	1.86	0.42
2:B:55:MET:HE1	2:B:63:LEU:HD21	2.02	0.42
23:C:1025:CLA:HMB3	26:C:1054:BCR:C27	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1035:CLA:HMD2	10:K:40:GLN:HE22	1.72	0.42
23:C:1032:CLA:H18	29:C:1056:DGD:HBH1	2.02	0.42
3:C:276:LEU:HD22	3:C:441:HIS:N	2.34	0.42
4:D:238:THR:HG22	4:D:239:GLN:HG2	2.01	0.42
4:D:69:GLU:HB3	5:E:55:TYR:OH	2.19	0.42
4:D:97:ALA:HB1	4:D:104:TRP:HB2	2.02	0.42
7:H:41:PHE:CD1	26:H:1049:BCR:H362	2.49	0.42
11:L:26:VAL:O	11:L:27:LEU:C	2.58	0.42
13:O:184:ASP:CG	13:O:188:ARG:NH1	2.74	0.42
13:O:76:PHE:CD1	13:O:261:ILE:HD12	2.54	0.42
16:V:156:TRP:HA	16:V:156:TRP:CE3	2.55	0.42
18:Y:35:ILE:CD1	18:Y:36:ILE:HD12	2.50	0.42
1:A:193:LEU:CD2	1:A:193:LEU:O	2.68	0.41
1:A:252:HIS:ND1	1:A:266:ASN:HB3	2.35	0.41
1:A:310:LYS:N	16:V:28:GLU:HB2	2.34	0.41
23:B:1023:CLA:HMA2	23:B:1023:CLA:H2	2.01	0.41
2:B:24:LEU:CG	2:B:111:ALA:HA	2.50	0.41
2:B:263:THR:O	2:B:263:THR:OG1	2.26	0.41
2:B:394:GLN:HB3	15:U:17:LEU:HD22	2.01	0.41
3:C:160:ILE:O	3:C:161:LEU:C	2.57	0.41
3:C:154:LYS:HE3	3:C:261:ARG:HE	1.83	0.41
3:C:224:ILE:HG22	3:C:289:PHE:CE1	2.55	0.41
3:C:451:ALA:O	3:C:454:GLY:N	2.53	0.41
3:C:79:LYS:O	3:C:84:GLN:NE2	2.53	0.41
24:D:1039:PHO:HMB2	23:D:1004:CLA:H111	2.02	0.41
5:E:34:GLY:O	5:E:37:PHE:HB3	2.20	0.41
4:D:54:PHE:CD1	5:E:47:PHE:HE1	2.38	0.41
6:F:24:HIS:C	6:F:26:LEU:N	2.73	0.41
23:B:1016:CLA:C19	23:H:1017:CLA:H191	2.16	0.41
8:I:4:LEU:O	8:I:5:LYS:C	2.58	0.41
26:K:1051:BCR:H371	26:K:1051:BCR:H24C	1.64	0.41
10:K:17:ILE:H	10:K:17:ILE:HG13	1.47	0.41
13:O:156:GLN:HA	13:O:157:PRO:HD3	1.86	0.41
13:O:163:THR:C	13:O:165:SER:N	2.72	0.41
13:O:175:PRO:HG2	13:O:176:SER:N	2.34	0.41
13:O:192:SER:OG	13:O:193:GLY:N	2.53	0.41
1:A:340:PRO:CD	15:U:103:TYR:CE2	3.03	0.41
15:U:45:LEU:HD12	15:U:45:LEU:HA	1.95	0.41
13:O:180:ALA:HB2	15:U:90:ALA:O	2.20	0.41
16:V:148:GLU:O	16:V:151:ILE:CD1	2.68	0.41
16:V:90:PRO:O	16:V:91:PRO:C	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:33:TRP:O	20:Z:37:LYS:HB3	2.19	0.41
1:A:183:MET:C	23:A:1003:CLA:CBC	2.88	0.41
23:B:1023:CLA:CMB	23:B:1023:CLA:HBB1	2.48	0.41
2:B:246:PHE:HB3	2:B:462:PHE:HB3	2.01	0.41
2:B:385:ARG:HE	2:B:385:ARG:HB2	1.14	0.41
23:C:1035:CLA:H2	23:C:1035:CLA:H93	2.02	0.41
3:C:157:MET:HB3	23:C:1031:CLA:CBC	2.49	0.41
3:C:165:LEU:HD21	23:C:1030:CLA:CBB	2.50	0.41
3:C:171:GLY:HA2	3:C:174:LEU:H	1.85	0.41
3:C:239:TRP:O	3:C:243:ILE:CG1	2.67	0.41
3:C:309:ALA:O	3:C:311:GLN:N	2.53	0.41
3:C:337:LEU:HA	3:C:337:LEU:HD23	1.80	0.41
3:C:56:HIS:HD2	3:C:57:ALA:CA	2.33	0.41
4:D:122:LEU:N	4:D:122:LEU:HD22	2.34	0.41
4:D:21:TRP:CE3	4:D:22:LEU:HB3	2.55	0.41
1:A:269:ARG:NE	4:D:222:LEU:HD21	2.35	0.41
4:D:267:LEU:HD23	4:D:268:HIS:N	2.35	0.41
4:D:46:GLY:HA2	26:D:1050:BCR:H10C	2.02	0.41
7:H:31:MET:SD	23:H:1017:CLA:CAA	3.04	0.41
7:H:35:MET:O	7:H:38:PHE:HB3	2.20	0.41
10:K:35:LEU:HD22	26:K:1051:BCR:H352	2.02	0.41
3:C:343:ARG:NH2	13:O:103:SER:O	2.47	0.41
13:O:231:ASP:CB	13:O:234:THR:OG1	2.65	0.41
3:C:348:GLU:CB	13:O:42:ALA:CB	2.84	0.41
26:T:6046:BCR:H371	26:T:6046:BCR:H24C	1.61	0.41
26:T:6048:BCR:C30	26:T:6048:BCR:C37	2.61	0.41
16:V:156:TRP:HE3	16:V:156:TRP:HA	1.85	0.41
1:A:215:HIS:HD2	1:A:275:LEU:CD1	2.33	0.41
1:A:278:TRP:CA	1:A:278:TRP:CE3	2.94	0.41
23:B:1012:CLA:C2C	23:B:1021:CLA:CBB	2.98	0.41
23:B:1021:CLA:HED2	23:B:1021:CLA:NA	2.20	0.41
2:B:56:TRP:HZ3	2:B:317:ASN:OD1	2.03	0.41
2:B:445:THR:OG1	2:B:449:GLY:HA3	2.20	0.41
23:C:1025:CLA:CMB	26:C:1054:BCR:C24	2.98	0.41
23:C:1026:CLA:CBD	23:C:1026:CLA:HAA1	2.50	0.41
23:C:1028:CLA:H161	23:C:1028:CLA:H202	1.61	0.41
25:D:1042:PQ9:H201	25:D:1042:PQ9:H162	1.84	0.41
4:D:236:ASN:OD1	4:D:239:GLN:O	2.37	0.41
4:D:269:PHE:C	4:D:271:MET:N	2.72	0.41
30:B:1060:MGE:H5B2	4:D:276:VAL:CG2	2.50	0.41
4:D:292:ASN:O	4:D:294:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:346:LEU:HA	4:D:347:PRO:HD2	1.86	0.41
5:E:77:GLU:C	5:E:79:PHE:N	2.74	0.41
7:H:40:VAL:HG12	7:H:44:ILE:HG12	2.03	0.41
8:I:3:THR:O	8:I:6:ILE:HG13	2.20	0.41
12:M:20:VAL:O	12:M:24:ILE:HG13	2.20	0.41
14:T:11:ALA:C	14:T:13:ILE:N	2.74	0.41
18:Y:43:ARG:CZ	20:Z:29:SER:HB3	2.49	0.41
1:A:183:MET:CB	23:A:1003:CLA:HBC3	2.35	0.41
1:A:107:TYR:O	1:A:109:GLY:N	2.53	0.41
1:A:142:TRP:CZ2	1:A:273:PHE:HD1	2.38	0.41
23:B:1016:CLA:H112	23:B:1016:CLA:H142	1.63	0.41
2:B:191:ASN:O	2:B:194:ASN:N	2.52	0.41
2:B:280:PHE:O	2:B:284:ILE:CG1	2.67	0.41
2:B:326:ARG:HG2	4:D:297:ASP:OD2	2.20	0.41
2:B:90:PHE:O	2:B:90:PHE:CD2	2.74	0.41
23:C:1025:CLA:HMB3	26:C:1054:BCR:H272	2.01	0.41
3:C:49:LEU:CG	23:C:1035:CLA:CMA	2.98	0.41
3:C:143:TYR:O	3:C:144:SER:C	2.59	0.41
3:C:343:ARG:HH11	3:C:348:GLU:CG	2.24	0.41
3:C:422:PRO:O	3:C:426:LEU:HD13	2.20	0.41
3:C:432:VAL:HG13	3:C:433:LEU:N	2.35	0.41
23:D:1004:CLA:H111	23:D:1004:CLA:H71	1.71	0.41
4:D:153:PHE:O	4:D:157:PHE:HB2	2.20	0.41
4:D:313:THR:H	4:D:316:THR:CG2	2.34	0.41
4:D:315:TYR:CZ	4:D:319:LEU:HD12	2.55	0.41
6:F:43:ILE:O	9:J:36:LEU:HG	2.20	0.41
11:L:25:LEU:HB3	14:T:13:ILE:HG12	2.01	0.41
13:O:183:LEU:HA	13:O:188:ARG:O	2.21	0.41
15:U:43:PRO:CG	16:V:109:ASP:CB	2.99	0.41
15:U:41:LEU:HD11	15:U:74:ILE:CG2	2.50	0.41
15:U:16:LYS:HZ2	15:U:85:THR:CB	2.34	0.41
1:A:107:TYR:C	1:A:109:GLY:N	2.74	0.41
1:A:193:LEU:O	4:D:179:PHE:CE2	2.73	0.41
1:A:202:VAL:HA	1:A:205:VAL:HG11	2.02	0.41
1:A:223:LEU:CG	4:D:265:ARG:HG2	2.51	0.41
1:A:187:GLN:HG2	1:A:328:MET:HE1	2.02	0.41
23:B:1010:CLA:H62	23:B:1010:CLA:H93	1.81	0.41
2:B:237:VAL:C	23:B:1020:CLA:CMD	2.89	0.41
2:B:98:LEU:O	2:B:102:VAL:HG22	2.20	0.41
2:B:33:TRP:HH2	2:B:62:VAL:CG2	2.33	0.41
3:C:100:GLY:O	3:C:101:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1025:CLA:H162	23:C:1025:CLA:H203	1.72	0.41
3:C:200:THR:OG1	3:C:201:ASN:N	2.53	0.41
3:C:237:HIS:O	3:C:238:ILE:C	2.58	0.41
3:C:304:PRO:HG3	3:C:398:HIS:O	2.21	0.41
3:C:350:ILE:CG2	3:C:359:TRP:HB2	2.31	0.41
3:C:386:PRO:C	3:C:388:GLN:N	2.73	0.41
3:C:443:TRP:CA	3:C:443:TRP:CE3	3.02	0.41
4:D:282:SER:HB2	23:D:1004:CLA:HED3	2.01	0.41
23:D:1008:CLA:H41	23:D:1008:CLA:H61	1.64	0.41
4:D:116:LEU:O	4:D:120:PHE:CD2	2.74	0.41
4:D:78:VAL:CG1	4:D:173:PHE:CB	2.99	0.41
4:D:273:PHE:O	4:D:276:VAL:HG22	2.21	0.41
4:D:27:PHE:HD1	6:F:19:ARG:HG3	1.85	0.41
6:F:24:HIS:O	6:F:25:THR:C	2.59	0.41
6:F:34:LEU:HD13	9:J:28:PHE:HZ	1.85	0.41
30:L:1061:MGE:H3B1	30:L:1061:MGE:H6B2	1.58	0.41
13:O:56:TYR:O	13:O:161:SER:HA	2.20	0.41
3:C:348:GLU:CB	13:O:42:ALA:HB3	2.49	0.41
14:T:22:PHE:HD1	14:T:22:PHE:N	2.17	0.41
16:V:105:PRO:HG2	16:V:115:ALA:CA	2.50	0.41
25:A:1043:PQ9:H311	25:A:1043:PQ9:H37	2.01	0.41
1:A:185:VAL:HG12	1:A:186:PHE:N	2.34	0.41
1:A:190:HIS:HA	1:A:298:ASN:HB3	2.03	0.41
1:A:272:HIS:HB3	4:D:218:VAL:CG1	2.50	0.41
23:B:1023:CLA:HAA2	23:B:1023:CLA:CBD	2.51	0.41
2:B:113:TRP:CZ2	23:B:1024:CLA:HBD	2.56	0.41
23:B:1024:CLA:O2A	23:B:1024:CLA:C2A	2.62	0.41
2:B:122:LEU:HD23	7:H:8:GLY:C	2.41	0.41
2:B:172:TYR:CD2	2:B:173:GLY:N	2.88	0.41
2:B:201:HIS:CD2	2:B:202:HIS:CD2	3.09	0.41
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.56	0.41
2:B:333:GLY:HA2	2:B:442:ILE:O	2.20	0.41
23:C:1025:CLA:CBB	23:C:1025:CLA:HMB1	2.47	0.41
26:C:1052:BCR:H331	26:C:1052:BCR:C8	2.49	0.41
3:C:305:THR:O	3:C:308:GLU:HB3	2.19	0.41
3:C:81:MET:O	3:C:86:LEU:HD12	2.20	0.41
4:D:176:ALA:O	4:D:179:PHE:N	2.52	0.41
4:D:29:PHE:CD2	4:D:29:PHE:C	2.93	0.41
6:F:15:ILE:HD12	31:F:1040:HEM:HMD1	2.02	0.41
9:J:34:ALA:O	9:J:35:GLY:O	2.39	0.41
10:K:21:LEU:C	10:K:23:ASP:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:162:ILE:HD13	13:O:269:ILE:HD12	2.02	0.41
16:V:32:GLU:HA	16:V:35:THR:CB	2.51	0.41
23:A:1003:CLA:CHD	23:A:1003:CLA:CBC	2.96	0.41
23:A:1007:CLA:H111	23:A:1007:CLA:H142	1.67	0.41
1:A:226:GLU:O	1:A:227:THR:HB	2.21	0.41
1:A:96:ILE:HG22	1:A:96:ILE:O	2.20	0.41
23:B:1010:CLA:C3D	23:B:1011:CLA:CMB	2.98	0.41
2:B:149:LEU:CB	23:B:1012:CLA:C20	2.95	0.41
23:B:1018:CLA:H8	23:B:1023:CLA:HBA2	2.01	0.41
2:B:472:ARG:CD	23:B:1019:CLA:HED3	2.50	0.41
2:B:121:GLU:O	2:B:124:ARG:N	2.35	0.41
2:B:346:PHE:HE1	2:B:421:ALA:HB2	1.84	0.41
2:B:469:HIS:O	2:B:473:THR:N	2.54	0.41
2:B:52:LEU:C	2:B:54:PRO:HD3	2.40	0.41
23:C:1026:CLA:H92	23:C:1026:CLA:H61	1.63	0.41
3:C:33:PHE:CD2	4:D:229:ALA:CB	3.04	0.41
3:C:401:LEU:O	3:C:409:GLY:N	2.48	0.41
1:A:184:ILE:CD1	4:D:186:GLN:NE2	2.84	0.41
1:A:323:ARG:CG	4:D:329:MET:HA	2.50	0.41
4:D:53:THR:HG22	4:D:67:TYR:HD2	1.85	0.41
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.55	0.41
4:D:92:LEU:HG	4:D:99:GLY:HA2	2.03	0.41
5:E:77:GLU:O	5:E:80:LEU:N	2.53	0.41
23:K:1034:CLA:CBA	23:K:1034:CLA:H43	2.44	0.41
3:C:62:PHE:CE2	10:K:29:PRO:HG3	2.55	0.41
13:O:216:PHE:CD2	13:O:216:PHE:C	2.94	0.41
16:V:118:HIS:NE2	31:V:1041:HEM:NB	2.69	0.41
26:A:1044:BCR:C30	26:A:1044:BCR:C37	2.61	0.41
1:A:96:ILE:HD12	23:A:1007:CLA:HMD3	2.01	0.41
23:B:1012:CLA:HBB1	23:B:1015:CLA:CAB	2.45	0.41
23:B:1013:CLA:C2B	23:B:1014:CLA:H11	2.51	0.41
23:B:1016:CLA:CHD	23:B:1016:CLA:CBC	2.97	0.41
23:B:1019:CLA:C19	23:B:1021:CLA:H71	2.50	0.41
23:B:1023:CLA:H112	23:B:1024:CLA:C11	2.51	0.41
2:B:125:ASP:OD1	2:B:126:PRO:HD2	2.21	0.41
2:B:12:LEU:CD2	2:B:19:LEU:HA	2.51	0.41
2:B:421:ALA:O	2:B:424:ALA:N	2.50	0.41
2:B:429:ILE:HG22	2:B:430:PHE:N	2.34	0.41
2:B:242:ILE:HG22	2:B:466:HIS:HB2	2.03	0.41
23:C:1028:CLA:H71	23:C:1028:CLA:H111	1.83	0.41
3:C:110:PRO:O	3:C:113:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:C	3:C:276:LEU:CD2	2.88	0.41
1:A:135:TYR:HE1	3:C:449:ARG:O	2.03	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HA	2.02	0.41
4:D:186:GLN:CB	23:D:1004:CLA:HBC1	2.51	0.41
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.41
5:E:23:HIS:O	5:E:27:ILE:HD13	2.21	0.41
5:E:34:GLY:CA	6:F:32:PHE:CD1	3.03	0.41
11:L:19:LEU:HD23	11:L:19:LEU:N	2.34	0.41
20:Z:43:GLY:O	20:Z:47:TRP:HB2	2.20	0.41
23:A:1006:CLA:HAA2	29:C:1057:DGD:HBN2	2.02	0.41
1:A:120:LEU:HD11	1:A:155:PHE:CD1	2.55	0.41
1:A:124:SER:OG	1:A:155:PHE:CE2	2.74	0.41
1:A:195:HIS:ND1	1:A:197:PHE:HB2	2.36	0.41
1:A:279:ARG:HG2	4:D:212:ALA:CB	2.50	0.41
23:B:1011:CLA:H92	23:B:1011:CLA:CBB	2.43	0.41
2:B:69:LEU:HD23	23:B:1013:CLA:H3A	2.03	0.41
2:B:153:PHE:HA	23:B:1014:CLA:HMC3	2.03	0.41
23:B:1016:CLA:H8	23:H:1017:CLA:H111	2.02	0.41
2:B:121:GLU:HB3	7:H:4:ARG:HA	2.01	0.41
2:B:137:LYS:HB3	2:B:137:LYS:NZ	2.36	0.41
2:B:192:PRO:HG3	7:H:49:TYR:CD1	2.55	0.41
2:B:271:THR:HG23	2:B:274:GLN:H	1.85	0.41
2:B:41:GLU:HB3	2:B:60:MET:SD	2.60	0.41
2:B:67:ALA:CB	2:B:267:LEU:HD21	2.50	0.41
23:C:1025:CLA:HBA2	23:C:1025:CLA:H3A	1.58	0.41
29:C:1056:DGD:HB21	29:C:1056:DGD:HG12	2.02	0.41
3:C:284:PHE:HB3	29:C:1055:DGD:C8B	2.50	0.41
3:C:49:LEU:HD23	3:C:133:ALA:HB2	2.03	0.41
26:D:1050:BCR:C16	26:D:1050:BCR:H351	2.48	0.41
4:D:129:GLN:NE2	4:D:142:ASN:OD1	2.54	0.41
4:D:144:ILE:O	4:D:145:ALA:C	2.59	0.41
1:A:180:PHE:HD1	4:D:192:THR:HB	1.73	0.41
4:D:103:ARG:HG3	5:E:73:LYS:CD	2.50	0.41
8:I:27:ASP:C	8:I:29:ALA:N	2.73	0.41
12:M:29:THR:C	12:M:31:SER:H	2.24	0.41
13:O:118:SER:HB3	13:O:157:PRO:HA	2.03	0.41
13:O:37:VAL:CG1	13:O:37:VAL:O	2.68	0.41
16:V:35:THR:HG23	16:V:46:THR:H	1.85	0.41
16:V:70:GLY:HA3	16:V:156:TRP:CE3	2.56	0.41
1:A:316:THR:CG2	4:D:75:THR:CG2	2.99	0.41
1:A:46:ILE:HD13	1:A:46:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ALA:O	2:B:113:TRP:HB3	2.21	0.41
2:B:341:LYS:O	2:B:404:GLY:HA3	2.20	0.41
23:C:1032:CLA:H2	23:K:1034:CLA:HMB1	2.03	0.41
3:C:376:ASP:OD1	3:C:379:LYS:HG3	2.20	0.41
3:C:404:LEU:C	3:C:406:SER:N	2.73	0.41
24:D:1039:PHO:H92	24:D:1039:PHO:H111	1.74	0.41
4:D:214:HIS:C	4:D:217:THR:HG22	2.41	0.41
1:A:331:MET:CG	4:D:320:LEU:HD22	2.51	0.41
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.96	0.41
13:O:131:PRO:HA	13:O:145:LEU:HD12	2.03	0.41
13:O:188:ARG:HD3	13:O:212:ASN:OD1	2.21	0.41
13:O:211:ALA:O	13:O:214:LYS:HD3	2.21	0.41
13:O:265:PHE:HD1	13:O:266:TYR:O	2.04	0.41
15:U:73:GLN:O	15:U:74:ILE:C	2.59	0.41
16:V:71:ILE:HG13	16:V:72:THR:N	2.35	0.41
20:Z:35:ARG:HG3	20:Z:36:SER:H	1.86	0.41
23:A:1007:CLA:H162	23:A:1007:CLA:H193	1.73	0.41
1:A:141:PRO:HG2	3:C:446:GLY:O	2.21	0.41
1:A:47:CYS:HA	26:A:1044:BCR:H372	2.02	0.41
1:A:76:ASN:HB2	1:A:79:THR:CG2	2.51	0.41
23:B:1021:CLA:CMA	23:B:1021:CLA:C2	2.99	0.41
23:B:1021:CLA:HED1	23:B:1021:CLA:H52	2.02	0.41
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.56	0.41
2:B:422:ARG:HG2	2:B:422:ARG:O	2.21	0.41
2:B:341:LYS:HD2	2:B:429:ILE:CG2	2.51	0.41
3:C:431:PHE:C	3:C:431:PHE:HD2	2.23	0.41
4:D:100:ASP:O	4:D:103:ARG:N	2.54	0.41
1:A:210:LEU:HD12	24:D:1039:PHO:NC	2.36	0.41
4:D:193:LEU:HA	4:D:198:MET:HE1	2.03	0.41
1:A:260:PHE:O	4:D:27:PHE:HE2	2.04	0.41
6:F:29:PRO:O	6:F:30:THR:C	2.58	0.41
6:F:37:ILE:C	6:F:39:ALA:N	2.74	0.41
8:I:4:LEU:HA	8:I:4:LEU:HD12	1.79	0.41
8:I:9:TYR:O	8:I:13:THR:N	2.36	0.41
3:C:60:ILE:CB	23:K:1034:CLA:HMD2	2.50	0.41
11:L:36:PHE:CD1	12:M:7:GLY:HA3	2.55	0.41
13:O:136:MET:HB2	13:O:140:GLU:HB2	2.02	0.41
13:O:185:PRO:O	13:O:186:LYS:CB	2.68	0.41
13:O:197:ALA:O	13:O:199:ALA:N	2.53	0.41
30:D:1062:MGE:H241	14:T:13:ILE:HG21	2.03	0.41
14:T:2:GLU:OE1	14:T:2:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:6046:BCR:C40	26:T:6046:BCR:H23C	2.36	0.41
15:U:75:LEU:O	15:U:76:ARG:C	2.59	0.41
24:A:1038:PHO:HBD	24:A:1038:PHO:HAA1	2.02	0.40
25:A:1043:PQ9:H401	25:A:1043:PQ9:H361	1.70	0.40
25:A:1043:PQ9:H37	25:A:1043:PQ9:C31	2.51	0.40
1:A:204:GLY:O	1:A:205:VAL:C	2.58	0.40
1:A:256:GLY:O	1:A:261:GLN:CA	2.69	0.40
1:A:309:ALA:HB3	16:V:28:GLU:CG	2.50	0.40
1:A:49:VAL:O	1:A:53:ILE:HG13	2.21	0.40
1:A:59:ASP:O	1:A:61:ASP:O	2.39	0.40
23:B:1016:CLA:HAA1	23:B:1016:CLA:CBD	2.49	0.40
23:B:1020:CLA:H112	23:B:1020:CLA:H91	1.56	0.40
2:B:238:LEU:HA	23:B:1020:CLA:HMD3	1.99	0.40
2:B:460:LEU:CA	29:B:1058:DGD:HAG1	2.38	0.40
2:B:135:LEU:H	2:B:136:PRO:CD	2.34	0.40
1:A:155:PHE:CE1	29:C:1055:DGD:HBN1	2.56	0.40
3:C:267:SER:O	3:C:268:GLY:C	2.59	0.40
3:C:321:ASP:OD1	3:C:340:TYR:CE1	2.74	0.40
3:C:464:GLU:HA	3:C:465:PRO:HD3	1.84	0.40
23:D:1005:CLA:C20	23:D:1005:CLA:C15	2.97	0.40
4:D:166:SER:C	4:D:168:PHE:N	2.75	0.40
4:D:209:LEU:O	4:D:210:LEU:C	2.59	0.40
4:D:21:TRP:CZ3	17:X:37:LEU:CD2	3.04	0.40
4:D:284:ILE:O	4:D:287:VAL:N	2.54	0.40
4:D:329:MET:O	4:D:330:ALA:C	2.59	0.40
4:D:68:LEU:CA	6:F:40:MET:SD	3.06	0.40
7:H:47:GLU:OE2	7:H:52:THR:HG21	2.21	0.40
9:J:21:VAL:CG1	9:J:22:ILE:N	2.84	0.40
9:J:24:ILE:HG23	9:J:25:VAL:N	2.36	0.40
12:M:28:GLN:HG3	12:M:29:THR:N	2.36	0.40
16:V:30:THR:HB	16:V:31:PRO:CD	2.52	0.40
20:Z:5:PHE:HD1	20:Z:57:LEU:HD13	1.87	0.40
1:A:172:MET:HE2	1:A:179:THR:HA	2.03	0.40
1:A:186:PHE:O	1:A:189:GLU:N	2.54	0.40
1:A:218:LEU:O	1:A:221:SER:N	2.52	0.40
1:A:78:ILE:HD13	11:L:33:SER:CB	2.50	0.40
1:A:85:SER:OG	1:A:168:PHE:HB2	2.21	0.40
2:B:102:VAL:O	2:B:106:LEU:HG	2.22	0.40
23:B:1019:CLA:CMD	30:B:1060:MGE:C1G	3.00	0.40
2:B:106:LEU:O	2:B:109:LEU:N	2.48	0.40
2:B:19:LEU:O	2:B:22:ALA:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:HD22	2:B:114:HIS:CD2	2.55	0.40
2:B:271:THR:HG22	2:B:274:GLN:CD	2.41	0.40
2:B:321:LYS:HA	2:B:321:LYS:NZ	2.37	0.40
2:B:52:LEU:CD1	2:B:339:ALA:HA	2.49	0.40
2:B:392:PHE:CE2	2:B:418:LYS:HA	2.55	0.40
2:B:5:TRP:CE2	30:L:1061:MGE:C2A	3.04	0.40
2:B:66:MET:O	2:B:71:VAL:N	2.54	0.40
23:C:1027:CLA:CGA	23:C:1027:CLA:H3A	2.50	0.40
26:C:1054:BCR:C31	26:C:1054:BCR:HC8	2.51	0.40
3:C:418:ASN:HD22	29:C:1057:DGD:HE61	1.84	0.40
3:C:65:GLY:HA3	3:C:119:LEU:CA	2.51	0.40
3:C:274:TYR:O	3:C:275:SER:C	2.59	0.40
3:C:327:ASN:ND2	3:C:330:SER:C	2.75	0.40
4:D:100:ASP:C	4:D:102:THR:H	2.25	0.40
4:D:199:MET:HG2	25:D:1042:PQ9:H352	2.02	0.40
30:D:1062:MGE:O1G	30:D:1062:MGE:C1B	2.69	0.40
4:D:170:ALA:O	4:D:171:PRO:C	2.57	0.40
12:M:6:LEU:O	12:M:7:GLY:C	2.56	0.40
13:O:183:LEU:CD1	13:O:183:LEU:N	2.84	0.40
13:O:252:GLY:O	13:O:253:ALA:C	2.59	0.40
13:O:79:LYS:HA	13:O:91:PHE:HA	2.03	0.40
14:T:14:ILE:CG2	14:T:15:ALA:N	2.84	0.40
26:T:6046:BCR:C23	26:T:6046:BCR:C39	2.83	0.40
4:D:21:TRP:CZ3	17:X:37:LEU:HD21	2.55	0.40
20:Z:20:VAL:O	20:Z:21:ILE:C	2.58	0.40
1:A:153:SER:O	1:A:156:ALA:N	2.55	0.40
1:A:316:THR:CG2	4:D:75:THR:HG23	2.51	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
1:A:31:GLY:HA3	1:A:132:GLU:CD	2.42	0.40
23:B:1012:CLA:HMB3	23:B:1015:CLA:CBB	2.46	0.40
23:B:1022:CLA:H143	23:B:1022:CLA:H71	1.94	0.40
23:B:1022:CLA:OBD	11:L:10:VAL:HG21	2.20	0.40
23:B:1023:CLA:C4D	23:B:1024:CLA:CMC	2.99	0.40
2:B:149:LEU:HD13	23:B:1012:CLA:H203	2.03	0.40
2:B:277:SER:C	2:B:279:TYR:N	2.71	0.40
2:B:468:TRP:CZ2	23:B:1019:CLA:HED2	2.56	0.40
3:C:257:PHE:O	3:C:261:ARG:HG3	2.21	0.40
4:D:111:TRP:CE2	4:D:173:PHE:HE2	2.38	0.40
4:D:171:PRO:HA	4:D:181:PHE:CE2	2.55	0.40
4:D:230:SER:C	4:D:232:PHE:N	2.74	0.40
4:D:71:CYS:HG	4:D:75:THR:HG22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:ARG:HH21	6:F:13:TYR:H	1.68	0.40
9:J:21:VAL:HG12	9:J:22:ILE:CD1	2.35	0.40
23:K:1034:CLA:H141	23:K:1034:CLA:H162	1.70	0.40
30:L:1061:MGE:H7B1	30:L:1061:MGE:C3B	2.51	0.40
13:O:223:ILE:HD13	13:O:225:LEU:CD1	2.50	0.40
15:U:74:ILE:O	15:U:75:LEU:C	2.58	0.40
15:U:9:LEU:H	15:U:9:LEU:HG	1.47	0.40
17:X:43:ILE:O	17:X:44:ASP:HB2	2.22	0.40
1:A:105:TRP:HZ3	26:A:1044:BCR:C39	2.33	0.40
1:A:133:LEU:HB3	4:D:252:PHE:CE2	2.57	0.40
1:A:137:LEU:CB	1:A:139:MET:HE3	2.51	0.40
1:A:213:ALA:HB3	24:D:1039:PHO:CBC	2.50	0.40
1:A:259:ILE:O	1:A:260:PHE:HB2	2.20	0.40
1:A:39:PRO:O	1:A:40:THR:C	2.59	0.40
2:B:103:LEU:HD22	23:B:1014:CLA:H61	2.04	0.40
2:B:115:TRP:HB2	28:B:1067:IOD:I	2.91	0.40
2:B:18:ARG:HH11	11:L:4:ASN:ND2	2.19	0.40
2:B:174:LEU:HD21	2:B:265:ILE:HB	2.04	0.40
23:C:1029:CLA:C1C	23:C:1029:CLA:H41	2.52	0.40
23:C:1031:CLA:CBD	23:C:1031:CLA:HAA2	2.51	0.40
23:C:1032:CLA:CHD	23:C:1032:CLA:HBC2	2.47	0.40
3:C:305:THR:O	3:C:305:THR:HG23	2.21	0.40
3:C:322:GLN:HB2	3:C:328:VAL:HG21	2.03	0.40
3:C:362:ARG:NH1	3:C:362:ARG:HG3	2.37	0.40
4:D:103:ARG:HA	4:D:106:GLN:HB2	2.04	0.40
4:D:103:ARG:HG3	4:D:103:ARG:HH11	1.87	0.40
4:D:180:ARG:C	4:D:180:ARG:HD2	2.41	0.40
4:D:54:PHE:HD1	5:E:47:PHE:HE1	1.68	0.40
5:E:49:THR:HA	5:E:50:PRO:HD3	1.88	0.40
8:I:6:ILE:O	8:I:10:ILE:CD1	2.70	0.40
8:I:11:VAL:O	8:I:15:PHE:HD1	2.04	0.40
9:J:24:ILE:O	9:J:27:LEU:HB3	2.21	0.40
11:L:15:THR:O	11:L:16:SER:C	2.60	0.40
13:O:41:LEU:C	13:O:43:ASN:H	2.24	0.40
31:V:1041:HEM:HHC	31:V:1041:HEM:CBB	2.51	0.40
16:V:47:LEU:HD23	16:V:48:THR:O	2.21	0.40
25:A:1043:PQ9:H112	25:A:1043:PQ9:H152	1.84	0.40
1:A:145:VAL:O	1:A:146:ALA:C	2.59	0.40
1:A:173:PRO:HG2	1:A:178:GLY:HA3	2.04	0.40
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.40
1:A:49:VAL:HG23	1:A:50:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:O	1:A:73:TYR:CD2	2.74	0.40
2:B:206:GLY:O	2:B:210:ILE:HG13	2.21	0.40
2:B:23:HIS:CD2	23:B:1020:CLA:HBA2	2.57	0.40
23:C:1028:CLA:H62	23:C:1028:CLA:H41	1.42	0.40
23:C:1029:CLA:CMD	23:C:1031:CLA:CBB	2.99	0.40
3:C:284:PHE:CB	29:C:1055:DGD:HB71	2.44	0.40
3:C:222:GLY:HA3	3:C:225:VAL:HG22	2.03	0.40
3:C:188:THR:CG2	3:C:300:GLU:OE1	2.69	0.40
3:C:321:ASP:C	3:C:324:LEU:H	2.23	0.40
3:C:459:ILE:O	4:D:223:PHE:HA	2.21	0.40
25:D:1042:PQ9:H361	25:D:1042:PQ9:H32	1.77	0.40
4:D:66:SER:N	4:D:71:CYS:SG	2.94	0.40
7:H:2:ALA:O	7:H:3:ARG:HB2	2.21	0.40
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.51	0.40
13:O:187:GLY:O	13:O:194:TYR:N	2.51	0.40
15:U:68:THR:HG23	15:U:71:GLN:H	1.80	0.40
16:V:62:ALA:O	31:V:1041:HEM:CBB	2.68	0.40
20:Z:48:ILE:O	20:Z:52:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	219 (66%)	75 (22%)	39 (12%)	0	8
1	a	333/344 (97%)	216 (65%)	76 (23%)	41 (12%)	0	7
2	B	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	11
2	b	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	11
3	C	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	17
3	c	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	338/340 (99%)	222 (66%)	78 (23%)	38 (11%)	0	9
4	d	338/340 (99%)	224 (66%)	77 (23%)	37 (11%)	0	9
5	E	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	8
5	e	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	8
6	F	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	7
6	f	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	7
7	H	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	6
7	h	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	6
8	I	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	3
8	i	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	3
9	J	32/40 (80%)	29 (91%)	0	3 (9%)	1	14
9	j	32/40 (80%)	29 (91%)	0	3 (9%)	1	14
10	K	34/36 (94%)	23 (68%)	5 (15%)	6 (18%)	0	3
10	k	34/36 (94%)	17 (50%)	8 (24%)	9 (26%)	0	1
11	L	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	2	26
11	l	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	2	26
12	M	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
12	m	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
13	O	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	8
13	o	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	8
14	T	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	4	37
14	t	28/30 (93%)	22 (79%)	4 (14%)	2 (7%)	1	20
15	U	96/98 (98%)	70 (73%)	17 (18%)	9 (9%)	1	14
15	u	96/98 (98%)	70 (73%)	18 (19%)	8 (8%)	1	16
16	V	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	19
16	v	135/137 (98%)	99 (73%)	26 (19%)	10 (7%)	1	19
17	X	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
17	x	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
18	Y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
18	y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
20	Z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	22
All	All	5124/5250 (98%)	3622 (71%)	986 (19%)	516 (10%)	1	12

All (516) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	61	ASP
1	A	100	ALA
1	A	224	ILE
1	A	226	GLU
1	A	337	HIS
2	B	11	VAL
2	B	36	SER
2	B	48	SER
2	B	93	PHE
2	B	112	CYS
2	B	171	PRO
2	B	230	ARG
2	B	250	PHE
2	B	278	SER
2	B	322	GLY
2	B	327	THR
2	B	330	MET
2	B	361	ALA
2	B	407	ASN
2	B	484	PRO
2	B	487	SER
3	C	85	GLY
3	C	132	HIS
3	C	144	SER
3	C	146	PHE
3	C	150	ASP
3	C	191	PRO
3	C	274	TYR
3	C	275	SER
3	C	416	SER
3	C	452	ALA
4	D	21	TRP
4	D	25	ASP
4	D	80	THR
4	D	101	PHE

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Mol	Chain	Res	Type
4	D	109	GLY
4	D	110	LEU
4	D	171	PRO
4	D	263	ASN
4	D	276	VAL
4	D	297	ASP
4	D	300	SER
4	D	351	ALA
6	F	23	VAL
6	F	41	GLN
6	F	43	ILE
7	H	18	TYR
7	H	64	ALA
8	I	26	GLY
8	I	34	ARG
9	J	39	SER
11	L	6	ASN
13	O	46	PRO
13	O	60	SER
13	O	88	GLU
13	O	115	SER
13	O	166	THR
13	O	182	PHE
13	O	207	GLU
13	O	253	ALA
15	U	37	GLN
15	U	42	TYR
15	U	43	PRO
15	U	53	ALA
16	V	160	LYS
18	Y	20	ALA
18	Y	21	GLN
18	Y	43	ARG
18	Y	44	GLY
1	a	5060	ILE
1	a	5061	ASP
1	a	5100	ALA
1	a	5224	ILE
1	a	5226	GLU
1	a	5337	HIS
2	b	5011	VAL
2	b	5036	SER

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Mol	Chain	Res	Type
2	b	5048	SER
2	b	5093	PHE
2	b	5112	CYS
2	b	5171	PRO
2	b	5230	ARG
2	b	5250	PHE
2	b	5278	SER
2	b	5322	GLY
2	b	5327	THR
2	b	5330	MET
2	b	5361	ALA
2	b	5407	ASN
2	b	5484	PRO
2	b	5487	SER
3	c	5085	GLY
3	c	5132	HIS
3	c	5144	SER
3	c	5146	PHE
3	c	5150	ASP
3	c	5191	PRO
3	c	5274	TYR
3	c	5275	SER
3	c	5416	SER
3	c	5452	ALA
4	d	5021	TRP
4	d	5025	ASP
4	d	5080	THR
4	d	5101	PHE
4	d	5109	GLY
4	d	5110	LEU
4	d	5171	PRO
4	d	5263	ASN
4	d	5276	VAL
4	d	5297	ASP
4	d	5300	SER
4	d	5351	ALA
6	f	5023	VAL
6	f	5041	GLN
6	f	5043	ILE
7	h	5018	TYR
7	h	5064	ALA
8	i	5026	GLY

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Mol	Chain	Res	Type
8	i	5034	ARG
9	j	5039	SER
10	k	5032	PHE
10	k	5034	ALA
11	l	5006	ASN
13	o	5046	PRO
13	o	5060	SER
13	o	5088	GLU
13	o	5115	SER
13	o	5166	THR
13	o	5182	PHE
13	o	5207	GLU
13	o	5253	ALA
15	u	5037	GLN
15	u	5042	TYR
15	u	5043	PRO
15	u	5053	ALA
16	v	5160	LYS
18	y	5020	ALA
18	y	5021	GLN
18	y	5043	ARG
18	y	5044	GLY
1	A	27	ARG
1	A	49	VAL
1	A	122	GLY
1	A	141	PRO
1	A	258	LEU
1	A	309	ALA
1	A	310	LYS
1	A	334	ARG
2	B	12	LEU
2	B	13	ILE
2	B	56	TRP
2	B	58	GLN
2	B	103	LEU
2	B	114	HIS
2	B	126	PRO
2	B	165	GLY
2	B	307	GLU
2	B	321	LYS
2	B	358	ARG
2	B	373	LYS

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Mol	Chain	Res	Type
2	B	415	PRO
3	C	145	SER
3	C	153	ASP
3	C	192	GLY
3	C	310	SER
3	C	398	HIS
4	D	34	GLY
4	D	79	SER
4	D	141	TYR
4	D	182	LEU
4	D	275	PRO
4	D	307	GLU
4	D	327	ALA
5	E	57	ALA
5	E	60	GLN
5	E	78	THR
5	E	81	GLU
7	H	3	ARG
7	H	51	SER
8	I	25	SER
8	I	30	ARG
9	J	31	GLY
10	K	31	LEU
10	K	44	GLY
11	L	14	ARG
13	O	50	ASP
13	O	64	TYR
13	O	138	GLY
13	O	164	THR
13	O	175	PRO
13	O	179	THR
13	O	194	TYR
13	O	198	ILE
13	O	222	GLN
13	O	267	ALA
15	U	30	THR
15	U	52	ASN
15	U	60	ASP
15	U	79	LEU
16	V	59	PHE
16	V	63	CYS
16	V	97	GLY

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Mol	Chain	Res	Type
20	Z	44	SER
20	Z	55	GLY
1	a	5027	ARG
1	a	5049	VAL
1	a	5122	GLY
1	a	5141	PRO
1	a	5258	LEU
1	a	5309	ALA
1	a	5310	LYS
1	a	5334	ARG
1	a	5336	ALA
2	b	5012	LEU
2	b	5013	ILE
2	b	5056	TRP
2	b	5058	GLN
2	b	5103	LEU
2	b	5114	HIS
2	b	5126	PRO
2	b	5165	GLY
2	b	5307	GLU
2	b	5321	LYS
2	b	5358	ARG
2	b	5373	LYS
2	b	5415	PRO
3	c	5145	SER
3	c	5153	ASP
3	c	5192	GLY
3	c	5310	SER
3	c	5398	HIS
4	d	5034	GLY
4	d	5079	SER
4	d	5141	TYR
4	d	5182	LEU
4	d	5275	PRO
4	d	5307	GLU
4	d	5327	ALA
5	e	5057	ALA
5	e	5060	GLN
5	e	5078	THR
5	e	5081	GLU
7	h	5003	ARG
7	h	5051	SER

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Mol	Chain	Res	Type
8	i	5025	SER
8	i	5030	ARG
9	j	5031	GLY
10	k	5033	PHE
10	k	5044	GLY
11	l	5014	ARG
13	o	5050	ASP
13	o	5064	TYR
13	o	5138	GLY
13	o	5164	THR
13	o	5175	PRO
13	o	5179	THR
13	o	5194	TYR
13	o	5198	ILE
13	o	5222	GLN
13	o	5267	ALA
14	t	5012	CYS
15	u	5030	THR
15	u	5052	ASN
15	u	5060	ASP
15	u	5079	LEU
16	v	5059	PHE
16	v	5063	CYS
16	v	5097	GLY
20	z	5044	SER
20	z	5055	GLY
1	A	35	VAL
1	A	48	PHE
1	A	108	ASN
1	A	120	LEU
1	A	260	PHE
1	A	298	ASN
2	B	75	TRP
2	B	111	ALA
2	B	146	ALA
2	B	249	ALA
2	B	319	PRO
2	B	483	ASP
3	C	29	GLU
3	C	57	ALA
3	C	309	ALA
3	C	429	SER

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Mol	Chain	Res	Type
3	C	430	HIS
4	D	19	ASP
4	D	22	LEU
4	D	111	TRP
4	D	183	LEU
4	D	192	THR
4	D	234	ALA
4	D	274	VAL
4	D	298	PHE
4	D	326	ARG
5	E	52	PRO
5	E	75	GLN
5	E	76	VAL
5	E	77	GLU
7	H	17	GLU
7	H	35	MET
8	I	2	GLU
10	K	16	ALA
13	O	53	ARG
13	O	68	ARG
13	O	252	GLY
16	V	107	THR
16	V	125	ASP
16	V	155	LYS
20	Z	22	GLY
1	a	5035	VAL
1	a	5048	PHE
1	a	5108	ASN
1	a	5120	LEU
1	a	5260	PHE
1	a	5298	ASN
2	b	5075	TRP
2	b	5111	ALA
2	b	5146	ALA
2	b	5249	ALA
2	b	5319	PRO
2	b	5483	ASP
3	c	5029	GLU
3	c	5057	ALA
3	c	5309	ALA
3	c	5429	SER
3	c	5430	HIS

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Mol	Chain	Res	Type
4	d	5019	ASP
4	d	5022	LEU
4	d	5111	TRP
4	d	5183	LEU
4	d	5192	THR
4	d	5234	ALA
4	d	5274	VAL
4	d	5298	PHE
4	d	5326	ARG
5	e	5052	PRO
5	e	5075	GLN
5	e	5076	VAL
5	e	5077	GLU
7	h	5017	GLU
7	h	5035	MET
8	i	5002	GLU
10	k	5016	ALA
10	k	5031	LEU
10	k	5036	ALA
13	o	5053	ARG
13	o	5068	ARG
13	o	5252	GLY
16	v	5107	THR
16	v	5125	ASP
16	v	5155	LYS
20	z	5022	GLY
1	A	37	MET
1	A	81	ALA
1	A	150	PRO
1	A	172	MET
1	A	183	MET
1	A	268	SER
1	A	276	ALA
2	B	99	ALA
2	B	197	GLY
2	B	418	LYS
3	C	39	ASN
3	C	217	PRO
3	C	328	VAL
3	C	397	THR
4	D	20	ASP
4	D	27	PHE

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Mol	Chain	Res	Type
4	D	90	LEU
4	D	113	PHE
4	D	268	HIS
4	D	299	ILE
4	D	343	GLU
6	F	14	PRO
13	O	212	ASN
16	V	47	LEU
1	a	5037	MET
1	a	5081	ALA
1	a	5150	PRO
1	a	5172	MET
1	a	5183	MET
1	a	5268	SER
1	a	5276	ALA
2	b	5099	ALA
2	b	5197	GLY
2	b	5418	LYS
3	c	5039	ASN
3	c	5217	PRO
3	c	5328	VAL
3	c	5397	THR
4	d	5020	ASP
4	d	5027	PHE
4	d	5090	LEU
4	d	5113	PHE
4	d	5299	ILE
4	d	5343	GLU
6	f	5014	PRO
13	o	5212	ASN
16	v	5047	LEU
1	A	112	TYR
1	A	148	SER
1	A	237	TYR
1	A	259	ILE
2	B	100	HIS
2	B	231	MET
2	B	408	GLY
2	B	419	SER
3	C	306	GLY
3	C	472	LEU
4	D	251	ARG

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Mol	Chain	Res	Type
5	E	48	GLY
10	K	36	ALA
13	O	143	PRO
13	O	192	SER
14	T	18	PHE
18	Y	45	ASN
1	a	5112	TYR
1	a	5148	SER
1	a	5237	TYR
1	a	5259	ILE
2	b	5100	HIS
2	b	5231	MET
2	b	5419	SER
3	c	5306	GLY
3	c	5472	LEU
4	d	5251	ARG
5	e	5048	GLY
7	h	5028	THR
13	o	5143	PRO
13	o	5192	SER
14	t	5018	PHE
18	y	5045	ASN
1	A	38	ILE
1	A	39	PRO
1	A	63	ILE
1	A	227	THR
1	A	342	ASP
2	B	47	PRO
2	B	169	SER
2	B	186	GLY
4	D	292	ASN
7	H	28	THR
8	I	27	ASP
13	O	42	ALA
13	O	73	PRO
13	O	98	THR
16	V	71	ILE
1	a	5038	ILE
1	a	5039	PRO
1	a	5063	ILE
1	a	5227	THR
1	a	5342	ASP

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Mol	Chain	Res	Type
2	b	5047	PRO
2	b	5169	SER
2	b	5408	GLY
4	d	5292	ASN
8	i	5027	ASP
13	o	5042	ALA
13	o	5073	PRO
13	o	5098	THR
16	v	5071	ILE
1	A	90	GLY
1	A	184	ILE
2	B	234	ILE
2	B	414	PRO
3	C	183	GLY
3	C	233	VAL
3	C	380	ILE
10	K	25	LEU
1	a	5090	GLY
1	a	5184	ILE
2	b	5186	GLY
2	b	5234	ILE
2	b	5414	PRO
3	c	5183	GLY
3	c	5211	GLY
3	c	5233	VAL
3	c	5380	ILE
10	k	5025	LEU
2	B	191	ASN
2	B	219	VAL
2	B	264	PRO
3	C	101	PRO
3	C	102	GLY
3	C	208	VAL
3	C	211	GLY
7	H	40	VAL
9	J	35	GLY
20	Z	20	VAL
2	b	5191	ASN
2	b	5219	VAL
2	b	5264	PRO
3	c	5101	PRO
3	c	5102	GLY

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Mol	Chain	Res	Type
3	c	5208	VAL
7	h	5040	VAL
9	j	5035	GLY
20	z	5020	VAL
3	C	205	ASP
16	V	76	PRO
3	c	5205	ASP
16	v	5076	PRO
4	D	195	PRO
4	d	5195	PRO
1	A	248	ILE
3	C	190	ALA
10	K	43	VAL
15	U	74	ILE
1	a	5236	GLY
1	a	5248	ILE
3	c	5190	ALA
10	k	5043	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	218 (81%)	52 (19%)	1	13
1	a	270/279 (97%)	217 (80%)	53 (20%)	1	12
2	B	388/388 (100%)	319 (82%)	69 (18%)	2	16
2	b	388/388 (100%)	319 (82%)	69 (18%)	2	16
3	C	349/349 (100%)	277 (79%)	72 (21%)	1	10
3	c	349/349 (100%)	276 (79%)	73 (21%)	1	10
4	D	275/275 (100%)	236 (86%)	39 (14%)	4	26
4	d	275/275 (100%)	237 (86%)	38 (14%)	4	27
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	12
5	e	72/73 (99%)	58 (81%)	14 (19%)	1	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	29/38 (76%)	23 (79%)	6 (21%)	1	10
6	f	29/38 (76%)	23 (79%)	6 (21%)	1	10
7	H	54/54 (100%)	44 (82%)	10 (18%)	2	14
7	h	54/54 (100%)	44 (82%)	10 (18%)	2	14
8	I	32/32 (100%)	23 (72%)	9 (28%)	0	3
8	i	32/32 (100%)	23 (72%)	9 (28%)	0	3
9	J	24/28 (86%)	19 (79%)	5 (21%)	1	10
9	j	24/28 (86%)	19 (79%)	5 (21%)	1	10
10	K	29/29 (100%)	24 (83%)	5 (17%)	2	17
10	k	29/29 (100%)	25 (86%)	4 (14%)	4	27
11	L	35/35 (100%)	29 (83%)	6 (17%)	2	17
11	l	35/35 (100%)	29 (83%)	6 (17%)	2	17
12	M	33/33 (100%)	31 (94%)	2 (6%)	22	58
12	m	33/33 (100%)	32 (97%)	1 (3%)	46	75
13	O	206/206 (100%)	168 (82%)	38 (18%)	2	14
13	o	206/206 (100%)	168 (82%)	38 (18%)	2	14
14	T	27/27 (100%)	23 (85%)	4 (15%)	3	23
14	t	27/27 (100%)	23 (85%)	4 (15%)	3	23
15	U	85/85 (100%)	74 (87%)	11 (13%)	5	28
15	u	85/85 (100%)	75 (88%)	10 (12%)	6	32
16	V	117/117 (100%)	96 (82%)	21 (18%)	2	15
16	v	117/117 (100%)	97 (83%)	20 (17%)	2	17
17	X	27/27 (100%)	17 (63%)	10 (37%)	0	1
17	x	27/27 (100%)	17 (63%)	10 (37%)	0	1
18	Y	21/21 (100%)	12 (57%)	9 (43%)	0	0
18	y	21/21 (100%)	12 (57%)	9 (43%)	0	0
20	Z	52/52 (100%)	40 (77%)	12 (23%)	1	7
20	z	52/52 (100%)	40 (77%)	12 (23%)	1	7
All	All	4250/4296 (99%)	3465 (82%)	785 (18%)	2	14

All (785) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	TRP
1	A	17	PHE
1	A	18	CYS
1	A	24	THR
1	A	28	LEU
1	A	30	VAL
1	A	42	LEU
1	A	63	ILE
1	A	70	SER
1	A	79	THR
1	A	83	VAL
1	A	101	SER
1	A	102	LEU
1	A	114	LEU
1	A	119	PHE
1	A	126	TYR
1	A	127	MET
1	A	131	TRP
1	A	142	TRP
1	A	144	CYS
1	A	150	PRO
1	A	151	LEU
1	A	155	PHE
1	A	192	ILE
1	A	193	LEU
1	A	197	PHE
1	A	199	GLN
1	A	206	PHE
1	A	218	LEU
1	A	223	LEU
1	A	224	ILE
1	A	225	ARG
1	A	230	THR
1	A	234	ASN
1	A	235	TYR
1	A	243	GLU
1	A	245	THR
1	A	246	TYR
1	A	254	TYR
1	A	260	PHE
1	A	267	ASN
1	A	268	SER

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	278	TRP
1	A	297	LEU
1	A	298	ASN
1	A	313	VAL
1	A	317	TRP
1	A	325	ASN
1	A	331	MET
1	A	335	ASN
2	B	6	TYR
2	B	7	ARG
2	B	8	VAL
2	B	12	LEU
2	B	13	ILE
2	B	27	THR
2	B	40	TYR
2	B	49	ASP
2	B	66	MET
2	B	69	LEU
2	B	71	VAL
2	B	81	THR
2	B	83	GLU
2	B	87	ASP
2	B	90	PHE
2	B	91	TRP
2	B	92	SER
2	B	102	VAL
2	B	113	TRP
2	B	120	LEU
2	B	122	LEU
2	B	127	ARG
2	B	135	LEU
2	B	143	LEU
2	B	156	PHE
2	B	172	TYR
2	B	174	LEU
2	B	185	TRP
2	B	191	ASN
2	B	215	PHE
2	B	226	TYR
2	B	230	ARG
2	B	246	PHE

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Mol	Chain	Res	Type
2	B	247	PHE
2	B	262	THR
2	B	265	ILE
2	B	266	GLU
2	B	271	THR
2	B	274	GLN
2	B	281	GLN
2	B	282	GLN
2	B	297	THR
2	B	311	PHE
2	B	321	LYS
2	B	334	ASP
2	B	338	GLN
2	B	350	GLU
2	B	355	PHE
2	B	359	MET
2	B	363	PHE
2	B	368	VAL
2	B	372	ASP
2	B	373	LYS
2	B	374	ASN
2	B	389	LYS
2	B	390	TYR
2	B	402	TYR
2	B	406	LEU
2	B	423	LYS
2	B	425	ILE
2	B	433	ASP
2	B	463	PHE
2	B	472	ARG
2	B	473	THR
2	B	475	PHE
2	B	476	ARG
2	B	485	GLU
2	B	486	LEU
2	B	489	GLU
3	C	27	ASP
3	C	31	SER
3	C	33	PHE
3	C	43	ILE
3	C	45	LEU
3	C	46	SER

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Mol	Chain	Res	Type
3	C	49	LEU
3	C	50	LEU
3	C	56	HIS
3	C	62	PHE
3	C	78	GLU
3	C	88	LEU
3	C	89	ILE
3	C	92	ILE
3	C	97	TRP
3	C	101	PRO
3	C	104	GLU
3	C	105	VAL
3	C	106	VAL
3	C	108	THR
3	C	117	VAL
3	C	122	SER
3	C	125	LEU
3	C	127	PHE
3	C	131	TYR
3	C	134	ILE
3	C	141	GLU
3	C	146	PHE
3	C	149	TYR
3	C	152	LYS
3	C	156	LYS
3	C	160	ILE
3	C	161	LEU
3	C	166	ILE
3	C	167	VAL
3	C	170	ILE
3	C	175	LEU
3	C	191	PRO
3	C	223	TRP
3	C	229	ASN
3	C	240	ILE
3	C	244	CYS
3	C	257	PHE
3	C	264	PHE
3	C	265	ILE
3	C	272	LEU
3	C	282	MET
3	C	288	CYS

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Mol	Chain	Res	Type
3	C	289	PHE
3	C	295	THR
3	C	318	LEU
3	C	328	VAL
3	C	334	PRO
3	C	335	THR
3	C	340	TYR
3	C	343	ARG
3	C	348	GLU
3	C	350	ILE
3	C	381	LYS
3	C	416	SER
3	C	417	VAL
3	C	418	ASN
3	C	419	PHE
3	C	420	VAL
3	C	431	PHE
3	C	436	PHE
3	C	443	TRP
3	C	444	HIS
3	C	456	GLU
3	C	467	LEU
3	C	472	LEU
3	C	473	ASP
4	D	14	TRP
4	D	22	LEU
4	D	24	ARG
4	D	25	ASP
4	D	26	ARG
4	D	32	TRP
4	D	36	LEU
4	D	43	LEU
4	D	50	THR
4	D	53	THR
4	D	83	ASN
4	D	87	HIS
4	D	88	SER
4	D	89	LEU
4	D	102	THR
4	D	138	VAL
4	D	178	ILE
4	D	180	ARG

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Mol	Chain	Res	Type
4	D	183	LEU
4	D	213	ILE
4	D	222	LEU
4	D	225	ASP
4	D	232	PHE
4	D	247	VAL
4	D	250	ASN
4	D	261	PHE
4	D	265	ARG
4	D	268	HIS
4	D	269	PHE
4	D	272	LEU
4	D	282	SER
4	D	295	SER
4	D	298	PHE
4	D	311	PHE
4	D	316	THR
4	D	320	LEU
4	D	338	ASN
4	D	345	VAL
4	D	352	LEU
5	E	8	ARG
5	E	15	THR
5	E	17	VAL
5	E	24	SER
5	E	32	ILE
5	E	39	SER
5	E	45	ASP
5	E	52	PRO
5	E	58	GLN
5	E	60	GLN
5	E	61	ARG
5	E	65	LEU
5	E	75	GLN
5	E	76	VAL
6	F	17	THR
6	F	19	ARG
6	F	24	HIS
6	F	32	PHE
6	F	43	ILE
6	F	45	ARG
7	H	4	ARG

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Mol	Chain	Res	Type
7	H	9	ASP
7	H	17	GLU
7	H	18	TYR
7	H	27	THR
7	H	35	MET
7	H	39	LEU
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	6	ILE
8	I	8	VAL
8	I	10	ILE
8	I	12	VAL
8	I	14	PHE
8	I	20	VAL
8	I	23	PHE
8	I	33	LYS
8	I	34	ARG
9	J	10	LEU
9	J	11	TRP
9	J	21	VAL
9	J	25	VAL
9	J	38	SER
10	K	21	LEU
10	K	23	ASP
10	K	33	PHE
10	K	39	VAL
10	K	40	GLN
11	L	6	ASN
11	L	8	GLN
11	L	11	GLU
11	L	17	LEU
11	L	26	VAL
11	L	35	PHE
12	M	8	PHE
12	M	28	GLN
13	O	34	ASP
13	O	46	PRO
13	O	47	THR
13	O	49	ASP
13	O	58	ILE
13	O	69	LEU

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Mol	Chain	Res	Type
13	O	73	PRO
13	O	83	LYS
13	O	84	ASN
13	O	85	LYS
13	O	86	ARG
13	O	87	GLN
13	O	90	GLU
13	O	91	PHE
13	O	99	ARG
13	O	101	THR
13	O	102	THR
13	O	116	ASP
13	O	125	ASP
13	O	129	PHE
13	O	130	GLN
13	O	136	MET
13	O	141	ARG
13	O	144	LEU
13	O	173	ASN
13	O	176	SER
13	O	181	ASN
13	O	183	LEU
13	O	186	LYS
13	O	194	TYR
13	O	195	ASP
13	O	213	VAL
13	O	215	ARG
13	O	216	PHE
13	O	237	ILE
13	O	254	HIS
13	O	264	VAL
13	O	265	PHE
14	T	2	GLU
14	T	4	ILE
14	T	12	CYS
14	T	24	ARG
15	U	9	LEU
15	U	31	ASN
15	U	55	TYR
15	U	60	ASP
15	U	63	ASN
15	U	68	THR

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Mol	Chain	Res	Type
15	U	69	GLU
15	U	79	LEU
15	U	82	PHE
15	U	87	VAL
15	U	89	THR
16	V	34	LEU
16	V	38	LEU
16	V	44	THR
16	V	45	ILE
16	V	47	LEU
16	V	49	GLU
16	V	63	CYS
16	V	65	SER
16	V	66	CYS
16	V	67	HIS
16	V	81	ARG
16	V	83	GLU
16	V	92	ARG
16	V	101	TYR
16	V	103	LYS
16	V	106	THR
16	V	108	TYR
16	V	119	PRO
16	V	122	ARG
16	V	126	ILE
16	V	151	ILE
17	X	12	ILE
17	X	13	THR
17	X	15	SER
17	X	24	LEU
17	X	32	LEU
17	X	33	THR
17	X	36	VAL
17	X	37	LEU
17	X	41	SER
17	X	42	GLN
18	Y	22	LEU
18	Y	28	ILE
18	Y	30	ILE
18	Y	35	ILE
18	Y	36	ILE
18	Y	41	VAL

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Mol	Chain	Res	Type
18	Y	42	ARG
18	Y	43	ARG
18	Y	45	ASN
20	Z	1	MET
20	Z	2	THR
20	Z	4	LEU
20	Z	6	GLN
20	Z	15	LEU
20	Z	17	PHE
20	Z	24	PRO
20	Z	27	TYR
20	Z	32	ASP
20	Z	38	GLN
20	Z	50	LEU
20	Z	60	PHE
1	a	5012	ASN
1	a	5014	TRP
1	a	5017	PHE
1	a	5018	CYS
1	a	5024	THR
1	a	5028	LEU
1	a	5030	VAL
1	a	5042	LEU
1	a	5063	ILE
1	a	5070	SER
1	a	5079	THR
1	a	5083	VAL
1	a	5101	SER
1	a	5102	LEU
1	a	5114	LEU
1	a	5119	PHE
1	a	5126	TYR
1	a	5127	MET
1	a	5131	TRP
1	a	5142	TRP
1	a	5144	CYS
1	a	5150	PRO
1	a	5151	LEU
1	a	5155	PHE
1	a	5192	ILE
1	a	5193	LEU
1	a	5197	PHE

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Mol	Chain	Res	Type
1	a	5199	GLN
1	a	5206	PHE
1	a	5218	LEU
1	a	5223	LEU
1	a	5224	ILE
1	a	5225	ARG
1	a	5230	THR
1	a	5234	ASN
1	a	5235	TYR
1	a	5243	GLU
1	a	5245	THR
1	a	5246	TYR
1	a	5254	TYR
1	a	5260	PHE
1	a	5267	ASN
1	a	5268	SER
1	a	5271	LEU
1	a	5278	TRP
1	a	5279	ARG
1	a	5297	LEU
1	a	5298	ASN
1	a	5313	VAL
1	a	5317	TRP
1	a	5325	ASN
1	a	5331	MET
1	a	5335	ASN
2	b	5006	TYR
2	b	5007	ARG
2	b	5008	VAL
2	b	5012	LEU
2	b	5013	ILE
2	b	5027	THR
2	b	5040	TYR
2	b	5049	ASP
2	b	5066	MET
2	b	5069	LEU
2	b	5071	VAL
2	b	5081	THR
2	b	5083	GLU
2	b	5087	ASP
2	b	5090	PHE
2	b	5091	TRP

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Mol	Chain	Res	Type
2	b	5092	SER
2	b	5102	VAL
2	b	5113	TRP
2	b	5120	LEU
2	b	5122	LEU
2	b	5127	ARG
2	b	5135	LEU
2	b	5143	LEU
2	b	5156	PHE
2	b	5172	TYR
2	b	5174	LEU
2	b	5185	TRP
2	b	5191	ASN
2	b	5215	PHE
2	b	5226	TYR
2	b	5230	ARG
2	b	5246	PHE
2	b	5247	PHE
2	b	5262	THR
2	b	5265	ILE
2	b	5266	GLU
2	b	5271	THR
2	b	5274	GLN
2	b	5281	GLN
2	b	5282	GLN
2	b	5297	THR
2	b	5311	PHE
2	b	5321	LYS
2	b	5334	ASP
2	b	5338	GLN
2	b	5350	GLU
2	b	5355	PHE
2	b	5359	MET
2	b	5363	PHE
2	b	5368	VAL
2	b	5372	ASP
2	b	5373	LYS
2	b	5374	ASN
2	b	5389	LYS
2	b	5390	TYR
2	b	5402	TYR
2	b	5406	LEU

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Mol	Chain	Res	Type
2	b	5423	LYS
2	b	5425	ILE
2	b	5433	ASP
2	b	5463	PHE
2	b	5472	ARG
2	b	5473	THR
2	b	5475	PHE
2	b	5476	ARG
2	b	5485	GLU
2	b	5486	LEU
2	b	5489	GLU
3	c	5027	ASP
3	c	5031	SER
3	c	5033	PHE
3	c	5042	LEU
3	c	5043	ILE
3	c	5045	LEU
3	c	5046	SER
3	c	5049	LEU
3	c	5050	LEU
3	c	5056	HIS
3	c	5062	PHE
3	c	5078	GLU
3	c	5088	LEU
3	c	5089	ILE
3	c	5092	ILE
3	c	5097	TRP
3	c	5101	PRO
3	c	5104	GLU
3	c	5105	VAL
3	c	5106	VAL
3	c	5108	THR
3	c	5117	VAL
3	c	5122	SER
3	c	5125	LEU
3	c	5127	PHE
3	c	5131	TYR
3	c	5134	ILE
3	c	5141	GLU
3	c	5146	PHE
3	c	5149	TYR
3	c	5152	LYS

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Mol	Chain	Res	Type
3	c	5156	LYS
3	c	5160	ILE
3	c	5161	LEU
3	c	5166	ILE
3	c	5167	VAL
3	c	5170	ILE
3	c	5175	LEU
3	c	5191	PRO
3	c	5223	TRP
3	c	5229	ASN
3	c	5240	ILE
3	c	5244	CYS
3	c	5257	PHE
3	c	5264	PHE
3	c	5265	ILE
3	c	5272	LEU
3	c	5282	MET
3	c	5288	CYS
3	c	5289	PHE
3	c	5295	THR
3	c	5318	LEU
3	c	5328	VAL
3	c	5334	PRO
3	c	5335	THR
3	c	5340	TYR
3	c	5343	ARG
3	c	5348	GLU
3	c	5350	ILE
3	c	5381	LYS
3	c	5416	SER
3	c	5417	VAL
3	c	5418	ASN
3	c	5419	PHE
3	c	5420	VAL
3	c	5431	PHE
3	c	5436	PHE
3	c	5443	TRP
3	c	5444	HIS
3	c	5456	GLU
3	c	5467	LEU
3	c	5472	LEU
3	c	5473	ASP

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Mol	Chain	Res	Type
4	d	5014	TRP
4	d	5022	LEU
4	d	5024	ARG
4	d	5025	ASP
4	d	5026	ARG
4	d	5032	TRP
4	d	5036	LEU
4	d	5043	LEU
4	d	5050	THR
4	d	5053	THR
4	d	5083	ASN
4	d	5087	HIS
4	d	5088	SER
4	d	5089	LEU
4	d	5102	THR
4	d	5138	VAL
4	d	5178	ILE
4	d	5180	ARG
4	d	5183	LEU
4	d	5213	ILE
4	d	5222	LEU
4	d	5225	ASP
4	d	5232	PHE
4	d	5247	VAL
4	d	5250	ASN
4	d	5261	PHE
4	d	5265	ARG
4	d	5269	PHE
4	d	5272	LEU
4	d	5282	SER
4	d	5295	SER
4	d	5298	PHE
4	d	5311	PHE
4	d	5316	THR
4	d	5320	LEU
4	d	5338	ASN
4	d	5345	VAL
4	d	5352	LEU
5	e	5008	ARG
5	e	5015	THR
5	e	5017	VAL
5	e	5024	SER

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Mol	Chain	Res	Type
5	e	5032	ILE
5	e	5039	SER
5	e	5045	ASP
5	e	5052	PRO
5	e	5058	GLN
5	e	5060	GLN
5	e	5061	ARG
5	e	5065	LEU
5	e	5075	GLN
5	e	5076	VAL
6	f	5017	THR
6	f	5019	ARG
6	f	5024	HIS
6	f	5032	PHE
6	f	5043	ILE
6	f	5045	ARG
7	h	5004	ARG
7	h	5009	ASP
7	h	5017	GLU
7	h	5018	TYR
7	h	5027	THR
7	h	5035	MET
7	h	5039	LEU
7	h	5049	TYR
7	h	5052	THR
7	h	5053	LEU
8	i	5006	ILE
8	i	5008	VAL
8	i	5010	ILE
8	i	5012	VAL
8	i	5014	PHE
8	i	5020	VAL
8	i	5023	PHE
8	i	5033	LYS
8	i	5034	ARG
9	j	5010	LEU
9	j	5011	TRP
9	j	5021	VAL
9	j	5025	VAL
9	j	5038	SER
10	k	5021	LEU
10	k	5023	ASP

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Mol	Chain	Res	Type
10	k	5033	PHE
10	k	5038	VAL
11	l	5006	ASN
11	l	5008	GLN
11	l	5011	GLU
11	l	5017	LEU
11	l	5026	VAL
11	l	5035	PHE
12	m	5028	GLN
13	o	5034	ASP
13	o	5046	PRO
13	o	5047	THR
13	o	5049	ASP
13	o	5058	ILE
13	o	5069	LEU
13	o	5073	PRO
13	o	5083	LYS
13	o	5084	ASN
13	o	5085	LYS
13	o	5086	ARG
13	o	5087	GLN
13	o	5090	GLU
13	o	5091	PHE
13	o	5099	ARG
13	o	5101	THR
13	o	5102	THR
13	o	5116	ASP
13	o	5125	ASP
13	o	5129	PHE
13	o	5130	GLN
13	o	5136	MET
13	o	5141	ARG
13	o	5144	LEU
13	o	5173	ASN
13	o	5176	SER
13	o	5181	ASN
13	o	5183	LEU
13	o	5186	LYS
13	o	5194	TYR
13	o	5195	ASP
13	o	5213	VAL
13	o	5215	ARG

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Mol	Chain	Res	Type
13	o	5216	PHE
13	o	5237	ILE
13	o	5254	HIS
13	o	5264	VAL
13	o	5265	PHE
14	t	5002	GLU
14	t	5004	ILE
14	t	5012	CYS
14	t	5024	ARG
15	u	5009	LEU
15	u	5031	ASN
15	u	5055	TYR
15	u	5060	ASP
15	u	5068	THR
15	u	5069	GLU
15	u	5079	LEU
15	u	5082	PHE
15	u	5087	VAL
15	u	5089	THR
16	v	5034	LEU
16	v	5038	LEU
16	v	5044	THR
16	v	5045	ILE
16	v	5047	LEU
16	v	5049	GLU
16	v	5063	CYS
16	v	5065	SER
16	v	5066	CYS
16	v	5067	HIS
16	v	5081	ARG
16	v	5083	GLU
16	v	5092	ARG
16	v	5101	TYR
16	v	5106	THR
16	v	5108	TYR
16	v	5119	PRO
16	v	5122	ARG
16	v	5126	ILE
16	v	5151	ILE
17	x	5012	ILE
17	x	5013	THR
17	x	5015	SER

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Mol	Chain	Res	Type
17	x	5024	LEU
17	x	5032	LEU
17	x	5033	THR
17	x	5036	VAL
17	x	5037	LEU
17	x	5041	SER
17	x	5042	GLN
18	y	5022	LEU
18	y	5028	ILE
18	y	5030	ILE
18	y	5035	ILE
18	y	5036	ILE
18	y	5041	VAL
18	y	5042	ARG
18	y	5043	ARG
18	y	5045	ASN
20	z	5001	MET
20	z	5002	THR
20	z	5004	LEU
20	z	5006	GLN
20	z	5015	LEU
20	z	5017	PHE
20	z	5024	PRO
20	z	5027	TYR
20	z	5032	ASP
20	z	5038	GLN
20	z	5050	LEU
20	z	5060	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	75	ASN
1	A	87	ASN
1	A	92	HIS
1	A	118	HIS
1	A	181	ASN
1	A	199	GLN
1	A	241	GLN
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	296	ASN
1	A	298	ASN
1	A	301	ASN
1	A	303	ASN
1	A	304	HIS
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
1	A	337	HIS
2	B	23	HIS
2	B	114	HIS
2	B	157	HIS
2	B	191	ASN
2	B	201	HIS
2	B	223	GLN
2	B	233	ASN
2	B	274	GLN
2	B	281	GLN
2	B	282	GLN
2	B	338	GLN
2	B	374	ASN
2	B	395	GLN
2	B	409	GLN
3	C	39	ASN
3	C	56	HIS
3	C	155	ASN
3	C	229	ASN
3	C	294	ASN
3	C	322	GLN
3	C	327	ASN
3	C	332	GLN
3	C	415	ASN
4	D	98	GLN
4	D	106	GLN
4	D	186	GLN
4	D	190	ASN
4	D	197	HIS
4	D	214	HIS
4	D	220	ASN
4	D	224	GLN
4	D	239	GLN

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Mol	Chain	Res	Type
4	D	255	GLN
4	D	292	ASN
4	D	301	GLN
4	D	322	ASN
4	D	332	GLN
4	D	334	GLN
5	E	75	GLN
6	F	24	HIS
7	H	15	ASN
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
12	M	28	GLN
12	M	32	GLN
13	O	62	GLN
13	O	72	GLN
13	O	84	ASN
13	O	150	ASN
13	O	173	ASN
13	O	254	HIS
13	O	262	GLN
15	U	28	ASN
15	U	29	ASN
15	U	31	ASN
15	U	99	ASN
16	V	39	ASN
16	V	60	GLN
16	V	67	HIS
16	V	94	ASN
16	V	112	GLN
18	Y	45	ASN
20	Z	6	GLN
20	Z	31	GLN
20	Z	38	GLN
1	a	5012	ASN
1	a	5019	ASN
1	a	5075	ASN
1	a	5087	ASN
1	a	5092	HIS
1	a	5118	HIS
1	a	5181	ASN
1	a	5199	GLN

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Mol	Chain	Res	Type
1	a	5241	GLN
1	a	5247	ASN
1	a	5267	ASN
1	a	5296	ASN
1	a	5298	ASN
1	a	5303	ASN
1	a	5304	HIS
1	a	5312	ASN
1	a	5322	ASN
1	a	5325	ASN
2	b	5023	HIS
2	b	5114	HIS
2	b	5157	HIS
2	b	5191	ASN
2	b	5201	HIS
2	b	5223	GLN
2	b	5233	ASN
2	b	5274	GLN
2	b	5281	GLN
2	b	5282	GLN
2	b	5338	GLN
2	b	5374	ASN
2	b	5395	GLN
3	c	5039	ASN
3	c	5056	HIS
3	c	5155	ASN
3	c	5229	ASN
3	c	5294	ASN
3	c	5322	GLN
3	c	5327	ASN
3	c	5332	GLN
3	c	5415	ASN
4	d	5098	GLN
4	d	5106	GLN
4	d	5186	GLN
4	d	5190	ASN
4	d	5197	HIS
4	d	5220	ASN
4	d	5224	GLN
4	d	5239	GLN
4	d	5255	GLN
4	d	5292	ASN

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Mol	Chain	Res	Type
4	d	5301	GLN
4	d	5322	ASN
4	d	5332	GLN
4	d	5334	GLN
4	d	5350	ASN
5	e	5075	GLN
6	f	5024	HIS
7	h	5015	ASN
11	l	5004	ASN
11	l	5006	ASN
11	l	5008	GLN
12	m	5028	GLN
12	m	5032	GLN
13	o	5062	GLN
13	o	5072	GLN
13	o	5084	ASN
13	o	5150	ASN
13	o	5173	ASN
13	o	5254	HIS
13	o	5262	GLN
15	u	5028	ASN
15	u	5029	ASN
15	u	5031	ASN
15	u	5099	ASN
16	v	5039	ASN
16	v	5060	GLN
16	v	5067	HIS
16	v	5094	ASN
16	v	5112	GLN
18	y	5045	ASN
20	z	5006	GLN
20	z	5031	GLN
20	z	5038	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 12 are monoatomic - leaving 124 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	$\# Z > 2$
21	OEC	A	1001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	A	1003	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	A	1006	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	A	1007	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
24	PHO	A	1038	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	A	1043	-	45,45,45	0.64	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	A	1044	-	41,41,41	4.14	16 (39%)	56,56,56	7.03	29 (51%)
27	LHG	A	1063	-	48,48,48	0.93	2 (4%)	49,54,54	1.08	3 (6%)
23	CLA	B	1009	-	56,73,73	1.78	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	B	1010	2	56,73,73	1.75	12 (21%)	65,113,113	2.40	19 (29%)
23	CLA	B	1011	-	56,73,73	1.76	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	B	1012	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	B	1013	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1014	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1015	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1016	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	B	1018	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1019	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	B	1020	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1021	2	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	B	1022	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1023	-	56,73,73	1.75	12 (21%)	65,113,113	2.37	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	1024	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	B	1045	-	41,41,41	4.25	17 (41%)	56,56,56	6.01	24 (42%)
26	BCR	B	1047	-	41,41,41	4.24	16 (39%)	56,56,56	5.34	28 (50%)
26	BCR	B	1048	-	41,41,41	4.24	16 (39%)	56,56,56	6.09	28 (50%)
29	DGD	B	1058	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
30	MGE	B	1060	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
23	CLA	C	1025	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1026	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	C	1027	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1028	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1029	-	56,73,73	1.75	12 (21%)	65,113,113	2.39	21 (32%)
23	CLA	C	1030	-	56,73,73	1.76	11 (19%)	65,113,113	2.35	20 (30%)
23	CLA	C	1031	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1032	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1033	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1035	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	C	1036	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1037	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
26	BCR	C	1052	-	41,41,41	4.25	16 (39%)	56,56,56	6.73	27 (48%)
26	BCR	C	1054	-	41,41,41	4.25	15 (36%)	56,56,56	5.26	24 (42%)
29	DGD	C	1055	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	C	1056	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	C	1057	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
23	CLA	D	1004	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	D	1005	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	D	1008	-	56,73,73	1.75	12 (21%)	65,113,113	2.38	21 (32%)
24	PHO	D	1039	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	D	1042	-	45,45,45	0.64	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	D	1050	-	41,41,41	4.25	15 (36%)	56,56,56	5.03	24 (42%)
30	MGE	D	1059	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
30	MGE	D	1062	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
31	HEM	F	1040	5	28,50,50	2.26	6 (21%)	17,82,82	1.39	1 (5%)
23	CLA	H	1017	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	H	1049	-	41,41,41	4.25	16 (39%)	56,56,56	5.13	24 (42%)
23	CLA	K	1034	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	K	1051	-	41,41,41	4.25	15 (36%)	56,56,56	4.83	24 (42%)
30	MGE	L	1061	-	48,48,48	0.94	2 (4%)	56,56,56	1.04	3 (5%)
26	BCR	T	6046	-	41,41,41	4.17	17 (41%)	56,56,56	5.87	27 (48%)
26	BCR	T	6048	-	41,41,41	4.24	16 (39%)	56,56,56	6.09	28 (50%)
31	HEM	V	1041	16	28,50,50	2.27	6 (21%)	17,82,82	1.41	1 (5%)
26	BCR	Z	1053	-	41,41,41	4.25	16 (39%)	56,56,56	5.83	24 (42%)
21	OEC	a	6001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	a	6003	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	a	6006	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	a	6007	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
24	PHO	a	6038	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	a	6043	-	45,45,45	0.65	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	a	6044	-	41,41,41	4.14	16 (39%)	56,56,56	7.04	30 (53%)
27	LHG	a	6063	-	48,48,48	0.93	2 (4%)	49,54,54	1.08	3 (6%)
23	CLA	b	6009	-	56,73,73	1.78	12 (21%)	65,113,113	2.39	21 (32%)
23	CLA	b	6010	2	56,73,73	1.75	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	b	6011	-	56,73,73	1.76	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	b	6012	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	b	6013	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	b	6014	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	b	6015	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6016	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	b	6018	-	56,73,73	1.80	12 (21%)	65,113,113	2.36	20 (30%)
23	CLA	b	6019	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6020	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6021	2	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	b	6022	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6023	-	56,73,73	1.75	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	b	6024	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
26	BCR	b	6045	-	41,41,41	4.25	16 (39%)	56,56,56	6.01	24 (42%)
26	BCR	b	6047	-	41,41,41	4.24	16 (39%)	56,56,56	5.34	28 (50%)
29	DGD	b	6058	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
30	MGE	b	6060	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
23	CLA	c	6025	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6026	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	6027	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6028	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	c	6029	-	56,73,73	1.75	12 (21%)	65,113,113	2.40	21 (32%)
23	CLA	c	6030	-	56,73,73	1.76	11 (19%)	65,113,113	2.35	20 (30%)
23	CLA	c	6031	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6032	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6033	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	c	6035	-	56,73,73	1.81	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	c	6036	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	c	6037	-	56,73,73	1.81	12 (21%)	65,113,113	2.36	19 (29%)
26	BCR	c	6054	-	41,41,41	4.25	15 (36%)	56,56,56	5.26	24 (42%)
29	DGD	c	6055	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	c	6056	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	c	6057	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
23	CLA	d	6004	-	56,73,73	1.80	12 (21%)	65,113,113	2.36	19 (29%)
23	CLA	d	6005	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	d	6008	-	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
24	PHO	d	6039	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	d	6042	-	45,45,45	0.64	1 (2%)	57,57,57	1.72	17 (29%)
26	BCR	d	6050	-	41,41,41	4.25	15 (36%)	56,56,56	5.03	24 (42%)
30	MGE	d	6059	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)
30	MGE	d	6062	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
31	HEM	f	6040	5	28,50,50	2.25	6 (21%)	17,82,82	1.39	1 (5%)
23	CLA	h	6017	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
26	BCR	h	6049	-	41,41,41	4.25	15 (36%)	56,56,56	5.13	24 (42%)
23	CLA	k	6034	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	k	6051	-	41,41,41	4.25	16 (39%)	56,56,56	4.83	24 (42%)
26	BCR	k	6052	-	41,41,41	4.25	16 (39%)	56,56,56	6.73	27 (48%)
30	MGE	l	6061	-	48,48,48	0.94	2 (4%)	56,56,56	1.04	3 (5%)
26	BCR	t	1046	-	41,41,41	4.17	17 (41%)	56,56,56	5.87	26 (46%)
31	HEM	v	6041	16	28,50,50	2.27	6 (21%)	17,82,82	1.41	1 (5%)
26	BCR	z	6053	-	41,41,41	4.26	17 (41%)	56,56,56	5.82	24 (42%)

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
21	OEC	A	1001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	A	1003	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	A	1006	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1007	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	1038	-	1/1/17/22	0/53/103/103	0/1/6/6
25	PQ9	A	1043	-	-	0/41/61/61	0/1/1/1
26	BCR	A	1044	-	-	0/29/63/63	0/2/2/2
27	LHG	A	1063	-	-	0/53/53/53	0/0/0/0
23	CLA	B	1009	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1010	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1011	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1012	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1013	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1014	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1015	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1018	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1019	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1020	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1021	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1022	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1023	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1024	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	1045	-	-	0/29/63/63	0/2/2/2
26	BCR	B	1047	-	-	1/29/63/63	0/2/2/2
26	BCR	B	1048	-	-	1/29/63/63	0/2/2/2
29	DGD	B	1058	-	-	0/55/95/95	0/2/2/2
30	MGE	B	1060	-	-	0/43/63/63	0/1/1/1
23	CLA	C	1025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1026	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1027	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1028	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1029	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1030	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	C	1031	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	1032	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1033	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1035	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1036	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1037	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	C	1052	-	-	0/29/63/63	0/2/2/2
26	BCR	C	1054	-	-	1/29/63/63	0/2/2/2
29	DGD	C	1055	-	-	1/55/95/95	0/2/2/2
29	DGD	C	1056	-	-	0/55/95/95	0/2/2/2
29	DGD	C	1057	-	-	0/55/95/95	0/2/2/2
23	CLA	D	1004	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1005	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1008	-	5/5/20/25	1/37/135/135	0/0/9/9
24	PHO	D	1039	-	3/3/17/22	0/53/103/103	0/1/6/6
25	PQ9	D	1042	-	-	0/41/61/61	0/1/1/1
26	BCR	D	1050	-	-	2/29/63/63	0/2/2/2
30	MGE	D	1059	-	-	0/43/63/63	0/1/1/1
30	MGE	D	1062	-	-	1/43/63/63	0/1/1/1
31	HEM	F	1040	5	-	2/6/54/54	0/0/8/8
23	CLA	H	1017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	H	1049	-	-	1/29/63/63	0/2/2/2
23	CLA	K	1034	-	7/7/20/25	0/37/135/135	0/0/9/9
26	BCR	K	1051	-	-	0/29/63/63	0/2/2/2
30	MGE	L	1061	-	-	0/43/63/63	0/1/1/1
26	BCR	T	6046	-	-	1/29/63/63	0/2/2/2
26	BCR	T	6048	-	-	1/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	0/6/54/54	0/0/8/8
26	BCR	Z	1053	-	-	0/29/63/63	0/2/2/2
21	OEC	a	6001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	a	6003	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	a	6006	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6007	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	6038	-	1/1/17/22	0/53/103/103	0/1/6/6
25	PQ9	a	6043	-	-	0/41/61/61	0/1/1/1
26	BCR	a	6044	-	-	0/29/63/63	0/2/2/2
27	LHG	a	6063	-	-	0/53/53/53	0/0/0/0
23	CLA	b	6009	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6010	2	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6011	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6012	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6013	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6014	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6015	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6018	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6019	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6020	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6021	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6022	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6023	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6024	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	6045	-	-	0/29/63/63	0/2/2/2
26	BCR	b	6047	-	-	1/29/63/63	0/2/2/2
29	DGD	b	6058	-	-	0/55/95/95	0/2/2/2
30	MGE	b	6060	-	-	0/43/63/63	0/1/1/1
23	CLA	c	6025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6026	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6027	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6028	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6029	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6030	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	c	6031	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6032	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6033	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6035	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6036	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6037	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	c	6054	-	-	1/29/63/63	0/2/2/2
29	DGD	c	6055	-	-	1/55/95/95	0/2/2/2
29	DGD	c	6056	-	-	0/55/95/95	0/2/2/2
29	DGD	c	6057	-	-	0/55/95/95	0/2/2/2
23	CLA	d	6004	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	d	6005	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	d	6008	-	5/5/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	d	6039	-	3/3/17/22	0/53/103/103	0/1/6/6
25	PQ9	d	6042	-	-	0/41/61/61	0/1/1/1
26	BCR	d	6050	-	-	2/29/63/63	0/2/2/2
30	MGE	d	6059	-	-	0/43/63/63	0/1/1/1
30	MGE	d	6062	-	-	1/43/63/63	0/1/1/1
31	HEM	f	6040	5	-	2/6/54/54	0/0/8/8
23	CLA	h	6017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	h	6049	-	-	1/29/63/63	0/2/2/2
23	CLA	k	6034	-	7/7/20/25	0/37/135/135	0/0/9/9
26	BCR	k	6051	-	-	0/29/63/63	0/2/2/2
26	BCR	k	6052	-	-	0/29/63/63	0/2/2/2
30	MGE	l	6061	-	-	0/43/63/63	0/1/1/1
26	BCR	t	1046	-	-	1/29/63/63	0/2/2/2
31	HEM	v	6041	16	-	0/6/54/54	0/0/8/8
26	BCR	z	6053	-	-	0/29/63/63	0/2/2/2

All (1344) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6047	BCR	C19-C18	-9.23	1.25	1.45
26	z	6053	BCR	C8-C9	-9.23	1.25	1.45
26	b	6047	BCR	C8-C9	-9.23	1.25	1.45
26	k	6051	BCR	C12-C13	-9.22	1.25	1.45
26	B	1047	BCR	C8-C9	-9.22	1.25	1.45
26	c	6054	BCR	C8-C9	-9.22	1.25	1.45
26	C	1054	BCR	C8-C9	-9.22	1.25	1.45
26	B	1047	BCR	C19-C18	-9.21	1.25	1.45
26	Z	1053	BCR	C8-C9	-9.21	1.25	1.45
26	k	6052	BCR	C12-C13	-9.21	1.25	1.45
26	h	6049	BCR	C19-C18	-9.21	1.25	1.45
26	B	1048	BCR	C8-C9	-9.21	1.25	1.45
26	K	1051	BCR	C12-C13	-9.21	1.25	1.45
26	C	1052	BCR	C12-C13	-9.20	1.25	1.45
26	B	1045	BCR	C19-C18	-9.20	1.25	1.45
26	T	6048	BCR	C8-C9	-9.20	1.25	1.45
26	H	1049	BCR	C19-C18	-9.20	1.25	1.45
26	B	1045	BCR	C8-C9	-9.20	1.25	1.45
26	Z	1053	BCR	C12-C13	-9.20	1.25	1.45
26	B	1048	BCR	C12-C13	-9.20	1.25	1.45
26	k	6051	BCR	C8-C9	-9.20	1.25	1.45
26	b	6045	BCR	C19-C18	-9.20	1.25	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	1050	BCR	C12-C13	-9.19	1.25	1.45
26	C	1054	BCR	C19-C18	-9.19	1.25	1.45
26	b	6045	BCR	C8-C9	-9.19	1.25	1.45
26	T	6048	BCR	C12-C13	-9.19	1.25	1.45
26	z	6053	BCR	C12-C13	-9.19	1.26	1.45
26	D	1050	BCR	C19-C18	-9.18	1.26	1.45
26	K	1051	BCR	C8-C9	-9.18	1.26	1.45
26	h	6049	BCR	C12-C13	-9.18	1.26	1.45
26	z	6053	BCR	C19-C18	-9.18	1.26	1.45
26	H	1049	BCR	C12-C13	-9.18	1.26	1.45
26	k	6052	BCR	C8-C9	-9.18	1.26	1.45
26	c	6054	BCR	C19-C18	-9.18	1.26	1.45
26	K	1051	BCR	C19-C18	-9.18	1.26	1.45
26	B	1047	BCR	C12-C13	-9.17	1.26	1.45
26	c	6054	BCR	C12-C13	-9.17	1.26	1.45
26	C	1052	BCR	C19-C18	-9.17	1.26	1.45
26	Z	1053	BCR	C19-C18	-9.17	1.26	1.45
26	C	1054	BCR	C12-C13	-9.17	1.26	1.45
26	d	6050	BCR	C12-C13	-9.17	1.26	1.45
26	d	6050	BCR	C19-C18	-9.17	1.26	1.45
26	k	6052	BCR	C19-C18	-9.16	1.26	1.45
26	h	6049	BCR	C8-C9	-9.16	1.26	1.45
26	C	1052	BCR	C8-C9	-9.16	1.26	1.45
26	b	6045	BCR	C12-C13	-9.16	1.26	1.45
26	k	6051	BCR	C19-C18	-9.16	1.26	1.45
26	H	1049	BCR	C8-C9	-9.16	1.26	1.45
26	b	6047	BCR	C12-C13	-9.16	1.26	1.45
26	B	1045	BCR	C12-C13	-9.15	1.26	1.45
26	B	1048	BCR	C19-C18	-9.15	1.26	1.45
26	T	6048	BCR	C19-C18	-9.15	1.26	1.45
26	D	1050	BCR	C8-C9	-9.15	1.26	1.45
26	d	6050	BCR	C8-C9	-9.15	1.26	1.45
26	a	6044	BCR	C19-C18	-9.11	1.26	1.45
26	T	6046	BCR	C12-C13	-9.11	1.26	1.45
26	A	1044	BCR	C19-C18	-9.11	1.26	1.45
26	t	1046	BCR	C12-C13	-9.10	1.26	1.45
26	t	1046	BCR	C8-C9	-9.08	1.26	1.45
26	T	6046	BCR	C8-C9	-9.06	1.26	1.45
26	T	6046	BCR	C19-C18	-9.04	1.26	1.45
26	t	1046	BCR	C19-C18	-9.04	1.26	1.45
26	A	1044	BCR	C8-C9	-8.98	1.26	1.45
26	a	6044	BCR	C8-C9	-8.96	1.26	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1044	BCR	C12-C13	-8.91	1.26	1.45
26	a	6044	BCR	C12-C13	-8.90	1.26	1.45
26	c	6054	BCR	C16-C17	-8.24	1.18	1.43
26	b	6047	BCR	C16-C17	-8.24	1.18	1.43
26	C	1054	BCR	C16-C17	-8.23	1.18	1.43
26	b	6047	BCR	C20-C21	-8.22	1.18	1.43
26	H	1049	BCR	C20-C21	-8.22	1.18	1.43
26	h	6049	BCR	C20-C21	-8.22	1.18	1.43
26	B	1048	BCR	C20-C21	-8.22	1.18	1.43
26	B	1047	BCR	C16-C17	-8.22	1.18	1.43
26	Z	1053	BCR	C16-C17	-8.21	1.18	1.43
26	B	1045	BCR	C16-C17	-8.21	1.18	1.43
26	K	1051	BCR	C20-C21	-8.21	1.18	1.43
26	b	6045	BCR	C16-C17	-8.21	1.18	1.43
26	k	6051	BCR	C16-C17	-8.21	1.18	1.43
26	B	1047	BCR	C20-C21	-8.21	1.18	1.43
26	C	1052	BCR	C20-C21	-8.21	1.18	1.43
26	b	6045	BCR	C20-C21	-8.21	1.18	1.43
26	K	1051	BCR	C16-C17	-8.21	1.18	1.43
26	C	1054	BCR	C20-C21	-8.21	1.18	1.43
26	z	6053	BCR	C16-C17	-8.21	1.18	1.43
26	B	1045	BCR	C20-C21	-8.20	1.18	1.43
26	c	6054	BCR	C20-C21	-8.20	1.18	1.43
26	k	6051	BCR	C20-C21	-8.20	1.18	1.43
26	z	6053	BCR	C20-C21	-8.20	1.18	1.43
26	d	6050	BCR	C16-C17	-8.20	1.18	1.43
26	H	1049	BCR	C16-C17	-8.20	1.18	1.43
26	T	6048	BCR	C16-C17	-8.20	1.18	1.43
26	k	6052	BCR	C20-C21	-8.20	1.18	1.43
26	C	1052	BCR	C16-C17	-8.20	1.18	1.43
26	D	1050	BCR	C16-C17	-8.20	1.18	1.43
26	Z	1053	BCR	C20-C21	-8.20	1.18	1.43
26	T	6048	BCR	C20-C21	-8.19	1.18	1.43
26	d	6050	BCR	C20-C21	-8.19	1.18	1.43
26	h	6049	BCR	C16-C17	-8.19	1.18	1.43
26	D	1050	BCR	C20-C21	-8.18	1.18	1.43
26	B	1048	BCR	C16-C17	-8.18	1.18	1.43
26	k	6052	BCR	C16-C17	-8.17	1.18	1.43
26	T	6046	BCR	C16-C17	-8.09	1.18	1.43
26	t	1046	BCR	C16-C17	-8.09	1.18	1.43
26	a	6044	BCR	C20-C21	-8.08	1.18	1.43
26	A	1044	BCR	C20-C21	-8.07	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	6044	BCR	C16-C17	-8.06	1.18	1.43
26	A	1044	BCR	C16-C17	-8.05	1.18	1.43
26	t	1046	BCR	C20-C21	-7.99	1.19	1.43
26	T	6046	BCR	C20-C21	-7.98	1.19	1.43
26	z	6053	BCR	C17-C18	-7.49	1.25	1.35
26	k	6052	BCR	C17-C18	-7.49	1.25	1.35
26	d	6050	BCR	C21-C22	-7.48	1.25	1.35
26	T	6048	BCR	C21-C22	-7.47	1.25	1.35
26	D	1050	BCR	C21-C22	-7.47	1.25	1.35
26	B	1048	BCR	C17-C18	-7.47	1.25	1.35
26	Z	1053	BCR	C21-C22	-7.46	1.25	1.35
26	b	6047	BCR	C21-C22	-7.45	1.25	1.35
26	z	6053	BCR	C21-C22	-7.44	1.25	1.35
26	Z	1053	BCR	C17-C18	-7.43	1.25	1.35
26	D	1050	BCR	C17-C18	-7.43	1.25	1.35
26	H	1049	BCR	C21-C22	-7.43	1.25	1.35
26	C	1054	BCR	C17-C18	-7.42	1.25	1.35
26	B	1045	BCR	C17-C18	-7.41	1.26	1.35
26	C	1052	BCR	C17-C18	-7.41	1.26	1.35
26	B	1048	BCR	C21-C22	-7.41	1.26	1.35
26	B	1047	BCR	C21-C22	-7.41	1.26	1.35
26	K	1051	BCR	C21-C22	-7.41	1.26	1.35
26	b	6045	BCR	C17-C18	-7.40	1.26	1.35
26	B	1047	BCR	C17-C18	-7.40	1.26	1.35
26	T	6048	BCR	C17-C18	-7.40	1.26	1.35
26	C	1054	BCR	C21-C22	-7.40	1.26	1.35
26	K	1051	BCR	C17-C18	-7.39	1.26	1.35
26	k	6051	BCR	C21-C22	-7.39	1.26	1.35
26	H	1049	BCR	C17-C18	-7.39	1.26	1.35
26	k	6051	BCR	C17-C18	-7.39	1.26	1.35
26	d	6050	BCR	C17-C18	-7.38	1.26	1.35
26	k	6052	BCR	C21-C22	-7.38	1.26	1.35
26	c	6054	BCR	C21-C22	-7.38	1.26	1.35
26	C	1052	BCR	C21-C22	-7.38	1.26	1.35
26	B	1045	BCR	C21-C22	-7.38	1.26	1.35
26	h	6049	BCR	C21-C22	-7.38	1.26	1.35
26	c	6054	BCR	C17-C18	-7.38	1.26	1.35
26	b	6045	BCR	C21-C22	-7.36	1.26	1.35
26	b	6047	BCR	C17-C18	-7.36	1.26	1.35
26	h	6049	BCR	C17-C18	-7.35	1.26	1.35
26	T	6046	BCR	C17-C18	-7.20	1.26	1.35
26	A	1044	BCR	C17-C18	-7.19	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	1046	BCR	C17-C18	-7.18	1.26	1.35
26	A	1044	BCR	C21-C22	-7.17	1.26	1.35
26	a	6044	BCR	C21-C22	-7.16	1.26	1.35
26	a	6044	BCR	C17-C18	-7.12	1.26	1.35
26	T	6046	BCR	C21-C22	-7.11	1.26	1.35
26	t	1046	BCR	C21-C22	-7.07	1.26	1.35
26	h	6049	BCR	C16-C15	-6.67	1.18	1.35
26	k	6052	BCR	C16-C15	-6.67	1.18	1.35
26	K	1051	BCR	C16-C15	-6.66	1.18	1.35
26	H	1049	BCR	C16-C15	-6.66	1.18	1.35
26	k	6051	BCR	C16-C15	-6.66	1.18	1.35
26	z	6053	BCR	C16-C15	-6.65	1.18	1.35
26	C	1052	BCR	C16-C15	-6.65	1.18	1.35
26	Z	1053	BCR	C16-C15	-6.65	1.18	1.35
26	B	1048	BCR	C16-C15	-6.64	1.18	1.35
26	b	6047	BCR	C16-C15	-6.63	1.18	1.35
26	B	1047	BCR	C16-C15	-6.63	1.18	1.35
26	C	1054	BCR	C16-C15	-6.62	1.18	1.35
26	B	1045	BCR	C16-C15	-6.62	1.18	1.35
26	T	6048	BCR	C16-C15	-6.62	1.18	1.35
26	b	6045	BCR	C16-C15	-6.61	1.18	1.35
26	D	1050	BCR	C16-C15	-6.61	1.18	1.35
26	d	6050	BCR	C16-C15	-6.61	1.18	1.35
26	c	6054	BCR	C16-C15	-6.60	1.18	1.35
26	t	1046	BCR	C16-C15	-6.45	1.18	1.35
26	T	6046	BCR	C16-C15	-6.45	1.18	1.35
26	a	6044	BCR	C16-C15	-6.38	1.19	1.35
26	A	1044	BCR	C16-C15	-6.36	1.19	1.35
26	b	6047	BCR	C11-C12	-6.26	1.18	1.34
26	c	6054	BCR	C20-C19	-6.26	1.18	1.34
26	T	6048	BCR	C20-C19	-6.26	1.18	1.34
26	k	6051	BCR	C20-C19	-6.25	1.18	1.34
26	d	6050	BCR	C20-C19	-6.25	1.18	1.34
26	C	1054	BCR	C11-C12	-6.25	1.18	1.34
26	B	1048	BCR	C20-C19	-6.25	1.18	1.34
26	z	6053	BCR	C11-C12	-6.25	1.18	1.34
26	k	6052	BCR	C20-C19	-6.24	1.18	1.34
26	B	1047	BCR	C11-C12	-6.24	1.18	1.34
26	b	6045	BCR	C11-C12	-6.24	1.18	1.34
26	k	6052	BCR	C11-C12	-6.23	1.18	1.34
26	D	1050	BCR	C20-C19	-6.23	1.18	1.34
26	c	6054	BCR	C11-C12	-6.23	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	1051	BCR	C20-C19	-6.23	1.18	1.34
26	C	1054	BCR	C20-C19	-6.23	1.18	1.34
26	B	1045	BCR	C11-C12	-6.23	1.18	1.34
26	H	1049	BCR	C11-C12	-6.23	1.18	1.34
26	Z	1053	BCR	C11-C12	-6.23	1.18	1.34
26	B	1048	BCR	C11-C12	-6.23	1.18	1.34
26	C	1052	BCR	C20-C19	-6.22	1.18	1.34
26	B	1045	BCR	C20-C19	-6.22	1.18	1.34
26	h	6049	BCR	C20-C19	-6.22	1.18	1.34
26	B	1047	BCR	C20-C19	-6.22	1.18	1.34
26	K	1051	BCR	C11-C12	-6.22	1.18	1.34
26	h	6049	BCR	C11-C12	-6.22	1.18	1.34
26	T	6048	BCR	C11-C12	-6.22	1.18	1.34
26	C	1052	BCR	C11-C12	-6.21	1.18	1.34
26	d	6050	BCR	C11-C12	-6.21	1.18	1.34
26	b	6045	BCR	C20-C19	-6.21	1.18	1.34
26	H	1049	BCR	C20-C19	-6.21	1.18	1.34
26	Z	1053	BCR	C20-C19	-6.21	1.18	1.34
26	D	1050	BCR	C11-C12	-6.20	1.18	1.34
26	k	6051	BCR	C11-C12	-6.20	1.18	1.34
26	z	6053	BCR	C20-C19	-6.20	1.18	1.34
26	b	6047	BCR	C20-C19	-6.19	1.18	1.34
26	T	6046	BCR	C11-C12	-6.06	1.18	1.34
26	A	1044	BCR	C20-C19	-6.06	1.18	1.34
26	t	1046	BCR	C11-C12	-6.05	1.18	1.34
26	a	6044	BCR	C20-C19	-6.04	1.18	1.34
26	T	6046	BCR	C20-C19	-6.03	1.19	1.34
26	A	1044	BCR	C11-C12	-6.02	1.19	1.34
26	t	1046	BCR	C20-C19	-6.02	1.19	1.34
26	a	6044	BCR	C11-C12	-6.02	1.19	1.34
26	d	6050	BCR	C11-C10	-5.78	1.25	1.43
26	T	6048	BCR	C11-C10	-5.78	1.25	1.43
26	D	1050	BCR	C11-C10	-5.77	1.25	1.43
26	C	1052	BCR	C11-C10	-5.77	1.25	1.43
26	b	6047	BCR	C15-C14	-5.77	1.25	1.43
26	B	1045	BCR	C11-C10	-5.76	1.25	1.43
26	h	6049	BCR	C11-C10	-5.76	1.25	1.43
26	B	1047	BCR	C15-C14	-5.76	1.25	1.43
26	B	1048	BCR	C15-C14	-5.76	1.25	1.43
26	B	1048	BCR	C11-C10	-5.76	1.25	1.43
26	k	6051	BCR	C11-C10	-5.76	1.25	1.43
26	D	1050	BCR	C15-C14	-5.76	1.25	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6045	BCR	C11-C10	-5.76	1.25	1.43
26	d	6050	BCR	C15-C14	-5.76	1.25	1.43
26	H	1049	BCR	C11-C10	-5.76	1.25	1.43
26	k	6051	BCR	C15-C14	-5.76	1.25	1.43
26	b	6045	BCR	C15-C14	-5.75	1.26	1.43
26	B	1045	BCR	C15-C14	-5.75	1.26	1.43
26	K	1051	BCR	C15-C14	-5.75	1.26	1.43
26	K	1051	BCR	C11-C10	-5.75	1.26	1.43
26	c	6054	BCR	C15-C14	-5.75	1.26	1.43
26	z	6053	BCR	C15-C14	-5.75	1.26	1.43
26	h	6049	BCR	C15-C14	-5.75	1.26	1.43
26	H	1049	BCR	C15-C14	-5.75	1.26	1.43
26	c	6054	BCR	C11-C10	-5.75	1.26	1.43
26	k	6052	BCR	C11-C10	-5.75	1.26	1.43
26	z	6053	BCR	C11-C10	-5.74	1.26	1.43
26	C	1054	BCR	C11-C10	-5.74	1.26	1.43
26	k	6052	BCR	C15-C14	-5.74	1.26	1.43
26	Z	1053	BCR	C11-C10	-5.74	1.26	1.43
26	Z	1053	BCR	C15-C14	-5.74	1.26	1.43
26	C	1054	BCR	C15-C14	-5.74	1.26	1.43
26	B	1047	BCR	C11-C10	-5.74	1.26	1.43
26	T	6048	BCR	C15-C14	-5.74	1.26	1.43
26	C	1052	BCR	C15-C14	-5.74	1.26	1.43
26	b	6047	BCR	C11-C10	-5.73	1.26	1.43
26	T	6046	BCR	C11-C10	-5.69	1.26	1.43
26	t	1046	BCR	C11-C10	-5.68	1.26	1.43
26	a	6044	BCR	C15-C14	-5.62	1.26	1.43
26	A	1044	BCR	C15-C14	-5.61	1.26	1.43
26	T	6046	BCR	C15-C14	-5.61	1.26	1.43
26	t	1046	BCR	C15-C14	-5.61	1.26	1.43
26	A	1044	BCR	C11-C10	-5.59	1.26	1.43
26	a	6044	BCR	C11-C10	-5.59	1.26	1.43
26	D	1050	BCR	C23-C22	-5.29	1.34	1.45
26	H	1049	BCR	C23-C22	-5.28	1.34	1.45
26	d	6050	BCR	C23-C22	-5.28	1.34	1.45
26	B	1045	BCR	C23-C22	-5.28	1.34	1.45
26	h	6049	BCR	C23-C22	-5.28	1.34	1.45
26	b	6045	BCR	C23-C22	-5.28	1.34	1.45
26	c	6054	BCR	C23-C22	-5.27	1.34	1.45
26	C	1054	BCR	C23-C22	-5.26	1.34	1.45
26	K	1051	BCR	C23-C22	-5.25	1.34	1.45
26	z	6053	BCR	C23-C22	-5.25	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	1053	BCR	C23-C22	-5.25	1.34	1.45
26	k	6051	BCR	C23-C22	-5.22	1.34	1.45
26	T	6046	BCR	C23-C22	-5.19	1.34	1.45
26	t	1046	BCR	C23-C22	-5.17	1.34	1.45
26	A	1044	BCR	C23-C22	-5.06	1.34	1.45
26	a	6044	BCR	C23-C22	-5.06	1.34	1.45
26	C	1052	BCR	C23-C22	-5.05	1.34	1.45
26	k	6052	BCR	C23-C22	-5.04	1.35	1.45
26	T	6048	BCR	C23-C22	-5.02	1.35	1.45
26	B	1048	BCR	C23-C22	-5.00	1.35	1.45
26	B	1047	BCR	C23-C22	-4.99	1.35	1.45
26	b	6047	BCR	C23-C22	-4.99	1.35	1.45
31	v	6041	HEM	C3B-C2B	-4.93	1.33	1.40
31	V	1041	HEM	C3B-C2B	-4.89	1.33	1.40
31	V	1041	HEM	C3C-C2C	-4.89	1.33	1.40
31	v	6041	HEM	C3C-C2C	-4.87	1.33	1.40
31	F	1040	HEM	C3B-C2B	-4.85	1.34	1.40
31	f	6040	HEM	C3B-C2B	-4.84	1.34	1.40
31	F	1040	HEM	C3C-C2C	-4.84	1.34	1.40
31	f	6040	HEM	C3C-C2C	-4.79	1.34	1.40
26	d	6050	BCR	C24-C25	-3.06	1.34	1.45
24	a	6038	PHO	O2D-CGD	-3.05	1.25	1.33
26	D	1050	BCR	C24-C25	-3.05	1.34	1.45
26	Z	1053	BCR	C24-C25	-3.05	1.34	1.45
26	z	6053	BCR	C24-C25	-3.05	1.34	1.45
24	A	1038	PHO	O2D-CGD	-3.05	1.25	1.33
26	k	6051	BCR	C24-C25	-3.04	1.34	1.45
24	D	1039	PHO	O2D-CGD	-3.04	1.25	1.33
24	d	6039	PHO	O2D-CGD	-3.03	1.25	1.33
26	b	6045	BCR	C24-C25	-3.03	1.34	1.45
26	K	1051	BCR	C24-C25	-3.03	1.34	1.45
26	B	1045	BCR	C24-C25	-3.03	1.34	1.45
26	C	1054	BCR	C24-C25	-3.02	1.34	1.45
26	c	6054	BCR	C24-C25	-3.00	1.34	1.45
26	h	6049	BCR	C24-C25	-3.00	1.34	1.45
26	t	1046	BCR	C24-C25	-3.00	1.34	1.45
26	H	1049	BCR	C24-C25	-3.00	1.34	1.45
26	T	6046	BCR	C24-C25	-2.99	1.34	1.45
26	k	6052	BCR	C24-C25	-2.86	1.35	1.45
24	D	1039	PHO	C1B-C2B	-2.86	1.39	1.45
26	C	1052	BCR	C24-C25	-2.85	1.35	1.45
24	d	6039	PHO	C1B-C2B	-2.84	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1038	PHO	C1B-C2B	-2.82	1.39	1.45
24	A	1038	PHO	C3D-C4D	-2.82	1.34	1.43
24	d	6039	PHO	C3D-C4D	-2.82	1.34	1.43
24	D	1039	PHO	C3D-C4D	-2.82	1.34	1.43
24	a	6038	PHO	C3D-C4D	-2.81	1.34	1.43
24	a	6038	PHO	C1B-C2B	-2.80	1.39	1.45
26	B	1047	BCR	C24-C25	-2.74	1.35	1.45
26	T	6048	BCR	C24-C25	-2.74	1.35	1.45
26	b	6047	BCR	C24-C25	-2.73	1.35	1.45
26	B	1048	BCR	C24-C25	-2.73	1.35	1.45
26	A	1044	BCR	C24-C25	-2.72	1.35	1.45
26	a	6044	BCR	C24-C25	-2.71	1.35	1.45
24	D	1039	PHO	O2A-CGA	-2.68	1.25	1.33
24	d	6039	PHO	O2A-CGA	-2.68	1.25	1.33
24	a	6038	PHO	O2A-CGA	-2.67	1.25	1.33
24	A	1038	PHO	O2A-CGA	-2.65	1.25	1.33
26	k	6052	BCR	C30-C25	-2.44	1.50	1.53
26	C	1052	BCR	C30-C25	-2.43	1.50	1.53
26	T	6046	BCR	C30-C25	-2.35	1.50	1.53
26	t	1046	BCR	C30-C25	-2.34	1.50	1.53
26	T	6046	BCR	C1-C6	-2.31	1.50	1.53
26	D	1050	BCR	C8-C7	-2.29	1.25	1.33
26	h	6049	BCR	C8-C7	-2.29	1.25	1.33
26	H	1049	BCR	C8-C7	-2.28	1.25	1.33
26	k	6052	BCR	C8-C7	-2.28	1.25	1.33
26	C	1052	BCR	C8-C7	-2.28	1.25	1.33
26	c	6054	BCR	C8-C7	-2.28	1.25	1.33
26	T	6048	BCR	C8-C7	-2.28	1.25	1.33
26	d	6050	BCR	C8-C7	-2.27	1.25	1.33
26	K	1051	BCR	C8-C7	-2.27	1.26	1.33
26	B	1047	BCR	C8-C7	-2.27	1.26	1.33
26	Z	1053	BCR	C8-C7	-2.27	1.26	1.33
26	k	6051	BCR	C8-C7	-2.27	1.26	1.33
26	C	1054	BCR	C8-C7	-2.26	1.26	1.33
26	b	6047	BCR	C8-C7	-2.26	1.26	1.33
26	B	1048	BCR	C8-C7	-2.26	1.26	1.33
26	b	6045	BCR	C8-C7	-2.26	1.26	1.33
26	t	1046	BCR	C1-C6	-2.26	1.50	1.53
26	B	1045	BCR	C8-C7	-2.26	1.26	1.33
26	z	6053	BCR	C8-C7	-2.25	1.26	1.33
24	D	1039	PHO	C1C-NC	-2.20	1.33	1.38
24	a	6038	PHO	C3B-C4B	-2.20	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	1039	PHO	C3B-C4B	-2.20	1.38	1.43
24	a	6038	PHO	C1C-NC	-2.19	1.33	1.38
24	d	6039	PHO	C1C-NC	-2.19	1.33	1.38
26	A	1044	BCR	C30-C25	-2.18	1.50	1.53
24	d	6039	PHO	C3B-C4B	-2.18	1.38	1.43
24	A	1038	PHO	C1C-NC	-2.17	1.33	1.38
26	t	1046	BCR	C8-C7	-2.16	1.26	1.33
26	a	6044	BCR	C30-C25	-2.16	1.50	1.53
26	T	6046	BCR	C8-C7	-2.16	1.26	1.33
24	A	1038	PHO	C3B-C4B	-2.15	1.38	1.43
24	D	1039	PHO	C1D-C2D	-2.15	1.41	1.45
24	A	1038	PHO	C1D-C2D	-2.15	1.41	1.45
24	a	6038	PHO	C1D-C2D	-2.14	1.41	1.45
26	a	6044	BCR	C8-C7	-2.14	1.26	1.33
26	A	1044	BCR	C8-C7	-2.14	1.26	1.33
24	d	6039	PHO	C1D-C2D	-2.13	1.41	1.45
26	b	6045	BCR	C30-C25	-2.08	1.50	1.53
26	k	6051	BCR	C1-C6	-2.05	1.51	1.53
24	D	1039	PHO	C4D-CHA	-2.04	1.38	1.44
26	b	6047	BCR	C30-C25	-2.04	1.51	1.53
26	z	6053	BCR	C30-C25	-2.04	1.51	1.53
24	d	6039	PHO	C4D-CHA	-2.04	1.38	1.44
26	B	1045	BCR	C30-C25	-2.03	1.51	1.53
24	a	6038	PHO	C4D-CHA	-2.03	1.38	1.44
26	z	6053	BCR	C1-C6	-2.03	1.51	1.53
24	A	1038	PHO	C4D-CHA	-2.03	1.38	1.44
26	H	1049	BCR	C1-C6	-2.03	1.51	1.53
26	Z	1053	BCR	C1-C6	-2.02	1.51	1.53
26	B	1048	BCR	C1-C6	-2.02	1.51	1.53
26	B	1047	BCR	C30-C25	-2.02	1.51	1.53
26	B	1045	BCR	C1-C6	-2.01	1.51	1.53
26	T	6048	BCR	C1-C6	-2.00	1.51	1.53
23	B	1011	CLA	C4C-C3C	2.03	1.48	1.45
23	b	6011	CLA	C4C-C3C	2.07	1.48	1.45
23	b	6011	CLA	C1C-C2C	2.07	1.48	1.44
23	B	1009	CLA	C1C-C2C	2.07	1.48	1.44
23	b	6009	CLA	C1C-C2C	2.07	1.48	1.44
23	B	1011	CLA	C1C-C2C	2.08	1.48	1.44
24	A	1038	PHO	C1C-C2C	2.11	1.50	1.45
23	b	6021	CLA	C4C-C3C	2.11	1.48	1.45
23	b	6010	CLA	C1C-C2C	2.11	1.48	1.44
24	a	6038	PHO	C1C-C2C	2.11	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1021	CLA	C4C-C3C	2.12	1.48	1.45
23	B	1010	CLA	C1C-C2C	2.12	1.48	1.44
24	d	6039	PHO	C1C-C2C	2.13	1.50	1.45
23	c	6029	CLA	C1C-C2C	2.14	1.48	1.44
23	D	1008	CLA	C1C-C2C	2.14	1.48	1.44
23	B	1023	CLA	C4C-C3C	2.14	1.48	1.45
23	b	6010	CLA	C4C-C3C	2.14	1.48	1.45
23	B	1023	CLA	C1C-C2C	2.14	1.48	1.44
23	B	1010	CLA	C4C-C3C	2.15	1.48	1.45
23	b	6023	CLA	C4C-C3C	2.15	1.48	1.45
24	D	1039	PHO	C1C-C2C	2.15	1.50	1.45
23	b	6023	CLA	C1C-C2C	2.16	1.48	1.44
23	c	6029	CLA	C4C-C3C	2.16	1.48	1.45
23	d	6008	CLA	C1C-C2C	2.16	1.48	1.44
23	c	6030	CLA	C1C-C2C	2.16	1.48	1.44
23	B	1021	CLA	C1C-C2C	2.17	1.48	1.44
23	D	1008	CLA	C4C-C3C	2.17	1.48	1.45
23	C	1029	CLA	C1C-C2C	2.17	1.48	1.44
23	b	6019	CLA	C4C-C3C	2.18	1.48	1.45
23	b	6021	CLA	C1C-C2C	2.19	1.48	1.44
23	H	1017	CLA	C4C-C3C	2.19	1.48	1.45
23	c	6035	CLA	C1C-C2C	2.19	1.48	1.44
23	k	6034	CLA	C4C-C3C	2.19	1.48	1.45
23	C	1030	CLA	C1C-C2C	2.20	1.48	1.44
23	C	1035	CLA	C1C-C2C	2.20	1.48	1.44
23	c	6027	CLA	C4C-C3C	2.20	1.48	1.45
23	c	6026	CLA	C4C-C3C	2.20	1.48	1.45
23	b	6016	CLA	C4C-C3C	2.21	1.48	1.45
23	C	1029	CLA	C4C-C3C	2.21	1.48	1.45
23	d	6004	CLA	C1C-C2C	2.21	1.48	1.44
23	b	6015	CLA	C4C-C3C	2.21	1.48	1.45
23	d	6008	CLA	C4C-C3C	2.21	1.48	1.45
23	a	6007	CLA	C4C-C3C	2.21	1.48	1.45
23	B	1016	CLA	C4C-C3C	2.21	1.48	1.45
23	A	1003	CLA	C1C-C2C	2.21	1.48	1.44
23	B	1019	CLA	C4C-C3C	2.21	1.48	1.45
23	h	6017	CLA	C4C-C3C	2.22	1.48	1.45
23	d	6004	CLA	C4C-C3C	2.22	1.48	1.45
23	B	1015	CLA	C4C-C3C	2.22	1.48	1.45
23	b	6020	CLA	C4C-C3C	2.22	1.49	1.45
23	c	6035	CLA	C4C-C3C	2.22	1.49	1.45
23	K	1034	CLA	C4C-C3C	2.22	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	1017	CLA	C1C-C2C	2.22	1.48	1.44
23	c	6032	CLA	C1C-C2C	2.22	1.48	1.44
23	C	1035	CLA	C4C-C3C	2.22	1.49	1.45
23	D	1004	CLA	C1C-C2C	2.23	1.48	1.44
23	a	6003	CLA	C1C-C2C	2.23	1.48	1.44
23	a	6006	CLA	C1C-C2C	2.23	1.48	1.44
23	B	1019	CLA	C1C-C2C	2.23	1.48	1.44
23	C	1027	CLA	C4C-C3C	2.23	1.49	1.45
23	A	1007	CLA	C4C-C3C	2.23	1.49	1.45
23	B	1018	CLA	C1C-C2C	2.23	1.48	1.44
23	B	1009	CLA	C4C-C3C	2.23	1.49	1.45
23	B	1014	CLA	C4C-C3C	2.23	1.49	1.45
23	a	6006	CLA	C4C-C3C	2.23	1.49	1.45
23	C	1037	CLA	C1C-C2C	2.23	1.48	1.44
23	D	1005	CLA	C4C-C3C	2.23	1.49	1.45
23	B	1020	CLA	C4C-C3C	2.24	1.49	1.45
23	a	6003	CLA	C4C-C3C	2.24	1.49	1.45
23	h	6017	CLA	C1C-C2C	2.24	1.48	1.44
23	b	6009	CLA	C4C-C3C	2.24	1.49	1.45
23	D	1004	CLA	C4C-C3C	2.24	1.49	1.45
23	A	1003	CLA	C4C-C3C	2.24	1.49	1.45
23	c	6037	CLA	C1C-C2C	2.24	1.48	1.44
23	C	1026	CLA	C4C-C3C	2.24	1.49	1.45
23	C	1032	CLA	C1C-C2C	2.24	1.48	1.44
23	b	6018	CLA	C1C-C2C	2.24	1.48	1.44
23	c	6028	CLA	C1C-C2C	2.24	1.48	1.44
23	C	1026	CLA	C1C-C2C	2.24	1.48	1.44
23	A	1006	CLA	C4C-C3C	2.24	1.49	1.45
23	c	6037	CLA	C4C-C3C	2.25	1.49	1.45
23	B	1015	CLA	C1C-C2C	2.25	1.48	1.44
23	B	1013	CLA	C1C-C2C	2.25	1.48	1.44
23	b	6014	CLA	C4C-C3C	2.25	1.49	1.45
23	b	6014	CLA	C1C-C2C	2.25	1.48	1.44
23	B	1024	CLA	C1C-C2C	2.25	1.48	1.44
23	C	1032	CLA	C4C-C3C	2.25	1.49	1.45
23	b	6012	CLA	C4C-C3C	2.25	1.49	1.45
23	b	6019	CLA	C1C-C2C	2.25	1.48	1.44
23	b	6016	CLA	C1C-C2C	2.25	1.48	1.44
23	A	1006	CLA	C1C-C2C	2.25	1.48	1.44
23	B	1016	CLA	C1C-C2C	2.25	1.48	1.44
23	B	1013	CLA	C4C-C3C	2.25	1.49	1.45
23	B	1012	CLA	C4C-C3C	2.25	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6033	CLA	C1C-C2C	2.26	1.48	1.44
23	C	1028	CLA	C1C-C2C	2.26	1.48	1.44
23	K	1034	CLA	C1C-C2C	2.26	1.48	1.44
23	B	1018	CLA	C4C-C3C	2.26	1.49	1.45
23	C	1037	CLA	C4C-C3C	2.26	1.49	1.45
23	b	6024	CLA	C1C-C2C	2.26	1.48	1.44
23	c	6032	CLA	C4C-C3C	2.26	1.49	1.45
23	C	1025	CLA	C4C-C3C	2.26	1.49	1.45
23	b	6013	CLA	C4C-C3C	2.26	1.49	1.45
23	b	6013	CLA	C1C-C2C	2.26	1.48	1.44
23	A	1007	CLA	C1C-C2C	2.26	1.48	1.44
23	c	6026	CLA	C1C-C2C	2.26	1.48	1.44
23	d	6005	CLA	C4C-C3C	2.26	1.49	1.45
23	C	1033	CLA	C4C-C3C	2.26	1.49	1.45
23	b	6022	CLA	C1C-C2C	2.26	1.48	1.44
23	c	6036	CLA	C4C-C3C	2.26	1.49	1.45
23	c	6033	CLA	C4C-C3C	2.27	1.49	1.45
23	B	1022	CLA	C1C-C2C	2.27	1.48	1.44
23	C	1025	CLA	C1C-C2C	2.27	1.48	1.44
23	C	1033	CLA	C1C-C2C	2.27	1.48	1.44
23	b	6015	CLA	C1C-C2C	2.27	1.48	1.44
23	D	1005	CLA	C1C-C2C	2.27	1.48	1.44
23	c	6025	CLA	C4C-C3C	2.27	1.49	1.45
23	B	1014	CLA	C1C-C2C	2.27	1.48	1.44
23	b	6018	CLA	C4C-C3C	2.27	1.49	1.45
23	C	1031	CLA	C1C-C2C	2.27	1.48	1.44
23	c	6028	CLA	C4C-C3C	2.27	1.49	1.45
23	k	6034	CLA	C1C-C2C	2.28	1.48	1.44
23	B	1022	CLA	C4C-C3C	2.28	1.49	1.45
23	c	6031	CLA	C1C-C2C	2.28	1.48	1.44
23	b	6012	CLA	C1C-C2C	2.28	1.48	1.44
23	B	1012	CLA	C1C-C2C	2.28	1.48	1.44
23	C	1028	CLA	C4C-C3C	2.29	1.49	1.45
23	B	1024	CLA	C4C-C3C	2.29	1.49	1.45
23	C	1036	CLA	C4C-C3C	2.29	1.49	1.45
23	C	1027	CLA	C1C-C2C	2.29	1.49	1.44
23	C	1036	CLA	C1C-C2C	2.29	1.49	1.44
23	c	6025	CLA	C1C-C2C	2.29	1.49	1.44
23	B	1020	CLA	C1C-C2C	2.29	1.49	1.44
23	b	6022	CLA	C4C-C3C	2.29	1.49	1.45
23	b	6020	CLA	C1C-C2C	2.29	1.49	1.44
23	a	6007	CLA	C1C-C2C	2.30	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6027	CLA	C1C-C2C	2.30	1.49	1.44
23	b	6024	CLA	C4C-C3C	2.30	1.49	1.45
23	d	6005	CLA	C1C-C2C	2.30	1.49	1.44
23	C	1031	CLA	C4C-C3C	2.30	1.49	1.45
23	c	6036	CLA	C1C-C2C	2.31	1.49	1.44
23	c	6031	CLA	C4C-C3C	2.32	1.49	1.45
23	c	6030	CLA	CHD-C4C	2.33	1.48	1.41
23	c	6029	CLA	CHD-C4C	2.35	1.48	1.41
23	B	1011	CLA	CHD-C4C	2.35	1.48	1.41
23	b	6011	CLA	CHD-C4C	2.35	1.48	1.41
23	b	6009	CLA	CHD-C4C	2.36	1.48	1.41
23	B	1009	CLA	CHD-C4C	2.36	1.48	1.41
23	C	1030	CLA	CHD-C4C	2.36	1.48	1.41
23	B	1023	CLA	CHD-C4C	2.36	1.48	1.41
23	b	6023	CLA	CHD-C4C	2.37	1.48	1.41
23	B	1010	CLA	CHD-C4C	2.37	1.48	1.41
23	C	1029	CLA	CHD-C4C	2.38	1.48	1.41
23	b	6021	CLA	CHD-C4C	2.39	1.48	1.41
23	D	1008	CLA	CHD-C4C	2.39	1.48	1.41
23	B	1021	CLA	CHD-C4C	2.39	1.48	1.41
23	d	6008	CLA	CHD-C4C	2.39	1.48	1.41
23	b	6010	CLA	CHD-C4C	2.40	1.48	1.41
23	B	1018	CLA	CHD-C4C	2.40	1.48	1.41
23	b	6012	CLA	CHD-C4C	2.41	1.48	1.41
23	a	6007	CLA	CHD-C4C	2.41	1.48	1.41
23	A	1007	CLA	CHD-C4C	2.41	1.48	1.41
23	d	6005	CLA	CHD-C4C	2.41	1.48	1.41
23	D	1005	CLA	CHD-C4C	2.41	1.48	1.41
23	b	6018	CLA	CHD-C4C	2.42	1.48	1.41
23	b	6024	CLA	CHD-C4C	2.42	1.48	1.41
23	c	6031	CLA	CHD-C4C	2.42	1.48	1.41
23	a	6006	CLA	CHD-C4C	2.42	1.48	1.41
23	A	1006	CLA	CHD-C4C	2.42	1.48	1.41
23	B	1012	CLA	CHD-C4C	2.43	1.48	1.41
23	b	6013	CLA	CHD-C4C	2.43	1.48	1.41
23	B	1019	CLA	CHD-C4C	2.43	1.48	1.41
23	B	1024	CLA	CHD-C4C	2.43	1.48	1.41
23	C	1026	CLA	CHD-C4C	2.43	1.48	1.41
23	A	1003	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1036	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1028	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1035	CLA	CHD-C4C	2.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6014	CLA	CHD-C4C	2.44	1.48	1.41
23	c	6037	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1037	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1031	CLA	CHD-C4C	2.44	1.48	1.41
23	c	6026	CLA	CHD-C4C	2.44	1.48	1.41
23	a	6003	CLA	CHD-C4C	2.44	1.48	1.41
23	b	6019	CLA	CHD-C4C	2.44	1.48	1.41
23	c	6032	CLA	CHD-C4C	2.44	1.48	1.41
23	C	1032	CLA	CHD-C4C	2.45	1.48	1.41
23	c	6036	CLA	CHD-C4C	2.45	1.48	1.41
23	C	1033	CLA	CHD-C4C	2.45	1.48	1.41
23	h	6017	CLA	CHD-C4C	2.45	1.48	1.41
23	B	1022	CLA	CHD-C4C	2.45	1.48	1.41
23	H	1017	CLA	CHD-C4C	2.45	1.48	1.41
23	B	1016	CLA	CHD-C4C	2.45	1.48	1.41
23	k	6034	CLA	CHD-C4C	2.45	1.48	1.41
23	c	6028	CLA	CHD-C4C	2.45	1.48	1.41
23	b	6016	CLA	CHD-C4C	2.45	1.48	1.41
23	C	1025	CLA	CHD-C4C	2.45	1.48	1.41
23	c	6025	CLA	CHD-C4C	2.45	1.48	1.41
23	K	1034	CLA	CHD-C4C	2.45	1.48	1.41
23	c	6033	CLA	CHD-C4C	2.46	1.48	1.41
23	B	1013	CLA	CHD-C4C	2.46	1.48	1.41
23	d	6004	CLA	CHD-C4C	2.46	1.48	1.41
23	B	1014	CLA	CHD-C4C	2.46	1.48	1.41
23	B	1020	CLA	CHD-C4C	2.46	1.48	1.41
23	b	6021	CLA	C1B-CHB	2.46	1.46	1.40
23	D	1004	CLA	CHD-C4C	2.46	1.48	1.41
23	c	6027	CLA	CHD-C4C	2.47	1.48	1.41
23	B	1015	CLA	CHD-C4C	2.47	1.48	1.41
23	b	6022	CLA	CHD-C4C	2.47	1.48	1.41
23	b	6020	CLA	CHD-C4C	2.47	1.48	1.41
23	C	1027	CLA	CHD-C4C	2.47	1.48	1.41
23	B	1021	CLA	C1B-CHB	2.47	1.46	1.40
23	c	6035	CLA	CHD-C4C	2.47	1.48	1.41
23	b	6022	CLA	C1B-CHB	2.47	1.46	1.40
23	b	6015	CLA	CHD-C4C	2.47	1.48	1.41
23	c	6030	CLA	C1B-CHB	2.48	1.46	1.40
23	C	1030	CLA	C1B-CHB	2.48	1.46	1.40
23	k	6034	CLA	C1B-CHB	2.48	1.46	1.40
31	v	6041	HEM	C4D-ND	2.49	1.39	1.36
23	B	1011	CLA	C1B-CHB	2.49	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6012	CLA	C1B-CHB	2.49	1.46	1.40
23	B	1022	CLA	C1B-CHB	2.49	1.46	1.40
23	c	6032	CLA	C1B-CHB	2.49	1.46	1.40
23	B	1012	CLA	C1B-CHB	2.49	1.46	1.40
23	a	6007	CLA	C1B-CHB	2.49	1.46	1.40
23	b	6016	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6015	CLA	C1B-CHB	2.50	1.46	1.40
23	C	1032	CLA	C1B-CHB	2.50	1.46	1.40
23	K	1034	CLA	C1B-CHB	2.50	1.46	1.40
23	B	1018	CLA	C1B-CHB	2.50	1.46	1.40
23	B	1015	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6018	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6013	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6010	CLA	C1B-CHB	2.50	1.46	1.40
23	C	1028	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6023	CLA	C1B-CHB	2.51	1.46	1.40
23	b	6020	CLA	C1B-CHB	2.51	1.46	1.40
23	b	6011	CLA	C1B-CHB	2.51	1.46	1.40
23	D	1004	CLA	C1B-CHB	2.51	1.46	1.40
23	c	6033	CLA	C1B-CHB	2.51	1.46	1.40
23	H	1017	CLA	C1B-CHB	2.51	1.46	1.40
23	C	1029	CLA	C1B-CHB	2.51	1.46	1.40
23	B	1023	CLA	C1B-CHB	2.51	1.46	1.40
23	c	6028	CLA	C1B-CHB	2.51	1.46	1.40
23	c	6036	CLA	C1B-CHB	2.51	1.46	1.40
23	B	1024	CLA	C1B-CHB	2.51	1.46	1.40
23	c	6029	CLA	C1B-CHB	2.52	1.46	1.40
23	C	1033	CLA	C1B-CHB	2.52	1.46	1.40
23	c	6026	CLA	C1B-CHB	2.52	1.46	1.40
23	C	1036	CLA	C1B-CHB	2.52	1.46	1.40
23	A	1006	CLA	C1B-CHB	2.52	1.46	1.40
23	c	6025	CLA	C1B-CHB	2.52	1.46	1.40
23	B	1010	CLA	C1B-CHB	2.52	1.46	1.40
23	B	1016	CLA	C1B-CHB	2.52	1.46	1.40
23	D	1005	CLA	C1B-CHB	2.52	1.46	1.40
23	A	1003	CLA	C1B-CHB	2.52	1.46	1.40
23	A	1007	CLA	C1B-CHB	2.52	1.46	1.40
23	d	6004	CLA	C1B-CHB	2.52	1.46	1.40
31	V	1041	HEM	C4D-ND	2.52	1.39	1.36
23	b	6019	CLA	C1B-CHB	2.52	1.46	1.40
23	c	6037	CLA	C1B-CHB	2.52	1.46	1.40
23	C	1031	CLA	C1B-CHB	2.53	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1020	CLA	C1B-CHB	2.53	1.46	1.40
23	a	6003	CLA	C1B-CHB	2.53	1.46	1.40
23	D	1008	CLA	C1B-CHB	2.53	1.46	1.40
23	c	6027	CLA	C1B-CHB	2.53	1.46	1.40
23	C	1026	CLA	C1B-CHB	2.53	1.46	1.40
23	C	1025	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1013	CLA	C1B-CHB	2.53	1.46	1.40
23	C	1027	CLA	C1B-CHB	2.53	1.46	1.40
23	C	1035	CLA	C1B-CHB	2.53	1.46	1.40
23	b	6024	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1019	CLA	C1B-CHB	2.53	1.46	1.40
23	c	6035	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1009	CLA	C1B-CHB	2.53	1.46	1.40
23	h	6017	CLA	C1B-CHB	2.54	1.46	1.40
23	C	1037	CLA	C1B-CHB	2.54	1.46	1.40
23	d	6008	CLA	C1B-CHB	2.54	1.46	1.40
23	a	6006	CLA	C1B-CHB	2.54	1.46	1.40
23	b	6014	CLA	C1B-CHB	2.54	1.46	1.40
23	c	6031	CLA	C1B-CHB	2.54	1.46	1.40
23	d	6005	CLA	C1B-CHB	2.54	1.46	1.40
23	B	1014	CLA	C1B-CHB	2.54	1.46	1.40
23	b	6009	CLA	C1B-CHB	2.55	1.46	1.40
25	D	1042	PQ9	C10-C5	2.55	1.48	1.35
25	d	6042	PQ9	C10-C5	2.56	1.48	1.35
23	c	6029	CLA	C4B-CHC	2.57	1.47	1.40
25	A	1043	PQ9	C10-C5	2.57	1.48	1.35
23	D	1008	CLA	C4B-CHC	2.57	1.47	1.40
23	C	1029	CLA	C4B-CHC	2.57	1.47	1.40
25	a	6043	PQ9	C10-C5	2.57	1.48	1.35
23	b	6021	CLA	C4B-CHC	2.57	1.47	1.40
23	c	6030	CLA	C4B-CHC	2.57	1.47	1.40
23	B	1010	CLA	C4B-CHC	2.58	1.47	1.40
23	d	6008	CLA	C4B-CHC	2.58	1.47	1.40
31	f	6040	HEM	C4D-ND	2.58	1.39	1.36
23	C	1030	CLA	C4B-CHC	2.58	1.47	1.40
23	B	1011	CLA	C4B-CHC	2.59	1.47	1.40
23	b	6010	CLA	C4B-CHC	2.60	1.47	1.40
23	B	1021	CLA	C4B-CHC	2.60	1.47	1.40
31	F	1040	HEM	C4D-ND	2.60	1.39	1.36
23	B	1009	CLA	C4B-CHC	2.60	1.47	1.40
23	b	6009	CLA	C4B-CHC	2.60	1.47	1.40
23	b	6011	CLA	C4B-CHC	2.62	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1023	CLA	C4B-CHC	2.64	1.47	1.40
23	d	6004	CLA	C4B-CHC	2.64	1.47	1.40
23	b	6024	CLA	C4B-CHC	2.65	1.47	1.40
23	d	6005	CLA	C4B-CHC	2.65	1.47	1.40
23	b	6014	CLA	C4B-CHC	2.65	1.47	1.40
23	C	1028	CLA	C4B-CHC	2.65	1.47	1.40
23	B	1024	CLA	C4B-CHC	2.66	1.47	1.40
23	c	6028	CLA	C4B-CHC	2.66	1.47	1.40
23	D	1005	CLA	C4B-CHC	2.66	1.47	1.40
23	b	6023	CLA	C4B-CHC	2.66	1.47	1.40
23	c	6032	CLA	C4B-CHC	2.66	1.47	1.40
23	c	6035	CLA	C4B-CHC	2.67	1.47	1.40
23	B	1014	CLA	C4B-CHC	2.67	1.47	1.40
23	C	1033	CLA	C4B-CHC	2.67	1.47	1.40
23	D	1004	CLA	C4B-CHC	2.67	1.47	1.40
23	K	1034	CLA	C4B-CHC	2.67	1.47	1.40
23	C	1032	CLA	C4B-CHC	2.67	1.47	1.40
23	c	6025	CLA	C4B-CHC	2.67	1.47	1.40
23	C	1025	CLA	C4B-CHC	2.67	1.47	1.40
23	b	6022	CLA	C4B-CHC	2.68	1.47	1.40
23	C	1031	CLA	C4B-CHC	2.68	1.47	1.40
23	A	1006	CLA	C4B-CHC	2.68	1.47	1.40
23	C	1036	CLA	C4B-CHC	2.68	1.47	1.40
23	B	1019	CLA	C4B-CHC	2.68	1.47	1.40
23	c	6031	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1026	CLA	C4B-CHC	2.69	1.47	1.40
23	b	6019	CLA	C4B-CHC	2.69	1.47	1.40
23	c	6026	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1027	CLA	C4B-CHC	2.69	1.47	1.40
23	c	6033	CLA	C4B-CHC	2.69	1.47	1.40
23	a	6006	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1035	CLA	C4B-CHC	2.69	1.47	1.40
23	B	1022	CLA	C4B-CHC	2.69	1.47	1.40
23	b	6013	CLA	C4B-CHC	2.70	1.47	1.40
23	h	6017	CLA	C4B-CHC	2.70	1.47	1.40
23	B	1018	CLA	C4B-CHC	2.70	1.47	1.40
23	A	1003	CLA	C4B-CHC	2.70	1.47	1.40
23	B	1020	CLA	C4B-CHC	2.70	1.47	1.40
23	B	1012	CLA	C4B-CHC	2.70	1.47	1.40
23	B	1016	CLA	C4B-CHC	2.70	1.47	1.40
23	B	1013	CLA	C4B-CHC	2.70	1.47	1.40
23	k	6034	CLA	C4B-CHC	2.70	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6016	CLA	C4B-CHC	2.70	1.47	1.40
23	b	6012	CLA	C4B-CHC	2.70	1.47	1.40
23	a	6003	CLA	C4B-CHC	2.70	1.47	1.40
23	c	6027	CLA	C4B-CHC	2.71	1.47	1.40
23	A	1007	CLA	C4B-CHC	2.71	1.47	1.40
23	c	6036	CLA	C4B-CHC	2.71	1.47	1.40
23	b	6018	CLA	C4B-CHC	2.71	1.47	1.40
23	C	1037	CLA	C4B-CHC	2.71	1.47	1.40
23	H	1017	CLA	C4B-CHC	2.72	1.47	1.40
23	B	1015	CLA	C4B-CHC	2.72	1.47	1.40
23	b	6020	CLA	C4B-CHC	2.72	1.47	1.40
23	b	6015	CLA	C4B-CHC	2.73	1.47	1.40
23	c	6037	CLA	C4B-CHC	2.74	1.47	1.40
23	a	6007	CLA	C4B-CHC	2.74	1.47	1.40
24	a	6038	PHO	C4C-C3C	2.79	1.50	1.45
24	A	1038	PHO	C4C-C3C	2.79	1.50	1.45
24	D	1039	PHO	C4C-C3C	2.81	1.50	1.45
24	d	6039	PHO	C4C-C3C	2.82	1.50	1.45
24	d	6039	PHO	CHD-C4C	2.92	1.47	1.40
24	D	1039	PHO	CHD-C4C	2.92	1.47	1.40
24	d	6039	PHO	CHB-C4A	2.94	1.47	1.40
24	A	1038	PHO	CHB-C4A	2.94	1.47	1.40
24	D	1039	PHO	CHB-C4A	2.94	1.47	1.40
24	A	1038	PHO	CHD-C4C	2.95	1.47	1.40
24	a	6038	PHO	CHB-C4A	2.96	1.47	1.40
24	a	6038	PHO	CHD-C4C	2.97	1.47	1.40
23	C	1029	CLA	C3D-C2D	3.25	1.46	1.39
23	c	6029	CLA	C3D-C2D	3.26	1.46	1.39
23	b	6011	CLA	C3D-C2D	3.29	1.47	1.39
23	B	1011	CLA	C3D-C2D	3.29	1.47	1.39
23	C	1030	CLA	C3D-C2D	3.30	1.47	1.39
23	D	1008	CLA	C3D-C2D	3.30	1.47	1.39
23	c	6030	CLA	C3D-C2D	3.30	1.47	1.39
23	B	1010	CLA	C3D-C2D	3.31	1.47	1.39
23	b	6010	CLA	C3D-C2D	3.32	1.47	1.39
23	B	1021	CLA	C3D-C2D	3.33	1.47	1.39
23	b	6021	CLA	C3D-C2D	3.33	1.47	1.39
23	d	6008	CLA	C3D-C2D	3.33	1.47	1.39
23	B	1023	CLA	C3D-C2D	3.33	1.47	1.39
23	b	6023	CLA	C3D-C2D	3.34	1.47	1.39
23	b	6009	CLA	C3D-C2D	3.36	1.47	1.39
24	D	1039	PHO	C3D-C2D	3.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	6038	PHO	C3D-C2D	3.36	1.47	1.38
23	a	6007	CLA	C3D-C2D	3.36	1.47	1.39
24	A	1038	PHO	C3D-C2D	3.37	1.47	1.38
23	B	1009	CLA	C3D-C2D	3.37	1.47	1.39
24	d	6039	PHO	C3D-C2D	3.38	1.47	1.38
23	c	6033	CLA	C3D-C2D	3.39	1.47	1.39
23	A	1007	CLA	C3D-C2D	3.40	1.47	1.39
23	c	6028	CLA	C3D-C2D	3.40	1.47	1.39
23	b	6013	CLA	C3D-C2D	3.41	1.47	1.39
23	b	6014	CLA	C3D-C2D	3.41	1.47	1.39
23	C	1028	CLA	C3D-C2D	3.41	1.47	1.39
23	c	6031	CLA	C3D-C2D	3.41	1.47	1.39
23	D	1004	CLA	C3D-C2D	3.41	1.47	1.39
23	b	6024	CLA	C3D-C2D	3.41	1.47	1.39
23	B	1013	CLA	C3D-C2D	3.41	1.47	1.39
23	C	1027	CLA	C3D-C2D	3.42	1.47	1.39
23	H	1017	CLA	C3D-C2D	3.42	1.47	1.39
23	h	6017	CLA	C3D-C2D	3.42	1.47	1.39
23	d	6004	CLA	C3D-C2D	3.42	1.47	1.39
23	b	6015	CLA	C3D-C2D	3.42	1.47	1.39
23	B	1014	CLA	C3D-C2D	3.42	1.47	1.39
23	C	1035	CLA	C3D-C2D	3.43	1.47	1.39
23	B	1024	CLA	C3D-C2D	3.43	1.47	1.39
23	A	1006	CLA	C3D-C2D	3.43	1.47	1.39
23	c	6027	CLA	C3D-C2D	3.43	1.47	1.39
23	B	1020	CLA	C3D-C2D	3.43	1.47	1.39
23	B	1015	CLA	C3D-C2D	3.43	1.47	1.39
23	c	6036	CLA	C3D-C2D	3.43	1.47	1.39
23	b	6020	CLA	C3D-C2D	3.43	1.47	1.39
23	B	1012	CLA	C3D-C2D	3.44	1.47	1.39
23	C	1033	CLA	C3D-C2D	3.44	1.47	1.39
23	d	6005	CLA	C3D-C2D	3.44	1.47	1.39
23	c	6025	CLA	C3D-C2D	3.44	1.47	1.39
23	B	1018	CLA	C3D-C2D	3.44	1.47	1.39
23	b	6016	CLA	C3D-C2D	3.44	1.47	1.39
23	A	1003	CLA	C3D-C2D	3.44	1.47	1.39
23	B	1019	CLA	C3D-C2D	3.44	1.47	1.39
23	B	1022	CLA	C3D-C2D	3.45	1.47	1.39
23	C	1032	CLA	C3D-C2D	3.45	1.47	1.39
23	c	6032	CLA	C3D-C2D	3.45	1.47	1.39
23	a	6006	CLA	C3D-C2D	3.45	1.47	1.39
23	C	1037	CLA	C3D-C2D	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6019	CLA	C3D-C2D	3.45	1.47	1.39
23	c	6037	CLA	C3D-C2D	3.45	1.47	1.39
23	C	1026	CLA	C3D-C2D	3.45	1.47	1.39
23	a	6003	CLA	C3D-C2D	3.45	1.47	1.39
23	K	1034	CLA	C3D-C2D	3.45	1.47	1.39
23	B	1016	CLA	C3D-C2D	3.45	1.47	1.39
23	C	1036	CLA	C3D-C2D	3.46	1.47	1.39
23	C	1031	CLA	C3D-C2D	3.46	1.47	1.39
23	b	6022	CLA	C3D-C2D	3.46	1.47	1.39
23	c	6035	CLA	C3D-C2D	3.46	1.47	1.39
23	D	1005	CLA	C3D-C2D	3.46	1.47	1.39
23	b	6018	CLA	C3D-C2D	3.46	1.47	1.39
23	c	6026	CLA	C3D-C2D	3.46	1.47	1.39
23	C	1025	CLA	C3D-C2D	3.46	1.47	1.39
23	k	6034	CLA	C3D-C2D	3.47	1.47	1.39
23	b	6012	CLA	C3D-C2D	3.47	1.47	1.39
31	f	6040	HEM	C3C-CAC	3.53	1.54	1.47
31	V	1041	HEM	C3B-CAB	3.54	1.54	1.47
31	F	1040	HEM	C3B-CAB	3.54	1.54	1.47
31	v	6041	HEM	C3B-CAB	3.54	1.54	1.47
31	f	6040	HEM	C3B-CAB	3.56	1.55	1.47
31	F	1040	HEM	C3C-CAC	3.57	1.54	1.47
31	V	1041	HEM	C3C-CAC	3.59	1.54	1.47
31	v	6041	HEM	C3C-CAC	3.60	1.54	1.47
24	A	1038	PHO	CBB-CAB	3.94	1.50	1.30
24	a	6038	PHO	CBB-CAB	3.95	1.50	1.30
29	C	1056	DGD	O2G-C1B	3.96	1.45	1.34
29	c	6057	DGD	O2G-C1B	3.96	1.45	1.34
24	D	1039	PHO	CBB-CAB	3.96	1.50	1.30
24	d	6039	PHO	CBB-CAB	3.97	1.50	1.30
29	C	1057	DGD	O2G-C1B	3.97	1.45	1.34
29	c	6056	DGD	O2G-C1B	3.98	1.45	1.34
30	B	1060	MGE	O2G-C1B	3.98	1.45	1.34
30	L	1061	MGE	O2G-C1B	3.98	1.45	1.34
29	b	6058	DGD	O2G-C1B	3.99	1.45	1.34
30	D	1062	MGE	O2G-C1B	3.99	1.45	1.34
30	b	6060	MGE	O2G-C1B	3.99	1.45	1.34
29	B	1058	DGD	O2G-C1B	3.99	1.45	1.34
29	C	1055	DGD	O2G-C1B	3.99	1.45	1.34
30	D	1059	MGE	O2G-C1B	4.00	1.45	1.34
30	d	6059	MGE	O2G-C1B	4.00	1.45	1.34
30	d	6062	MGE	O2G-C1B	4.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	l	6061	MGE	O2G-C1B	4.00	1.45	1.34
29	c	6055	DGD	O2G-C1B	4.00	1.45	1.34
27	a	6063	LHG	O7-C7	4.01	1.45	1.34
27	A	1063	LHG	O7-C7	4.02	1.45	1.34
23	b	6009	CLA	CHC-C1C	4.03	1.47	1.35
23	B	1009	CLA	CHC-C1C	4.04	1.47	1.35
23	b	6011	CLA	CHC-C1C	4.04	1.47	1.35
23	D	1008	CLA	CHC-C1C	4.06	1.47	1.35
23	B	1011	CLA	CHC-C1C	4.06	1.47	1.35
23	d	6008	CLA	CHC-C1C	4.07	1.47	1.35
23	b	6010	CLA	CHC-C1C	4.07	1.47	1.35
23	c	6029	CLA	CHC-C1C	4.08	1.47	1.35
23	B	1010	CLA	CHC-C1C	4.08	1.47	1.35
23	B	1023	CLA	CHC-C1C	4.08	1.47	1.35
23	C	1029	CLA	CHC-C1C	4.09	1.47	1.35
23	b	6023	CLA	CHC-C1C	4.10	1.47	1.35
23	B	1021	CLA	CHC-C1C	4.11	1.47	1.35
23	b	6021	CLA	CHC-C1C	4.11	1.47	1.35
23	b	6015	CLA	CHC-C1C	4.13	1.47	1.35
23	c	6037	CLA	CHC-C1C	4.13	1.47	1.35
23	h	6017	CLA	CHC-C1C	4.14	1.47	1.35
23	C	1030	CLA	CHC-C1C	4.14	1.47	1.35
23	C	1036	CLA	CHC-C1C	4.14	1.47	1.35
23	c	6027	CLA	CHC-C1C	4.14	1.47	1.35
23	c	6030	CLA	CHC-C1C	4.15	1.47	1.35
23	C	1037	CLA	CHC-C1C	4.15	1.47	1.35
23	B	1015	CLA	CHC-C1C	4.15	1.47	1.35
23	d	6004	CLA	CHC-C1C	4.15	1.47	1.35
23	b	6022	CLA	CHC-C1C	4.15	1.47	1.35
23	A	1006	CLA	CHC-C1C	4.16	1.47	1.35
23	B	1022	CLA	CHC-C1C	4.16	1.47	1.35
23	C	1027	CLA	CHC-C1C	4.16	1.47	1.35
23	c	6036	CLA	CHC-C1C	4.16	1.47	1.35
23	c	6032	CLA	CHC-C1C	4.16	1.47	1.35
23	C	1032	CLA	CHC-C1C	4.16	1.47	1.35
23	B	1012	CLA	CHC-C1C	4.16	1.47	1.35
23	b	6018	CLA	CHC-C1C	4.16	1.47	1.35
23	b	6020	CLA	CHC-C1C	4.16	1.47	1.35
23	b	6019	CLA	CHC-C1C	4.16	1.47	1.35
23	b	6016	CLA	CHC-C1C	4.16	1.47	1.35
23	H	1017	CLA	CHC-C1C	4.16	1.47	1.35
23	c	6025	CLA	CHC-C1C	4.16	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6012	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1018	CLA	CHC-C1C	4.17	1.47	1.35
23	A	1003	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1019	CLA	CHC-C1C	4.17	1.47	1.35
23	c	6031	CLA	CHC-C1C	4.17	1.47	1.35
23	c	6028	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1013	CLA	CHC-C1C	4.17	1.47	1.35
23	C	1026	CLA	CHC-C1C	4.17	1.47	1.35
23	C	1031	CLA	CHC-C1C	4.17	1.47	1.35
23	C	1025	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1014	CLA	CHC-C1C	4.17	1.47	1.35
23	C	1028	CLA	CHC-C1C	4.17	1.47	1.35
23	a	6003	CLA	CHC-C1C	4.17	1.47	1.35
23	K	1034	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1020	CLA	CHC-C1C	4.17	1.47	1.35
23	a	6006	CLA	CHC-C1C	4.17	1.47	1.35
23	D	1004	CLA	CHC-C1C	4.17	1.47	1.35
23	B	1024	CLA	CHC-C1C	4.17	1.47	1.35
23	b	6013	CLA	CHC-C1C	4.17	1.47	1.35
23	k	6034	CLA	CHC-C1C	4.18	1.47	1.35
23	b	6014	CLA	CHC-C1C	4.18	1.47	1.35
23	b	6021	CLA	O2A-CGA	4.18	1.45	1.33
23	c	6026	CLA	CHC-C1C	4.18	1.47	1.35
23	C	1033	CLA	CHC-C1C	4.18	1.47	1.35
23	a	6007	CLA	CHC-C1C	4.18	1.47	1.35
23	B	1011	CLA	O2A-CGA	4.18	1.45	1.33
23	A	1007	CLA	CHC-C1C	4.19	1.47	1.35
23	B	1016	CLA	CHC-C1C	4.19	1.47	1.35
23	b	6023	CLA	O2A-CGA	4.19	1.45	1.33
23	b	6024	CLA	CHC-C1C	4.19	1.47	1.35
23	c	6035	CLA	CHC-C1C	4.20	1.47	1.35
23	C	1035	CLA	CHC-C1C	4.20	1.47	1.35
23	b	6011	CLA	O2A-CGA	4.20	1.45	1.33
23	b	6009	CLA	O2A-CGA	4.20	1.45	1.33
23	b	6010	CLA	O2A-CGA	4.20	1.45	1.33
23	D	1005	CLA	CHC-C1C	4.20	1.47	1.35
23	c	6033	CLA	CHC-C1C	4.21	1.47	1.35
23	B	1023	CLA	O2A-CGA	4.21	1.45	1.33
23	B	1021	CLA	O2A-CGA	4.21	1.45	1.33
23	C	1029	CLA	O2A-CGA	4.21	1.45	1.33
23	a	6003	CLA	O2A-CGA	4.21	1.45	1.33
23	d	6005	CLA	CHC-C1C	4.21	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	6008	CLA	O2A-CGA	4.21	1.45	1.33
23	h	6017	CLA	O2A-CGA	4.22	1.45	1.33
23	c	6027	CLA	O2A-CGA	4.22	1.45	1.33
23	D	1008	CLA	O2A-CGA	4.22	1.45	1.33
23	A	1003	CLA	O2A-CGA	4.22	1.45	1.33
23	B	1010	CLA	O2A-CGA	4.22	1.45	1.33
23	B	1009	CLA	O2A-CGA	4.22	1.45	1.33
23	c	6026	CLA	O2A-CGA	4.22	1.45	1.33
23	c	6028	CLA	O2A-CGA	4.23	1.45	1.33
23	c	6029	CLA	O2A-CGA	4.23	1.45	1.33
30	l	6061	MGE	O1G-C1A	4.23	1.45	1.33
23	b	6020	CLA	O2A-CGA	4.23	1.45	1.33
23	C	1027	CLA	O2A-CGA	4.23	1.45	1.33
23	A	1007	CLA	O2A-CGA	4.23	1.45	1.33
23	H	1017	CLA	O2A-CGA	4.23	1.45	1.33
23	C	1028	CLA	O2A-CGA	4.23	1.45	1.33
23	c	6036	CLA	O2A-CGA	4.23	1.45	1.33
23	c	6025	CLA	O2A-CGA	4.23	1.45	1.33
23	A	1006	CLA	O2A-CGA	4.24	1.45	1.33
23	c	6035	CLA	O2A-CGA	4.24	1.45	1.33
23	B	1014	CLA	O2A-CGA	4.24	1.45	1.33
23	a	6007	CLA	O2A-CGA	4.24	1.45	1.33
23	K	1034	CLA	O2A-CGA	4.24	1.45	1.33
23	b	6018	CLA	O2A-CGA	4.24	1.45	1.33
23	c	6030	CLA	O2A-CGA	4.24	1.45	1.33
29	C	1056	DGD	O1G-C1A	4.24	1.45	1.33
29	c	6056	DGD	O1G-C1A	4.24	1.45	1.33
23	C	1026	CLA	O2A-CGA	4.24	1.45	1.33
23	B	1018	CLA	O2A-CGA	4.24	1.45	1.33
23	C	1035	CLA	O2A-CGA	4.24	1.45	1.33
23	B	1019	CLA	O2A-CGA	4.24	1.45	1.33
23	B	1015	CLA	O2A-CGA	4.24	1.45	1.33
23	C	1036	CLA	O2A-CGA	4.24	1.45	1.33
30	d	6059	MGE	O1G-C1A	4.24	1.45	1.33
23	a	6006	CLA	O2A-CGA	4.25	1.45	1.33
23	C	1031	CLA	O2A-CGA	4.25	1.45	1.33
30	B	1060	MGE	O1G-C1A	4.25	1.45	1.33
23	B	1024	CLA	O2A-CGA	4.25	1.45	1.33
23	b	6019	CLA	O2A-CGA	4.25	1.45	1.33
30	L	1061	MGE	O1G-C1A	4.25	1.45	1.33
23	b	6014	CLA	O2A-CGA	4.25	1.45	1.33
23	B	1012	CLA	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	1057	DGD	O1G-C1A	4.25	1.45	1.33
23	c	6032	CLA	O2A-CGA	4.25	1.45	1.33
30	D	1059	MGE	O1G-C1A	4.25	1.45	1.33
27	a	6063	LHG	O8-C23	4.25	1.45	1.33
23	b	6013	CLA	O2A-CGA	4.25	1.45	1.33
23	B	1020	CLA	O2A-CGA	4.25	1.45	1.33
23	C	1030	CLA	O2A-CGA	4.25	1.45	1.33
23	k	6034	CLA	O2A-CGA	4.25	1.45	1.33
23	C	1033	CLA	O2A-CGA	4.25	1.45	1.33
23	B	1016	CLA	O2A-CGA	4.25	1.45	1.33
23	C	1025	CLA	O2A-CGA	4.25	1.45	1.33
23	B	1013	CLA	O2A-CGA	4.26	1.45	1.33
30	D	1062	MGE	O1G-C1A	4.26	1.45	1.33
29	C	1055	DGD	O1G-C1A	4.26	1.45	1.33
23	D	1004	CLA	O2A-CGA	4.26	1.45	1.33
23	d	6004	CLA	O2A-CGA	4.26	1.45	1.33
27	A	1063	LHG	O8-C23	4.26	1.45	1.33
23	b	6022	CLA	O2A-CGA	4.26	1.45	1.33
23	B	1022	CLA	O2A-CGA	4.26	1.45	1.33
23	b	6012	CLA	O2A-CGA	4.26	1.45	1.33
23	b	6024	CLA	O2A-CGA	4.26	1.45	1.33
23	C	1037	CLA	O2A-CGA	4.26	1.45	1.33
23	C	1032	CLA	O2A-CGA	4.26	1.45	1.33
30	d	6062	MGE	O1G-C1A	4.26	1.45	1.33
30	b	6060	MGE	O1G-C1A	4.26	1.45	1.33
23	c	6031	CLA	O2A-CGA	4.27	1.45	1.33
29	B	1058	DGD	O1G-C1A	4.27	1.45	1.33
23	c	6033	CLA	O2A-CGA	4.27	1.45	1.33
23	b	6016	CLA	O2A-CGA	4.27	1.45	1.33
23	b	6015	CLA	O2A-CGA	4.27	1.45	1.33
23	c	6037	CLA	O2A-CGA	4.27	1.45	1.33
29	b	6058	DGD	O1G-C1A	4.27	1.45	1.33
23	D	1005	CLA	O2A-CGA	4.28	1.45	1.33
29	c	6055	DGD	O1G-C1A	4.28	1.45	1.33
29	c	6057	DGD	O1G-C1A	4.28	1.45	1.33
23	d	6005	CLA	O2A-CGA	4.29	1.46	1.33
23	B	1010	CLA	OBD-CAD	4.31	1.28	1.22
23	c	6030	CLA	OBD-CAD	4.31	1.28	1.22
24	D	1039	PHO	CHC-C4B	4.32	1.50	1.40
24	d	6039	PHO	CHC-C4B	4.32	1.50	1.40
24	A	1038	PHO	CHC-C4B	4.32	1.50	1.40
24	a	6038	PHO	CHC-C4B	4.33	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1029	CLA	OBD-CAD	4.36	1.28	1.22
23	d	6008	CLA	OBD-CAD	4.36	1.28	1.22
23	b	6010	CLA	OBD-CAD	4.36	1.28	1.22
23	D	1008	CLA	OBD-CAD	4.37	1.28	1.22
23	C	1030	CLA	OBD-CAD	4.38	1.28	1.22
23	B	1009	CLA	OBD-CAD	4.38	1.28	1.22
23	c	6029	CLA	OBD-CAD	4.39	1.28	1.22
23	b	6023	CLA	OBD-CAD	4.40	1.28	1.22
23	B	1023	CLA	OBD-CAD	4.40	1.28	1.22
23	b	6009	CLA	OBD-CAD	4.41	1.28	1.22
23	B	1011	CLA	OBD-CAD	4.44	1.28	1.22
23	b	6011	CLA	OBD-CAD	4.48	1.28	1.22
23	C	1026	CLA	OBD-CAD	4.50	1.28	1.22
23	a	6006	CLA	OBD-CAD	4.50	1.28	1.22
23	b	6013	CLA	OBD-CAD	4.51	1.28	1.22
23	c	6026	CLA	OBD-CAD	4.53	1.28	1.22
23	A	1003	CLA	OBD-CAD	4.53	1.28	1.22
23	A	1007	CLA	OBD-CAD	4.53	1.28	1.22
23	K	1034	CLA	OBD-CAD	4.53	1.28	1.22
23	a	6007	CLA	OBD-CAD	4.53	1.28	1.22
23	c	6036	CLA	OBD-CAD	4.54	1.28	1.22
23	b	6020	CLA	OBD-CAD	4.54	1.28	1.22
23	b	6012	CLA	OBD-CAD	4.54	1.28	1.22
23	d	6005	CLA	OBD-CAD	4.54	1.28	1.22
23	B	1016	CLA	OBD-CAD	4.54	1.28	1.22
23	b	6016	CLA	OBD-CAD	4.54	1.28	1.22
23	C	1027	CLA	OBD-CAD	4.54	1.28	1.22
23	b	6022	CLA	OBD-CAD	4.54	1.28	1.22
23	A	1006	CLA	OBD-CAD	4.55	1.28	1.22
23	c	6028	CLA	OBD-CAD	4.55	1.28	1.22
23	D	1005	CLA	OBD-CAD	4.55	1.28	1.22
23	a	6003	CLA	OBD-CAD	4.55	1.28	1.22
23	B	1012	CLA	OBD-CAD	4.55	1.28	1.22
23	B	1013	CLA	OBD-CAD	4.55	1.28	1.22
23	c	6027	CLA	OBD-CAD	4.56	1.28	1.22
23	b	6024	CLA	OBD-CAD	4.56	1.28	1.22
23	C	1031	CLA	OBD-CAD	4.56	1.28	1.22
23	B	1022	CLA	OBD-CAD	4.56	1.28	1.22
23	B	1021	CLA	OBD-CAD	4.56	1.28	1.22
23	c	6031	CLA	OBD-CAD	4.56	1.28	1.22
23	C	1033	CLA	OBD-CAD	4.57	1.28	1.22
23	B	1020	CLA	OBD-CAD	4.57	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1028	CLA	OBD-CAD	4.57	1.29	1.22
23	H	1017	CLA	OBD-CAD	4.57	1.29	1.22
23	B	1018	CLA	OBD-CAD	4.57	1.29	1.22
23	B	1019	CLA	OBD-CAD	4.58	1.29	1.22
23	B	1015	CLA	OBD-CAD	4.58	1.29	1.22
23	k	6034	CLA	OBD-CAD	4.58	1.29	1.22
23	C	1036	CLA	OBD-CAD	4.58	1.29	1.22
23	c	6033	CLA	OBD-CAD	4.58	1.29	1.22
23	B	1024	CLA	OBD-CAD	4.58	1.29	1.22
23	d	6004	CLA	OBD-CAD	4.58	1.29	1.22
23	b	6021	CLA	OBD-CAD	4.59	1.29	1.22
23	b	6018	CLA	OBD-CAD	4.59	1.29	1.22
23	b	6019	CLA	OBD-CAD	4.59	1.29	1.22
23	b	6015	CLA	OBD-CAD	4.60	1.29	1.22
23	c	6025	CLA	OBD-CAD	4.60	1.29	1.22
23	C	1035	CLA	OBD-CAD	4.60	1.29	1.22
23	C	1032	CLA	OBD-CAD	4.60	1.29	1.22
24	A	1038	PHO	CHC-C1C	4.60	1.47	1.38
23	D	1004	CLA	OBD-CAD	4.60	1.29	1.22
23	C	1037	CLA	OBD-CAD	4.61	1.29	1.22
23	C	1025	CLA	OBD-CAD	4.61	1.29	1.22
23	c	6032	CLA	OBD-CAD	4.61	1.29	1.22
24	d	6039	PHO	CHC-C1C	4.62	1.47	1.38
24	D	1039	PHO	CHC-C1C	4.62	1.47	1.38
23	h	6017	CLA	OBD-CAD	4.63	1.29	1.22
23	B	1014	CLA	OBD-CAD	4.63	1.29	1.22
24	a	6038	PHO	CHC-C1C	4.63	1.47	1.38
23	C	1029	CLA	C3B-C2B	4.63	1.46	1.40
23	c	6035	CLA	OBD-CAD	4.63	1.29	1.22
23	c	6029	CLA	C3B-C2B	4.64	1.46	1.40
23	B	1011	CLA	C3B-C2B	4.66	1.46	1.40
23	b	6014	CLA	OBD-CAD	4.66	1.29	1.22
23	c	6037	CLA	OBD-CAD	4.66	1.29	1.22
23	b	6021	CLA	C3B-C2B	4.67	1.46	1.40
23	d	6008	CLA	C3C-C2C	4.67	1.46	1.36
23	D	1008	CLA	C3B-C2B	4.67	1.46	1.40
23	b	6011	CLA	C3B-C2B	4.68	1.46	1.40
23	B	1010	CLA	C3B-C2B	4.68	1.46	1.40
23	D	1008	CLA	C3C-C2C	4.68	1.46	1.36
23	b	6010	CLA	C3B-C2B	4.69	1.46	1.40
23	B	1021	CLA	C3B-C2B	4.70	1.46	1.40
23	d	6008	CLA	C3B-C2B	4.70	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1023	CLA	C3C-C2C	4.70	1.46	1.36
23	b	6023	CLA	C3B-C2B	4.71	1.46	1.40
23	b	6023	CLA	C3C-C2C	4.71	1.46	1.36
23	c	6029	CLA	C3C-C2C	4.72	1.46	1.36
23	B	1023	CLA	C3B-C2B	4.72	1.46	1.40
23	C	1029	CLA	C3C-C2C	4.73	1.46	1.36
23	b	6010	CLA	C3C-C2C	4.76	1.46	1.36
23	B	1021	CLA	C3C-C2C	4.76	1.46	1.36
23	B	1011	CLA	C3C-C2C	4.76	1.46	1.36
23	b	6021	CLA	C3C-C2C	4.76	1.47	1.36
23	b	6011	CLA	C3C-C2C	4.77	1.47	1.36
23	C	1030	CLA	C3C-C2C	4.78	1.47	1.36
23	c	6030	CLA	C3C-C2C	4.78	1.47	1.36
23	B	1010	CLA	C3C-C2C	4.78	1.47	1.36
23	b	6021	CLA	O2D-CGD	4.80	1.45	1.33
23	b	6019	CLA	C3C-C2C	4.80	1.47	1.36
23	b	6009	CLA	C3C-C2C	4.81	1.47	1.36
23	B	1009	CLA	C3C-C2C	4.82	1.47	1.36
23	c	6037	CLA	C3C-C2C	4.83	1.47	1.36
23	B	1019	CLA	C3C-C2C	4.83	1.47	1.36
23	c	6033	CLA	C3C-C2C	4.83	1.47	1.36
23	B	1021	CLA	O2D-CGD	4.83	1.45	1.33
23	b	6023	CLA	O2D-CGD	4.83	1.45	1.33
23	C	1028	CLA	C3C-C2C	4.83	1.47	1.36
23	c	6036	CLA	C3C-C2C	4.83	1.47	1.36
23	C	1033	CLA	C3C-C2C	4.84	1.47	1.36
23	B	1023	CLA	O2D-CGD	4.84	1.45	1.33
23	b	6022	CLA	C3C-C2C	4.84	1.47	1.36
23	b	6024	CLA	C3C-C2C	4.84	1.47	1.36
23	b	6013	CLA	C3C-C2C	4.84	1.47	1.36
23	c	6028	CLA	C3C-C2C	4.85	1.47	1.36
23	D	1005	CLA	C3C-C2C	4.85	1.47	1.36
23	C	1037	CLA	C3C-C2C	4.85	1.47	1.36
23	c	6026	CLA	C3C-C2C	4.85	1.47	1.36
23	c	6025	CLA	C3C-C2C	4.85	1.47	1.36
23	C	1035	CLA	C3C-C2C	4.85	1.47	1.36
23	A	1006	CLA	C3C-C2C	4.85	1.47	1.36
23	C	1032	CLA	C3C-C2C	4.85	1.47	1.36
23	C	1036	CLA	C3C-C2C	4.85	1.47	1.36
23	b	6016	CLA	C3C-C2C	4.85	1.47	1.36
23	B	1015	CLA	C3C-C2C	4.85	1.47	1.36
23	B	1012	CLA	C3C-C2C	4.86	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	6005	CLA	C3C-C2C	4.86	1.47	1.36
23	C	1031	CLA	C3C-C2C	4.86	1.47	1.36
23	B	1020	CLA	C3C-C2C	4.86	1.47	1.36
23	c	6031	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1022	CLA	C3C-C2C	4.87	1.47	1.36
23	C	1026	CLA	C3C-C2C	4.87	1.47	1.36
23	A	1007	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1013	CLA	C3C-C2C	4.87	1.47	1.36
23	c	6032	CLA	C3C-C2C	4.87	1.47	1.36
23	b	6020	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1018	CLA	C3C-C2C	4.87	1.47	1.36
23	b	6012	CLA	C3C-C2C	4.87	1.47	1.36
23	C	1030	CLA	C3B-C2B	4.87	1.46	1.40
23	d	6004	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1024	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1016	CLA	C3C-C2C	4.87	1.47	1.36
23	C	1025	CLA	C3C-C2C	4.88	1.47	1.36
23	c	6030	CLA	C3B-C2B	4.88	1.46	1.40
23	c	6035	CLA	C3C-C2C	4.88	1.47	1.36
23	C	1030	CLA	O2D-CGD	4.88	1.45	1.33
23	C	1027	CLA	C3C-C2C	4.88	1.47	1.36
23	c	6030	CLA	O2D-CGD	4.88	1.45	1.33
23	H	1017	CLA	C3C-C2C	4.88	1.47	1.36
23	b	6018	CLA	C3C-C2C	4.88	1.47	1.36
23	h	6017	CLA	C3C-C2C	4.88	1.47	1.36
23	a	6006	CLA	C3C-C2C	4.88	1.47	1.36
23	B	1014	CLA	C3C-C2C	4.88	1.47	1.36
23	C	1029	CLA	O2D-CGD	4.88	1.45	1.33
23	a	6007	CLA	C3C-C2C	4.89	1.47	1.36
23	D	1004	CLA	C3C-C2C	4.89	1.47	1.36
23	A	1003	CLA	C3C-C2C	4.89	1.47	1.36
23	c	6027	CLA	C3C-C2C	4.89	1.47	1.36
23	K	1034	CLA	C3C-C2C	4.89	1.47	1.36
23	b	6015	CLA	C3C-C2C	4.89	1.47	1.36
23	b	6014	CLA	C3C-C2C	4.90	1.47	1.36
23	k	6034	CLA	C3C-C2C	4.90	1.47	1.36
23	c	6029	CLA	O2D-CGD	4.90	1.45	1.33
23	B	1009	CLA	O2D-CGD	4.91	1.45	1.33
23	a	6007	CLA	C3B-C2B	4.91	1.46	1.40
23	a	6003	CLA	C3C-C2C	4.92	1.47	1.36
23	C	1037	CLA	C3B-C2B	4.92	1.46	1.40
23	D	1005	CLA	C3B-C2B	4.93	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1012	CLA	C3B-C2B	4.93	1.46	1.40
23	b	6012	CLA	C3B-C2B	4.93	1.46	1.40
23	b	6009	CLA	O2D-CGD	4.93	1.45	1.33
23	b	6018	CLA	C3B-C2B	4.94	1.46	1.40
23	c	6033	CLA	C3B-C2B	4.94	1.46	1.40
23	B	1009	CLA	C3B-C2B	4.95	1.46	1.40
23	b	6015	CLA	O2D-CGD	4.95	1.45	1.33
23	D	1008	CLA	O2D-CGD	4.95	1.45	1.33
23	C	1033	CLA	C3B-C2B	4.95	1.46	1.40
23	B	1016	CLA	C3B-C2B	4.96	1.46	1.40
23	C	1036	CLA	C3B-C2B	4.96	1.46	1.40
23	B	1015	CLA	O2D-CGD	4.96	1.45	1.33
23	d	6005	CLA	C3B-C2B	4.96	1.46	1.40
23	c	6031	CLA	O2D-CGD	4.96	1.45	1.33
23	b	6009	CLA	C3B-C2B	4.96	1.46	1.40
23	d	6008	CLA	O2D-CGD	4.96	1.45	1.33
23	C	1028	CLA	C3B-C2B	4.96	1.46	1.40
23	B	1014	CLA	O2D-CGD	4.96	1.45	1.33
23	c	6031	CLA	C3B-C2B	4.96	1.46	1.40
23	B	1018	CLA	C3B-C2B	4.96	1.46	1.40
23	a	6006	CLA	O2D-CGD	4.96	1.45	1.33
23	k	6034	CLA	O2D-CGD	4.96	1.45	1.33
23	A	1006	CLA	C3B-C2B	4.96	1.46	1.40
23	B	1024	CLA	C3B-C2B	4.97	1.46	1.40
23	b	6018	CLA	O2D-CGD	4.97	1.45	1.33
23	A	1007	CLA	C3B-C2B	4.97	1.46	1.40
23	C	1037	CLA	O2D-CGD	4.97	1.45	1.33
23	c	6032	CLA	C3B-C2B	4.97	1.46	1.40
23	C	1025	CLA	C3B-C2B	4.97	1.46	1.40
23	A	1003	CLA	O2D-CGD	4.97	1.45	1.33
23	c	6035	CLA	O2D-CGD	4.97	1.45	1.33
23	b	6019	CLA	C3B-C2B	4.97	1.46	1.40
23	a	6006	CLA	C3B-C2B	4.97	1.46	1.40
23	C	1031	CLA	C3B-C2B	4.97	1.46	1.40
23	b	6016	CLA	C3B-C2B	4.97	1.46	1.40
23	c	6037	CLA	O2D-CGD	4.97	1.45	1.33
23	b	6019	CLA	O2D-CGD	4.97	1.45	1.33
23	d	6005	CLA	O2D-CGD	4.97	1.45	1.33
23	h	6017	CLA	O2D-CGD	4.98	1.45	1.33
23	b	6016	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1022	CLA	C3B-C2B	4.98	1.46	1.40
23	B	1015	CLA	C3B-C2B	4.98	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	6004	CLA	O2D-CGD	4.98	1.45	1.33
23	H	1017	CLA	O2D-CGD	4.98	1.45	1.33
23	c	6028	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1018	CLA	O2D-CGD	4.98	1.45	1.33
23	C	1032	CLA	C3B-C2B	4.98	1.46	1.40
23	b	6013	CLA	O2D-CGD	4.98	1.45	1.33
23	a	6003	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1022	CLA	O2D-CGD	4.98	1.45	1.33
23	c	6027	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1016	CLA	O2D-CGD	4.98	1.45	1.33
23	C	1026	CLA	O2D-CGD	4.98	1.45	1.33
23	K	1034	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1019	CLA	O2D-CGD	4.98	1.45	1.33
23	c	6036	CLA	O2D-CGD	4.98	1.45	1.33
23	c	6025	CLA	C3B-C2B	4.98	1.46	1.40
23	C	1028	CLA	O2D-CGD	4.98	1.45	1.33
23	B	1010	CLA	O2D-CGD	4.98	1.45	1.33
23	a	6003	CLA	C3B-C2B	4.99	1.46	1.40
23	D	1005	CLA	O2D-CGD	4.99	1.45	1.33
23	B	1012	CLA	O2D-CGD	4.99	1.45	1.33
23	b	6014	CLA	O2D-CGD	4.99	1.45	1.33
23	D	1004	CLA	O2D-CGD	4.99	1.45	1.33
23	B	1013	CLA	C3B-C2B	4.99	1.46	1.40
23	h	6017	CLA	C3B-C2B	4.99	1.46	1.40
23	b	6020	CLA	O2D-CGD	4.99	1.45	1.33
23	b	6012	CLA	O2D-CGD	4.99	1.45	1.33
23	c	6025	CLA	O2D-CGD	4.99	1.45	1.33
23	B	1014	CLA	C3B-C2B	4.99	1.46	1.40
23	c	6037	CLA	C3B-C2B	4.99	1.46	1.40
23	B	1020	CLA	O2D-CGD	4.99	1.45	1.33
23	C	1027	CLA	C3B-C2B	4.99	1.46	1.40
23	c	6026	CLA	O2D-CGD	4.99	1.45	1.33
23	C	1027	CLA	O2D-CGD	4.99	1.45	1.33
23	A	1006	CLA	O2D-CGD	4.99	1.45	1.33
23	C	1031	CLA	O2D-CGD	4.99	1.45	1.33
23	b	6013	CLA	C3B-C2B	4.99	1.46	1.40
23	b	6010	CLA	O2D-CGD	4.99	1.45	1.33
23	B	1019	CLA	C3B-C2B	4.99	1.46	1.40
23	b	6024	CLA	C3B-C2B	5.00	1.47	1.40
23	c	6026	CLA	C3B-C2B	5.00	1.47	1.40
23	B	1013	CLA	O2D-CGD	5.00	1.45	1.33
23	b	6020	CLA	C3B-C2B	5.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1035	CLA	O2D-CGD	5.00	1.45	1.33
23	A	1003	CLA	C3B-C2B	5.00	1.47	1.40
23	C	1035	CLA	C3B-C2B	5.00	1.47	1.40
23	c	6027	CLA	C3B-C2B	5.00	1.47	1.40
23	c	6036	CLA	C3B-C2B	5.00	1.47	1.40
23	H	1017	CLA	C3B-C2B	5.00	1.47	1.40
23	C	1025	CLA	O2D-CGD	5.00	1.45	1.33
23	C	1032	CLA	O2D-CGD	5.01	1.45	1.33
23	B	1024	CLA	O2D-CGD	5.01	1.45	1.33
23	C	1026	CLA	C3B-C2B	5.01	1.47	1.40
23	b	6022	CLA	O2D-CGD	5.01	1.45	1.33
23	C	1033	CLA	O2D-CGD	5.02	1.45	1.33
23	c	6033	CLA	O2D-CGD	5.02	1.45	1.33
23	a	6007	CLA	O2D-CGD	5.02	1.45	1.33
23	D	1004	CLA	C3B-C2B	5.02	1.47	1.40
23	b	6022	CLA	C3B-C2B	5.02	1.47	1.40
23	K	1034	CLA	C3B-C2B	5.02	1.47	1.40
23	c	6028	CLA	C3B-C2B	5.02	1.47	1.40
23	b	6014	CLA	C3B-C2B	5.02	1.47	1.40
23	C	1036	CLA	O2D-CGD	5.03	1.45	1.33
23	c	6032	CLA	O2D-CGD	5.03	1.46	1.33
23	b	6024	CLA	O2D-CGD	5.03	1.46	1.33
23	A	1007	CLA	O2D-CGD	5.03	1.46	1.33
23	B	1020	CLA	C3B-C2B	5.04	1.47	1.40
23	c	6035	CLA	C3B-C2B	5.04	1.47	1.40
23	b	6015	CLA	C3B-C2B	5.04	1.47	1.40
23	b	6011	CLA	O2D-CGD	5.04	1.46	1.33
23	B	1011	CLA	O2D-CGD	5.05	1.46	1.33
23	d	6004	CLA	C3B-C2B	5.05	1.47	1.40
23	k	6034	CLA	C3B-C2B	5.07	1.47	1.40
31	f	6040	HEM	C3D-C2D	5.41	1.53	1.37
31	F	1040	HEM	C3D-C2D	5.43	1.53	1.37
31	v	6041	HEM	C3D-C2D	5.46	1.53	1.37
31	V	1041	HEM	C3D-C2D	5.48	1.53	1.37
24	a	6038	PHO	C2-C3	5.77	1.47	1.33
24	A	1038	PHO	C2-C3	5.77	1.47	1.33
24	D	1039	PHO	C2-C3	5.79	1.47	1.33
24	d	6039	PHO	C2-C3	5.81	1.47	1.33
24	d	6039	PHO	CHD-C1D	5.89	1.50	1.38
24	D	1039	PHO	CHD-C1D	5.90	1.50	1.38
24	a	6038	PHO	CHD-C1D	5.91	1.50	1.38
24	A	1038	PHO	CHD-C1D	5.91	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	1039	PHO	CHB-C1B	6.13	1.50	1.38
24	d	6039	PHO	CHB-C1B	6.13	1.50	1.38
24	a	6038	PHO	CHB-C1B	6.13	1.50	1.38
24	A	1038	PHO	CHB-C1B	6.16	1.50	1.38
24	a	6038	PHO	O1A-CGA	6.30	1.41	1.22
24	D	1039	PHO	O1A-CGA	6.31	1.41	1.22
24	d	6039	PHO	O1A-CGA	6.31	1.41	1.22
24	A	1038	PHO	O1A-CGA	6.32	1.41	1.22
24	d	6039	PHO	C3C-C2C	7.38	1.52	1.36
24	a	6038	PHO	C3C-C2C	7.38	1.52	1.36
24	D	1039	PHO	C3C-C2C	7.39	1.52	1.36
24	A	1038	PHO	C3C-C2C	7.39	1.52	1.36
24	d	6039	PHO	O1D-CGD	8.01	1.41	1.21
24	A	1038	PHO	O1D-CGD	8.03	1.41	1.21
24	D	1039	PHO	O1D-CGD	8.03	1.41	1.21
24	a	6038	PHO	O1D-CGD	8.05	1.41	1.21
24	a	6038	PHO	OBD-CAD	10.85	1.41	1.22
24	A	1038	PHO	OBD-CAD	10.85	1.41	1.22
24	D	1039	PHO	OBD-CAD	10.85	1.41	1.22
24	d	6039	PHO	OBD-CAD	10.86	1.41	1.22

All (2174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	1039	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	a	6038	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	A	1038	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	d	6039	PHO	CAC-C3C-C4C	-13.38	109.50	125.21
24	D	1039	PHO	CMC-C2C-C1C	-9.99	109.47	125.04
24	d	6039	PHO	CMC-C2C-C1C	-9.99	109.48	125.04
24	a	6038	PHO	CMC-C2C-C1C	-9.97	109.52	125.04
24	A	1038	PHO	CMC-C2C-C1C	-9.96	109.52	125.04
24	a	6038	PHO	CAC-C3C-C2C	-9.54	110.96	127.49
24	A	1038	PHO	CAC-C3C-C2C	-9.53	110.98	127.49
24	d	6039	PHO	CAC-C3C-C2C	-9.49	111.04	127.49
24	D	1039	PHO	CAC-C3C-C2C	-9.49	111.04	127.49
24	a	6038	PHO	CMD-C2D-C3D	-8.21	107.97	127.86
24	A	1038	PHO	CMD-C2D-C3D	-8.21	107.97	127.86
24	d	6039	PHO	CMD-C2D-C3D	-8.20	107.99	127.86
24	D	1039	PHO	CMD-C2D-C3D	-8.20	107.99	127.86
23	b	6009	CLA	C1C-NC-C4C	-8.19	102.34	107.06
23	B	1009	CLA	C1C-NC-C4C	-8.18	102.35	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1011	CLA	C1C-NC-C4C	-8.08	102.41	107.06
23	B	1010	CLA	C1C-NC-C4C	-8.08	102.41	107.06
23	b	6010	CLA	C1C-NC-C4C	-8.07	102.41	107.06
23	c	6029	CLA	C1C-NC-C4C	-8.07	102.41	107.06
23	b	6011	CLA	C1C-NC-C4C	-8.06	102.42	107.06
23	c	6035	CLA	C1C-NC-C4C	-8.06	102.42	107.06
23	B	1019	CLA	C1C-NC-C4C	-8.06	102.42	107.06
23	b	6019	CLA	C1C-NC-C4C	-8.04	102.43	107.06
23	B	1015	CLA	C1C-NC-C4C	-8.04	102.43	107.06
23	C	1035	CLA	C1C-NC-C4C	-8.03	102.43	107.06
23	d	6005	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	b	6015	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	D	1008	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	H	1017	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	h	6017	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	D	1005	CLA	C1C-NC-C4C	-8.03	102.44	107.06
23	B	1024	CLA	C1C-NC-C4C	-8.02	102.44	107.06
23	c	6033	CLA	C1C-NC-C4C	-8.02	102.44	107.06
23	K	1034	CLA	C1C-NC-C4C	-8.02	102.44	107.06
23	b	6022	CLA	C1C-NC-C4C	-8.01	102.45	107.06
23	b	6013	CLA	C1C-NC-C4C	-8.01	102.45	107.06
23	B	1013	CLA	C1C-NC-C4C	-8.00	102.45	107.06
23	C	1029	CLA	C1C-NC-C4C	-8.00	102.45	107.06
23	c	6036	CLA	C1C-NC-C4C	-8.00	102.45	107.06
23	a	6003	CLA	C1C-NC-C4C	-7.99	102.46	107.06
23	b	6023	CLA	C1C-NC-C4C	-7.99	102.46	107.06
23	C	1025	CLA	C1C-NC-C4C	-7.99	102.46	107.06
23	C	1026	CLA	C1C-NC-C4C	-7.99	102.46	107.06
23	k	6034	CLA	C1C-NC-C4C	-7.99	102.46	107.06
23	b	6020	CLA	C1C-NC-C4C	-7.98	102.46	107.06
23	B	1016	CLA	C1C-NC-C4C	-7.98	102.46	107.06
23	c	6028	CLA	C1C-NC-C4C	-7.98	102.47	107.06
23	b	6014	CLA	C1C-NC-C4C	-7.98	102.47	107.06
23	d	6008	CLA	C1C-NC-C4C	-7.97	102.47	107.06
23	a	6007	CLA	C1C-NC-C4C	-7.97	102.47	107.06
23	b	6024	CLA	C1C-NC-C4C	-7.97	102.47	107.06
23	C	1033	CLA	C1C-NC-C4C	-7.96	102.47	107.06
23	D	1004	CLA	C1C-NC-C4C	-7.96	102.47	107.06
23	c	6026	CLA	C1C-NC-C4C	-7.96	102.48	107.06
23	C	1027	CLA	C1C-NC-C4C	-7.96	102.48	107.06
23	c	6025	CLA	C1C-NC-C4C	-7.96	102.48	107.06
23	B	1020	CLA	C1C-NC-C4C	-7.95	102.48	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1030	CLA	C1C-NC-C4C	-7.95	102.48	107.06
23	B	1022	CLA	C1C-NC-C4C	-7.95	102.48	107.06
23	C	1036	CLA	C1C-NC-C4C	-7.95	102.48	107.06
23	c	6032	CLA	C1C-NC-C4C	-7.95	102.48	107.06
23	A	1007	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	a	6006	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	A	1006	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	B	1014	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	c	6027	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	A	1003	CLA	C1C-NC-C4C	-7.94	102.49	107.06
23	C	1032	CLA	C1C-NC-C4C	-7.93	102.49	107.06
23	b	6016	CLA	C1C-NC-C4C	-7.93	102.49	107.06
23	B	1023	CLA	C1C-NC-C4C	-7.93	102.50	107.06
23	d	6004	CLA	C1C-NC-C4C	-7.92	102.50	107.06
23	C	1028	CLA	C1C-NC-C4C	-7.92	102.50	107.06
23	B	1018	CLA	C1C-NC-C4C	-7.92	102.50	107.06
23	c	6030	CLA	C1C-NC-C4C	-7.90	102.51	107.06
23	C	1037	CLA	C1C-NC-C4C	-7.90	102.51	107.06
23	b	6012	CLA	C1C-NC-C4C	-7.90	102.51	107.06
23	B	1021	CLA	C1C-NC-C4C	-7.89	102.52	107.06
23	B	1012	CLA	C1C-NC-C4C	-7.89	102.52	107.06
23	c	6037	CLA	C1C-NC-C4C	-7.89	102.52	107.06
23	C	1031	CLA	C1C-NC-C4C	-7.88	102.52	107.06
23	c	6031	CLA	C1C-NC-C4C	-7.87	102.53	107.06
23	b	6018	CLA	C1C-NC-C4C	-7.84	102.54	107.06
23	b	6021	CLA	C1C-NC-C4C	-7.83	102.55	107.06
26	C	1052	BCR	C30-C25-C26	-5.97	114.21	122.59
26	k	6052	BCR	C30-C25-C26	-5.94	114.25	122.59
24	A	1038	PHO	CMC-C2C-C3C	-5.45	111.01	126.09
24	d	6039	PHO	CMC-C2C-C3C	-5.45	111.01	126.09
24	D	1039	PHO	CMC-C2C-C3C	-5.44	111.03	126.09
24	a	6038	PHO	CMC-C2C-C3C	-5.43	111.05	126.09
26	h	6049	BCR	C15-C14-C13	-5.18	119.92	127.31
26	c	6054	BCR	C15-C14-C13	-5.17	119.94	127.31
26	C	1054	BCR	C15-C14-C13	-5.16	119.95	127.31
26	k	6051	BCR	C11-C10-C9	-5.15	119.95	127.31
26	k	6052	BCR	C11-C10-C9	-5.15	119.95	127.31
26	B	1045	BCR	C15-C14-C13	-5.15	119.96	127.31
26	C	1052	BCR	C11-C10-C9	-5.15	119.97	127.31
26	D	1050	BCR	C11-C10-C9	-5.14	119.97	127.31
26	b	6045	BCR	C15-C14-C13	-5.14	119.97	127.31
26	H	1049	BCR	C15-C14-C13	-5.14	119.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	1053	BCR	C15-C14-C13	-5.13	119.98	127.31
26	B	1045	BCR	C11-C10-C9	-5.13	119.98	127.31
26	z	6053	BCR	C15-C14-C13	-5.13	119.98	127.31
26	b	6045	BCR	C11-C10-C9	-5.13	119.99	127.31
26	K	1051	BCR	C11-C10-C9	-5.13	119.99	127.31
26	d	6050	BCR	C11-C10-C9	-5.13	119.99	127.31
26	b	6047	BCR	C15-C14-C13	-5.13	119.99	127.31
26	B	1047	BCR	C15-C14-C13	-5.13	119.99	127.31
26	Z	1053	BCR	C11-C10-C9	-5.13	120.00	127.31
26	b	6047	BCR	C11-C10-C9	-5.12	120.00	127.31
26	d	6050	BCR	C15-C14-C13	-5.12	120.00	127.31
26	H	1049	BCR	C11-C10-C9	-5.12	120.00	127.31
26	C	1052	BCR	C15-C14-C13	-5.12	120.01	127.31
26	T	6048	BCR	C15-C14-C13	-5.11	120.02	127.31
26	K	1051	BCR	C15-C14-C13	-5.11	120.02	127.31
26	D	1050	BCR	C15-C14-C13	-5.11	120.02	127.31
26	T	6048	BCR	C11-C10-C9	-5.11	120.02	127.31
26	c	6054	BCR	C11-C10-C9	-5.10	120.03	127.31
26	B	1048	BCR	C11-C10-C9	-5.10	120.03	127.31
26	B	1047	BCR	C11-C10-C9	-5.10	120.03	127.31
26	k	6051	BCR	C15-C14-C13	-5.10	120.03	127.31
26	B	1048	BCR	C15-C14-C13	-5.10	120.03	127.31
26	h	6049	BCR	C11-C10-C9	-5.09	120.04	127.31
26	k	6052	BCR	C15-C14-C13	-5.09	120.05	127.31
26	z	6053	BCR	C11-C10-C9	-5.08	120.06	127.31
26	C	1054	BCR	C11-C10-C9	-5.08	120.06	127.31
26	t	1046	BCR	C15-C14-C13	-4.67	120.64	127.31
26	T	6046	BCR	C15-C14-C13	-4.66	120.67	127.31
26	C	1052	BCR	C28-C27-C26	-4.63	105.81	113.78
26	k	6052	BCR	C28-C27-C26	-4.63	105.82	113.78
26	a	6044	BCR	C11-C10-C9	-4.57	120.79	127.31
26	T	6046	BCR	C11-C10-C9	-4.57	120.79	127.31
26	t	1046	BCR	C11-C10-C9	-4.56	120.80	127.31
26	A	1044	BCR	C11-C10-C9	-4.53	120.84	127.31
26	A	1044	BCR	C30-C25-C26	-4.47	116.31	122.59
26	a	6044	BCR	C30-C25-C26	-4.46	116.32	122.59
26	C	1052	BCR	C27-C26-C25	-4.24	116.52	122.74
26	k	6052	BCR	C27-C26-C25	-4.23	116.53	122.74
26	c	6054	BCR	C24-C23-C22	-4.17	119.95	126.21
26	k	6051	BCR	C24-C23-C22	-4.17	119.95	126.21
26	T	6046	BCR	C24-C23-C22	-4.16	119.96	126.21
26	h	6049	BCR	C24-C23-C22	-4.16	119.96	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	1054	BCR	C24-C23-C22	-4.16	119.97	126.21
26	H	1049	BCR	C24-C23-C22	-4.15	119.97	126.21
26	K	1051	BCR	C24-C23-C22	-4.15	119.97	126.21
26	t	1046	BCR	C24-C23-C22	-4.15	119.97	126.21
26	h	6049	BCR	C38-C26-C25	-4.15	119.86	124.51
24	a	6038	PHO	C3D-C2D-C1D	-4.14	99.68	105.82
26	D	1050	BCR	C24-C23-C22	-4.14	120.00	126.21
26	B	1047	BCR	C30-C25-C26	-4.13	116.79	122.59
26	z	6053	BCR	C24-C23-C22	-4.13	120.01	126.21
26	H	1049	BCR	C38-C26-C25	-4.13	119.89	124.51
26	b	6047	BCR	C30-C25-C26	-4.12	116.80	122.59
26	B	1048	BCR	C30-C25-C26	-4.12	116.80	122.59
26	Z	1053	BCR	C24-C23-C22	-4.12	120.02	126.21
24	A	1038	PHO	C3D-C2D-C1D	-4.12	99.71	105.82
24	D	1039	PHO	C3D-C2D-C1D	-4.11	99.72	105.82
26	B	1045	BCR	C24-C23-C22	-4.11	120.03	126.21
26	b	6045	BCR	C24-C23-C22	-4.11	120.03	126.21
24	d	6039	PHO	C3D-C2D-C1D	-4.11	99.72	105.82
26	T	6048	BCR	C30-C25-C26	-4.11	116.81	122.59
26	b	6045	BCR	C33-C5-C6	-4.10	119.91	124.51
26	C	1054	BCR	C38-C26-C25	-4.10	119.92	124.51
26	d	6050	BCR	C38-C26-C25	-4.09	119.93	124.51
26	d	6050	BCR	C24-C23-C22	-4.09	120.07	126.21
26	B	1045	BCR	C33-C5-C6	-4.08	119.94	124.51
26	c	6054	BCR	C38-C26-C25	-4.08	119.95	124.51
26	H	1049	BCR	C33-C5-C6	-4.06	119.96	124.51
26	k	6052	BCR	C33-C5-C6	-4.06	119.96	124.51
26	D	1050	BCR	C38-C26-C25	-4.06	119.96	124.51
26	k	6051	BCR	C33-C5-C6	-4.06	119.97	124.51
26	h	6049	BCR	C33-C5-C6	-4.06	119.97	124.51
26	K	1051	BCR	C38-C26-C25	-4.06	119.97	124.51
26	k	6051	BCR	C38-C26-C25	-4.05	119.97	124.51
26	K	1051	BCR	C33-C5-C6	-4.05	119.97	124.51
23	C	1030	CLA	CHD-C4C-C3C	-4.05	118.81	124.92
26	B	1047	BCR	C33-C5-C6	-4.05	119.97	124.51
23	c	6030	CLA	CHD-C4C-C3C	-4.05	118.82	124.92
26	b	6045	BCR	C38-C26-C25	-4.05	119.98	124.51
26	Z	1053	BCR	C38-C26-C25	-4.04	119.98	124.51
24	a	6038	PHO	C4C-C3C-C2C	-4.04	102.27	106.81
26	A	1044	BCR	C15-C14-C13	-4.04	121.54	127.31
24	A	1038	PHO	C4C-C3C-C2C	-4.04	102.27	106.81
26	T	6048	BCR	C33-C5-C6	-4.03	119.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	1048	BCR	C33-C5-C6	-4.03	120.00	124.51
26	B	1045	BCR	C38-C26-C25	-4.03	120.00	124.51
26	z	6053	BCR	C38-C26-C25	-4.02	120.00	124.51
26	C	1052	BCR	C33-C5-C6	-4.02	120.00	124.51
26	c	6054	BCR	C33-C5-C6	-4.02	120.00	124.51
26	D	1050	BCR	C33-C5-C6	-4.02	120.01	124.51
24	D	1039	PHO	C4C-C3C-C2C	-4.01	102.30	106.81
26	a	6044	BCR	C15-C14-C13	-4.01	121.58	127.31
26	B	1048	BCR	C38-C26-C25	-4.01	120.02	124.51
26	b	6047	BCR	C33-C5-C6	-4.01	120.02	124.51
26	z	6053	BCR	C33-C5-C6	-4.01	120.02	124.51
26	A	1044	BCR	C33-C5-C6	-4.01	120.02	124.51
26	Z	1053	BCR	C33-C5-C6	-4.01	120.02	124.51
26	C	1054	BCR	C33-C5-C6	-4.00	120.03	124.51
26	b	6047	BCR	C38-C26-C25	-4.00	120.03	124.51
24	d	6039	PHO	C4C-C3C-C2C	-4.00	102.32	106.81
26	d	6050	BCR	C33-C5-C6	-4.00	120.03	124.51
26	B	1047	BCR	C38-C26-C25	-4.00	120.03	124.51
26	a	6044	BCR	C33-C5-C6	-3.98	120.05	124.51
26	T	6048	BCR	C38-C26-C25	-3.96	120.08	124.51
23	b	6021	CLA	C1C-C2C-C3C	-3.95	102.54	106.92
23	b	6011	CLA	CHD-C4C-C3C	-3.94	118.98	124.92
23	B	1021	CLA	C1C-C2C-C3C	-3.94	102.55	106.92
23	B	1011	CLA	CHD-C4C-C3C	-3.94	118.99	124.92
23	B	1009	CLA	C1C-C2C-C3C	-3.91	102.58	106.92
23	k	6034	CLA	C1C-C2C-C3C	-3.90	102.59	106.92
23	a	6007	CLA	C1C-C2C-C3C	-3.90	102.59	106.92
23	b	6009	CLA	C1C-C2C-C3C	-3.90	102.60	106.92
23	A	1007	CLA	C1C-C2C-C3C	-3.87	102.62	106.92
23	b	6012	CLA	C1C-C2C-C3C	-3.86	102.63	106.92
23	K	1034	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	b	6023	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	D	1005	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	b	6023	CLA	CHD-C4C-C3C	-3.86	119.10	124.92
23	c	6027	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	d	6005	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	b	6014	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	C	1030	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	B	1012	CLA	C1C-C2C-C3C	-3.86	102.64	106.92
23	c	6031	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	D	1008	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	d	6008	CLA	C1C-C2C-C3C	-3.85	102.65	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1021	CLA	CHD-C4C-C3C	-3.85	119.12	124.92
23	B	1020	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	b	6019	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	c	6026	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	a	6006	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	b	6020	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	b	6022	CLA	C1C-C2C-C3C	-3.85	102.66	106.92
23	B	1014	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	b	6018	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	b	6021	CLA	CHD-C4C-C3C	-3.84	119.13	124.92
23	b	6024	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	B	1010	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	B	1016	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	C	1027	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	B	1023	CLA	CHD-C4C-C3C	-3.84	119.13	124.92
23	B	1022	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	A	1006	CLA	C1C-C2C-C3C	-3.84	102.67	106.92
23	B	1024	CLA	C1C-C2C-C3C	-3.84	102.67	106.92
23	c	6030	CLA	C1C-C2C-C3C	-3.84	102.67	106.92
23	C	1029	CLA	CHD-C4C-C3C	-3.83	119.14	124.92
23	c	6036	CLA	C1C-C2C-C3C	-3.83	102.67	106.92
23	C	1033	CLA	C1C-C2C-C3C	-3.83	102.67	106.92
23	B	1009	CLA	CHD-C4C-C3C	-3.83	119.14	124.92
23	H	1017	CLA	C1C-C2C-C3C	-3.83	102.67	106.92
23	B	1013	CLA	CHD-C4C-C3C	-3.83	119.15	124.92
23	b	6010	CLA	C1C-C2C-C3C	-3.83	102.68	106.92
23	b	6015	CLA	C1C-C2C-C3C	-3.83	102.68	106.92
23	b	6013	CLA	C1C-C2C-C3C	-3.83	102.68	106.92
23	B	1023	CLA	C1C-C2C-C3C	-3.83	102.68	106.92
23	b	6016	CLA	CHD-C4C-C3C	-3.82	119.15	124.92
23	b	6009	CLA	CHD-C4C-C3C	-3.82	119.15	124.92
23	B	1019	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	c	6033	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	B	1013	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	C	1037	CLA	CHD-C4C-C3C	-3.82	119.16	124.92
23	b	6016	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	c	6035	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	C	1031	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	C	1025	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
23	b	6020	CLA	CHD-C4C-C3C	-3.82	119.16	124.92
23	C	1036	CLA	C1C-C2C-C3C	-3.82	102.69	106.92
23	C	1031	CLA	CHD-C4C-C3C	-3.82	119.17	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6022	CLA	CHD-C4C-C3C	-3.82	119.17	124.92
23	b	6015	CLA	CHD-C4C-C3C	-3.82	119.17	124.92
23	C	1026	CLA	C1C-C2C-C3C	-3.82	102.69	106.92
23	B	1015	CLA	C1C-C2C-C3C	-3.82	102.69	106.92
23	d	6005	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	c	6032	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	D	1004	CLA	C1C-C2C-C3C	-3.81	102.69	106.92
23	B	1014	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	C	1027	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	c	6029	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	B	1018	CLA	C1C-C2C-C3C	-3.81	102.69	106.92
23	b	6013	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
23	C	1032	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	c	6025	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	c	6031	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	B	1022	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	b	6014	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	B	1024	CLA	CHD-C4C-C3C	-3.81	119.18	124.92
23	B	1016	CLA	CHD-C4C-C3C	-3.80	119.18	124.92
23	c	6035	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	h	6017	CLA	C1C-C2C-C3C	-3.80	102.70	106.92
23	c	6029	CLA	C1C-C2C-C3C	-3.80	102.70	106.92
23	d	6008	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	C	1029	CLA	C1C-C2C-C3C	-3.80	102.70	106.92
23	C	1028	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	B	1020	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	c	6025	CLA	C1C-C2C-C3C	-3.80	102.70	106.92
23	c	6037	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	D	1004	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	b	6018	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	C	1035	CLA	C1C-C2C-C3C	-3.80	102.71	106.92
23	a	6007	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	A	1003	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	c	6028	CLA	C1C-C2C-C3C	-3.80	102.71	106.92
23	B	1018	CLA	CHD-C4C-C3C	-3.80	119.19	124.92
23	a	6003	CLA	CHD-C4C-C3C	-3.80	119.20	124.92
23	a	6003	CLA	C1C-C2C-C3C	-3.80	102.71	106.92
23	C	1028	CLA	C1C-C2C-C3C	-3.80	102.71	106.92
23	b	6010	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	h	6017	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	H	1017	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	K	1034	CLA	CHD-C4C-C3C	-3.79	119.20	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1003	CLA	C1C-C2C-C3C	-3.79	102.71	106.92
23	C	1032	CLA	C1C-C2C-C3C	-3.79	102.71	106.92
23	A	1007	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	B	1010	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	D	1005	CLA	CHD-C4C-C3C	-3.79	119.20	124.92
23	C	1025	CLA	CHD-C4C-C3C	-3.79	119.21	124.92
23	c	6027	CLA	CHD-C4C-C3C	-3.79	119.21	124.92
23	c	6028	CLA	CHD-C4C-C3C	-3.79	119.21	124.92
23	C	1035	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	B	1015	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	C	1037	CLA	C1C-C2C-C3C	-3.78	102.72	106.92
23	k	6034	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	a	6006	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	d	6004	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	C	1036	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	C	1026	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	C	1033	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	c	6032	CLA	C1C-C2C-C3C	-3.78	102.73	106.92
23	B	1012	CLA	CHD-C4C-C3C	-3.78	119.22	124.92
23	A	1006	CLA	CHD-C4C-C3C	-3.78	119.23	124.92
23	B	1011	CLA	C1C-C2C-C3C	-3.77	102.73	106.92
23	d	6004	CLA	C1C-C2C-C3C	-3.77	102.74	106.92
23	D	1008	CLA	CHD-C4C-C3C	-3.77	119.24	124.92
23	b	6024	CLA	CHD-C4C-C3C	-3.77	119.24	124.92
23	c	6026	CLA	CHD-C4C-C3C	-3.77	119.24	124.92
23	c	6036	CLA	CHD-C4C-C3C	-3.76	119.24	124.92
23	b	6019	CLA	CHD-C4C-C3C	-3.76	119.25	124.92
23	c	6033	CLA	CHD-C4C-C3C	-3.76	119.26	124.92
23	b	6012	CLA	CHD-C4C-C3C	-3.76	119.26	124.92
23	B	1019	CLA	CHD-C4C-C3C	-3.75	119.27	124.92
23	c	6037	CLA	C1C-C2C-C3C	-3.75	102.77	106.92
23	b	6011	CLA	C1C-C2C-C3C	-3.74	102.78	106.92
25	a	6043	PQ9	C11-C12-C13	-3.73	120.47	126.71
25	A	1043	PQ9	C11-C12-C13	-3.72	120.48	126.71
25	d	6042	PQ9	C11-C12-C13	-3.71	120.50	126.71
26	B	1047	BCR	C37-C22-C21	-3.71	117.72	122.92
25	D	1042	PQ9	C11-C12-C13	-3.71	120.51	126.71
26	t	1046	BCR	C1-C6-C5	-3.71	117.38	122.59
26	b	6047	BCR	C37-C22-C21	-3.70	117.75	122.92
26	a	6044	BCR	C38-C26-C25	-3.69	120.38	124.51
26	B	1048	BCR	C37-C22-C21	-3.68	117.77	122.92
26	T	6048	BCR	C37-C22-C21	-3.67	117.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	6046	BCR	C1-C6-C5	-3.67	117.43	122.59
26	A	1044	BCR	C38-C26-C25	-3.67	120.41	124.51
23	b	6023	CLA	C2A-C1A-CHA	-3.51	117.70	123.92
23	B	1023	CLA	C2A-C1A-CHA	-3.50	117.71	123.92
26	T	6046	BCR	C38-C26-C25	-3.50	120.59	124.51
23	d	6008	CLA	C2A-C1A-CHA	-3.50	117.72	123.92
23	b	6022	CLA	C2A-C1A-CHA	-3.50	117.72	123.92
26	t	1046	BCR	C38-C26-C25	-3.50	120.59	124.51
23	b	6014	CLA	C2A-C1A-CHA	-3.49	117.73	123.92
23	b	6016	CLA	C2A-C1A-CHA	-3.49	117.73	123.92
23	c	6025	CLA	C2A-C1A-CHA	-3.49	117.73	123.92
23	B	1014	CLA	C2A-C1A-CHA	-3.49	117.73	123.92
23	D	1008	CLA	C2A-C1A-CHA	-3.49	117.74	123.92
23	C	1037	CLA	C2A-C1A-CHA	-3.49	117.74	123.92
23	c	6037	CLA	C2A-C1A-CHA	-3.48	117.74	123.92
23	a	6006	CLA	C2A-C1A-CHA	-3.48	117.75	123.92
23	C	1025	CLA	C2A-C1A-CHA	-3.48	117.75	123.92
23	b	6013	CLA	C2A-C1A-CHA	-3.48	117.75	123.92
23	c	6035	CLA	C2A-C1A-CHA	-3.48	117.75	123.92
23	k	6034	CLA	C2A-C1A-CHA	-3.48	117.76	123.92
23	c	6033	CLA	C2A-C1A-CHA	-3.47	117.76	123.92
23	d	6005	CLA	C2A-C1A-CHA	-3.47	117.76	123.92
23	D	1005	CLA	C2A-C1A-CHA	-3.47	117.76	123.92
23	A	1006	CLA	C2A-C1A-CHA	-3.47	117.76	123.92
23	B	1022	CLA	C2A-C1A-CHA	-3.47	117.77	123.92
23	C	1033	CLA	C2A-C1A-CHA	-3.47	117.77	123.92
23	a	6007	CLA	C2A-C1A-CHA	-3.47	117.77	123.92
23	b	6019	CLA	C2A-C1A-CHA	-3.47	117.77	123.92
23	B	1019	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	H	1017	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	A	1003	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	B	1015	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	B	1021	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	C	1031	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	b	6015	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	B	1013	CLA	C2A-C1A-CHA	-3.46	117.78	123.92
23	A	1007	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
23	D	1004	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
23	K	1034	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
23	C	1027	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
23	C	1036	CLA	C2A-C1A-CHA	-3.46	117.79	123.92
23	c	6036	CLA	C2A-C1A-CHA	-3.45	117.79	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1028	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	d	6004	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	C	1035	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	B	1020	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	B	1016	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	B	1012	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	c	6032	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	c	6027	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	B	1018	CLA	C2A-C1A-CHA	-3.45	117.80	123.92
23	B	1024	CLA	C2A-C1A-CHA	-3.45	117.81	123.92
23	C	1032	CLA	C2A-C1A-CHA	-3.45	117.81	123.92
23	b	6024	CLA	C2A-C1A-CHA	-3.45	117.81	123.92
23	c	6031	CLA	C2A-C1A-CHA	-3.45	117.81	123.92
23	b	6021	CLA	C2A-C1A-CHA	-3.45	117.81	123.92
23	c	6028	CLA	C2A-C1A-CHA	-3.44	117.81	123.92
23	h	6017	CLA	C2A-C1A-CHA	-3.44	117.82	123.92
23	b	6012	CLA	C2A-C1A-CHA	-3.44	117.82	123.92
23	a	6003	CLA	C2A-C1A-CHA	-3.44	117.82	123.92
23	C	1026	CLA	C2A-C1A-CHA	-3.44	117.82	123.92
23	b	6018	CLA	C2A-C1A-CHA	-3.43	117.84	123.92
23	b	6020	CLA	C2A-C1A-CHA	-3.42	117.85	123.92
23	c	6030	CLA	C2A-C1A-CHA	-3.42	117.85	123.92
26	A	1044	BCR	C37-C22-C21	-3.42	118.13	122.92
23	b	6010	CLA	C2A-C1A-CHA	-3.42	117.85	123.92
26	a	6044	BCR	C37-C22-C21	-3.42	118.13	122.92
23	c	6026	CLA	C2A-C1A-CHA	-3.42	117.86	123.92
23	B	1010	CLA	C2A-C1A-CHA	-3.41	117.86	123.92
23	B	1011	CLA	C2A-C1A-CHA	-3.41	117.87	123.92
23	b	6011	CLA	C2A-C1A-CHA	-3.40	117.88	123.92
23	C	1030	CLA	C2A-C1A-CHA	-3.40	117.89	123.92
23	c	6029	CLA	C2A-C1A-CHA	-3.39	117.90	123.92
23	C	1029	CLA	C2A-C1A-CHA	-3.39	117.91	123.92
23	b	6011	CLA	O1D-CGD-CBD	-3.38	118.53	124.60
23	B	1011	CLA	O1D-CGD-CBD	-3.37	118.55	124.60
23	B	1009	CLA	C2A-C1A-CHA	-3.35	117.98	123.92
23	b	6009	CLA	C2A-C1A-CHA	-3.35	117.98	123.92
26	t	1046	BCR	C33-C5-C6	-3.32	120.79	124.51
26	T	6046	BCR	C33-C5-C6	-3.29	120.82	124.51
24	a	6038	PHO	C1C-C2C-C3C	-3.26	102.73	106.51
24	d	6039	PHO	C1C-C2C-C3C	-3.26	102.73	106.51
24	D	1039	PHO	C1C-C2C-C3C	-3.25	102.73	106.51
24	A	1038	PHO	C1C-C2C-C3C	-3.25	102.74	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	1039	PHO	OBD-CAD-C3D	-3.23	120.49	128.43
24	A	1038	PHO	OBD-CAD-C3D	-3.23	120.49	128.43
24	d	6039	PHO	OBD-CAD-C3D	-3.22	120.51	128.43
26	k	6052	BCR	C37-C22-C21	-3.22	118.41	122.92
24	a	6038	PHO	OBD-CAD-C3D	-3.22	120.52	128.43
26	C	1052	BCR	C37-C22-C21	-3.20	118.44	122.92
23	D	1008	CLA	O1D-CGD-CBD	-3.19	118.88	124.60
23	d	6008	CLA	O1D-CGD-CBD	-3.16	118.93	124.60
23	B	1011	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
23	b	6011	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
23	d	6008	CLA	O2D-CGD-O1D	-3.01	117.75	123.82
23	D	1008	CLA	O2D-CGD-O1D	-3.01	117.76	123.82
23	C	1029	CLA	O1D-CGD-CBD	-3.01	119.20	124.60
23	b	6022	CLA	C1-C2-C3	-3.00	120.43	125.96
23	c	6028	CLA	C1-C2-C3	-3.00	120.43	125.96
23	a	6003	CLA	C1-C2-C3	-3.00	120.43	125.96
23	c	6029	CLA	O1D-CGD-CBD	-3.00	119.21	124.60
23	c	6037	CLA	C1-C2-C3	-2.99	120.44	125.96
23	B	1009	CLA	C1-C2-C3	-2.99	120.45	125.96
23	c	6032	CLA	C1-C2-C3	-2.99	120.45	125.96
23	b	6009	CLA	C1-C2-C3	-2.99	120.45	125.96
23	d	6004	CLA	C1-C2-C3	-2.99	120.46	125.96
23	B	1022	CLA	C1-C2-C3	-2.98	120.46	125.96
23	c	6027	CLA	C1-C2-C3	-2.98	120.46	125.96
23	C	1028	CLA	C1-C2-C3	-2.98	120.47	125.96
23	C	1033	CLA	C1-C2-C3	-2.98	120.47	125.96
23	C	1032	CLA	C1-C2-C3	-2.98	120.47	125.96
23	c	6031	CLA	C1-C2-C3	-2.98	120.47	125.96
23	A	1003	CLA	C1-C2-C3	-2.97	120.48	125.96
23	b	6024	CLA	C1-C2-C3	-2.97	120.48	125.96
23	B	1016	CLA	C1-C2-C3	-2.97	120.48	125.96
23	c	6035	CLA	C1-C2-C3	-2.97	120.48	125.96
23	D	1005	CLA	C1-C2-C3	-2.97	120.48	125.96
23	B	1014	CLA	C1-C2-C3	-2.97	120.49	125.96
23	C	1037	CLA	C1-C2-C3	-2.97	120.49	125.96
23	C	1036	CLA	C1-C2-C3	-2.97	120.49	125.96
23	b	6014	CLA	C1-C2-C3	-2.97	120.49	125.96
23	b	6015	CLA	C1-C2-C3	-2.97	120.49	125.96
23	C	1031	CLA	C1-C2-C3	-2.97	120.49	125.96
23	H	1017	CLA	C1-C2-C3	-2.97	120.49	125.96
23	K	1034	CLA	C1-C2-C3	-2.97	120.49	125.96
23	c	6026	CLA	C1-C2-C3	-2.97	120.49	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6007	CLA	C1-C2-C3	-2.97	120.49	125.96
23	d	6005	CLA	C1-C2-C3	-2.97	120.49	125.96
23	a	6006	CLA	C1-C2-C3	-2.97	120.49	125.96
23	A	1006	CLA	C1-C2-C3	-2.97	120.49	125.96
23	C	1035	CLA	C1-C2-C3	-2.97	120.49	125.96
24	D	1039	PHO	C1-C2-C3	-2.97	120.49	125.96
23	B	1019	CLA	C1-C2-C3	-2.97	120.49	125.96
26	T	6046	BCR	C4-C5-C6	-2.96	118.39	122.74
23	C	1026	CLA	C1-C2-C3	-2.96	120.50	125.96
23	A	1007	CLA	C1-C2-C3	-2.96	120.50	125.96
23	B	1012	CLA	C1-C2-C3	-2.96	120.50	125.96
23	h	6017	CLA	C1-C2-C3	-2.96	120.50	125.96
23	k	6034	CLA	C1-C2-C3	-2.96	120.50	125.96
23	B	1015	CLA	C1-C2-C3	-2.96	120.50	125.96
23	b	6018	CLA	C1-C2-C3	-2.96	120.50	125.96
23	C	1027	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	6036	CLA	C1-C2-C3	-2.96	120.51	125.96
23	b	6016	CLA	C1-C2-C3	-2.96	120.51	125.96
23	c	6033	CLA	C1-C2-C3	-2.96	120.51	125.96
23	B	1013	CLA	C1-C2-C3	-2.96	120.51	125.96
23	c	6025	CLA	C1-C2-C3	-2.96	120.51	125.96
23	D	1004	CLA	C1-C2-C3	-2.96	120.51	125.96
23	B	1020	CLA	C1-C2-C3	-2.95	120.51	125.96
23	B	1018	CLA	C1-C2-C3	-2.95	120.51	125.96
23	b	6012	CLA	C1-C2-C3	-2.95	120.52	125.96
23	b	6019	CLA	C1-C2-C3	-2.95	120.52	125.96
23	B	1024	CLA	C1-C2-C3	-2.95	120.52	125.96
24	A	1038	PHO	C1-C2-C3	-2.95	120.52	125.96
23	C	1025	CLA	C1-C2-C3	-2.95	120.52	125.96
24	d	6039	PHO	C1-C2-C3	-2.95	120.52	125.96
26	A	1044	BCR	C28-C27-C26	-2.95	108.71	113.78
24	D	1039	PHO	CHD-C1D-ND	-2.95	118.86	124.64
24	a	6038	PHO	C1-C2-C3	-2.94	120.53	125.96
23	b	6013	CLA	C1-C2-C3	-2.94	120.54	125.96
26	a	6044	BCR	C28-C27-C26	-2.94	108.72	113.78
24	d	6039	PHO	CHD-C1D-ND	-2.94	118.88	124.64
23	b	6020	CLA	C1-C2-C3	-2.93	120.56	125.96
26	t	1046	BCR	C4-C5-C6	-2.92	118.45	122.74
24	A	1038	PHO	CHD-C1D-ND	-2.91	118.92	124.64
24	a	6038	PHO	CHD-C1D-ND	-2.91	118.93	124.64
23	b	6010	CLA	C1-C2-C3	-2.89	120.63	125.96
25	d	6042	PQ9	C26-C27-C28	-2.88	120.44	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	6042	PQ9	C16-C17-C18	-2.88	120.45	127.68
25	d	6042	PQ9	C31-C32-C33	-2.88	120.46	127.68
25	D	1042	PQ9	C31-C32-C33	-2.87	120.47	127.68
25	d	6042	PQ9	C36-C37-C38	-2.87	120.47	127.68
23	B	1010	CLA	C1-C2-C3	-2.87	120.67	125.96
25	D	1042	PQ9	C26-C27-C28	-2.87	120.47	127.68
25	d	6042	PQ9	C21-C22-C23	-2.86	120.48	127.68
26	t	1046	BCR	C30-C25-C26	-2.86	118.57	122.59
25	D	1042	PQ9	C16-C17-C18	-2.86	120.49	127.68
25	a	6043	PQ9	C21-C22-C23	-2.86	120.49	127.68
25	A	1043	PQ9	C31-C32-C33	-2.86	120.49	127.68
25	D	1042	PQ9	C21-C22-C23	-2.86	120.50	127.68
25	a	6043	PQ9	C31-C32-C33	-2.86	120.50	127.68
25	A	1043	PQ9	C21-C22-C23	-2.86	120.50	127.68
25	D	1042	PQ9	C36-C37-C38	-2.86	120.50	127.68
23	D	1008	CLA	C1-C2-C3	-2.86	120.70	125.96
25	A	1043	PQ9	C26-C27-C28	-2.85	120.52	127.68
25	a	6043	PQ9	C26-C27-C28	-2.85	120.53	127.68
23	c	6029	CLA	C1-C2-C3	-2.85	120.71	125.96
25	a	6043	PQ9	C16-C17-C18	-2.84	120.53	127.68
25	A	1043	PQ9	C16-C17-C18	-2.84	120.54	127.68
25	a	6043	PQ9	C36-C37-C38	-2.84	120.55	127.68
25	A	1043	PQ9	C36-C37-C38	-2.84	120.55	127.68
23	C	1029	CLA	C1-C2-C3	-2.84	120.73	125.96
26	T	6046	BCR	C30-C25-C26	-2.83	118.61	122.59
23	d	6008	CLA	C1-C2-C3	-2.83	120.74	125.96
23	b	6021	CLA	C1-C2-C3	-2.79	120.81	125.96
23	B	1021	CLA	C1-C2-C3	-2.78	120.83	125.96
23	B	1023	CLA	C1-C2-C3	-2.78	120.83	125.96
26	C	1052	BCR	C38-C26-C25	-2.78	121.40	124.51
26	k	6052	BCR	C38-C26-C25	-2.77	121.41	124.51
23	b	6023	CLA	C1-C2-C3	-2.77	120.86	125.96
26	B	1048	BCR	C28-C27-C26	-2.77	109.03	113.78
26	T	6048	BCR	C28-C27-C26	-2.76	109.04	113.78
26	a	6044	BCR	C3-C4-C5	-2.75	109.06	113.78
23	c	6030	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
26	B	1047	BCR	C28-C27-C26	-2.73	109.08	113.78
26	A	1044	BCR	C3-C4-C5	-2.73	109.08	113.78
23	b	6011	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
26	b	6047	BCR	C28-C27-C26	-2.72	109.10	113.78
23	C	1030	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
23	C	1029	CLA	O2D-CGD-O1D	-2.71	118.36	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6030	CLA	C1-C2-C3	-2.71	120.97	125.96
23	B	1011	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
23	c	6029	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
23	C	1030	CLA	C1-C2-C3	-2.70	120.99	125.96
23	a	6003	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
23	c	6032	CLA	C4C-C3C-C2C	-2.65	102.84	106.91
23	C	1029	CLA	C4C-C3C-C2C	-2.65	102.85	106.91
23	B	1010	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
23	A	1003	CLA	C4C-C3C-C2C	-2.64	102.85	106.91
23	b	6009	CLA	C4C-C3C-C2C	-2.64	102.85	106.91
23	b	6010	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
23	d	6004	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	c	6035	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	c	6028	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	B	1009	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	b	6015	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	C	1035	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	B	1010	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	C	1032	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
23	B	1013	CLA	C4C-C3C-C2C	-2.64	102.87	106.91
23	b	6010	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
23	D	1004	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
23	C	1026	CLA	C4C-C3C-C2C	-2.63	102.87	106.91
23	C	1028	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
23	c	6037	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
23	C	1031	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
23	C	1027	CLA	C4C-C3C-C2C	-2.63	102.88	106.91
23	b	6016	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
23	c	6025	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
23	b	6009	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
23	B	1022	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
23	C	1037	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
23	c	6033	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	6020	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	B	1024	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	B	1016	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	B	1014	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	K	1034	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	6011	CLA	C1-C2-C3	-2.62	121.13	125.96
23	h	6017	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	C	1025	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	a	6006	CLA	C4C-C3C-C2C	-2.62	102.89	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1033	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	6022	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	c	6029	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	6014	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	6013	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
23	B	1015	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
23	B	1009	CLA	O2D-CGD-O1D	-2.61	118.56	123.82
23	B	1011	CLA	C1-C2-C3	-2.61	121.14	125.96
23	B	1018	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
26	D	1050	BCR	C8-C7-C6	-2.61	119.94	127.25
23	C	1036	CLA	C4C-C3C-C2C	-2.61	102.90	106.91
23	H	1017	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
23	c	6030	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
23	B	1020	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
23	d	6005	CLA	C4C-C3C-C2C	-2.60	102.91	106.91
26	b	6047	BCR	C8-C7-C6	-2.60	119.96	127.25
23	C	1030	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	c	6031	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	c	6027	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	c	6036	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	B	1012	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
26	d	6050	BCR	C8-C7-C6	-2.60	119.97	127.25
26	K	1051	BCR	C23-C24-C25	-2.60	119.97	127.25
23	B	1009	CLA	O1D-CGD-CBD	-2.60	119.93	124.60
23	b	6024	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	k	6034	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
23	c	6026	CLA	C4C-C3C-C2C	-2.60	102.92	106.91
26	k	6051	BCR	C23-C24-C25	-2.60	119.98	127.25
26	k	6052	BCR	C8-C7-C6	-2.60	119.99	127.25
23	D	1005	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
23	A	1006	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
23	b	6018	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
26	B	1045	BCR	C8-C7-C6	-2.59	119.99	127.25
23	A	1007	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
23	B	1019	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
23	b	6012	CLA	C4C-C3C-C2C	-2.59	102.93	106.91
26	h	6049	BCR	C8-C7-C6	-2.59	119.99	127.25
30	l	6061	MGE	C2G-O2G-C1B	-2.59	111.75	117.88
26	H	1049	BCR	C8-C7-C6	-2.59	120.00	127.25
26	C	1052	BCR	C8-C7-C6	-2.59	120.00	127.25
26	D	1050	BCR	C23-C24-C25	-2.59	120.00	127.25
26	C	1054	BCR	C8-C7-C6	-2.59	120.00	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1023	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
26	b	6045	BCR	C8-C7-C6	-2.59	120.00	127.25
26	T	6048	BCR	C8-C7-C6	-2.59	120.00	127.25
26	B	1048	BCR	C8-C7-C6	-2.59	120.01	127.25
26	B	1045	BCR	C23-C24-C25	-2.59	120.01	127.25
30	L	1061	MGE	C2G-O2G-C1B	-2.59	111.76	117.88
23	b	6023	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
26	H	1049	BCR	C28-C27-C26	-2.59	109.33	113.78
26	z	6053	BCR	C8-C7-C6	-2.59	120.01	127.25
23	b	6019	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
26	B	1047	BCR	C8-C7-C6	-2.59	120.01	127.25
26	K	1051	BCR	C8-C7-C6	-2.59	120.01	127.25
26	b	6045	BCR	C23-C24-C25	-2.59	120.01	127.25
23	d	6008	CLA	C4C-C3C-C2C	-2.58	102.94	106.91
23	a	6007	CLA	C4C-C3C-C2C	-2.58	102.94	106.91
26	Z	1053	BCR	C23-C24-C25	-2.58	120.02	127.25
26	C	1054	BCR	C28-C27-C26	-2.58	109.34	113.78
26	Z	1053	BCR	C8-C7-C6	-2.58	120.03	127.25
29	c	6055	DGD	C2G-O2G-C1B	-2.58	111.78	117.88
26	d	6050	BCR	C23-C24-C25	-2.58	120.03	127.25
26	k	6051	BCR	C8-C7-C6	-2.58	120.03	127.25
29	C	1057	DGD	C2G-O2G-C1B	-2.58	111.78	117.88
29	C	1055	DGD	C2G-O2G-C1B	-2.58	111.78	117.88
29	B	1058	DGD	C2G-O2G-C1B	-2.58	111.79	117.88
23	B	1021	CLA	C4C-C3C-C2C	-2.58	102.96	106.91
26	c	6054	BCR	C28-C27-C26	-2.58	109.35	113.78
30	b	6060	MGE	C2G-O2G-C1B	-2.58	111.79	117.88
23	b	6021	CLA	C4C-C3C-C2C	-2.58	102.96	106.91
26	z	6053	BCR	C23-C24-C25	-2.58	120.04	127.25
23	b	6009	CLA	O1D-CGD-CBD	-2.57	119.98	124.60
27	a	6063	LHG	C5-O7-C7	-2.57	111.79	117.88
23	D	1008	CLA	C4C-C3C-C2C	-2.57	102.96	106.91
27	A	1063	LHG	C5-O7-C7	-2.57	111.80	117.88
26	c	6054	BCR	C8-C7-C6	-2.57	120.06	127.25
26	h	6049	BCR	C28-C27-C26	-2.57	109.36	113.78
30	B	1060	MGE	C2G-O2G-C1B	-2.57	111.81	117.88
29	c	6056	DGD	C2G-O2G-C1B	-2.57	111.81	117.88
29	c	6057	DGD	C2G-O2G-C1B	-2.57	111.81	117.88
29	C	1056	DGD	C2G-O2G-C1B	-2.56	111.82	117.88
26	C	1054	BCR	C3-C4-C5	-2.56	109.38	113.78
29	b	6058	DGD	C2G-O2G-C1B	-2.56	111.83	117.88
26	T	6048	BCR	C3-C4-C5	-2.56	109.38	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	6054	BCR	C3-C4-C5	-2.56	109.38	113.78
26	b	6045	BCR	C28-C27-C26	-2.56	109.39	113.78
30	D	1059	MGE	C2G-O2G-C1B	-2.56	111.84	117.88
26	z	6053	BCR	C3-C4-C5	-2.55	109.39	113.78
23	b	6023	CLA	O2D-CGD-O1D	-2.55	118.68	123.82
30	d	6062	MGE	C2G-O2G-C1B	-2.55	111.85	117.88
26	B	1048	BCR	C3-C4-C5	-2.55	109.39	113.78
30	D	1062	MGE	C2G-O2G-C1B	-2.55	111.86	117.88
26	Z	1053	BCR	C3-C4-C5	-2.55	109.40	113.78
25	d	6042	PQ9	C11-C2-C3	-2.55	119.61	123.23
30	d	6059	MGE	C2G-O2G-C1B	-2.54	111.86	117.88
25	a	6043	PQ9	C11-C2-C3	-2.54	119.61	123.23
23	C	1030	CLA	O1D-CGD-CBD	-2.54	120.04	124.60
23	B	1023	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
23	c	6030	CLA	O1D-CGD-CBD	-2.54	120.04	124.60
25	A	1043	PQ9	C11-C2-C3	-2.53	119.62	123.23
25	D	1042	PQ9	C11-C2-C3	-2.53	119.63	123.23
26	B	1045	BCR	C28-C27-C26	-2.53	109.43	113.78
26	k	6052	BCR	C3-C4-C5	-2.53	109.43	113.78
26	d	6050	BCR	C3-C4-C5	-2.53	109.44	113.78
26	D	1050	BCR	C3-C4-C5	-2.52	109.44	113.78
26	C	1052	BCR	C3-C4-C5	-2.52	109.45	113.78
26	b	6047	BCR	C3-C4-C5	-2.51	109.46	113.78
24	D	1039	PHO	C4D-ND-C1D	-2.51	102.45	106.98
24	d	6039	PHO	C4D-ND-C1D	-2.51	102.45	106.98
26	d	6050	BCR	C28-C27-C26	-2.51	109.47	113.78
23	B	1009	CLA	O2A-CGA-O1A	-2.50	117.33	123.55
26	D	1050	BCR	C28-C27-C26	-2.50	109.48	113.78
26	B	1047	BCR	C3-C4-C5	-2.50	109.48	113.78
26	B	1045	BCR	C3-C4-C5	-2.50	109.48	113.78
24	a	6038	PHO	C4D-ND-C1D	-2.50	102.47	106.98
26	b	6045	BCR	C3-C4-C5	-2.50	109.49	113.78
24	A	1038	PHO	C4D-ND-C1D	-2.50	102.48	106.98
26	h	6049	BCR	C3-C4-C5	-2.49	109.49	113.78
26	t	1046	BCR	C36-C18-C17	-2.49	119.43	122.92
26	H	1049	BCR	C3-C4-C5	-2.49	109.50	113.78
26	k	6051	BCR	C3-C4-C5	-2.49	109.50	113.78
26	K	1051	BCR	C3-C4-C5	-2.49	109.50	113.78
26	Z	1053	BCR	C28-C27-C26	-2.48	109.51	113.78
23	b	6009	CLA	O2A-CGA-O1A	-2.48	117.39	123.55
26	T	6046	BCR	C36-C18-C17	-2.47	119.46	122.92
23	B	1010	CLA	O1D-CGD-CBD	-2.47	120.17	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6011	CLA	O2A-CGA-O1A	-2.47	117.43	123.55
26	z	6053	BCR	C28-C27-C26	-2.47	109.54	113.78
23	b	6010	CLA	O1D-CGD-CBD	-2.46	120.19	124.60
26	K	1051	BCR	C28-C27-C26	-2.45	109.57	113.78
23	B	1011	CLA	O2A-CGA-O1A	-2.45	117.48	123.55
23	b	6009	CLA	CHC-C1C-C2C	-2.43	120.01	126.65
26	k	6051	BCR	C28-C27-C26	-2.43	109.60	113.78
23	d	6005	CLA	O2D-CGD-O1D	-2.43	118.93	123.82
23	B	1009	CLA	CHC-C1C-C2C	-2.43	120.03	126.65
23	b	6024	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
23	B	1024	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
23	b	6018	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
23	C	1036	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
23	C	1037	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
23	B	1022	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
23	D	1005	CLA	O2D-CGD-O1D	-2.41	118.96	123.82
23	C	1026	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	C	1033	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	B	1023	CLA	O1D-CGD-CBD	-2.41	120.27	124.60
23	A	1006	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	c	6035	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	b	6022	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	c	6033	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
23	C	1027	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
23	b	6021	CLA	O1D-CGD-CBD	-2.41	120.28	124.60
23	B	1018	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
23	a	6006	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
23	c	6036	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
23	K	1034	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
23	B	1016	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
23	b	6023	CLA	O1D-CGD-CBD	-2.40	120.29	124.60
23	a	6007	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
23	c	6037	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
23	b	6019	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
23	C	1032	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
26	k	6052	BCR	C29-C30-C25	-2.40	106.72	110.48
23	a	6003	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
23	b	6020	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
23	A	1003	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
23	B	1021	CLA	O1D-CGD-CBD	-2.39	120.30	124.60
23	B	1012	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
23	B	1019	CLA	O2D-CGD-O1D	-2.39	119.00	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6026	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
23	b	6012	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
23	B	1020	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
23	k	6034	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
23	C	1025	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
23	C	1035	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
23	c	6025	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
26	h	6049	BCR	C23-C24-C25	-2.38	120.58	127.25
23	A	1007	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
26	C	1052	BCR	C29-C30-C25	-2.38	106.75	110.48
23	c	6032	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	c	6031	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	D	1004	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	b	6016	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	c	6027	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	B	1015	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
26	H	1049	BCR	C23-C24-C25	-2.38	120.59	127.25
23	B	1014	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
23	C	1031	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
23	b	6014	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
23	B	1013	CLA	O2D-CGD-O1D	-2.37	119.04	123.82
23	b	6013	CLA	O2D-CGD-O1D	-2.37	119.04	123.82
23	H	1017	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
23	d	6004	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
23	h	6017	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
23	b	6015	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
26	A	1044	BCR	C34-C9-C10	-2.37	119.60	122.92
26	a	6044	BCR	C34-C9-C10	-2.37	119.61	122.92
26	c	6054	BCR	C23-C24-C25	-2.36	120.64	127.25
26	C	1054	BCR	C23-C24-C25	-2.36	120.64	127.25
23	c	6037	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
23	C	1028	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
23	B	1021	CLA	O2A-CGA-O1A	-2.34	117.73	123.55
24	A	1038	PHO	O2D-CGD-O1D	-2.34	119.11	123.82
23	C	1037	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
23	a	6006	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
23	d	6004	CLA	O1D-CGD-CBD	-2.33	120.41	124.60
23	d	6008	CLA	CHC-C1C-C2C	-2.33	120.29	126.65
23	b	6021	CLA	O2A-CGA-O1A	-2.33	117.76	123.55
26	T	6046	BCR	C23-C24-C25	-2.33	120.73	127.25
23	b	6023	CLA	CHC-C1C-C2C	-2.33	120.30	126.65
23	D	1008	CLA	CHC-C1C-C2C	-2.33	120.30	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1006	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
24	D	1039	PHO	O2D-CGD-O1D	-2.33	119.14	123.82
24	a	6038	PHO	O2D-CGD-O1D	-2.33	119.14	123.82
26	t	1046	BCR	C23-C24-C25	-2.33	120.74	127.25
23	c	6035	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
26	t	1046	BCR	C28-C27-C26	-2.32	109.78	113.78
23	k	6034	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
23	c	6028	CLA	O2D-CGD-O1D	-2.32	119.14	123.82
23	B	1021	CLA	CHC-C1C-C2C	-2.32	120.31	126.65
23	C	1035	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
23	K	1034	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
23	b	6021	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
23	B	1023	CLA	CHC-C1C-C2C	-2.32	120.32	126.65
23	k	6034	CLA	CHC-C1C-C2C	-2.32	120.33	126.65
26	T	6046	BCR	C28-C27-C26	-2.32	109.80	113.78
23	b	6021	CLA	CHC-C1C-C2C	-2.32	120.33	126.65
24	d	6039	PHO	O2D-CGD-O1D	-2.32	119.16	123.82
23	D	1004	CLA	O1D-CGD-CBD	-2.32	120.44	124.60
23	c	6026	CLA	O1D-CGD-CBD	-2.31	120.44	124.60
23	B	1010	CLA	CHC-C1C-C2C	-2.31	120.34	126.65
23	b	6010	CLA	CHC-C1C-C2C	-2.31	120.34	126.65
23	B	1021	CLA	O2D-CGD-O1D	-2.31	119.16	123.82
26	t	1046	BCR	C37-C22-C21	-2.31	119.68	122.92
26	T	6046	BCR	C37-C22-C21	-2.31	119.68	122.92
23	c	6027	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
23	b	6020	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
23	C	1029	CLA	CHC-C1C-C2C	-2.31	120.35	126.65
23	c	6027	CLA	CHC-C1C-C2C	-2.31	120.36	126.65
23	a	6007	CLA	CHC-C1C-C2C	-2.31	120.36	126.65
23	C	1027	CLA	O1D-CGD-CBD	-2.31	120.46	124.60
23	c	6031	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	B	1022	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	b	6022	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	B	1020	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	b	6012	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
23	B	1022	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
23	C	1026	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	c	6036	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	B	1018	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	B	1012	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	K	1034	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	b	6022	CLA	CHC-C1C-C2C	-2.30	120.38	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6031	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	h	6017	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	c	6033	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	a	6003	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	C	1033	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
23	D	1005	CLA	O1D-CGD-CBD	-2.30	120.48	124.60
23	A	1007	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	B	1011	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	b	6018	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	C	1027	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	b	6011	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	B	1014	CLA	O1D-CGD-CBD	-2.30	120.48	124.60
23	b	6020	CLA	CHC-C1C-C2C	-2.30	120.39	126.65
23	b	6018	CLA	O1D-CGD-CBD	-2.30	120.48	124.60
23	c	6029	CLA	CHC-C1C-C2C	-2.29	120.39	126.65
23	b	6016	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	c	6025	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	a	6006	CLA	CHC-C1C-C2C	-2.29	120.39	126.65
23	B	1014	CLA	CHC-C1C-C2C	-2.29	120.39	126.65
23	a	6007	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	H	1017	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	B	1016	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	C	1026	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	b	6019	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	b	6015	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	c	6025	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	C	1032	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	b	6014	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	b	6013	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
23	B	1013	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
23	C	1025	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	c	6026	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	d	6005	CLA	CHC-C1C-C2C	-2.29	120.40	126.65
23	c	6036	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	B	1020	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	D	1005	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	b	6024	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	A	1007	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
23	A	1003	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	B	1024	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
23	d	6005	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
23	c	6032	CLA	O1D-CGD-CBD	-2.29	120.49	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1016	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	C	1031	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
23	B	1018	CLA	CHC-C1C-C2C	-2.29	120.42	126.65
23	b	6013	CLA	CHC-C1C-C2C	-2.29	120.42	126.65
23	B	1013	CLA	CHC-C1C-C2C	-2.28	120.42	126.65
23	C	1036	CLA	CHC-C1C-C2C	-2.28	120.42	126.65
23	b	6014	CLA	O1D-CGD-CBD	-2.28	120.50	124.60
23	b	6015	CLA	CHC-C1C-C2C	-2.28	120.42	126.65
23	C	1032	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
23	B	1019	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
23	A	1006	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
23	D	1004	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
23	C	1036	CLA	O1D-CGD-CBD	-2.28	120.51	124.60
23	C	1025	CLA	O1D-CGD-CBD	-2.28	120.51	124.60
23	H	1017	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
23	C	1035	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
23	c	6032	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
23	C	1031	CLA	O1D-CGD-CBD	-2.28	120.51	124.60
23	B	1019	CLA	O1D-CGD-CBD	-2.28	120.51	124.60
23	c	6028	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
23	C	1028	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
23	h	6017	CLA	CHC-C1C-C2C	-2.27	120.45	126.65
23	B	1024	CLA	CHC-C1C-C2C	-2.27	120.45	126.65
23	b	6019	CLA	O1D-CGD-CBD	-2.27	120.52	124.60
23	B	1015	CLA	O1D-CGD-CBD	-2.27	120.52	124.60
23	B	1015	CLA	CHC-C1C-C2C	-2.27	120.45	126.65
23	b	6024	CLA	O1D-CGD-CBD	-2.27	120.53	124.60
23	b	6016	CLA	CHC-C1C-C2C	-2.27	120.46	126.65
23	c	6035	CLA	CHC-C1C-C2C	-2.26	120.47	126.65
23	d	6004	CLA	CHC-C1C-C2C	-2.26	120.47	126.65
23	A	1003	CLA	O1D-CGD-CBD	-2.26	120.53	124.60
23	C	1033	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
23	c	6037	CLA	CHC-C1C-C2C	-2.26	120.49	126.65
23	B	1012	CLA	O1D-CGD-CBD	-2.26	120.55	124.60
23	c	6028	CLA	O1D-CGD-CBD	-2.25	120.55	124.60
23	C	1037	CLA	CHC-C1C-C2C	-2.25	120.50	126.65
23	c	6033	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
23	a	6003	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
23	b	6012	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
23	C	1030	CLA	CHC-C1C-C2C	-2.25	120.52	126.65
23	c	6030	CLA	CHC-C1C-C2C	-2.24	120.55	126.65
23	C	1028	CLA	O1D-CGD-CBD	-2.23	120.59	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	6038	PHO	O1D-CGD-CBD	-2.21	120.64	124.60
23	C	1030	CLA	O2A-CGA-O1A	-2.21	118.07	123.55
26	T	6046	BCR	C35-C13-C14	-2.20	119.84	122.92
24	A	1038	PHO	O1D-CGD-CBD	-2.19	120.67	124.60
23	c	6030	CLA	O2A-CGA-O1A	-2.19	118.12	123.55
26	a	6044	BCR	C36-C18-C17	-2.19	119.86	122.92
31	V	1041	HEM	C1D-C2D-C3D	-2.19	105.47	107.00
26	t	1046	BCR	C35-C13-C14	-2.19	119.86	122.92
26	A	1044	BCR	C35-C13-C14	-2.18	119.87	122.92
26	A	1044	BCR	C36-C18-C17	-2.18	119.87	122.92
26	t	1046	BCR	C8-C7-C6	-2.17	121.16	127.25
26	a	6044	BCR	C35-C13-C14	-2.17	119.88	122.92
23	b	6023	CLA	O2A-CGA-O1A	-2.17	118.15	123.55
23	B	1023	CLA	O2A-CGA-O1A	-2.17	118.16	123.55
24	D	1039	PHO	CBB-CAB-C3B	-2.17	116.50	127.39
31	v	6041	HEM	C1D-C2D-C3D	-2.17	105.49	107.00
24	A	1038	PHO	CBB-CAB-C3B	-2.17	116.51	127.39
23	c	6029	CLA	O2A-CGA-O1A	-2.17	118.17	123.55
24	d	6039	PHO	CBB-CAB-C3B	-2.17	116.53	127.39
24	D	1039	PHO	O1D-CGD-CBD	-2.16	120.71	124.60
24	a	6038	PHO	CBB-CAB-C3B	-2.16	116.54	127.39
23	C	1029	CLA	O2A-CGA-O1A	-2.15	118.20	123.55
26	T	6046	BCR	C8-C7-C6	-2.15	121.23	127.25
24	d	6039	PHO	O1D-CGD-CBD	-2.15	120.74	124.60
26	b	6047	BCR	C24-C25-C26	-2.14	116.43	121.54
26	A	1044	BCR	C1-C6-C5	-2.13	119.59	122.59
26	B	1047	BCR	C24-C25-C26	-2.13	116.46	121.54
26	z	6053	BCR	C34-C9-C10	-2.13	119.94	122.92
26	a	6044	BCR	C1-C6-C5	-2.12	119.61	122.59
26	h	6049	BCR	C36-C18-C17	-2.12	119.96	122.92
26	k	6051	BCR	C35-C13-C14	-2.12	119.96	122.92
26	b	6047	BCR	C36-C18-C17	-2.11	119.97	122.92
31	F	1040	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
31	f	6040	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
26	T	6048	BCR	C24-C25-C26	-2.11	116.51	121.54
26	B	1048	BCR	C34-C9-C10	-2.11	119.97	122.92
26	k	6052	BCR	C35-C13-C14	-2.11	119.97	122.92
26	b	6047	BCR	C34-C9-C10	-2.11	119.97	122.92
26	K	1051	BCR	C35-C13-C14	-2.10	119.97	122.92
26	t	1046	BCR	C34-C9-C10	-2.10	119.98	122.92
26	T	6048	BCR	C34-C9-C10	-2.10	119.98	122.92
26	H	1049	BCR	C36-C18-C17	-2.10	119.98	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	6047	BCR	C35-C13-C14	-2.10	119.98	122.92
26	B	1048	BCR	C24-C25-C26	-2.10	116.53	121.54
26	B	1047	BCR	C36-C18-C17	-2.10	119.98	122.92
26	D	1050	BCR	C37-C22-C21	-2.10	119.98	122.92
26	D	1050	BCR	C36-C18-C17	-2.10	119.98	122.92
26	B	1047	BCR	C35-C13-C14	-2.10	119.99	122.92
26	B	1047	BCR	C34-C9-C10	-2.09	119.99	122.92
26	Z	1053	BCR	C34-C9-C10	-2.09	119.99	122.92
26	Z	1053	BCR	C35-C13-C14	-2.09	119.99	122.92
26	K	1051	BCR	C36-C18-C17	-2.09	119.99	122.92
26	C	1054	BCR	C34-C9-C10	-2.09	120.00	122.92
26	B	1048	BCR	C35-C13-C14	-2.09	120.00	122.92
26	b	6045	BCR	C35-C13-C14	-2.09	120.00	122.92
26	k	6052	BCR	C34-C9-C10	-2.09	120.00	122.92
23	c	6029	CLA	CMD-C2D-C3D	-2.09	121.02	124.89
26	h	6049	BCR	C34-C9-C10	-2.09	120.00	122.92
26	z	6053	BCR	C35-C13-C14	-2.08	120.00	122.92
23	d	6008	CLA	CMD-C2D-C3D	-2.08	121.03	124.89
26	H	1049	BCR	C37-C22-C21	-2.08	120.00	122.92
26	C	1052	BCR	C35-C13-C14	-2.08	120.00	122.92
26	k	6051	BCR	C36-C18-C17	-2.08	120.00	122.92
23	D	1008	CLA	CMD-C2D-C3D	-2.08	121.03	124.89
26	C	1052	BCR	C34-C9-C10	-2.08	120.01	122.92
26	B	1045	BCR	C34-C9-C10	-2.08	120.01	122.92
26	Z	1053	BCR	C36-C18-C17	-2.08	120.01	122.92
26	d	6050	BCR	C37-C22-C21	-2.08	120.01	122.92
26	T	6046	BCR	C34-C9-C10	-2.08	120.01	122.92
26	K	1051	BCR	C37-C22-C21	-2.08	120.01	122.92
26	k	6052	BCR	C36-C18-C17	-2.08	120.01	122.92
23	C	1029	CLA	CMD-C2D-C3D	-2.08	121.04	124.89
26	d	6050	BCR	C36-C18-C17	-2.08	120.02	122.92
26	z	6053	BCR	C36-C18-C17	-2.08	120.02	122.92
26	C	1054	BCR	C36-C18-C17	-2.07	120.02	122.92
26	H	1049	BCR	C34-C9-C10	-2.07	120.02	122.92
26	C	1052	BCR	C36-C18-C17	-2.07	120.02	122.92
26	c	6054	BCR	C34-C9-C10	-2.07	120.02	122.92
26	b	6045	BCR	C34-C9-C10	-2.07	120.03	122.92
26	B	1045	BCR	C37-C22-C21	-2.07	120.03	122.92
26	D	1050	BCR	C34-C9-C10	-2.07	120.03	122.92
26	Z	1053	BCR	C37-C22-C21	-2.07	120.03	122.92
26	c	6054	BCR	C36-C18-C17	-2.06	120.03	122.92
26	D	1050	BCR	C35-C13-C14	-2.06	120.03	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	6048	BCR	C35-C13-C14	-2.06	120.03	122.92
26	b	6045	BCR	C36-C18-C17	-2.06	120.04	122.92
26	C	1054	BCR	C35-C13-C14	-2.06	120.04	122.92
23	B	1021	CLA	CMD-C2D-C3D	-2.06	121.07	124.89
26	b	6045	BCR	C37-C22-C21	-2.06	120.04	122.92
26	B	1048	BCR	C36-C18-C17	-2.06	120.04	122.92
26	B	1045	BCR	C36-C18-C17	-2.06	120.04	122.92
26	h	6049	BCR	C37-C22-C21	-2.06	120.04	122.92
26	K	1051	BCR	C34-C9-C10	-2.06	120.04	122.92
25	d	6042	PQ9	C41-C42-C43	-2.06	120.45	127.80
26	c	6054	BCR	C35-C13-C14	-2.06	120.04	122.92
26	T	6048	BCR	C36-C18-C17	-2.06	120.04	122.92
26	z	6053	BCR	C37-C22-C21	-2.06	120.04	122.92
26	k	6051	BCR	C34-C9-C10	-2.06	120.04	122.92
26	B	1045	BCR	C35-C13-C14	-2.06	120.04	122.92
23	k	6034	CLA	CMD-C2D-C3D	-2.05	121.08	124.89
26	H	1049	BCR	C35-C13-C14	-2.05	120.05	122.92
23	b	6021	CLA	CMD-C2D-C3D	-2.05	121.08	124.89
26	d	6050	BCR	C35-C13-C14	-2.05	120.05	122.92
26	C	1054	BCR	C37-C22-C21	-2.05	120.05	122.92
26	c	6054	BCR	C37-C22-C21	-2.05	120.05	122.92
25	A	1043	PQ9	C41-C42-C43	-2.05	120.49	127.80
26	A	1044	BCR	C8-C7-C6	-2.05	121.52	127.25
25	a	6043	PQ9	C41-C42-C43	-2.05	120.50	127.80
26	k	6051	BCR	C37-C22-C21	-2.05	120.06	122.92
25	D	1042	PQ9	C41-C42-C43	-2.05	120.50	127.80
26	d	6050	BCR	C34-C9-C10	-2.05	120.06	122.92
26	a	6044	BCR	C8-C7-C6	-2.04	121.53	127.25
23	c	6035	CLA	CMD-C2D-C3D	-2.04	121.10	124.89
23	c	6026	CLA	CMD-C2D-C3D	-2.04	121.10	124.89
24	a	6038	PHO	C1B-NB-C4B	-2.04	102.48	106.52
23	d	6008	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
23	D	1008	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
23	A	1003	CLA	CMD-C2D-C3D	-2.04	121.11	124.89
23	b	6023	CLA	CMD-C2D-C3D	-2.03	121.12	124.89
24	A	1038	PHO	C1B-NB-C4B	-2.03	102.50	106.52
23	a	6003	CLA	CMD-C2D-C3D	-2.03	121.12	124.89
23	C	1033	CLA	CMD-C2D-C3D	-2.03	121.12	124.89
23	K	1034	CLA	CMD-C2D-C3D	-2.03	121.13	124.89
23	b	6024	CLA	CMD-C2D-C3D	-2.03	121.13	124.89
23	B	1015	CLA	CMD-C2D-C3D	-2.02	121.14	124.89
23	b	6018	CLA	CMD-C2D-C3D	-2.02	121.14	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6033	CLA	CMD-C2D-C3D	-2.02	121.14	124.89
23	C	1035	CLA	CMD-C2D-C3D	-2.02	121.14	124.89
23	B	1020	CLA	CMD-C2D-C3D	-2.02	121.14	124.89
23	C	1026	CLA	CMD-C2D-C3D	-2.02	121.14	124.89
23	B	1024	CLA	CMD-C2D-C3D	-2.02	121.15	124.89
26	h	6049	BCR	C35-C13-C14	-2.02	120.10	122.92
23	b	6015	CLA	CMD-C2D-C3D	-2.02	121.15	124.89
23	d	6005	CLA	CMD-C2D-C3D	-2.02	121.15	124.89
24	D	1039	PHO	C1B-NB-C4B	-2.01	102.53	106.52
24	d	6039	PHO	C1B-NB-C4B	-2.01	102.53	106.52
23	B	1023	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	A	1007	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	c	6032	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	C	1031	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	c	6025	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	B	1022	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	C	1025	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	B	1018	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
23	b	6022	CLA	CMD-C2D-C3D	-2.01	121.16	124.89
26	T	6046	BCR	C2-C1-C6	-2.01	107.33	110.48
26	a	6044	BCR	C27-C26-C25	-2.01	119.79	122.74
23	B	1013	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	D	1005	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	b	6020	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	b	6010	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
26	a	6044	BCR	C29-C30-C25	-2.01	107.34	110.48
23	c	6031	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	B	1014	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	b	6012	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	a	6006	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	b	6019	CLA	CMD-C2D-C3D	-2.01	121.17	124.89
23	b	6009	CLA	CMD-C2D-C3D	-2.00	121.17	124.89
23	c	6027	CLA	CMD-C2D-C3D	-2.00	121.18	124.89
23	H	1017	CLA	CMD-C2D-C3D	-2.00	121.18	124.89
26	A	1044	BCR	C27-C26-C25	-2.00	119.80	122.74
23	C	1027	CLA	CMD-C2D-C3D	-2.00	121.18	124.89
24	A	1038	PHO	C2C-C1C-NC	2.01	112.80	109.82
24	D	1039	PHO	C2C-C1C-NC	2.02	112.80	109.82
24	a	6038	PHO	C2C-C1C-NC	2.02	112.81	109.82
24	d	6039	PHO	C2C-C1C-NC	2.02	112.81	109.82
26	k	6052	BCR	C24-C25-C26	2.04	126.41	121.54
26	C	1052	BCR	C24-C25-C26	2.06	126.45	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6009	CLA	O2A-CGA-CBA	2.21	118.32	111.90
23	B	1009	CLA	O2A-CGA-CBA	2.21	118.33	111.90
23	B	1011	CLA	CMC-C2C-C1C	2.31	128.52	125.02
23	C	1030	CLA	CAC-C3C-C4C	2.31	128.09	124.83
25	D	1042	PQ9	C45-C43-C44	2.31	120.00	114.60
25	d	6042	PQ9	C45-C43-C44	2.31	120.00	114.60
23	b	6011	CLA	CMC-C2C-C1C	2.32	128.53	125.02
23	c	6030	CLA	CAC-C3C-C4C	2.32	128.10	124.83
23	B	1009	CLA	CMC-C2C-C1C	2.33	128.56	125.02
25	a	6043	PQ9	C45-C43-C44	2.33	120.05	114.60
25	A	1043	PQ9	C45-C43-C44	2.33	120.05	114.60
23	b	6009	CLA	CMC-C2C-C1C	2.35	128.59	125.02
26	b	6047	BCR	C23-C24-C25	2.36	133.85	127.25
23	B	1015	CLA	CMC-C2C-C1C	2.36	128.60	125.02
26	B	1047	BCR	C23-C24-C25	2.37	133.90	127.25
23	c	6025	CLA	CMC-C2C-C1C	2.37	128.62	125.02
23	b	6015	CLA	CMC-C2C-C1C	2.38	128.63	125.02
23	C	1031	CLA	CMC-C2C-C1C	2.38	128.63	125.02
23	b	6016	CLA	CMC-C2C-C1C	2.38	128.64	125.02
23	b	6023	CLA	O2A-CGA-CBA	2.38	118.84	111.90
23	b	6013	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	c	6036	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	b	6019	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	C	1027	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	C	1036	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	B	1019	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	B	1013	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	C	1028	CLA	CMC-C2C-C1C	2.39	128.64	125.02
23	A	1006	CLA	CMC-C2C-C1C	2.39	128.65	125.02
23	c	6028	CLA	CMC-C2C-C1C	2.39	128.65	125.02
26	B	1048	BCR	C23-C24-C25	2.39	133.94	127.25
23	B	1020	CLA	CMC-C2C-C1C	2.39	128.65	125.02
23	B	1023	CLA	O2A-CGA-CBA	2.39	118.86	111.90
23	h	6017	CLA	CMC-C2C-C1C	2.39	128.65	125.02
23	A	1003	CLA	CMC-C2C-C1C	2.40	128.65	125.02
23	d	6005	CLA	CMC-C2C-C1C	2.40	128.65	125.02
23	B	1024	CLA	CMC-C2C-C1C	2.40	128.65	125.02
23	H	1017	CLA	CMC-C2C-C1C	2.40	128.65	125.02
23	c	6035	CLA	CMC-C2C-C1C	2.40	128.65	125.02
26	T	6048	BCR	C23-C24-C25	2.40	133.96	127.25
23	a	6003	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	C	1035	CLA	CMC-C2C-C1C	2.40	128.66	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1025	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	B	1022	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	b	6020	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	C	1032	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	D	1005	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	C	1033	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	a	6007	CLA	CMC-C2C-C1C	2.41	128.67	125.02
23	c	6032	CLA	CMC-C2C-C1C	2.41	128.67	125.02
23	B	1016	CLA	CMC-C2C-C1C	2.41	128.67	125.02
23	b	6022	CLA	CMC-C2C-C1C	2.41	128.67	125.02
23	c	6037	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	c	6027	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	b	6024	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	B	1014	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	c	6033	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	A	1007	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	b	6012	CLA	CMC-C2C-C1C	2.41	128.68	125.02
23	C	1026	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	c	6031	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	d	6004	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	B	1018	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	c	6026	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	c	6029	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	a	6006	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	B	1012	CLA	CMC-C2C-C1C	2.42	128.69	125.02
23	C	1037	CLA	CMC-C2C-C1C	2.43	128.70	125.02
23	K	1034	CLA	CMC-C2C-C1C	2.43	128.70	125.02
23	D	1004	CLA	CMC-C2C-C1C	2.43	128.70	125.02
23	b	6014	CLA	CMC-C2C-C1C	2.43	128.71	125.02
23	k	6034	CLA	CMC-C2C-C1C	2.44	128.72	125.02
23	C	1029	CLA	CMC-C2C-C1C	2.44	128.72	125.02
23	d	6008	CLA	CMB-C2B-C3B	2.44	129.42	124.89
23	b	6010	CLA	CMB-C2B-C3B	2.45	129.43	124.89
23	b	6018	CLA	CMC-C2C-C1C	2.45	128.73	125.02
23	b	6021	CLA	CMC-C2C-C1C	2.45	128.74	125.02
23	D	1008	CLA	CMB-C2B-C3B	2.45	129.44	124.89
23	b	6010	CLA	CMC-C2C-C1C	2.45	128.74	125.02
23	B	1010	CLA	CMB-C2B-C3B	2.46	129.46	124.89
23	B	1010	CLA	CMC-C2C-C1C	2.46	128.75	125.02
23	B	1021	CLA	CMC-C2C-C1C	2.47	128.77	125.02
23	b	6021	CLA	O2A-CGA-CBA	2.48	119.11	111.90
23	b	6011	CLA	CAC-C3C-C4C	2.48	128.33	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1011	CLA	CAC-C3C-C4C	2.49	128.34	124.83
23	B	1021	CLA	O2A-CGA-CBA	2.49	119.14	111.90
23	c	6030	CLA	CMC-C2C-C1C	2.49	128.79	125.02
23	B	1021	CLA	CMB-C2B-C3B	2.49	129.51	124.89
23	B	1023	CLA	CMC-C2C-C1C	2.49	128.80	125.02
23	C	1030	CLA	CMC-C2C-C1C	2.49	128.80	125.02
23	B	1011	CLA	CMB-C2B-C3B	2.49	129.52	124.89
23	b	6023	CLA	CMC-C2C-C1C	2.50	128.81	125.02
23	b	6011	CLA	CMB-C2B-C3B	2.50	129.53	124.89
23	b	6023	CLA	CMB-C2B-C3B	2.51	129.55	124.89
23	b	6021	CLA	CMB-C2B-C3B	2.51	129.56	124.89
23	B	1023	CLA	CMB-C2B-C3B	2.52	129.56	124.89
23	d	6008	CLA	CMC-C2C-C1C	2.53	128.85	125.02
23	D	1008	CLA	CMC-C2C-C1C	2.53	128.85	125.02
23	B	1021	CLA	CAC-C3C-C4C	2.56	128.45	124.83
23	b	6021	CLA	CAC-C3C-C4C	2.58	128.47	124.83
23	C	1029	CLA	CMB-C2B-C3B	2.58	129.68	124.89
23	c	6029	CLA	CMB-C2B-C3B	2.59	129.69	124.89
23	b	6020	CLA	CMB-C2B-C3B	2.59	129.69	124.89
23	b	6024	CLA	CAC-C3C-C4C	2.59	128.48	124.83
23	c	6026	CLA	CMB-C2B-C3B	2.59	129.69	124.89
23	c	6030	CLA	O2A-CGA-CBA	2.59	119.45	111.90
23	b	6015	CLA	CMB-C2B-C3B	2.60	129.71	124.89
26	a	6044	BCR	C23-C24-C25	2.60	134.52	127.25
23	b	6018	CLA	CAC-C3C-C4C	2.60	128.49	124.83
23	c	6031	CLA	CAC-C3C-C4C	2.60	128.49	124.83
23	C	1026	CLA	CMB-C2B-C3B	2.60	129.71	124.89
26	A	1044	BCR	C23-C24-C25	2.60	134.53	127.25
23	b	6024	CLA	CMB-C2B-C3B	2.60	129.72	124.89
23	C	1030	CLA	O2A-CGA-CBA	2.60	119.47	111.90
23	c	6037	CLA	CAC-C3C-C4C	2.60	128.50	124.83
23	b	6014	CLA	CMB-C2B-C3B	2.60	129.72	124.89
23	b	6016	CLA	CMB-C2B-C3B	2.60	129.72	124.89
23	c	6027	CLA	CMB-C2B-C3B	2.60	129.72	124.89
23	D	1005	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	B	1015	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	B	1020	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	b	6013	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	B	1024	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	a	6003	CLA	CMB-C2B-C3B	2.61	129.73	124.89
23	d	6005	CLA	CMB-C2B-C3B	2.61	129.74	124.89
23	c	6036	CLA	CMB-C2B-C3B	2.61	129.74	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	6017	CLA	CMB-C2B-C3B	2.61	129.74	124.89
23	c	6033	CLA	CAC-C3C-C4C	2.61	128.51	124.83
23	c	6028	CLA	CMB-C2B-C3B	2.61	129.74	124.89
23	c	6032	CLA	CMB-C2B-C3B	2.61	129.74	124.89
23	B	1014	CLA	CMB-C2B-C3B	2.61	129.74	124.89
23	b	6012	CLA	CAC-C3C-C4C	2.62	128.52	124.83
23	b	6018	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	A	1003	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	C	1032	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	c	6036	CLA	CAC-C3C-C4C	2.62	128.52	124.83
23	B	1018	CLA	CAC-C3C-C4C	2.62	128.52	124.83
23	a	6007	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	b	6019	CLA	CAC-C3C-C4C	2.62	128.52	124.83
23	B	1019	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	A	1007	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	C	1033	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	d	6004	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	K	1034	CLA	CMB-C2B-C3B	2.62	129.76	124.89
23	C	1027	CLA	CMB-C2B-C3B	2.62	129.76	124.89
23	C	1028	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	k	6034	CLA	CMB-C2B-C3B	2.62	129.76	124.89
23	B	1016	CLA	CMB-C2B-C3B	2.62	129.76	124.89
23	B	1012	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	C	1037	CLA	CAC-C3C-C4C	2.62	128.53	124.83
23	b	6012	CLA	CMB-C2B-C3B	2.63	129.76	124.89
23	d	6005	CLA	CAC-C3C-C4C	2.63	128.53	124.83
23	C	1036	CLA	CMB-C2B-C3B	2.63	129.77	124.89
23	B	1018	CLA	CMB-C2B-C3B	2.63	129.77	124.89
23	D	1005	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	C	1036	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	B	1013	CLA	CMB-C2B-C3B	2.63	129.78	124.89
23	b	6013	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	C	1031	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	H	1017	CLA	CMB-C2B-C3B	2.63	129.78	124.89
23	b	6019	CLA	CMB-C2B-C3B	2.63	129.78	124.89
23	c	6030	CLA	C4-C3-C5	2.63	119.86	115.29
23	c	6025	CLA	CMB-C2B-C3B	2.63	129.78	124.89
23	D	1004	CLA	CMB-C2B-C3B	2.64	129.78	124.89
23	C	1031	CLA	CMB-C2B-C3B	2.64	129.78	124.89
23	A	1007	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	c	6025	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	d	6004	CLA	CMB-C2B-C3B	2.64	129.79	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6033	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	B	1012	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	A	1006	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	C	1028	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	B	1015	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	C	1035	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	C	1025	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	b	6022	CLA	CAC-C3C-C4C	2.64	128.55	124.83
23	B	1019	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	C	1035	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	C	1037	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	b	6009	CLA	C4-C3-C5	2.64	119.87	115.29
23	b	6020	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	C	1025	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	D	1004	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	B	1009	CLA	C4-C3-C5	2.64	119.88	115.29
23	c	6037	CLA	CMB-C2B-C3B	2.64	129.80	124.89
23	B	1020	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	B	1024	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	c	6032	CLA	CAC-C3C-C4C	2.64	128.56	124.83
23	c	6028	CLA	CAC-C3C-C4C	2.65	128.56	124.83
23	b	6014	CLA	CAC-C3C-C4C	2.65	128.56	124.83
23	c	6027	CLA	CAC-C3C-C4C	2.65	128.56	124.83
25	d	6042	PQ9	C6-C5-C4	2.65	120.46	114.84
23	C	1032	CLA	CAC-C3C-C4C	2.65	128.56	124.83
23	c	6035	CLA	CMB-C2B-C3B	2.65	129.81	124.89
23	k	6034	CLA	CAC-C3C-C4C	2.65	128.56	124.83
23	C	1030	CLA	C4-C3-C5	2.65	119.88	115.29
23	C	1026	CLA	CAC-C3C-C4C	2.65	128.57	124.83
23	c	6026	CLA	CAC-C3C-C4C	2.65	128.57	124.83
23	A	1006	CLA	CMB-C2B-C3B	2.65	129.81	124.89
23	B	1022	CLA	CAC-C3C-C4C	2.65	128.57	124.83
23	B	1022	CLA	CMB-C2B-C3B	2.65	129.81	124.89
23	b	6016	CLA	CAC-C3C-C4C	2.65	128.57	124.83
23	h	6017	CLA	CAC-C3C-C4C	2.65	128.57	124.83
23	a	6006	CLA	CAC-C3C-C4C	2.66	128.57	124.83
23	B	1014	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	B	1013	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	K	1034	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	H	1017	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	C	1033	CLA	CMB-C2B-C3B	2.66	129.83	124.89
25	D	1042	PQ9	C6-C5-C4	2.66	120.49	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6007	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	c	6031	CLA	CMB-C2B-C3B	2.66	129.83	124.89
23	B	1016	CLA	CAC-C3C-C4C	2.66	128.59	124.83
23	b	6022	CLA	CMB-C2B-C3B	2.66	129.84	124.89
23	A	1003	CLA	CAC-C3C-C4C	2.67	128.59	124.83
23	c	6035	CLA	CAC-C3C-C4C	2.67	128.59	124.83
23	a	6006	CLA	CMB-C2B-C3B	2.67	129.84	124.89
23	C	1027	CLA	CAC-C3C-C4C	2.67	128.59	124.83
23	a	6003	CLA	CAC-C3C-C4C	2.68	128.60	124.83
23	b	6015	CLA	CAC-C3C-C4C	2.68	128.60	124.83
23	b	6019	CLA	C4-C3-C5	2.68	119.94	115.29
23	C	1030	CLA	CMB-C2B-C3B	2.68	129.87	124.89
23	b	6009	CLA	CAC-C3C-C4C	2.68	128.61	124.83
23	b	6016	CLA	C4-C3-C5	2.68	119.94	115.29
23	B	1023	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	a	6043	PQ9	C34-C33-C35	2.69	119.95	115.29
23	c	6025	CLA	C4-C3-C5	2.69	119.95	115.29
23	c	6028	CLA	C4-C3-C5	2.69	119.96	115.29
23	b	6009	CLA	CMB-C2B-C3B	2.69	129.89	124.89
23	B	1016	CLA	C4-C3-C5	2.69	119.96	115.29
25	d	6042	PQ9	C14-C13-C15	2.69	119.96	115.29
23	C	1028	CLA	C4-C3-C5	2.69	119.96	115.29
23	d	6005	CLA	C4-C3-C5	2.69	119.96	115.29
25	a	6043	PQ9	C29-C28-C30	2.69	119.96	115.29
23	b	6023	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	A	1043	PQ9	C6-C5-C4	2.69	120.56	114.84
23	B	1011	CLA	O2A-CGA-CBA	2.69	119.74	111.90
23	C	1025	CLA	C4-C3-C5	2.69	119.96	115.29
23	C	1037	CLA	C4-C3-C5	2.70	119.97	115.29
23	b	6011	CLA	O2A-CGA-CBA	2.70	119.74	111.90
23	b	6012	CLA	C4-C3-C5	2.70	119.97	115.29
25	A	1043	PQ9	C29-C28-C30	2.70	119.97	115.29
25	A	1043	PQ9	C34-C33-C35	2.70	119.97	115.29
25	a	6043	PQ9	C6-C5-C4	2.70	120.57	114.84
23	d	6004	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	b	6018	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	1009	CLA	CAC-C3C-C4C	2.70	128.64	124.83
24	a	6038	PHO	C4-C3-C5	2.70	119.97	115.29
23	D	1005	CLA	C4-C3-C5	2.70	119.97	115.29
23	c	6030	CLA	CMB-C2B-C3B	2.70	129.91	124.89
23	b	6020	CLA	C4-C3-C5	2.70	119.98	115.29
25	D	1042	PQ9	C34-C33-C35	2.70	119.98	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1010	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	1019	CLA	C4-C3-C5	2.71	119.98	115.29
23	c	6033	CLA	C4-C3-C5	2.71	119.98	115.29
23	b	6023	CLA	C4-C3-C5	2.71	119.98	115.29
25	A	1043	PQ9	C24-C23-C25	2.71	119.98	115.29
23	c	6035	CLA	C4-C3-C5	2.71	119.99	115.29
25	A	1043	PQ9	C19-C18-C20	2.71	119.99	115.29
23	B	1023	CLA	CAC-C3C-C4C	2.71	128.65	124.83
23	B	1020	CLA	C4-C3-C5	2.71	119.99	115.29
23	b	6024	CLA	C4-C3-C5	2.71	119.99	115.29
23	c	6036	CLA	C4-C3-C5	2.71	119.99	115.29
23	B	1022	CLA	C4-C3-C5	2.71	119.99	115.29
23	B	1012	CLA	C4-C3-C5	2.71	119.99	115.29
25	a	6043	PQ9	C19-C18-C20	2.71	119.99	115.29
23	K	1034	CLA	C4-C3-C5	2.71	119.99	115.29
23	c	6028	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	C	1035	CLA	C4-C3-C5	2.71	119.99	115.29
23	b	6010	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	C	1027	CLA	C4-C3-C5	2.71	119.99	115.29
23	B	1011	CLA	C4-C3-C5	2.71	119.99	115.29
23	B	1009	CLA	CMB-C2B-C3B	2.71	129.93	124.89
23	b	6011	CLA	C4-C3-C5	2.71	119.99	115.29
23	b	6018	CLA	C4-C3-C5	2.71	119.99	115.29
23	C	1033	CLA	C4-C3-C5	2.71	119.99	115.29
23	D	1004	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	C	1031	CLA	C4-C3-C5	2.71	120.00	115.29
23	c	6027	CLA	C4-C3-C5	2.71	120.00	115.29
23	B	1018	CLA	C4-C3-C5	2.71	120.00	115.29
23	b	6013	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	C	1026	CLA	C4-C3-C5	2.72	120.00	115.29
23	c	6037	CLA	C4-C3-C5	2.72	120.00	115.29
23	C	1032	CLA	C4-C3-C5	2.72	120.00	115.29
23	B	1014	CLA	C4-C3-C5	2.72	120.00	115.29
23	a	6003	CLA	C4-C3-C5	2.72	120.00	115.29
25	a	6043	PQ9	C24-C23-C25	2.72	120.00	115.29
23	c	6031	CLA	C4-C3-C5	2.72	120.00	115.29
23	c	6026	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	A	1003	CLA	C4-C3-C5	2.72	120.00	115.29
25	A	1043	PQ9	C39-C38-C40	2.72	120.00	115.29
23	c	6029	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	A	1006	CLA	C4-C3-C5	2.72	120.01	115.29
23	a	6006	CLA	C4-C3-C5	2.72	120.01	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6004	CLA	C4-C3-C5	2.72	120.01	115.29
23	h	6017	CLA	C4-C3-C5	2.72	120.01	115.29
23	C	1028	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	B	1018	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	D	1042	PQ9	C14-C13-C15	2.72	120.01	115.29
25	a	6043	PQ9	C14-C13-C15	2.72	120.01	115.29
23	B	1023	CLA	C4-C3-C5	2.72	120.01	115.29
24	A	1038	PHO	C4-C3-C5	2.72	120.01	115.29
23	k	6034	CLA	C4-C3-C5	2.72	120.01	115.29
25	A	1043	PQ9	C14-C13-C15	2.72	120.01	115.29
23	d	6008	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	H	1017	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	1029	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	c	6026	CLA	C4-C3-C5	2.72	120.02	115.29
23	c	6032	CLA	C4-C3-C5	2.73	120.02	115.29
25	d	6042	PQ9	C24-C23-C25	2.73	120.02	115.29
25	D	1042	PQ9	C24-C23-C25	2.73	120.02	115.29
23	D	1008	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	D	1004	CLA	C4-C3-C5	2.73	120.02	115.29
23	b	6023	CLA	CAC-C3C-C4C	2.73	128.68	124.83
23	B	1024	CLA	C4-C3-C5	2.73	120.02	115.29
25	d	6042	PQ9	C34-C33-C35	2.73	120.02	115.29
23	b	6022	CLA	C4-C3-C5	2.73	120.02	115.29
25	D	1042	PQ9	C29-C28-C30	2.73	120.02	115.29
23	b	6015	CLA	C4-C3-C5	2.73	120.02	115.29
25	D	1042	PQ9	C39-C38-C40	2.73	120.02	115.29
25	a	6043	PQ9	C39-C38-C40	2.73	120.02	115.29
25	d	6042	PQ9	C39-C38-C40	2.73	120.03	115.29
23	b	6024	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	C	1036	CLA	C4-C3-C5	2.73	120.03	115.29
23	C	1025	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	d	6042	PQ9	C19-C18-C20	2.73	120.03	115.29
24	D	1039	PHO	C4-C3-C5	2.73	120.03	115.29
23	H	1017	CLA	C4-C3-C5	2.74	120.03	115.29
23	a	6007	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	B	1013	CLA	C4-C3-C5	2.74	120.04	115.29
23	d	6008	CLA	C4-C3-C5	2.74	120.04	115.29
25	D	1042	PQ9	C19-C18-C20	2.74	120.04	115.29
23	C	1032	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	C	1033	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	c	6025	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	d	6042	PQ9	C29-C28-C30	2.74	120.04	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1015	CLA	C4-C3-C5	2.74	120.04	115.29
23	B	1021	CLA	C4-C3-C5	2.74	120.04	115.29
23	b	6014	CLA	C4-C3-C5	2.74	120.04	115.29
23	K	1034	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	D	1008	CLA	C4-C3-C5	2.74	120.04	115.29
23	b	6021	CLA	C4-C3-C5	2.74	120.05	115.29
23	B	1015	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	C	1027	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	B	1009	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	C	1026	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	A	1006	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	b	6009	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	h	6017	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	A	1007	CLA	C4-C3-C5	2.75	120.05	115.29
23	b	6010	CLA	C4-C3-C5	2.75	120.05	115.29
23	A	1003	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	a	6007	CLA	C4-C3-C5	2.75	120.06	115.29
23	B	1013	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	C	1035	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	c	6037	CLA	O2A-CGA-CBA	2.75	119.90	111.90
23	c	6032	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	b	6020	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	B	1020	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	d	6039	PHO	C4-C3-C5	2.75	120.06	115.29
23	C	1037	CLA	O2A-CGA-CBA	2.75	119.91	111.90
23	B	1022	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	a	6006	CLA	O2A-CGA-CBA	2.75	119.91	111.90
23	b	6013	CLA	C4-C3-C5	2.75	120.07	115.29
23	C	1031	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	B	1024	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	b	6010	CLA	CAC-C3C-C4C	2.75	128.72	124.83
23	k	6034	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	c	6036	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	a	6003	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	B	1012	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	B	1010	CLA	CAC-C3C-C4C	2.76	128.72	124.83
23	B	1010	CLA	C4-C3-C5	2.76	120.08	115.29
23	b	6016	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	c	6035	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	c	6029	CLA	CAC-C3C-C4C	2.76	128.72	124.83
23	c	6030	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	B	1016	CLA	CHB-C4A-NA	2.76	128.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1036	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	a	6006	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	A	1007	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	b	6022	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	C	1029	CLA	CAC-C3C-C4C	2.76	128.73	124.83
23	b	6012	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6037	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	b	6015	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	B	1014	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6036	CLA	O2A-CGA-CBA	2.77	119.95	111.90
23	D	1004	CLA	O2A-CGA-CBA	2.77	119.95	111.90
23	D	1005	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6033	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6027	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	b	6018	CLA	O2A-CGA-CBA	2.77	119.96	111.90
23	C	1037	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	b	6024	CLA	O2A-CGA-CBA	2.77	119.96	111.90
23	d	6004	CLA	O2A-CGA-CBA	2.77	119.96	111.90
23	d	6005	CLA	O2A-CGA-CBA	2.77	119.96	111.90
23	A	1006	CLA	O2A-CGA-CBA	2.77	119.97	111.90
23	b	6014	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	C	1036	CLA	O2A-CGA-CBA	2.77	119.97	111.90
23	C	1026	CLA	O2A-CGA-CBA	2.78	119.98	111.90
23	B	1024	CLA	O2A-CGA-CBA	2.78	119.98	111.90
23	C	1030	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	B	1019	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	b	6019	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	D	1005	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	c	6026	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	b	6012	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	B	1010	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	K	1034	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	b	6011	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	B	1013	CLA	O2A-CGA-CBA	2.78	119.99	111.90
23	B	1022	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	B	1015	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	c	6031	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	C	1031	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	b	6013	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	B	1012	CLA	O2A-CGA-CBA	2.78	120.00	111.90
23	c	6031	CLA	CHB-C4A-NA	2.79	128.36	124.51
23	A	1003	CLA	O2A-CGA-CBA	2.79	120.00	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6032	CLA	O2A-CGA-CBA	2.79	120.01	111.90
23	C	1032	CLA	O2A-CGA-CBA	2.79	120.01	111.90
23	D	1008	CLA	O2A-CGA-CBA	2.79	120.01	111.90
23	d	6008	CLA	O2A-CGA-CBA	2.79	120.01	111.90
23	b	6019	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	c	6035	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	b	6015	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	b	6016	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	B	1018	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	c	6028	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	b	6010	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	C	1028	CLA	O2A-CGA-CBA	2.79	120.02	111.90
23	B	1019	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	C	1035	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	a	6003	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	k	6034	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	a	6007	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	B	1016	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	c	6029	CLA	C4-C3-C5	2.79	120.14	115.29
23	C	1027	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	c	6027	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	c	6033	CLA	O2A-CGA-CBA	2.79	120.03	111.90
23	H	1017	CLA	O2A-CGA-CBA	2.80	120.03	111.90
23	d	6005	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	b	6022	CLA	O2A-CGA-CBA	2.80	120.04	111.90
23	C	1033	CLA	O2A-CGA-CBA	2.80	120.04	111.90
23	b	6021	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	C	1025	CLA	O2A-CGA-CBA	2.80	120.05	111.90
23	h	6017	CLA	O2A-CGA-CBA	2.80	120.05	111.90
23	C	1029	CLA	C4-C3-C5	2.80	120.15	115.29
23	A	1007	CLA	O2A-CGA-CBA	2.80	120.06	111.90
23	b	6014	CLA	O2A-CGA-CBA	2.81	120.06	111.90
23	B	1020	CLA	O2A-CGA-CBA	2.81	120.06	111.90
23	c	6025	CLA	O2A-CGA-CBA	2.81	120.06	111.90
23	B	1014	CLA	O2A-CGA-CBA	2.81	120.06	111.90
23	B	1021	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	b	6020	CLA	O2A-CGA-CBA	2.81	120.08	111.90
29	c	6057	DGD	O1G-C1A-C2A	2.81	120.09	111.90
23	B	1011	CLA	CHB-C4A-NA	2.82	128.41	124.51
30	d	6059	MGE	O1G-C1A-C2A	2.83	120.12	111.90
29	C	1057	DGD	O1G-C1A-C2A	2.83	120.13	111.90
29	c	6056	DGD	O1G-C1A-C2A	2.84	120.16	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	6062	MGE	O1G-C1A-C2A	2.84	120.17	111.90
30	L	1061	MGE	O1G-C1A-C2A	2.84	120.17	111.90
23	c	6029	CLA	O2A-CGA-CBA	2.84	120.17	111.90
27	a	6063	LHG	O8-C23-C24	2.84	120.17	111.90
30	l	6061	MGE	O1G-C1A-C2A	2.84	120.17	111.90
29	B	1058	DGD	O1G-C1A-C2A	2.84	120.17	111.90
23	C	1029	CLA	O2A-CGA-CBA	2.84	120.17	111.90
24	a	6038	PHO	O2A-CGA-CBA	2.84	120.17	111.90
24	A	1038	PHO	O2A-CGA-CBA	2.84	120.17	111.90
30	D	1059	MGE	O1G-C1A-C2A	2.84	120.17	111.90
29	C	1056	DGD	O1G-C1A-C2A	2.85	120.18	111.90
29	b	6058	DGD	O1G-C1A-C2A	2.85	120.19	111.90
30	b	6060	MGE	O1G-C1A-C2A	2.85	120.19	111.90
29	C	1055	DGD	O1G-C1A-C2A	2.85	120.20	111.90
27	A	1063	LHG	O8-C23-C24	2.85	120.20	111.90
29	c	6055	DGD	O1G-C1A-C2A	2.85	120.20	111.90
30	D	1062	MGE	O1G-C1A-C2A	2.85	120.20	111.90
30	B	1060	MGE	O1G-C1A-C2A	2.85	120.20	111.90
24	d	6039	PHO	O2A-CGA-CBA	2.86	120.21	111.90
24	D	1039	PHO	O2A-CGA-CBA	2.86	120.21	111.90
23	d	6008	CLA	CAC-C3C-C4C	2.89	128.90	124.83
23	D	1008	CLA	CAC-C3C-C4C	2.90	128.92	124.83
26	C	1052	BCR	C37-C22-C23	3.16	123.13	118.10
26	k	6052	BCR	C37-C22-C23	3.18	123.16	118.10
26	t	1046	BCR	C38-C26-C27	3.18	119.48	113.45
26	T	6046	BCR	C38-C26-C27	3.18	119.49	113.45
24	a	6038	PHO	C2B-C1B-NB	3.34	114.77	109.82
24	d	6039	PHO	C2B-C1B-NB	3.34	114.77	109.82
26	A	1044	BCR	C38-C26-C27	3.34	119.79	113.45
24	D	1039	PHO	C2B-C1B-NB	3.35	114.77	109.82
25	A	1043	PQ9	C11-C2-C1	3.36	119.61	116.88
26	a	6044	BCR	C38-C26-C27	3.36	119.84	113.45
25	a	6043	PQ9	C11-C2-C1	3.37	119.61	116.88
25	D	1042	PQ9	C11-C2-C1	3.37	119.61	116.88
24	A	1038	PHO	C2B-C1B-NB	3.37	114.81	109.82
26	c	6054	BCR	C38-C26-C27	3.39	119.88	113.45
26	C	1054	BCR	C38-C26-C27	3.39	119.89	113.45
26	H	1049	BCR	C38-C26-C27	3.41	119.91	113.45
26	h	6049	BCR	C38-C26-C27	3.41	119.92	113.45
25	d	6042	PQ9	C11-C2-C1	3.42	119.66	116.88
26	k	6051	BCR	C38-C26-C27	3.44	119.97	113.45
26	K	1051	BCR	C38-C26-C27	3.44	119.97	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	6049	BCR	C33-C5-C4	3.44	119.98	113.45
26	H	1049	BCR	C33-C5-C4	3.44	119.98	113.45
26	d	6050	BCR	C33-C5-C4	3.44	119.99	113.45
26	C	1052	BCR	C33-C5-C4	3.45	119.99	113.45
26	k	6052	BCR	C33-C5-C4	3.46	120.01	113.45
26	D	1050	BCR	C33-C5-C4	3.46	120.01	113.45
26	Z	1053	BCR	C38-C26-C27	3.46	120.01	113.45
26	B	1045	BCR	C38-C26-C27	3.46	120.01	113.45
26	b	6045	BCR	C38-C26-C27	3.46	120.02	113.45
26	K	1051	BCR	C33-C5-C4	3.46	120.02	113.45
26	B	1047	BCR	C33-C5-C4	3.46	120.02	113.45
26	b	6045	BCR	C33-C5-C4	3.46	120.02	113.45
26	k	6051	BCR	C33-C5-C4	3.46	120.02	113.45
26	z	6053	BCR	C33-C5-C4	3.46	120.02	113.45
26	B	1047	BCR	C38-C26-C27	3.46	120.02	113.45
26	C	1054	BCR	C33-C5-C4	3.46	120.02	113.45
26	b	6047	BCR	C33-C5-C4	3.47	120.03	113.45
26	Z	1053	BCR	C33-C5-C4	3.47	120.03	113.45
26	B	1045	BCR	C33-C5-C4	3.47	120.03	113.45
26	D	1050	BCR	C38-C26-C27	3.47	120.03	113.45
26	A	1044	BCR	C37-C22-C23	3.47	123.63	118.10
26	T	6048	BCR	C33-C5-C4	3.47	120.04	113.45
26	b	6047	BCR	C38-C26-C27	3.47	120.04	113.45
26	d	6050	BCR	C38-C26-C27	3.47	120.04	113.45
26	B	1048	BCR	C33-C5-C4	3.47	120.04	113.45
26	z	6053	BCR	C38-C26-C27	3.47	120.04	113.45
26	a	6044	BCR	C37-C22-C23	3.47	123.63	118.10
26	c	6054	BCR	C33-C5-C4	3.48	120.05	113.45
26	T	6048	BCR	C38-C26-C27	3.49	120.07	113.45
26	B	1048	BCR	C38-C26-C27	3.49	120.08	113.45
26	a	6044	BCR	C33-C5-C4	3.51	120.12	113.45
26	A	1044	BCR	C33-C5-C4	3.52	120.13	113.45
23	d	6008	CLA	O2D-CGD-CBD	3.57	117.67	111.30
23	D	1008	CLA	O2D-CGD-CBD	3.58	117.69	111.30
23	B	1011	CLA	C3B-C4B-NB	3.73	114.03	109.21
23	b	6022	CLA	C3B-C4B-NB	3.74	114.05	109.21
23	b	6011	CLA	C3B-C4B-NB	3.75	114.05	109.21
23	C	1030	CLA	O2D-CGD-CBD	3.75	117.99	111.30
23	C	1029	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	d	6005	CLA	C3B-C4B-NB	3.76	114.07	109.21
23	B	1024	CLA	C3B-C4B-NB	3.76	114.07	109.21
23	c	6025	CLA	C3B-C4B-NB	3.76	114.07	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1006	CLA	C3B-C4B-NB	3.76	114.07	109.21
23	D	1005	CLA	C3B-C4B-NB	3.76	114.07	109.21
23	K	1034	CLA	C3B-C4B-NB	3.76	114.07	109.21
23	C	1025	CLA	C3B-C4B-NB	3.76	114.08	109.21
23	c	6030	CLA	O2D-CGD-CBD	3.76	118.03	111.30
23	b	6024	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	c	6029	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	d	6004	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	B	1023	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	c	6031	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	k	6034	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	C	1028	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	b	6014	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	B	1022	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	B	1014	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	a	6003	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	c	6032	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	C	1027	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	b	6023	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	C	1033	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	c	6030	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	c	6028	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	B	1012	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	a	6006	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	C	1036	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	B	1019	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	b	6012	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	h	6017	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	B	1018	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	A	1003	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	C	1031	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	b	6019	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	C	1037	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	b	6021	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	c	6027	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	b	6018	CLA	C3B-C4B-NB	3.79	114.12	109.21
23	A	1007	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	B	1016	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	c	6037	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	B	1021	CLA	C3B-C4B-NB	3.80	114.13	109.21
23	D	1004	CLA	C3B-C4B-NB	3.80	114.13	109.21
23	a	6007	CLA	C3B-C4B-NB	3.80	114.13	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1030	CLA	C3B-C4B-NB	3.80	114.13	109.21
23	c	6035	CLA	C3B-C4B-NB	3.80	114.13	109.21
23	c	6026	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	C	1026	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	C	1032	CLA	C3B-C4B-NB	3.81	114.14	109.21
23	b	6013	CLA	C3B-C4B-NB	3.81	114.14	109.21
23	B	1013	CLA	C3B-C4B-NB	3.81	114.14	109.21
23	b	6016	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	H	1017	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	C	1035	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	c	6033	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	B	1015	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	B	1010	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	B	1009	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	b	6009	CLA	C3B-C4B-NB	3.83	114.17	109.21
23	b	6015	CLA	C3B-C4B-NB	3.83	114.17	109.21
23	c	6036	CLA	C3B-C4B-NB	3.84	114.17	109.21
23	B	1020	CLA	C3B-C4B-NB	3.84	114.17	109.21
23	b	6010	CLA	C3B-C4B-NB	3.84	114.18	109.21
24	A	1038	PHO	C2D-C1D-ND	3.84	115.51	109.82
26	t	1046	BCR	C33-C5-C4	3.85	120.75	113.45
23	b	6020	CLA	C3B-C4B-NB	3.85	114.19	109.21
24	D	1039	PHO	C2D-C1D-ND	3.85	115.52	109.82
24	d	6039	PHO	C2D-C1D-ND	3.85	115.53	109.82
24	a	6038	PHO	C2D-C1D-ND	3.86	115.54	109.82
26	T	6046	BCR	C33-C5-C4	3.87	120.79	113.45
23	D	1008	CLA	C3B-C4B-NB	3.88	114.22	109.21
26	a	6044	BCR	C30-C25-C24	3.88	126.65	115.73
26	A	1044	BCR	C30-C25-C24	3.89	126.65	115.73
26	t	1046	BCR	C7-C8-C9	3.89	132.06	126.21
26	T	6048	BCR	C30-C25-C24	3.89	126.67	115.73
26	B	1048	BCR	C30-C25-C24	3.89	126.67	115.73
23	d	6008	CLA	C3B-C4B-NB	3.90	114.25	109.21
23	B	1011	CLA	O2D-CGD-CBD	3.91	118.28	111.30
26	T	6046	BCR	C7-C8-C9	3.91	132.09	126.21
23	b	6011	CLA	O2D-CGD-CBD	3.92	118.30	111.30
26	B	1047	BCR	C30-C25-C24	3.92	126.75	115.73
26	b	6047	BCR	C30-C25-C24	3.93	126.77	115.73
26	b	6047	BCR	C37-C22-C23	3.99	124.46	118.10
26	T	6048	BCR	C37-C22-C23	4.00	124.47	118.10
26	B	1048	BCR	C37-C22-C23	4.01	124.48	118.10
26	B	1047	BCR	C37-C22-C23	4.01	124.49	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6009	CLA	O2D-CGD-CBD	4.07	118.58	111.30
23	B	1009	CLA	O2D-CGD-CBD	4.08	118.60	111.30
30	d	6059	MGE	O2G-C1B-C2B	4.11	120.08	111.55
30	D	1059	MGE	O2G-C1B-C2B	4.12	120.10	111.55
29	b	6058	DGD	O2G-C1B-C2B	4.13	120.12	111.55
29	c	6055	DGD	O2G-C1B-C2B	4.14	120.14	111.55
27	A	1063	LHG	O7-C7-C8	4.14	120.14	111.55
29	B	1058	DGD	O2G-C1B-C2B	4.14	120.14	111.55
29	C	1055	DGD	O2G-C1B-C2B	4.14	120.15	111.55
30	L	1061	MGE	O2G-C1B-C2B	4.15	120.16	111.55
30	B	1060	MGE	O2G-C1B-C2B	4.15	120.17	111.55
30	b	6060	MGE	O2G-C1B-C2B	4.15	120.18	111.55
27	a	6063	LHG	O7-C7-C8	4.15	120.18	111.55
30	l	6061	MGE	O2G-C1B-C2B	4.16	120.18	111.55
29	C	1057	DGD	O2G-C1B-C2B	4.16	120.19	111.55
29	c	6057	DGD	O2G-C1B-C2B	4.17	120.20	111.55
30	D	1062	MGE	O2G-C1B-C2B	4.17	120.21	111.55
29	C	1056	DGD	O2G-C1B-C2B	4.18	120.22	111.55
29	c	6056	DGD	O2G-C1B-C2B	4.18	120.24	111.55
23	c	6029	CLA	O2D-CGD-CBD	4.19	118.78	111.30
30	d	6062	MGE	O2G-C1B-C2B	4.19	120.25	111.55
26	T	6048	BCR	C24-C23-C22	4.19	132.50	126.21
26	B	1048	BCR	C24-C23-C22	4.20	132.53	126.21
23	C	1029	CLA	O2D-CGD-CBD	4.20	118.81	111.30
26	B	1047	BCR	C24-C23-C22	4.21	132.53	126.21
26	A	1044	BCR	C24-C23-C22	4.22	132.55	126.21
26	a	6044	BCR	C24-C23-C22	4.23	132.57	126.21
26	b	6047	BCR	C24-C23-C22	4.24	132.59	126.21
26	k	6052	BCR	C7-C8-C9	4.34	132.74	126.21
26	C	1052	BCR	C7-C8-C9	4.34	132.74	126.21
26	k	6052	BCR	C38-C26-C27	4.44	121.88	113.45
26	C	1052	BCR	C38-C26-C27	4.46	121.91	113.45
24	a	6038	PHO	C4D-C3D-CAD	4.59	113.92	105.41
24	A	1038	PHO	C4D-C3D-CAD	4.60	113.94	105.41
24	D	1039	PHO	C4D-C3D-CAD	4.61	113.97	105.41
24	d	6039	PHO	C4D-C3D-CAD	4.63	114.00	105.41
23	b	6010	CLA	O2D-CGD-CBD	4.77	119.82	111.30
23	B	1010	CLA	O2D-CGD-CBD	4.79	119.87	111.30
23	k	6034	CLA	O2D-CGD-CBD	4.82	119.91	111.30
23	B	1021	CLA	O2D-CGD-CBD	4.82	119.91	111.30
23	K	1034	CLA	O2D-CGD-CBD	4.83	119.92	111.30
23	b	6021	CLA	O2D-CGD-CBD	4.83	119.92	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6016	CLA	O2D-CGD-CBD	4.83	119.92	111.30
23	c	6032	CLA	O2D-CGD-CBD	4.83	119.92	111.30
23	D	1005	CLA	O2D-CGD-CBD	4.84	119.94	111.30
23	c	6033	CLA	O2D-CGD-CBD	4.84	119.94	111.30
23	C	1036	CLA	O2D-CGD-CBD	4.84	119.95	111.30
23	b	6022	CLA	O2D-CGD-CBD	4.85	119.96	111.30
23	B	1018	CLA	O2D-CGD-CBD	4.85	119.96	111.30
23	d	6005	CLA	O2D-CGD-CBD	4.85	119.96	111.30
23	c	6036	CLA	O2D-CGD-CBD	4.85	119.96	111.30
23	C	1032	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	c	6027	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	b	6024	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	C	1033	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	B	1016	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	B	1020	CLA	O2D-CGD-CBD	4.85	119.97	111.30
23	b	6018	CLA	O2D-CGD-CBD	4.86	119.98	111.30
23	B	1022	CLA	O2D-CGD-CBD	4.86	119.98	111.30
23	B	1024	CLA	O2D-CGD-CBD	4.86	119.98	111.30
23	c	6026	CLA	O2D-CGD-CBD	4.86	119.99	111.30
23	D	1004	CLA	O2D-CGD-CBD	4.86	119.99	111.30
23	C	1026	CLA	O2D-CGD-CBD	4.86	119.99	111.30
23	C	1025	CLA	O2D-CGD-CBD	4.87	120.00	111.30
23	B	1019	CLA	O2D-CGD-CBD	4.87	120.00	111.30
23	b	6014	CLA	O2D-CGD-CBD	4.87	120.00	111.30
23	C	1035	CLA	O2D-CGD-CBD	4.87	120.00	111.30
23	A	1007	CLA	O2D-CGD-CBD	4.87	120.00	111.30
23	b	6020	CLA	O2D-CGD-CBD	4.87	120.01	111.30
23	d	6004	CLA	O2D-CGD-CBD	4.87	120.01	111.30
23	b	6019	CLA	O2D-CGD-CBD	4.88	120.01	111.30
23	b	6013	CLA	O2D-CGD-CBD	4.88	120.01	111.30
23	C	1027	CLA	O2D-CGD-CBD	4.88	120.02	111.30
23	c	6025	CLA	O2D-CGD-CBD	4.88	120.02	111.30
23	B	1013	CLA	O2D-CGD-CBD	4.88	120.02	111.30
23	b	6012	CLA	O2D-CGD-CBD	4.89	120.03	111.30
23	B	1014	CLA	O2D-CGD-CBD	4.89	120.03	111.30
23	A	1006	CLA	O2D-CGD-CBD	4.89	120.03	111.30
23	a	6007	CLA	O2D-CGD-CBD	4.89	120.04	111.30
23	a	6006	CLA	O2D-CGD-CBD	4.89	120.05	111.30
23	c	6035	CLA	O2D-CGD-CBD	4.90	120.05	111.30
23	C	1031	CLA	O2D-CGD-CBD	4.90	120.05	111.30
23	B	1012	CLA	O2D-CGD-CBD	4.90	120.05	111.30
23	B	1015	CLA	O2D-CGD-CBD	4.90	120.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6015	CLA	O2D-CGD-CBD	4.90	120.06	111.30
23	H	1017	CLA	O2D-CGD-CBD	4.91	120.07	111.30
23	a	6003	CLA	O2D-CGD-CBD	4.91	120.07	111.30
23	c	6028	CLA	O2D-CGD-CBD	4.91	120.08	111.30
23	h	6017	CLA	O2D-CGD-CBD	4.91	120.08	111.30
23	C	1028	CLA	O2D-CGD-CBD	4.92	120.08	111.30
23	c	6037	CLA	O2D-CGD-CBD	4.92	120.09	111.30
23	A	1003	CLA	O2D-CGD-CBD	4.92	120.09	111.30
24	d	6039	PHO	O2D-CGD-CBD	4.92	120.10	111.30
23	c	6031	CLA	O2D-CGD-CBD	4.92	120.10	111.30
23	C	1037	CLA	O2D-CGD-CBD	4.93	120.10	111.30
24	D	1039	PHO	O2D-CGD-CBD	4.95	120.15	111.30
24	A	1038	PHO	O2D-CGD-CBD	4.99	120.22	111.30
24	a	6038	PHO	O2D-CGD-CBD	4.99	120.22	111.30
23	b	6023	CLA	O2D-CGD-CBD	5.05	120.32	111.30
23	B	1023	CLA	O2D-CGD-CBD	5.05	120.32	111.30
26	t	1046	BCR	C11-C12-C13	5.09	140.73	126.42
26	T	6046	BCR	C11-C12-C13	5.12	140.79	126.42
26	a	6044	BCR	C20-C19-C18	5.14	140.86	126.42
26	A	1044	BCR	C20-C19-C18	5.14	140.87	126.42
23	b	6018	CLA	C3C-C4C-NC	5.27	115.55	110.21
23	c	6031	CLA	C3C-C4C-NC	5.27	115.55	110.21
23	d	6008	CLA	C3C-C4C-NC	5.29	115.57	110.21
23	D	1008	CLA	C3C-C4C-NC	5.29	115.57	110.21
23	b	6024	CLA	C3C-C4C-NC	5.29	115.57	110.21
23	b	6012	CLA	C3C-C4C-NC	5.30	115.58	110.21
23	B	1018	CLA	C3C-C4C-NC	5.31	115.59	110.21
23	B	1023	CLA	C3C-C4C-NC	5.32	115.60	110.21
23	C	1031	CLA	C3C-C4C-NC	5.32	115.60	110.21
23	A	1006	CLA	C3C-C4C-NC	5.32	115.60	110.21
23	B	1012	CLA	C3C-C4C-NC	5.32	115.60	110.21
23	C	1037	CLA	C3C-C4C-NC	5.32	115.60	110.21
23	c	6037	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	C	1028	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	A	1007	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	b	6021	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	c	6026	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	C	1036	CLA	C3C-C4C-NC	5.33	115.61	110.21
23	B	1021	CLA	C3C-C4C-NC	5.34	115.62	110.21
23	b	6023	CLA	C3C-C4C-NC	5.34	115.62	110.21
23	a	6006	CLA	C3C-C4C-NC	5.34	115.62	110.21
23	C	1033	CLA	C3C-C4C-NC	5.35	115.63	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6004	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	B	1019	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	C	1025	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	D	1005	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	c	6029	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	c	6028	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	c	6033	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	b	6013	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	B	1020	CLA	C3C-C4C-NC	5.35	115.63	110.21
23	b	6014	CLA	C3C-C4C-NC	5.35	115.63	110.21
26	t	1046	BCR	C20-C19-C18	5.35	141.46	126.42
23	D	1004	CLA	C3C-C4C-NC	5.35	115.64	110.21
23	a	6007	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	B	1024	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	d	6005	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	A	1003	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	B	1014	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	C	1026	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	c	6036	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	c	6025	CLA	C3C-C4C-NC	5.36	115.64	110.21
23	b	6019	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	C	1032	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	B	1022	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	b	6022	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	k	6034	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	C	1029	CLA	C3C-C4C-NC	5.37	115.65	110.21
23	H	1017	CLA	C3C-C4C-NC	5.37	115.66	110.21
23	C	1035	CLA	C3C-C4C-NC	5.38	115.66	110.21
26	T	6046	BCR	C20-C19-C18	5.38	141.54	126.42
23	B	1015	CLA	C3C-C4C-NC	5.38	115.66	110.21
23	B	1013	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	h	6017	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	c	6030	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	c	6032	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	b	6020	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	c	6027	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	b	6010	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	B	1016	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	B	1009	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	K	1034	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	b	6009	CLA	C3C-C4C-NC	5.39	115.67	110.21
23	B	1010	CLA	C3C-C4C-NC	5.39	115.67	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6003	CLA	C3C-C4C-NC	5.40	115.68	110.21
23	b	6016	CLA	C3C-C4C-NC	5.40	115.68	110.21
23	c	6035	CLA	C3C-C4C-NC	5.40	115.69	110.21
23	C	1027	CLA	C3C-C4C-NC	5.41	115.69	110.21
26	z	6053	BCR	C20-C19-C18	5.41	141.62	126.42
26	B	1045	BCR	C11-C12-C13	5.42	141.63	126.42
26	b	6045	BCR	C11-C12-C13	5.42	141.65	126.42
23	C	1030	CLA	C3C-C4C-NC	5.42	115.71	110.21
26	Z	1053	BCR	C20-C19-C18	5.43	141.66	126.42
26	C	1052	BCR	C20-C19-C18	5.43	141.66	126.42
26	K	1051	BCR	C20-C19-C18	5.43	141.66	126.42
26	k	6051	BCR	C20-C19-C18	5.44	141.69	126.42
23	b	6015	CLA	C3C-C4C-NC	5.44	115.72	110.21
26	k	6052	BCR	C20-C19-C18	5.44	141.71	126.42
26	H	1049	BCR	C20-C19-C18	5.45	141.74	126.42
26	b	6047	BCR	C11-C12-C13	5.45	141.74	126.42
26	h	6049	BCR	C20-C19-C18	5.46	141.74	126.42
26	B	1047	BCR	C11-C12-C13	5.47	141.78	126.42
23	B	1011	CLA	C3C-C4C-NC	5.51	115.79	110.21
23	b	6011	CLA	C3C-C4C-NC	5.52	115.80	110.21
26	b	6045	BCR	C20-C19-C18	5.67	142.34	126.42
26	B	1045	BCR	C20-C19-C18	5.69	142.39	126.42
26	d	6050	BCR	C20-C19-C18	5.93	143.07	126.42
26	D	1050	BCR	C20-C19-C18	5.94	143.10	126.42
26	b	6047	BCR	C20-C19-C18	6.14	143.67	126.42
26	B	1047	BCR	C20-C19-C18	6.15	143.68	126.42
26	b	6047	BCR	C10-C11-C12	6.92	144.47	123.23
26	B	1047	BCR	C10-C11-C12	6.93	144.48	123.23
26	h	6049	BCR	C7-C8-C9	7.53	137.53	126.21
26	H	1049	BCR	C7-C8-C9	7.55	137.56	126.21
26	D	1050	BCR	C7-C8-C9	7.68	137.75	126.21
26	d	6050	BCR	C7-C8-C9	7.69	137.77	126.21
26	C	1054	BCR	C20-C19-C18	7.95	148.74	126.42
26	c	6054	BCR	C20-C19-C18	7.96	148.77	126.42
26	T	6048	BCR	C10-C11-C12	8.30	148.68	123.23
26	B	1048	BCR	C10-C11-C12	8.30	148.70	123.23
26	t	1046	BCR	C10-C11-C12	8.51	149.35	123.23
26	T	6046	BCR	C10-C11-C12	8.52	149.38	123.23
26	B	1047	BCR	C16-C15-C14	8.64	141.91	123.46
26	b	6047	BCR	C16-C15-C14	8.65	141.93	123.46
26	z	6053	BCR	C11-C12-C13	8.66	150.74	126.42
26	Z	1053	BCR	C11-C12-C13	8.66	150.74	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6037	CLA	C2C-C1C-NC	8.74	116.23	110.22
23	c	6030	CLA	C2C-C1C-NC	8.76	116.25	110.22
23	C	1030	CLA	C2C-C1C-NC	8.77	116.25	110.22
23	b	6016	CLA	C2C-C1C-NC	8.79	116.27	110.22
26	C	1054	BCR	C7-C8-C9	8.80	139.44	126.21
23	c	6032	CLA	C2C-C1C-NC	8.80	116.28	110.22
23	C	1037	CLA	C2C-C1C-NC	8.80	116.28	110.22
23	d	6004	CLA	C2C-C1C-NC	8.81	116.28	110.22
23	b	6011	CLA	C2C-C1C-NC	8.82	116.28	110.22
23	C	1032	CLA	C2C-C1C-NC	8.82	116.28	110.22
23	c	6027	CLA	C2C-C1C-NC	8.82	116.29	110.22
26	c	6054	BCR	C7-C8-C9	8.82	139.47	126.21
23	c	6025	CLA	C2C-C1C-NC	8.83	116.29	110.22
23	B	1023	CLA	C2C-C1C-NC	8.83	116.30	110.22
23	C	1027	CLA	C2C-C1C-NC	8.84	116.30	110.22
23	C	1028	CLA	C2C-C1C-NC	8.84	116.30	110.22
23	h	6017	CLA	C2C-C1C-NC	8.84	116.30	110.22
23	A	1003	CLA	C2C-C1C-NC	8.85	116.31	110.22
23	b	6015	CLA	C2C-C1C-NC	8.85	116.31	110.22
23	B	1011	CLA	C2C-C1C-NC	8.85	116.31	110.22
23	C	1036	CLA	C2C-C1C-NC	8.86	116.31	110.22
23	C	1031	CLA	C2C-C1C-NC	8.86	116.32	110.22
23	A	1006	CLA	C2C-C1C-NC	8.86	116.32	110.22
23	c	6036	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	B	1015	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	B	1018	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	B	1012	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	B	1016	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	B	1020	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	a	6003	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	b	6018	CLA	C2C-C1C-NC	8.87	116.32	110.22
23	H	1017	CLA	C2C-C1C-NC	8.88	116.33	110.22
23	B	1022	CLA	C2C-C1C-NC	8.88	116.33	110.22
23	B	1014	CLA	C2C-C1C-NC	8.88	116.33	110.22
23	D	1004	CLA	C2C-C1C-NC	8.88	116.33	110.22
23	b	6020	CLA	C2C-C1C-NC	8.88	116.33	110.22
23	b	6019	CLA	C2C-C1C-NC	8.89	116.33	110.22
23	B	1013	CLA	C2C-C1C-NC	8.89	116.33	110.22
23	c	6026	CLA	C2C-C1C-NC	8.89	116.33	110.22
23	c	6028	CLA	C2C-C1C-NC	8.89	116.34	110.22
23	C	1026	CLA	C2C-C1C-NC	8.89	116.34	110.22
23	C	1025	CLA	C2C-C1C-NC	8.89	116.34	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1035	CLA	C2C-C1C-NC	8.89	116.34	110.22
23	C	1033	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	b	6012	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	b	6013	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	b	6021	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	B	1019	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	a	6006	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	b	6023	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	C	1029	CLA	C2C-C1C-NC	8.91	116.35	110.22
23	a	6007	CLA	C2C-C1C-NC	8.91	116.35	110.22
23	A	1007	CLA	C2C-C1C-NC	8.91	116.35	110.22
23	b	6022	CLA	C2C-C1C-NC	8.92	116.35	110.22
26	H	1049	BCR	C11-C12-C13	8.92	151.46	126.42
23	c	6035	CLA	C2C-C1C-NC	8.92	116.36	110.22
23	B	1021	CLA	C2C-C1C-NC	8.92	116.36	110.22
23	c	6033	CLA	C2C-C1C-NC	8.92	116.36	110.22
23	c	6031	CLA	C2C-C1C-NC	8.92	116.36	110.22
23	K	1034	CLA	C2C-C1C-NC	8.93	116.36	110.22
23	c	6029	CLA	C2C-C1C-NC	8.93	116.36	110.22
23	b	6014	CLA	C2C-C1C-NC	8.93	116.36	110.22
23	D	1005	CLA	C2C-C1C-NC	8.93	116.37	110.22
26	h	6049	BCR	C11-C12-C13	8.94	151.52	126.42
23	d	6008	CLA	C2C-C1C-NC	8.94	116.37	110.22
23	k	6034	CLA	C2C-C1C-NC	8.94	116.37	110.22
23	d	6005	CLA	C2C-C1C-NC	8.94	116.37	110.22
23	B	1024	CLA	C2C-C1C-NC	8.94	116.37	110.22
23	b	6010	CLA	C2C-C1C-NC	8.94	116.37	110.22
23	b	6024	CLA	C2C-C1C-NC	8.95	116.37	110.22
23	D	1008	CLA	C2C-C1C-NC	8.95	116.38	110.22
23	B	1010	CLA	C2C-C1C-NC	8.98	116.39	110.22
26	b	6047	BCR	C7-C8-C9	9.08	139.86	126.21
26	B	1047	BCR	C7-C8-C9	9.11	139.90	126.21
23	b	6009	CLA	C2C-C1C-NC	9.18	116.53	110.22
23	B	1009	CLA	C2C-C1C-NC	9.18	116.53	110.22
26	k	6051	BCR	C10-C11-C12	9.21	151.48	123.23
26	K	1051	BCR	C10-C11-C12	9.22	151.51	123.23
26	T	6048	BCR	C11-C12-C13	9.62	153.43	126.42
26	B	1048	BCR	C11-C12-C13	9.62	153.45	126.42
26	B	1048	BCR	C7-C8-C9	9.78	140.91	126.21
26	T	6048	BCR	C7-C8-C9	9.82	140.96	126.21
26	K	1051	BCR	C7-C8-C9	9.89	141.07	126.21
26	k	6051	BCR	C7-C8-C9	9.93	141.13	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	6045	BCR	C20-C21-C22	10.01	141.59	127.31
26	z	6053	BCR	C20-C21-C22	10.01	141.60	127.31
26	Z	1053	BCR	C20-C21-C22	10.03	141.63	127.31
26	B	1045	BCR	C20-C21-C22	10.04	141.63	127.31
26	Z	1053	BCR	C21-C20-C19	10.04	154.04	123.23
26	k	6051	BCR	C21-C20-C19	10.05	154.07	123.23
26	h	6049	BCR	C20-C21-C22	10.05	141.66	127.31
26	Z	1053	BCR	C16-C17-C18	10.06	141.67	127.31
26	K	1051	BCR	C21-C20-C19	10.06	154.09	123.23
26	z	6053	BCR	C21-C20-C19	10.06	154.11	123.23
26	B	1045	BCR	C21-C20-C19	10.07	154.11	123.23
26	b	6047	BCR	C16-C17-C18	10.07	141.68	127.31
26	H	1049	BCR	C21-C20-C19	10.07	154.13	123.23
26	z	6053	BCR	C16-C17-C18	10.08	141.69	127.31
26	B	1047	BCR	C16-C17-C18	10.08	141.69	127.31
26	b	6045	BCR	C21-C20-C19	10.08	154.16	123.23
26	h	6049	BCR	C21-C20-C19	10.09	154.17	123.23
26	d	6050	BCR	C16-C17-C18	10.09	141.71	127.31
26	k	6051	BCR	C16-C17-C18	10.10	141.72	127.31
26	D	1050	BCR	C16-C17-C18	10.11	141.74	127.31
26	K	1051	BCR	C16-C17-C18	10.11	141.74	127.31
26	H	1049	BCR	C20-C21-C22	10.12	141.75	127.31
26	C	1054	BCR	C21-C20-C19	10.12	154.27	123.23
26	B	1047	BCR	C21-C20-C19	10.12	154.27	123.23
26	c	6054	BCR	C21-C20-C19	10.12	154.29	123.23
26	b	6047	BCR	C21-C20-C19	10.13	154.30	123.23
26	D	1050	BCR	C21-C20-C19	10.18	154.47	123.23
26	d	6050	BCR	C21-C20-C19	10.19	154.49	123.23
26	c	6054	BCR	C20-C21-C22	10.19	141.86	127.31
26	C	1054	BCR	C20-C21-C22	10.20	141.87	127.31
26	h	6049	BCR	C16-C17-C18	10.24	141.93	127.31
26	H	1049	BCR	C16-C17-C18	10.24	141.93	127.31
26	c	6054	BCR	C16-C17-C18	10.24	141.93	127.31
26	C	1054	BCR	C16-C17-C18	10.26	141.95	127.31
26	K	1051	BCR	C20-C21-C22	10.35	142.08	127.31
26	k	6051	BCR	C20-C21-C22	10.38	142.12	127.31
26	T	6048	BCR	C20-C19-C18	10.52	155.97	126.42
26	B	1048	BCR	C20-C19-C18	10.53	156.01	126.42
26	K	1051	BCR	C11-C12-C13	10.58	156.14	126.42
26	k	6051	BCR	C11-C12-C13	10.59	156.17	126.42
26	C	1052	BCR	C11-C12-C13	10.63	156.29	126.42
26	k	6052	BCR	C11-C12-C13	10.64	156.30	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	1049	BCR	C10-C11-C12	10.76	156.24	123.23
26	h	6049	BCR	C10-C11-C12	10.77	156.29	123.23
26	A	1044	BCR	C10-C11-C12	10.86	156.55	123.23
26	a	6044	BCR	C10-C11-C12	10.86	156.56	123.23
26	D	1050	BCR	C10-C11-C12	11.03	157.08	123.23
26	d	6050	BCR	C10-C11-C12	11.04	157.10	123.23
26	T	6046	BCR	C16-C17-C18	11.54	143.78	127.31
26	t	1046	BCR	C16-C17-C18	11.57	143.82	127.31
26	Z	1053	BCR	C10-C11-C12	11.81	159.45	123.23
26	z	6053	BCR	C10-C11-C12	11.82	159.48	123.23
26	z	6053	BCR	C7-C8-C9	11.86	144.02	126.21
26	Z	1053	BCR	C7-C8-C9	11.88	144.06	126.21
26	B	1045	BCR	C16-C15-C14	11.93	148.92	123.46
26	b	6045	BCR	C16-C15-C14	11.93	148.92	123.46
26	T	6048	BCR	C16-C17-C18	12.20	144.72	127.31
26	d	6050	BCR	C11-C12-C13	12.20	160.70	126.42
26	D	1050	BCR	C11-C12-C13	12.20	160.70	126.42
26	B	1048	BCR	C16-C17-C18	12.24	144.78	127.31
26	a	6044	BCR	C11-C12-C13	12.25	160.83	126.42
26	A	1044	BCR	C11-C12-C13	12.26	160.85	126.42
26	C	1052	BCR	C16-C17-C18	12.42	145.04	127.31
26	k	6052	BCR	C16-C17-C18	12.44	145.06	127.31
26	B	1045	BCR	C7-C8-C9	12.46	144.93	126.21
26	b	6045	BCR	C7-C8-C9	12.48	144.97	126.21
26	B	1048	BCR	C20-C21-C22	12.95	145.79	127.31
26	T	6048	BCR	C20-C21-C22	12.95	145.79	127.31
26	C	1054	BCR	C11-C12-C13	13.59	164.60	126.42
26	c	6054	BCR	C11-C12-C13	13.60	164.62	126.42
26	A	1044	BCR	C16-C15-C14	13.72	152.74	123.46
26	a	6044	BCR	C16-C15-C14	13.75	152.81	123.46
26	C	1054	BCR	C16-C15-C14	13.88	153.09	123.46
26	c	6054	BCR	C16-C15-C14	13.89	153.11	123.46
26	h	6049	BCR	C16-C15-C14	14.05	153.46	123.46
26	H	1049	BCR	C16-C15-C14	14.06	153.48	123.46
26	K	1051	BCR	C15-C16-C17	14.37	154.14	123.46
26	d	6050	BCR	C15-C16-C17	14.39	154.18	123.46
26	D	1050	BCR	C15-C16-C17	14.39	154.18	123.46
26	k	6051	BCR	C15-C16-C17	14.39	154.18	123.46
26	B	1047	BCR	C15-C16-C17	14.49	154.38	123.46
26	b	6047	BCR	C15-C16-C17	14.50	154.41	123.46
26	b	6045	BCR	C10-C11-C12	14.59	168.01	123.23
26	B	1045	BCR	C10-C11-C12	14.61	168.05	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	1050	BCR	C20-C21-C22	14.62	148.17	127.31
26	d	6050	BCR	C20-C21-C22	14.65	148.22	127.31
26	D	1050	BCR	C16-C15-C14	14.76	154.98	123.46
26	d	6050	BCR	C16-C15-C14	14.79	155.04	123.46
26	b	6045	BCR	C15-C16-C17	14.81	155.08	123.46
26	B	1045	BCR	C15-C16-C17	14.84	155.15	123.46
26	T	6048	BCR	C16-C15-C14	14.85	155.15	123.46
26	B	1048	BCR	C16-C15-C14	14.85	155.16	123.46
26	C	1054	BCR	C10-C11-C12	15.73	171.50	123.23
26	c	6054	BCR	C10-C11-C12	15.74	171.52	123.23
26	k	6052	BCR	C21-C20-C19	15.80	171.69	123.23
26	C	1052	BCR	C21-C20-C19	15.80	171.71	123.23
26	A	1044	BCR	C16-C17-C18	15.95	150.07	127.31
26	a	6044	BCR	C16-C17-C18	15.95	150.07	127.31
26	k	6051	BCR	C16-C15-C14	16.13	157.90	123.46
26	K	1051	BCR	C16-C15-C14	16.14	157.91	123.46
26	A	1044	BCR	C21-C20-C19	16.24	173.04	123.23
26	a	6044	BCR	C21-C20-C19	16.25	173.08	123.23
26	c	6054	BCR	C15-C16-C17	16.28	158.21	123.46
26	C	1054	BCR	C15-C16-C17	16.29	158.24	123.46
26	B	1048	BCR	C21-C20-C19	16.36	173.41	123.23
26	T	6048	BCR	C21-C20-C19	16.36	173.41	123.23
26	k	6052	BCR	C10-C11-C12	16.77	174.69	123.23
26	C	1052	BCR	C10-C11-C12	16.78	174.71	123.23
26	t	1046	BCR	C21-C20-C19	17.13	175.79	123.23
26	T	6046	BCR	C21-C20-C19	17.14	175.81	123.23
26	t	1046	BCR	C16-C15-C14	17.66	161.16	123.46
26	T	6046	BCR	C16-C15-C14	17.68	161.19	123.46
26	k	6052	BCR	C20-C21-C22	18.90	154.28	127.31
26	C	1052	BCR	C20-C21-C22	18.90	154.29	127.31
26	A	1044	BCR	C20-C21-C22	19.25	154.78	127.31
26	a	6044	BCR	C20-C21-C22	19.25	154.78	127.31
26	z	6053	BCR	C16-C15-C14	19.50	165.08	123.46
26	Z	1053	BCR	C16-C15-C14	19.51	165.11	123.46
26	T	6046	BCR	C15-C16-C17	20.14	166.45	123.46
26	t	1046	BCR	C15-C16-C17	20.16	166.48	123.46
26	t	1046	BCR	C20-C21-C22	20.83	157.04	127.31
26	T	6046	BCR	C20-C21-C22	20.88	157.12	127.31
26	C	1052	BCR	C16-C15-C14	21.25	168.82	123.46
26	k	6052	BCR	C16-C15-C14	21.28	168.88	123.46
26	h	6049	BCR	C15-C16-C17	21.95	170.32	123.46
26	H	1049	BCR	C15-C16-C17	21.96	170.34	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1044	BCR	C15-C16-C17	23.07	172.71	123.46
26	a	6044	BCR	C15-C16-C17	23.09	172.74	123.46
26	C	1052	BCR	C15-C16-C17	24.76	176.31	123.46
26	k	6052	BCR	C15-C16-C17	24.78	176.36	123.46
26	A	1044	BCR	C7-C8-C9	24.89	163.62	126.21
26	a	6044	BCR	C7-C8-C9	24.92	163.66	126.21
26	z	6053	BCR	C15-C16-C17	25.05	176.92	123.46
26	Z	1053	BCR	C15-C16-C17	25.05	176.94	123.46
26	B	1048	BCR	C15-C16-C17	25.35	177.57	123.46
26	T	6048	BCR	C15-C16-C17	25.38	177.62	123.46
26	B	1047	BCR	C20-C21-C22	25.41	163.57	127.31
26	b	6047	BCR	C20-C21-C22	25.41	163.58	127.31
26	B	1045	BCR	C16-C17-C18	28.73	168.32	127.31
26	b	6045	BCR	C16-C17-C18	28.75	168.34	127.31

All (302) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	6013	CLA	C8
23	b	6013	CLA	NC
23	b	6013	CLA	ND
23	b	6013	CLA	NA
23	C	1026	CLA	NC
23	C	1026	CLA	ND
23	C	1026	CLA	NA
23	b	6011	CLA	CBD
23	b	6011	CLA	C8
23	b	6011	CLA	NC
23	b	6011	CLA	ND
23	b	6011	CLA	NA
23	c	6033	CLA	C8
23	c	6033	CLA	NC
23	c	6033	CLA	ND
23	c	6033	CLA	NA
24	D	1039	PHO	C8
24	D	1039	PHO	C13
24	D	1039	PHO	C3A
23	B	1013	CLA	C8
23	B	1013	CLA	NC
23	B	1013	CLA	ND
23	B	1013	CLA	NA
23	a	6007	CLA	NC

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Mol	Chain	Res	Type	Atom
23	a	6007	CLA	ND
23	a	6007	CLA	NA
23	B	1020	CLA	C8
23	B	1020	CLA	C13
23	B	1020	CLA	NC
23	B	1020	CLA	ND
23	B	1020	CLA	NA
23	k	6034	CLA	C8
23	k	6034	CLA	NA
23	k	6034	CLA	NC
23	k	6034	CLA	C2A
23	k	6034	CLA	C13
23	k	6034	CLA	ND
23	k	6034	CLA	C3A
23	b	6024	CLA	NC
23	b	6024	CLA	ND
23	b	6024	CLA	NA
24	A	1038	PHO	C8
23	d	6005	CLA	C8
23	d	6005	CLA	NC
23	d	6005	CLA	ND
23	d	6005	CLA	NA
23	c	6036	CLA	C8
23	c	6036	CLA	NC
23	c	6036	CLA	ND
23	c	6036	CLA	NA
24	d	6039	PHO	C8
24	d	6039	PHO	C13
24	d	6039	PHO	C3A
23	A	1007	CLA	NC
23	A	1007	CLA	ND
23	A	1007	CLA	NA
23	a	6003	CLA	C8
23	a	6003	CLA	NC
23	a	6003	CLA	ND
23	a	6003	CLA	NA
23	a	6006	CLA	C8
23	a	6006	CLA	NC
23	a	6006	CLA	ND
23	a	6006	CLA	NA
23	b	6019	CLA	C13
23	b	6019	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	6019	CLA	ND
23	b	6019	CLA	NA
23	C	1030	CLA	C8
23	C	1030	CLA	NC
23	C	1030	CLA	ND
23	C	1030	CLA	NA
23	b	6016	CLA	NC
23	b	6016	CLA	ND
23	b	6016	CLA	NA
23	C	1028	CLA	C8
23	C	1028	CLA	NC
23	C	1028	CLA	ND
23	C	1028	CLA	NA
23	b	6009	CLA	CBD
23	b	6009	CLA	NC
23	b	6009	CLA	ND
23	b	6009	CLA	NA
23	c	6032	CLA	C8
23	c	6032	CLA	C13
23	c	6032	CLA	NC
23	c	6032	CLA	ND
23	c	6032	CLA	NA
23	A	1006	CLA	C8
23	A	1006	CLA	NC
23	A	1006	CLA	ND
23	A	1006	CLA	NA
23	D	1008	CLA	C8
23	D	1008	CLA	NC
23	D	1008	CLA	ND
23	D	1008	CLA	NA
23	D	1008	CLA	C3A
23	c	6025	CLA	C8
23	c	6025	CLA	NC
23	c	6025	CLA	ND
23	c	6025	CLA	NA
23	B	1010	CLA	C8
23	B	1010	CLA	NC
23	B	1010	CLA	ND
23	B	1010	CLA	NA
23	H	1017	CLA	C8
23	H	1017	CLA	NC
23	H	1017	CLA	ND

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Mol	Chain	Res	Type	Atom
23	H	1017	CLA	NA
23	B	1021	CLA	C8
23	B	1021	CLA	NC
23	B	1021	CLA	ND
23	B	1021	CLA	NA
23	c	6031	CLA	C8
23	c	6031	CLA	NC
23	c	6031	CLA	ND
23	c	6031	CLA	NA
23	c	6028	CLA	C8
23	c	6028	CLA	NC
23	c	6028	CLA	ND
23	c	6028	CLA	NA
23	h	6017	CLA	C8
23	h	6017	CLA	NC
23	h	6017	CLA	ND
23	h	6017	CLA	NA
23	B	1022	CLA	CBD
23	B	1022	CLA	C13
23	B	1022	CLA	NC
23	B	1022	CLA	ND
23	B	1022	CLA	NA
23	b	6014	CLA	C8
23	b	6014	CLA	NC
23	b	6014	CLA	ND
23	b	6014	CLA	NA
23	B	1014	CLA	C8
23	B	1014	CLA	NC
23	B	1014	CLA	ND
23	B	1014	CLA	NA
23	B	1012	CLA	C8
23	B	1012	CLA	NC
23	B	1012	CLA	ND
23	B	1012	CLA	NA
23	B	1024	CLA	NC
23	B	1024	CLA	ND
23	B	1024	CLA	NA
23	b	6020	CLA	C8
23	b	6020	CLA	C13
23	b	6020	CLA	NC
23	b	6020	CLA	ND
23	b	6020	CLA	NA

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Mol	Chain	Res	Type	Atom
23	A	1003	CLA	C8
23	A	1003	CLA	NC
23	A	1003	CLA	ND
23	A	1003	CLA	NA
23	c	6030	CLA	C8
23	c	6030	CLA	NC
23	c	6030	CLA	ND
23	c	6030	CLA	NA
23	c	6027	CLA	C8
23	c	6027	CLA	C13
23	c	6027	CLA	NC
23	c	6027	CLA	ND
23	c	6027	CLA	NA
23	C	1029	CLA	C8
23	C	1029	CLA	NC
23	C	1029	CLA	ND
23	C	1029	CLA	NA
23	C	1029	CLA	C3A
23	b	6010	CLA	C8
23	b	6010	CLA	NC
23	b	6010	CLA	ND
23	b	6010	CLA	NA
24	a	6038	PHO	C8
23	C	1031	CLA	C8
23	C	1031	CLA	NC
23	C	1031	CLA	ND
23	C	1031	CLA	NA
23	K	1034	CLA	C8
23	K	1034	CLA	NA
23	K	1034	CLA	NC
23	K	1034	CLA	C2A
23	K	1034	CLA	C13
23	K	1034	CLA	ND
23	K	1034	CLA	C3A
23	C	1025	CLA	C8
23	C	1025	CLA	NC
23	C	1025	CLA	ND
23	C	1025	CLA	NA
23	d	6004	CLA	C8
23	d	6004	CLA	NC
23	d	6004	CLA	ND
23	d	6004	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	1016	CLA	NC
23	B	1016	CLA	ND
23	B	1016	CLA	NA
23	B	1019	CLA	C13
23	B	1019	CLA	NC
23	B	1019	CLA	ND
23	B	1019	CLA	NA
23	b	6023	CLA	C8
23	b	6023	CLA	C13
23	b	6023	CLA	NC
23	b	6023	CLA	ND
23	b	6023	CLA	NA
23	b	6015	CLA	C8
23	b	6015	CLA	NC
23	b	6015	CLA	ND
23	b	6015	CLA	NA
23	C	1035	CLA	C8
23	C	1035	CLA	NC
23	C	1035	CLA	ND
23	C	1035	CLA	NA
23	D	1005	CLA	C8
23	D	1005	CLA	NC
23	D	1005	CLA	ND
23	D	1005	CLA	NA
23	c	6035	CLA	C8
23	c	6035	CLA	NC
23	c	6035	CLA	ND
23	c	6035	CLA	NA
23	C	1037	CLA	C8
23	C	1037	CLA	NC
23	C	1037	CLA	ND
23	C	1037	CLA	NA
23	B	1015	CLA	C8
23	B	1015	CLA	NC
23	B	1015	CLA	ND
23	B	1015	CLA	NA
23	b	6018	CLA	C8
23	b	6018	CLA	NC
23	b	6018	CLA	ND
23	b	6018	CLA	NA
23	d	6008	CLA	C8
23	d	6008	CLA	NC

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Mol	Chain	Res	Type	Atom
23	d	6008	CLA	ND
23	d	6008	CLA	NA
23	d	6008	CLA	C3A
23	b	6021	CLA	C8
23	b	6021	CLA	NC
23	b	6021	CLA	ND
23	b	6021	CLA	NA
23	B	1011	CLA	CBD
23	B	1011	CLA	C8
23	B	1011	CLA	NC
23	B	1011	CLA	ND
23	B	1011	CLA	NA
23	B	1023	CLA	C8
23	B	1023	CLA	C13
23	B	1023	CLA	NC
23	B	1023	CLA	ND
23	B	1023	CLA	NA
23	c	6029	CLA	C8
23	c	6029	CLA	NC
23	c	6029	CLA	ND
23	c	6029	CLA	NA
23	c	6029	CLA	C3A
23	c	6026	CLA	NC
23	c	6026	CLA	ND
23	c	6026	CLA	NA
23	C	1033	CLA	C8
23	C	1033	CLA	NC
23	C	1033	CLA	ND
23	C	1033	CLA	NA
23	C	1032	CLA	C8
23	C	1032	CLA	C13
23	C	1032	CLA	NC
23	C	1032	CLA	ND
23	C	1032	CLA	NA
23	B	1018	CLA	C8
23	B	1018	CLA	NC
23	B	1018	CLA	ND
23	B	1018	CLA	NA
23	b	6012	CLA	C8
23	b	6012	CLA	NC
23	b	6012	CLA	ND
23	b	6012	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	6037	CLA	C8
23	c	6037	CLA	NC
23	c	6037	CLA	ND
23	c	6037	CLA	NA
23	b	6022	CLA	CBD
23	b	6022	CLA	C13
23	b	6022	CLA	NC
23	b	6022	CLA	ND
23	b	6022	CLA	NA
23	D	1004	CLA	C8
23	D	1004	CLA	NC
23	D	1004	CLA	ND
23	D	1004	CLA	NA
23	C	1027	CLA	C8
23	C	1027	CLA	C13
23	C	1027	CLA	NC
23	C	1027	CLA	ND
23	C	1027	CLA	NA
23	B	1009	CLA	CBD
23	B	1009	CLA	NC
23	B	1009	CLA	ND
23	B	1009	CLA	NA
23	C	1036	CLA	C8
23	C	1036	CLA	NC
23	C	1036	CLA	ND
23	C	1036	CLA	NA

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	H	1049	BCR	C10-C11-C12-C13
26	h	6049	BCR	C10-C11-C12-C13
31	f	6040	HEM	C1A-C2A-CAA-CBA
31	F	1040	HEM	C1A-C2A-CAA-CBA
31	f	6040	HEM	C3A-C2A-CAA-CBA
31	F	1040	HEM	C3A-C2A-CAA-CBA
26	D	1050	BCR	C17-C16-C15-C14
26	d	6050	BCR	C17-C16-C15-C14
26	T	6046	BCR	C17-C16-C15-C14
26	t	1046	BCR	C17-C16-C15-C14
26	C	1054	BCR	C10-C11-C12-C13
26	c	6054	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	B	1048	BCR	C10-C11-C12-C13
26	T	6048	BCR	C10-C11-C12-C13
29	c	6055	DGD	C3G-O3G-C1D-O6D
26	D	1050	BCR	C21-C20-C19-C18
26	d	6050	BCR	C21-C20-C19-C18
29	C	1055	DGD	C3G-O3G-C1D-O6D
26	b	6047	BCR	C21-C20-C19-C18
26	B	1047	BCR	C21-C20-C19-C18
23	d	6008	CLA	CED-O2D-CGD-CBD
23	D	1008	CLA	CED-O2D-CGD-CBD
23	b	6015	CLA	CED-O2D-CGD-CBD
23	B	1015	CLA	CED-O2D-CGD-CBD
30	d	6062	MGE	C1D-O3G-C3G-C2G
30	D	1062	MGE	C1D-O3G-C3G-C2G
23	B	1022	CLA	CED-O2D-CGD-CBD
23	b	6022	CLA	CED-O2D-CGD-CBD
23	B	1009	CLA	CED-O2D-CGD-CBD
23	b	6009	CLA	CED-O2D-CGD-CBD
23	c	6030	CLA	CED-O2D-CGD-CBD
23	C	1030	CLA	CED-O2D-CGD-CBD
23	a	6003	CLA	CED-O2D-CGD-CBD
23	A	1003	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

62 monomers are involved in 2123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1003	CLA	55	0
23	A	1006	CLA	45	0
23	A	1007	CLA	40	0
24	A	1038	PHO	63	0
25	A	1043	PQ9	39	0
26	A	1044	BCR	25	0
27	A	1063	LHG	36	0
23	B	1009	CLA	63	0
23	B	1010	CLA	38	0
23	B	1011	CLA	89	0
23	B	1012	CLA	61	0
23	B	1013	CLA	67	0
23	B	1014	CLA	49	0
23	B	1015	CLA	45	0
23	B	1016	CLA	49	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1018	CLA	34	0
23	B	1019	CLA	40	0
23	B	1020	CLA	54	0
23	B	1021	CLA	63	0
23	B	1022	CLA	75	0
23	B	1023	CLA	70	0
23	B	1024	CLA	45	0
26	B	1045	BCR	21	0
26	B	1047	BCR	31	0
26	B	1048	BCR	23	0
29	B	1058	DGD	32	0
30	B	1060	MGE	39	0
23	C	1025	CLA	67	0
23	C	1026	CLA	29	0
23	C	1027	CLA	37	0
23	C	1028	CLA	34	0
23	C	1029	CLA	62	0
23	C	1030	CLA	38	0
23	C	1031	CLA	63	0
23	C	1032	CLA	43	0
23	C	1033	CLA	65	0
23	C	1035	CLA	56	0
23	C	1036	CLA	24	0
23	C	1037	CLA	23	0
26	C	1052	BCR	40	0
26	C	1054	BCR	41	0
29	C	1055	DGD	26	0
29	C	1056	DGD	55	0
29	C	1057	DGD	41	0
23	D	1004	CLA	57	0
23	D	1005	CLA	58	0
23	D	1008	CLA	48	0
24	D	1039	PHO	53	0
25	D	1042	PQ9	52	0
26	D	1050	BCR	40	0
30	D	1059	MGE	45	0
30	D	1062	MGE	21	0
31	F	1040	HEM	17	0
23	H	1017	CLA	45	0
26	H	1049	BCR	36	0
23	K	1034	CLA	87	0
26	K	1051	BCR	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	L	1061	MGE	29	0
26	T	6046	BCR	25	0
26	T	6048	BCR	15	0
31	V	1041	HEM	12	0
26	Z	1053	BCR	18	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.57	0 100 100	135, 156, 186, 200	0
1	a	335/344 (97%)	-0.62	1 (0%) 93 91	135, 156, 186, 200	0
2	B	488/488 (100%)	-0.56	0 100 100	133, 156, 180, 191	0
2	b	488/488 (100%)	-0.54	1 (0%) 94 93	133, 156, 180, 191	0
3	C	447/447 (100%)	-0.55	2 (0%) 92 88	138, 165, 181, 193	0
3	c	447/447 (100%)	-0.43	1 (0%) 94 93	138, 165, 181, 193	0
4	D	340/340 (100%)	-0.59	3 (0%) 84 77	134, 156, 179, 192	0
4	d	340/340 (100%)	-0.60	0 100 100	134, 156, 179, 192	0
5	E	82/83 (98%)	-0.48	0 100 100	153, 172, 191, 198	0
5	e	82/83 (98%)	-0.32	3 (3%) 42 33	153, 172, 191, 198	0
6	F	35/44 (79%)	-0.42	1 (2%) 52 42	153, 167, 187, 191	0
6	f	35/44 (79%)	-0.39	2 (5%) 24 19	153, 167, 187, 191	0
7	H	64/64 (100%)	-0.48	0 100 100	154, 163, 175, 185	0
7	h	64/64 (100%)	-0.33	1 (1%) 72 63	154, 163, 175, 185	0
8	I	35/35 (100%)	-0.12	2 (5%) 24 19	152, 169, 196, 201	0
8	i	35/35 (100%)	-0.08	0 100 100	152, 169, 196, 201	0
9	J	34/40 (85%)	-0.65	0 100 100	155, 162, 184, 192	0
9	j	34/40 (85%)	-0.65	0 100 100	155, 162, 184, 192	0
10	K	36/36 (100%)	-0.66	0 100 100	144, 168, 182, 185	0
10	k	36/36 (100%)	-0.52	0 100 100	156, 170, 182, 192	0
11	L	37/37 (100%)	-0.42	0 100 100	138, 160, 191, 197	0
11	l	37/37 (100%)	-0.31	1 (2%) 55 44	138, 160, 191, 197	0
12	M	36/36 (100%)	-0.35	1 (2%) 53 43	131, 146, 188, 194	0
12	m	36/36 (100%)	-0.56	0 100 100	131, 146, 188, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.45	1 (0%) 92 88	139, 160, 181, 187	0
13	o	242/242 (100%)	-0.46	2 (0%) 86 79	139, 160, 181, 187	0
14	T	30/30 (100%)	-0.68	0 100 100	124, 143, 186, 191	0
14	t	30/30 (100%)	-0.78	0 100 100	131, 143, 186, 191	0
15	U	98/98 (100%)	-0.57	0 100 100	139, 155, 165, 173	0
15	u	98/98 (100%)	-0.63	1 (1%) 82 74	139, 155, 165, 173	0
16	V	137/137 (100%)	-0.54	0 100 100	144, 162, 173, 178	0
16	v	137/137 (100%)	-0.56	0 100 100	144, 162, 173, 178	0
17	X	34/34 (100%)	-0.76	0 100 100	173, 181, 198, 201	0
17	x	34/34 (100%)	-0.47	1 (2%) 52 42	173, 181, 198, 201	0
18	Y	28/28 (100%)	0.08	0 100 100	187, 199, 208, 210	0
18	y	28/28 (100%)	-0.29	0 100 100	187, 199, 208, 210	0
19	N	0/23	-	-	-	-
19	n	0/23	-	-	-	-
20	Z	62/62 (100%)	-0.55	1 (1%) 72 63	159, 173, 188, 196	0
20	z	62/62 (100%)	-0.36	2 (3%) 48 38	159, 173, 188, 196	0
All	All	5200/5296 (98%)	-0.52	27 (0%) 90 86	124, 161, 185, 210	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	45	LEU	6.7
3	C	44	ASN	5.3
4	D	228	GLY	3.6
5	e	5006	GLY	3.2
5	e	5084	LYS	3.1
13	o	5233	ARG	3.0
20	z	5034	ASP	2.8
6	f	5013	TYR	2.7
13	o	5049	ASP	2.6
7	h	5023	PRO	2.5
1	a	5012	ASN	2.5
17	x	5011	THR	2.4
4	D	13	GLY	2.4
5	e	5004	THR	2.4
11	l	5001	MET	2.3
15	u	5008	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	227	GLU	2.3
20	z	5042	LEU	2.2
12	M	33	GLN	2.2
8	I	34	ARG	2.2
2	b	5172	TYR	2.2
13	O	87	GLN	2.2
3	c	5462	GLU	2.2
6	f	5012	SER	2.1
6	F	12	SER	2.0
8	I	35	LYS	2.0
20	Z	33	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	IOD	D	1068	1/1	0.69	1.30	14.01	198,198,198,198	0
26	BCR	h	6049	40/40	0.71	0.44	9.17	177,182,188,189	0
26	BCR	a	6044	40/40	0.71	0.52	6.32	155,177,185,185	0
30	MGE	d	6059	48/48	0.67	0.47	6.17	179,190,215,216	0
26	BCR	B	1045	40/40	0.77	0.51	6.15	163,196,216,216	0
26	BCR	T	6046	40/40	0.70	0.51	5.98	179,185,188,189	0
23	CLA	C	1027	65/65	0.65	0.51	5.87	192,198,204,216	0
28	IOD	d	6068	1/1	0.76	0.63	5.61	199,199,199,199	0
26	BCR	A	1044	40/40	0.73	0.61	5.54	155,177,185,185	0
26	BCR	z	6053	40/40	0.64	0.53	5.16	190,214,216,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	BCR	D	1050	40/40	0.79	0.49	5.09	184,193,198,199	0
26	BCR	T	6048	40/40	0.74	0.65	4.89	179,184,203,204	0
26	BCR	H	1049	40/40	0.72	0.40	4.87	177,182,188,189	0
26	BCR	d	6050	40/40	0.79	0.47	4.82	184,193,198,199	0
26	BCR	b	6047	40/40	0.77	0.43	4.48	155,171,200,202	0
30	MGE	D	1059	48/48	0.71	0.41	4.36	179,190,215,216	0
23	CLA	K	1034	65/65	0.64	0.48	4.22	138,189,216,216	0
26	BCR	b	6045	40/40	0.74	0.50	4.19	163,196,216,216	0
26	BCR	Z	1053	40/40	0.60	0.59	4.11	190,214,216,216	0
23	CLA	d	6008	65/65	0.72	0.47	4.07	184,188,216,216	0
23	CLA	k	6034	65/65	0.69	0.43	4.05	138,189,216,216	0
26	BCR	B	1048	40/40	0.75	0.58	4.00	179,184,203,204	0
26	BCR	k	6052	40/40	0.59	0.41	3.95	191,195,202,203	0
26	BCR	t	1046	40/40	0.75	0.40	3.91	179,185,188,189	0
23	CLA	A	1007	65/65	0.73	0.45	3.89	129,174,204,205	0
23	CLA	a	6007	65/65	0.66	0.50	3.83	129,174,204,205	0
26	BCR	k	6051	40/40	0.72	0.42	3.76	192,202,210,210	0
23	CLA	D	1008	65/65	0.73	0.45	3.67	184,188,216,216	0
29	DGD	c	6056	66/66	0.75	0.43	3.42	190,201,216,216	0
25	PQ9	d	6042	45/45	0.68	0.43	3.37	171,173,185,187	0
23	CLA	D	1005	65/65	0.83	0.35	3.35	135,162,169,173	0
23	CLA	C	1037	65/65	0.71	0.49	3.19	201,211,214,216	0
23	CLA	C	1028	65/65	0.88	0.29	3.19	178,182,201,202	0
23	CLA	c	6029	65/65	0.87	0.36	3.17	177,187,190,201	0
29	DGD	C	1056	66/66	0.73	0.38	2.91	190,201,216,216	0
23	CLA	H	1017	65/65	0.79	0.35	2.89	169,197,201,208	0
30	MGE	B	1060	48/48	0.69	0.50	2.88	186,199,213,216	0
30	MGE	D	1062	48/48	0.74	0.37	2.82	187,202,208,210	0
26	BCR	K	1051	40/40	0.67	0.46	2.77	192,202,210,210	0
23	CLA	c	6027	65/65	0.66	0.51	2.77	192,198,204,216	0
23	CLA	b	6021	65/65	0.85	0.30	2.66	154,164,172,176	0
24	PHO	D	1039	64/64	0.80	0.34	2.66	184,187,196,198	0
29	DGD	c	6055	66/66	0.73	0.41	2.61	184,192,202,203	0
23	CLA	c	6026	65/65	0.85	0.34	2.54	138,171,178,183	0
26	BCR	B	1047	40/40	0.80	0.35	2.50	155,171,200,202	0
29	DGD	b	6058	66/66	0.82	0.32	2.50	175,188,196,203	0
30	MGE	b	6060	48/48	0.76	0.41	2.37	186,199,213,216	0
23	CLA	h	6017	65/65	0.72	0.42	2.35	169,197,201,208	0
23	CLA	C	1026	65/65	0.86	0.29	2.35	138,171,178,183	0
23	CLA	B	1018	65/65	0.86	0.30	2.33	172,186,191,192	0
30	MGE	L	1061	48/48	0.74	0.45	2.29	177,191,195,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	b	6012	65/65	0.84	0.34	2.27	160,167,172,174	0
24	PHO	a	6038	64/64	0.85	0.34	2.26	166,176,178,181	0
23	CLA	d	6005	65/65	0.83	0.33	2.23	135,162,169,173	0
29	DGD	C	1055	66/66	0.80	0.36	2.22	184,192,202,203	0
23	CLA	A	1006	65/65	0.84	0.33	2.18	166,181,211,213	0
30	MGE	d	6062	48/48	0.67	0.42	2.17	187,202,208,210	0
23	CLA	B	1024	65/65	0.74	0.39	2.09	165,193,197,198	0
23	CLA	c	6028	65/65	0.88	0.28	2.06	178,182,201,202	0
23	CLA	c	6037	65/65	0.63	0.56	2.04	201,211,214,216	0
25	PQ9	D	1042	45/45	0.82	0.32	2.02	171,173,185,187	0
23	CLA	b	6016	65/65	0.89	0.29	1.91	130,172,175,180	0
23	CLA	b	6013	65/65	0.89	0.29	1.90	146,173,183,184	0
23	CLA	d	6004	65/65	0.92	0.24	1.88	130,168,179,181	0
26	BCR	C	1052	40/40	0.78	0.28	1.87	191,195,202,203	0
26	BCR	C	1054	40/40	0.68	0.43	1.80	197,201,216,216	0
23	CLA	D	1004	65/65	0.91	0.27	1.79	130,168,179,181	0
25	PQ9	A	1043	45/45	0.71	0.42	1.77	171,172,193,197	30
23	CLA	C	1029	65/65	0.89	0.31	1.68	177,187,190,201	0
23	CLA	a	6003	65/65	0.89	0.29	1.64	160,169,175,212	0
25	PQ9	a	6043	45/45	0.75	0.39	1.64	171,172,193,197	30
29	DGD	C	1057	66/66	0.82	0.33	1.62	177,190,206,207	0
27	LHG	a	6063	49/49	0.58	0.53	1.61	199,213,216,216	0
30	MGE	l	6061	48/48	0.77	0.39	1.59	177,191,195,199	0
23	CLA	B	1010	65/65	0.85	0.29	1.57	160,183,186,189	0
23	CLA	c	6031	65/65	0.79	0.41	1.56	181,185,202,216	0
26	BCR	c	6054	40/40	0.70	0.42	1.53	197,201,216,216	0
23	CLA	C	1036	65/65	0.73	0.38	1.52	186,190,203,216	0
23	CLA	C	1033	65/65	0.89	0.32	1.51	138,185,199,200	0
24	PHO	A	1038	64/64	0.87	0.30	1.50	166,176,178,181	0
23	CLA	b	6015	65/65	0.82	0.31	1.49	177,182,185,216	0
23	CLA	b	6014	65/65	0.72	0.40	1.48	178,187,197,216	0
23	CLA	a	6006	65/65	0.89	0.24	1.45	166,181,211,213	0
31	HEM	f	6040	43/43	0.85	0.37	1.44	186,215,216,216	0
23	CLA	C	1025	65/65	0.89	0.27	1.43	156,187,191,194	0
23	CLA	B	1019	65/65	0.89	0.30	1.43	167,172,175,180	0
23	CLA	b	6018	65/65	0.88	0.27	1.42	172,186,191,192	0
24	PHO	d	6039	64/64	0.87	0.24	1.41	184,187,196,198	0
27	LHG	A	1063	49/49	0.52	0.59	1.41	199,213,216,216	0
23	CLA	b	6011	65/65	0.86	0.31	1.36	168,178,184,188	0
23	CLA	C	1032	65/65	0.81	0.37	1.31	184,188,192,216	0
23	CLA	c	6035	65/65	0.77	0.42	1.26	189,202,210,216	0
23	CLA	b	6009	65/65	0.74	0.43	1.26	143,192,213,213	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	1009	65/65	0.80	0.35	1.25	143,192,213,213	0
23	CLA	B	1014	65/65	0.76	0.37	1.21	178,187,197,216	0
29	DGD	c	6057	66/66	0.77	0.36	1.13	177,190,206,207	0
29	DGD	B	1058	66/66	0.86	0.29	1.10	175,188,196,203	0
31	HEM	F	1040	43/43	0.83	0.37	1.09	186,215,216,216	0
23	CLA	C	1031	65/65	0.83	0.33	1.09	181,185,202,216	0
23	CLA	B	1015	65/65	0.89	0.27	1.05	177,182,185,216	0
23	CLA	B	1020	65/65	0.94	0.24	1.04	167,175,180,197	0
23	CLA	c	6033	65/65	0.85	0.33	0.99	138,185,199,200	0
23	CLA	C	1035	65/65	0.82	0.36	0.98	189,202,210,216	0
23	CLA	C	1030	65/65	0.79	0.34	0.96	185,197,216,216	0
23	CLA	b	6010	65/65	0.89	0.26	0.94	160,183,186,189	0
23	CLA	B	1012	65/65	0.86	0.29	0.82	160,167,172,174	0
23	CLA	A	1003	65/65	0.90	0.25	0.81	160,169,175,212	0
23	CLA	c	6032	65/65	0.82	0.34	0.79	186,189,200,216	0
23	CLA	b	6024	65/65	0.73	0.37	0.78	165,193,197,198	0
23	CLA	c	6025	65/65	0.87	0.26	0.77	156,187,191,194	0
23	CLA	B	1011	65/65	0.89	0.25	0.75	168,178,184,188	0
23	CLA	B	1016	65/65	0.93	0.21	0.75	130,172,175,180	0
23	CLA	c	6036	65/65	0.78	0.36	0.75	186,190,203,216	0
31	HEM	V	1041	43/43	0.94	0.28	0.72	131,181,185,187	0
23	CLA	b	6019	65/65	0.89	0.25	0.69	167,172,175,180	0
23	CLA	B	1021	65/65	0.87	0.25	0.67	154,164,172,176	0
23	CLA	b	6020	65/65	0.92	0.24	0.62	167,175,180,197	0
23	CLA	B	1013	65/65	0.92	0.22	0.61	146,173,183,184	0
31	HEM	v	6041	43/43	0.93	0.25	0.60	131,181,185,187	0
23	CLA	B	1023	65/65	0.88	0.25	0.53	174,179,181,191	0
23	CLA	b	6023	65/65	0.87	0.27	0.51	174,179,181,191	0
23	CLA	c	6030	65/65	0.81	0.28	0.06	185,197,216,216	0
23	CLA	b	6022	65/65	0.90	0.25	0.03	138,180,198,200	0
23	CLA	B	1022	65/65	0.91	0.23	-0.26	138,180,198,200	0
22	FE2	D	1002	1/1	0.93	0.17	-1.03	148,148,148,148	0
21	OEC	A	1001	5/9	0.97	0.14	-1.42	132,148,162,172	0
21	OEC	a	6001	5/9	0.98	0.17	-1.58	132,148,162,172	0
28	IOD	A	1065	1/1	0.98	0.13	-1.99	158,158,158,158	0
22	FE2	a	6002	1/1	0.80	0.24	-2.10	148,148,148,148	0
28	IOD	a	6065	1/1	0.99	0.13	-2.54	158,158,158,158	0
28	IOD	T	1066	1/1	0.65	0.23	-	199,199,199,199	0
28	IOD	t	6066	1/1	0.99	0.08	-	199,199,199,199	0
28	IOD	b	6067	1/1	0.84	0.51	-	199,199,199,199	0
28	IOD	D	1064	1/1	0.98	0.04	-	160,160,160,160	0
28	IOD	d	6064	1/1	0.98	0.12	-	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	IOD	B	1067	1/1	0.59	0.51	-	198,198,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.