



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:56 am GMT

PDB ID : 3A0B
Title : Crystal structure of Br-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-16
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

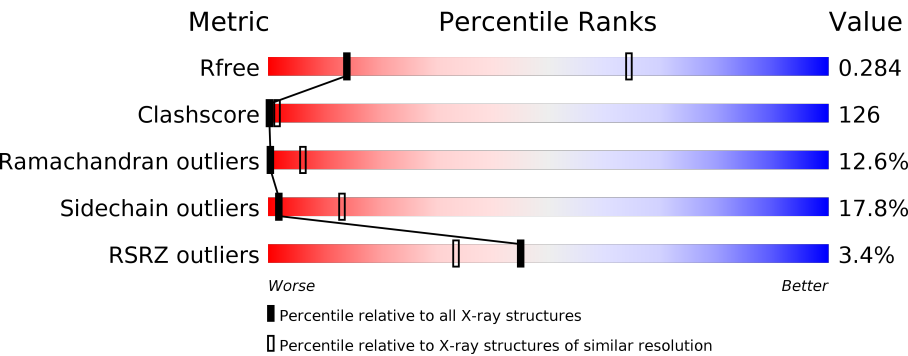
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1413 (3.90-3.50)
Clashscore	122126	1524 (3.90-3.50)
Ramachandran outliers	120053	1470 (3.90-3.50)
Sidechain outliers	120020	1467 (3.90-3.50)
RSRZ outliers	108989	1298 (3.90-3.50)

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	<div><div></div><div>9%66%22%..</div></div>
1	a	344	<div><div></div><div>71%24%..</div></div>
2	B	488	<div><div>2%</div><div>16%64%18%..</div></div>
2	b	488	<div><div>3%</div><div>77%20%..</div></div>
3	C	447	<div><div>2%</div><div>16%62%21%.</div></div>
3	c	447	<div><div>5%</div><div>78%21%.</div></div>

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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	24	
19	n	24	
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	-
23	CLA	A	1007	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	-
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	-
23	CLA	C	1027	X	-	X	X
23	CLA	C	1028	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	X
23	CLA	C	1033	X	-	X	-
23	CLA	C	1034	X	-	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	-	-	-
23	CLA	D	1005	X	-	X	-
23	CLA	D	1008	X	-	X	-
23	CLA	H	1017	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	-	-	-
23	CLA	b	6013	X	-	-	-
23	CLA	b	6014	X	-	-	-
23	CLA	b	6015	X	-	-	-
23	CLA	b	6016	X	-	-	-
23	CLA	b	6017	X	-	-	-
23	CLA	b	6018	X	-	-	-
23	CLA	b	6019	X	-	-	-
23	CLA	b	6020	X	-	-	-
23	CLA	b	6021	X	-	-	-
23	CLA	b	6022	X	-	-	-
23	CLA	b	6023	X	-	-	-
23	CLA	b	6024	X	-	-	X
23	CLA	c	6025	X	-	-	-
23	CLA	c	6026	X	-	-	-
23	CLA	c	6027	X	-	-	X
23	CLA	c	6028	X	-	-	-
23	CLA	c	6029	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	6034	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6035	X	-	-	-
23	CLA	c	6036	X	-	-	X
23	CLA	c	6037	X	-	-	X
23	CLA	d	6004	X	-	-	-
23	CLA	d	6005	X	-	-	-
23	CLA	d	6008	X	-	-	X
24	PHO	A	1038	X	-	X	-
24	PHO	A	1039	X	-	X	-
24	PHO	a	6039	X	-	-	-
24	PHO	d	6038	X	-	-	X
25	PQ9	D	1042	-	-	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	1054	-	-	X	X
26	BCR	D	1050	-	-	X	-
26	BCR	H	1049	-	-	X	X
26	BCR	K	1051	-	-	X	X
26	BCR	K	1052	-	-	X	X
26	BCR	T	6046	-	-	-	X
26	BCR	Z	1053	-	-	X	X
26	BCR	a	6044	-	-	-	X
26	BCR	b	6047	-	-	-	X
26	BCR	b	6048	-	-	-	X
26	BCR	c	6054	-	-	-	X
26	BCR	d	6050	-	-	-	X
26	BCR	h	6049	-	-	-	X
26	BCR	t	1046	-	-	-	X
26	BCR	z	6053	-	-	-	X
27	LHG	A	1063	-	-	X	X
27	LHG	a	6063	-	-	-	X
28	BR	A	1065	-	-	X	-
29	MGE	B	1060	-	-	X	-
29	MGE	D	1062	-	-	X	-
29	MGE	J	1059	-	-	X	-
29	MGE	L	1061	-	-	X	-
29	MGE	d	6059	-	-	-	X
30	DGD	C	1055	-	-	X	-
30	DGD	C	1056	-	-	X	X
30	DGD	C	1057	-	-	X	X
30	DGD	H	1058	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	DGD	c	6056	-	-	-	X
30	DGD	c	6057	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 47988 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	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	13			
2	b	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	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
			1841	1152	311	374	4			
13	o	242	Total	C	N	O	S	0	0	0
			1841	1152	311	374	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			

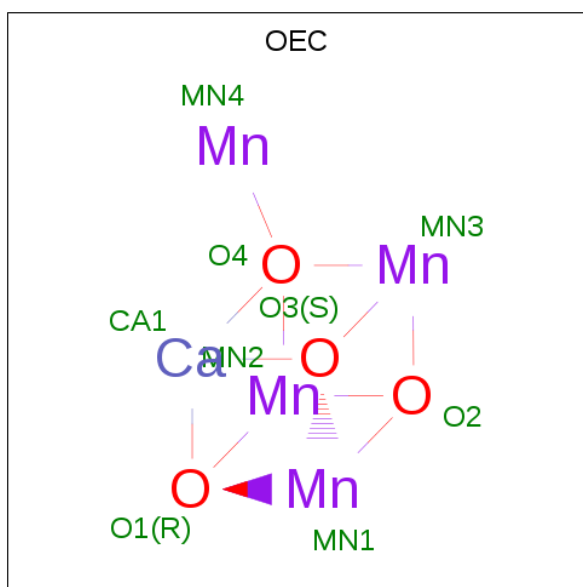
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	24	Total	C	N	O	0	0	0
			121	72	24	25			
19	n	24	Total	C	N	O	0	0	0
			121	72	24	25			

- 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	a	1	Total	Fe	0	0
			1	1		

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



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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	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	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
23	D	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

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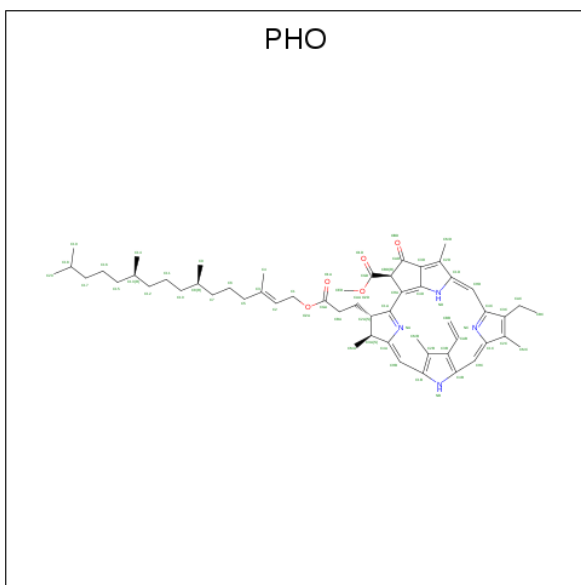
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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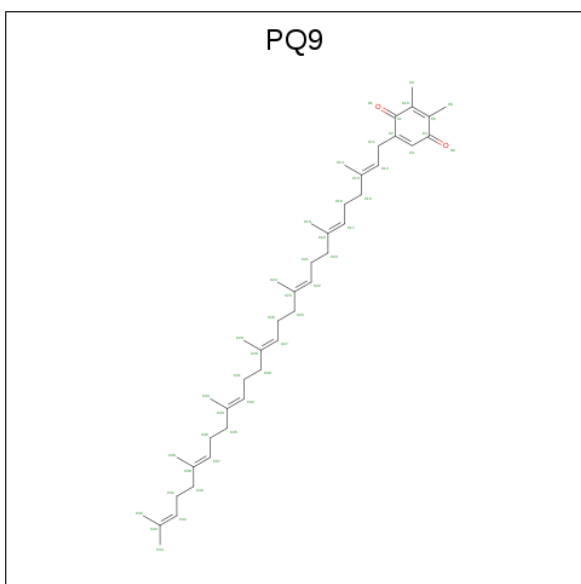
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



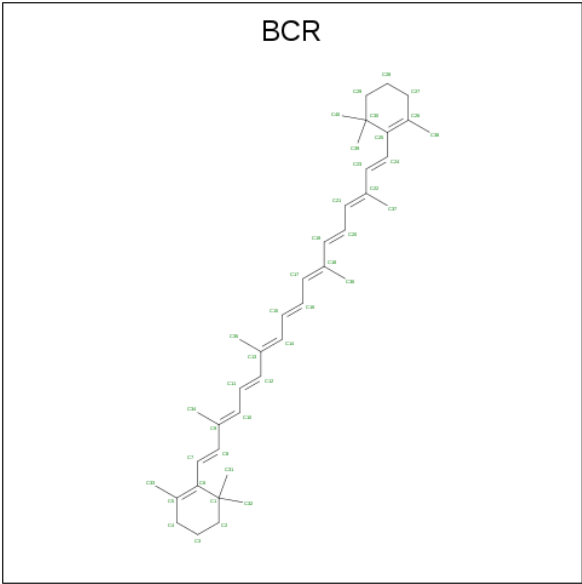
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- 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: $C_{43}H_{64}O_2$).



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).



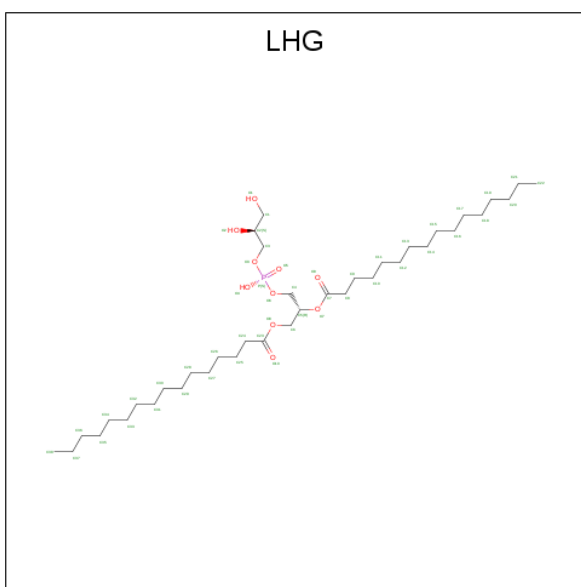
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		
26	H	1	Total	C	0	0
			40	40		
26	K	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	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	b	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	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

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

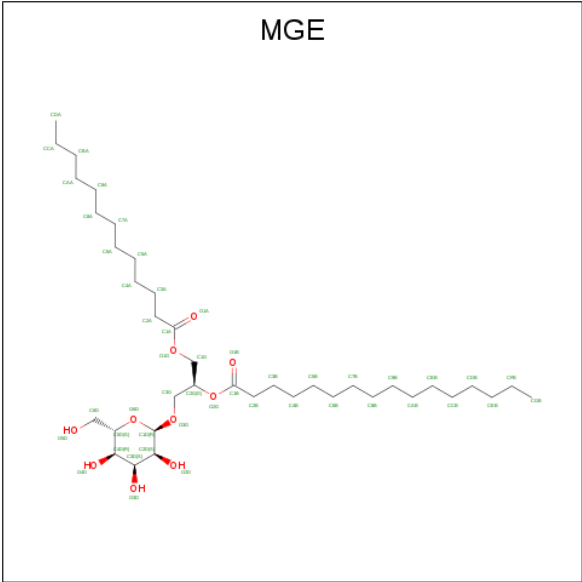


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is BROMIDE ION (three-letter code: BR) (formula: Br).

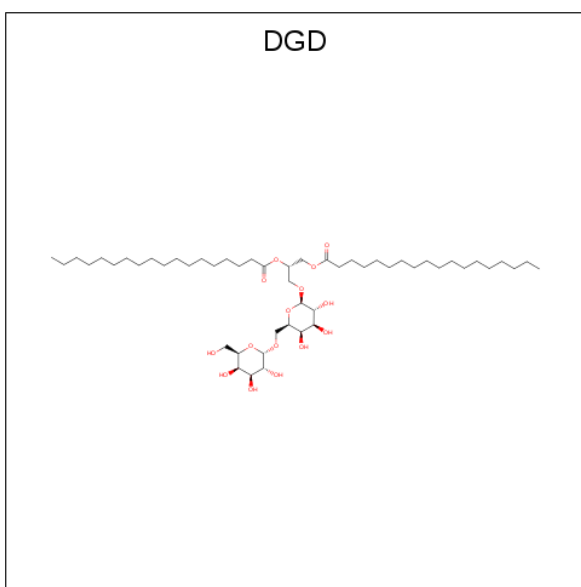
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	2	Total	Br	0	0
			2	2		
28	d	1	Total	Br	0	0
			1	1		
28	a	1	Total	Br	0	0
			1	1		

- Molecule 29 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



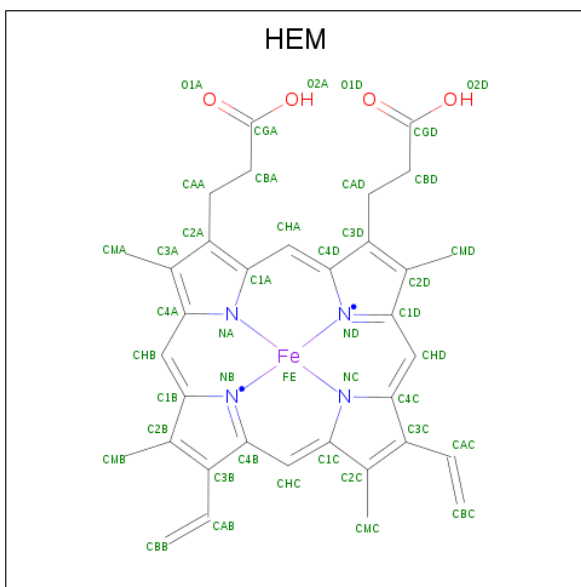
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	J	1	Total	C	O	0	0
			48	38	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	h	1	Total	C	O	0	0
			66	51	15		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

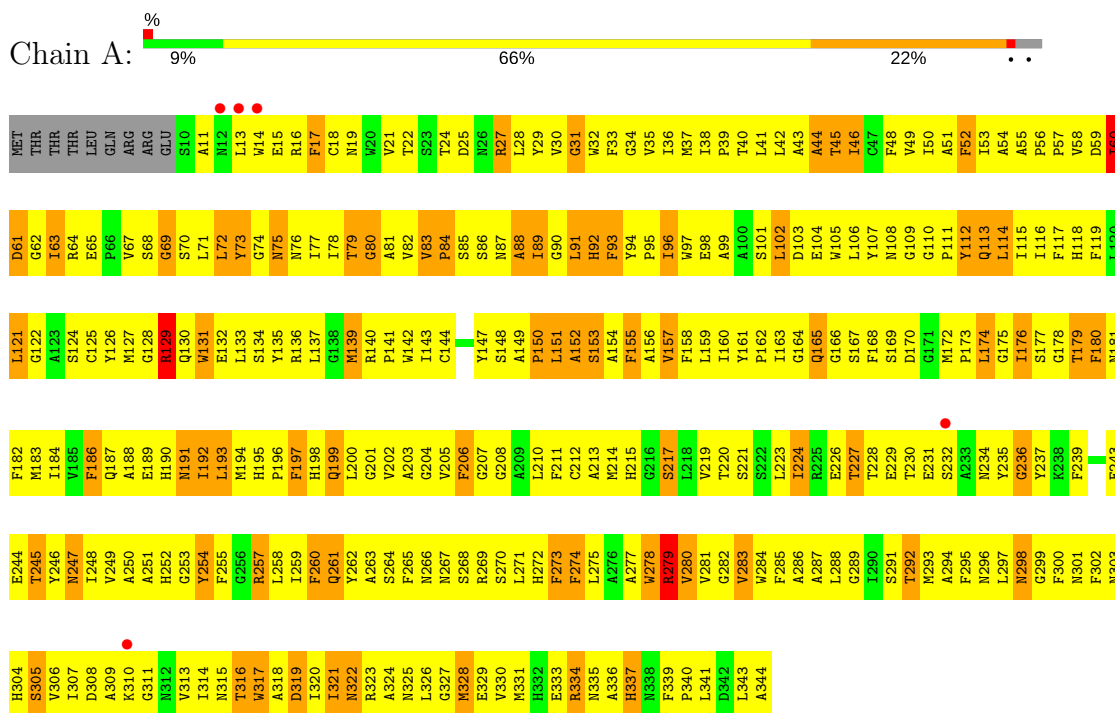


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
31	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

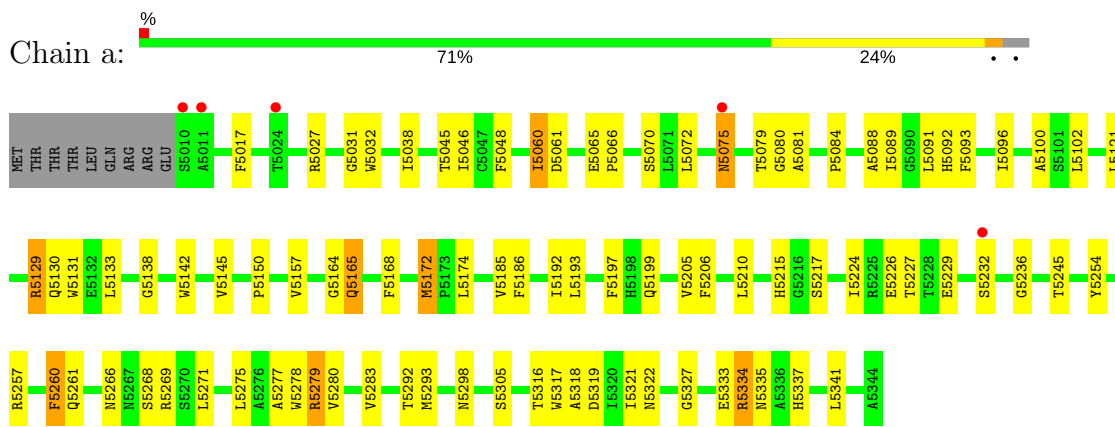
3 Residue-property plots

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.

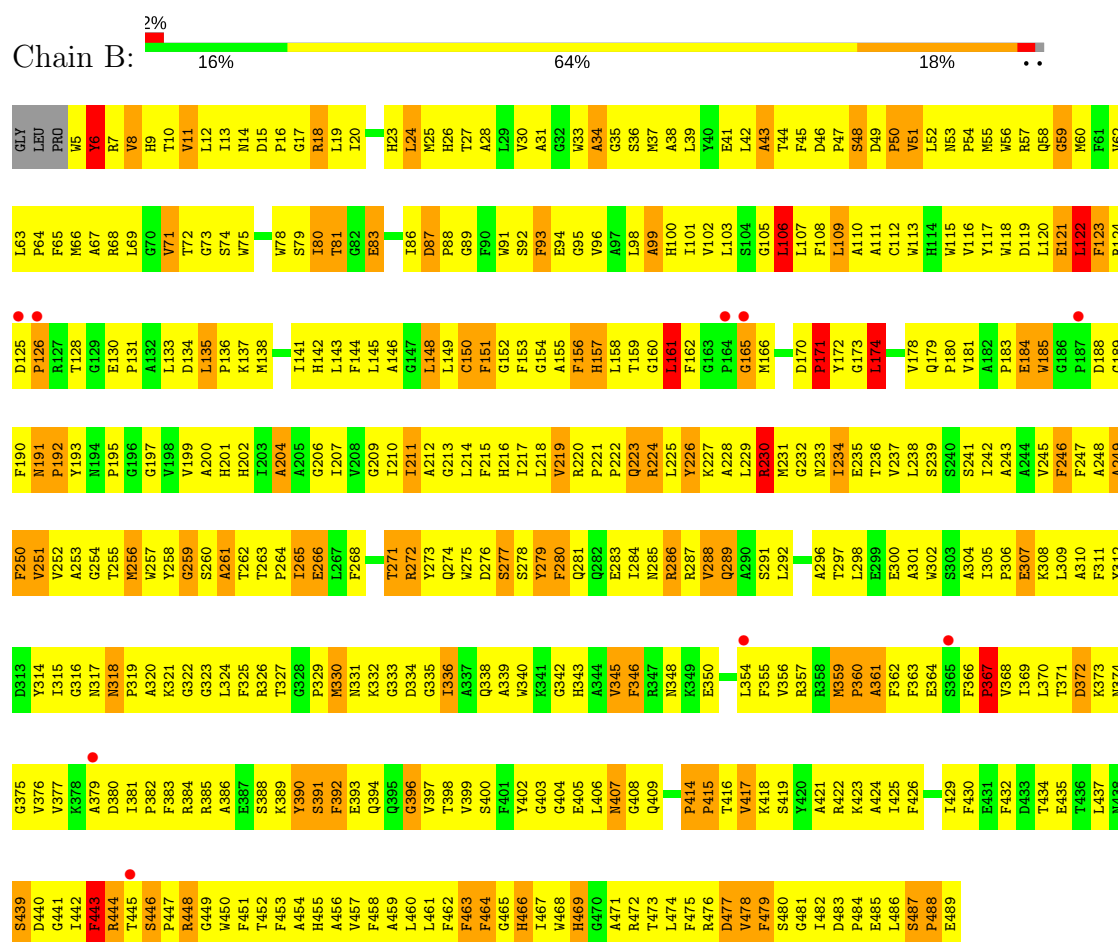
- Molecule 1: Photosystem Q(B) protein



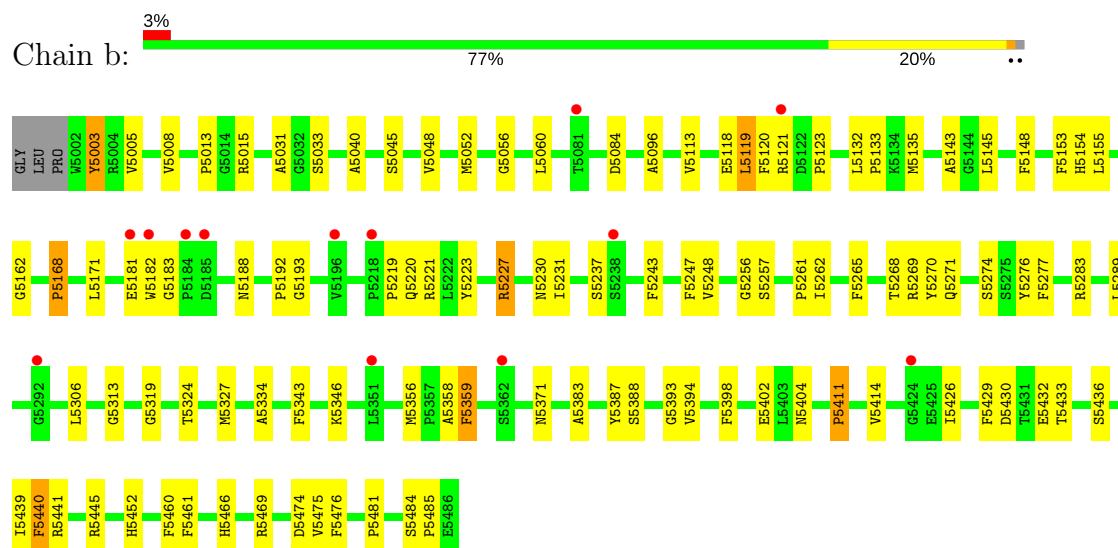
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II core light harvesting protein

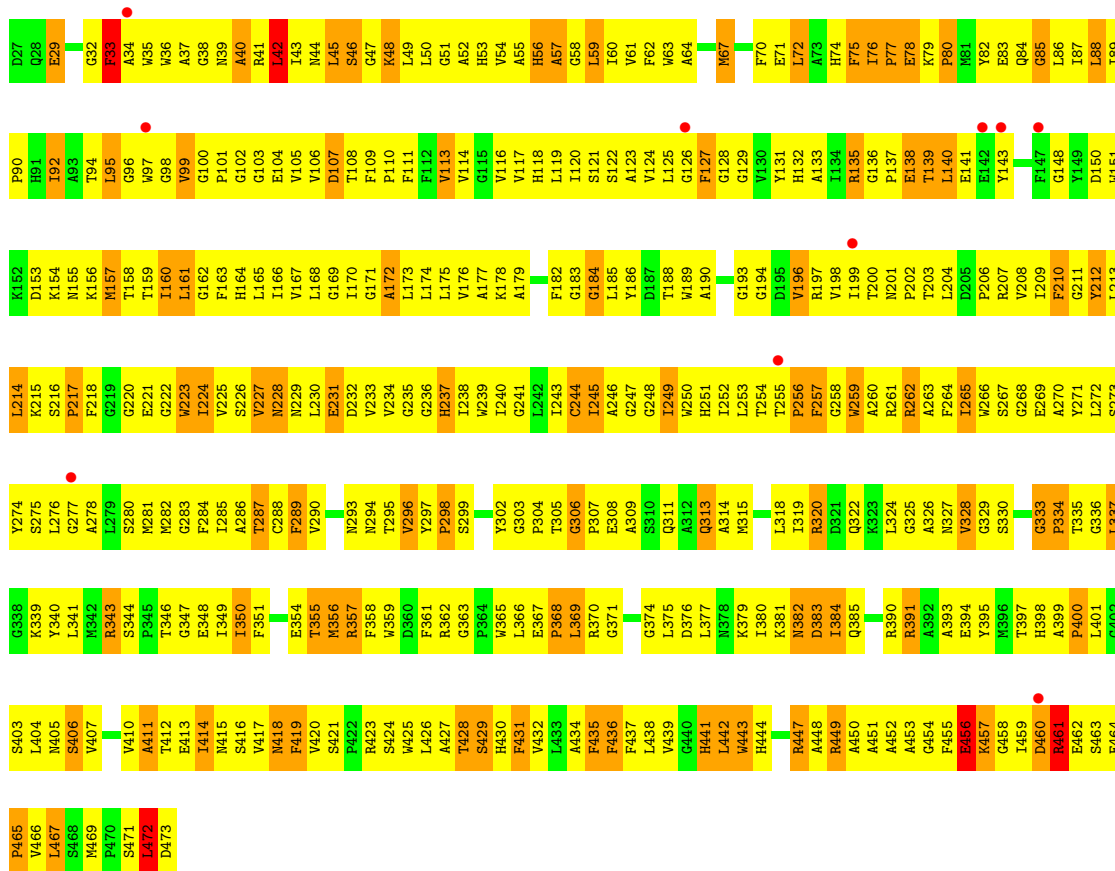


• Molecule 2: Photosystem II core light harvesting protein

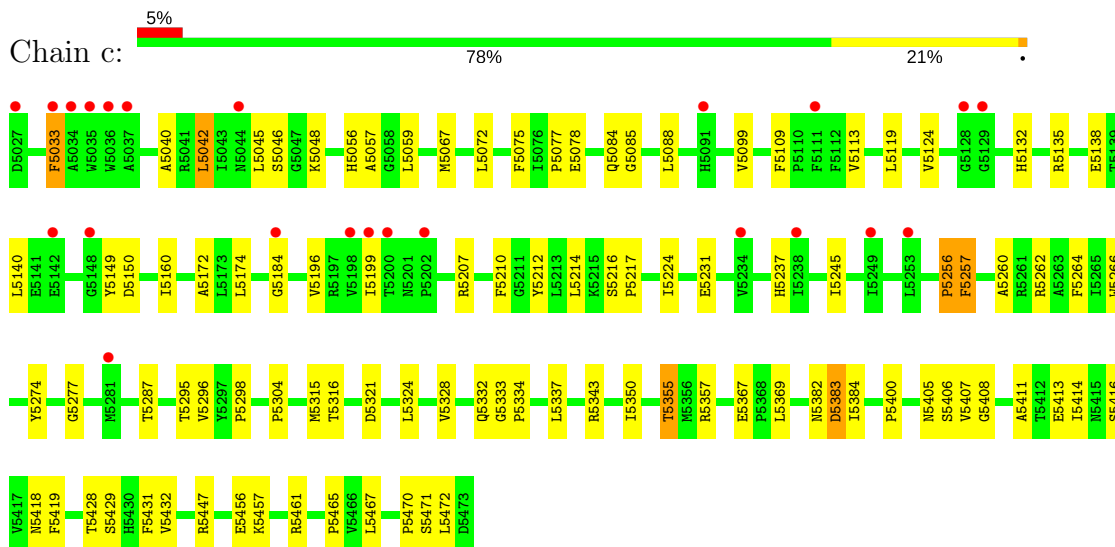


• Molecule 3: Photosystem II CP43 protein

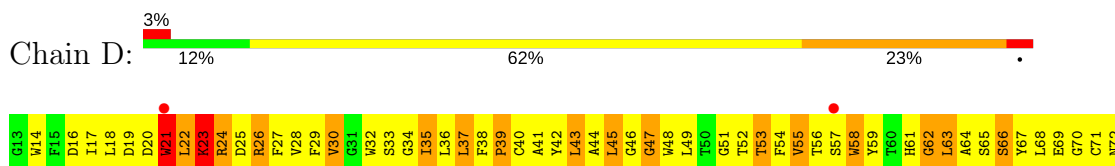


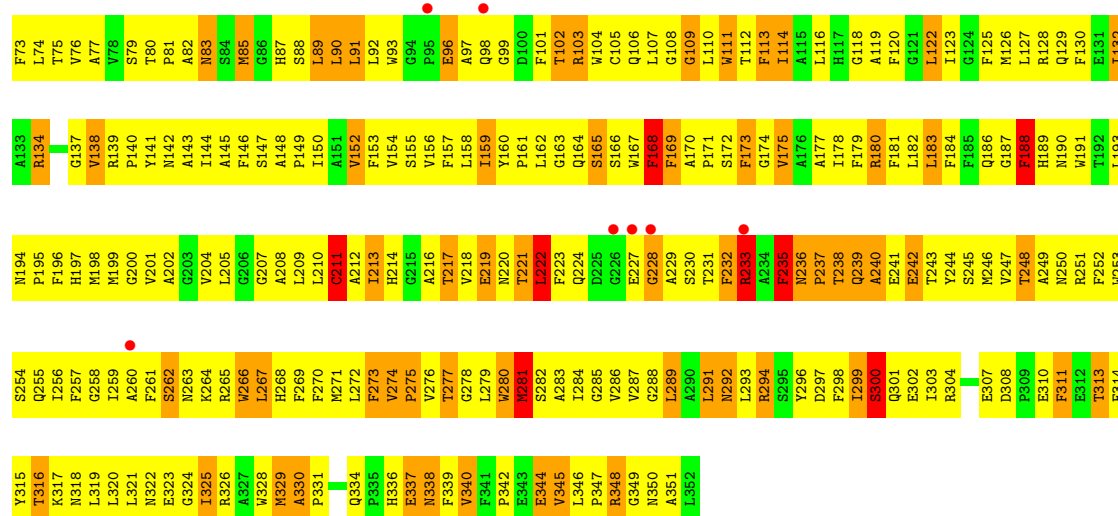


- Molecule 3: Photosystem II CP43 protein

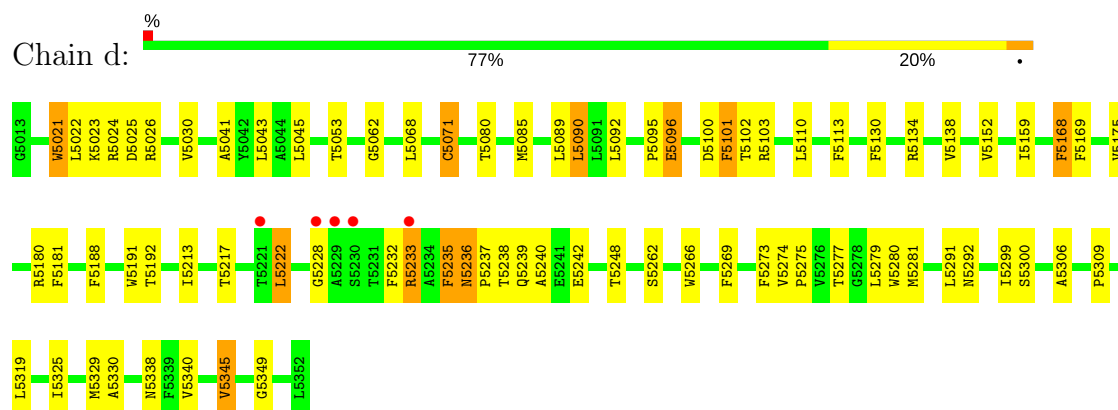


- Molecule 4: Photosystem II D2 protein

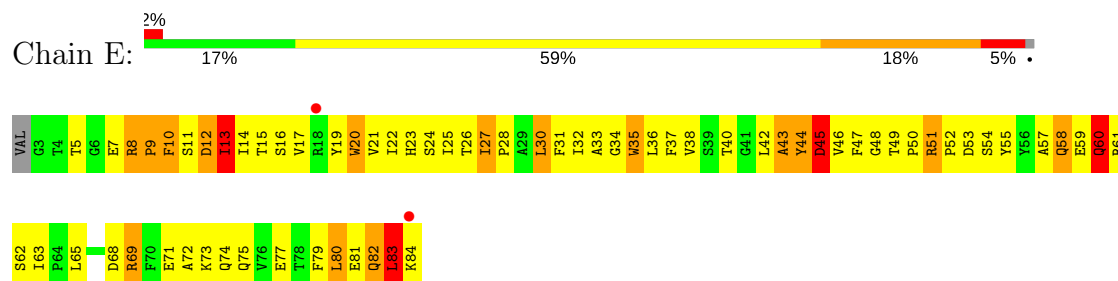




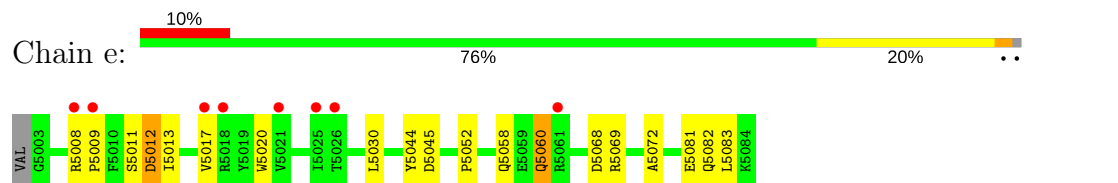
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

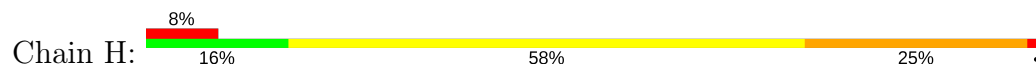




- Molecule 6: Cytochrome b559 subunit beta



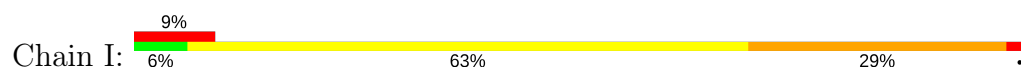
- Molecule 7: Photosystem II reaction center protein H



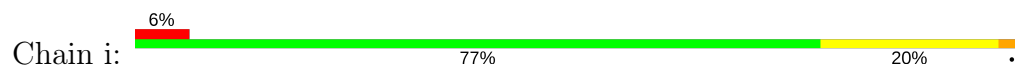
- Molecule 7: Photosystem II reaction center protein H



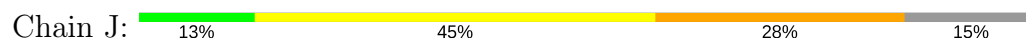
- Molecule 8: Photosystem II reaction center protein I



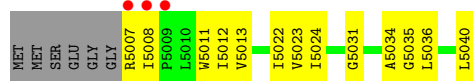
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



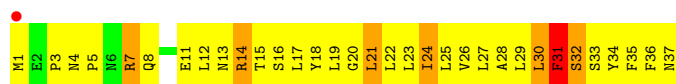
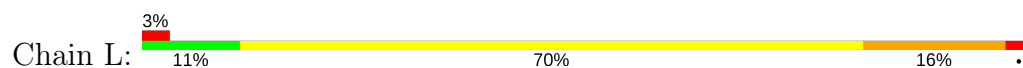
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



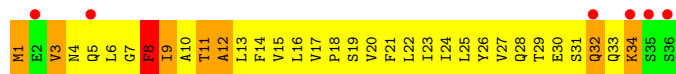
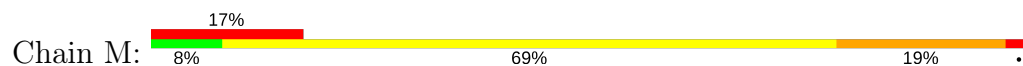
- Molecule 11: Photosystem II reaction center protein L



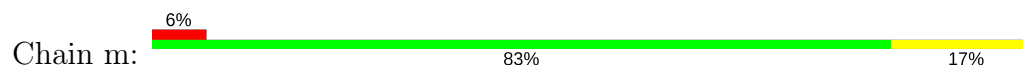
- Molecule 11: Photosystem II reaction center protein L



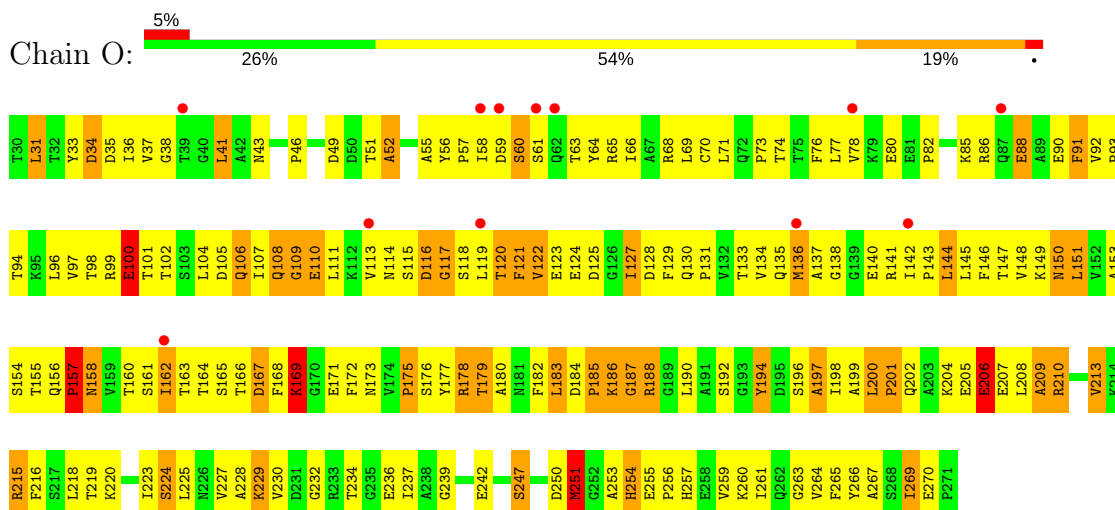
- Molecule 12: Photosystem II reaction center protein M



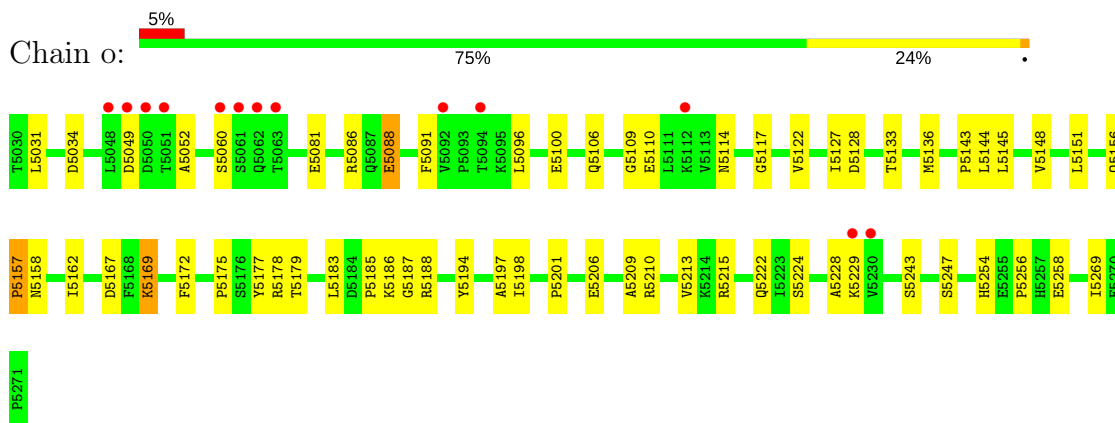
- Molecule 12: Photosystem II reaction center protein M



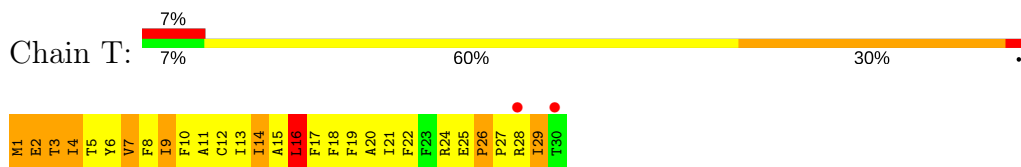
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



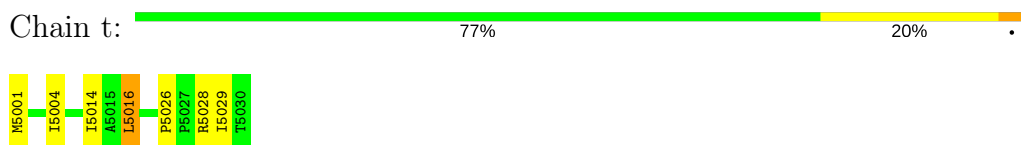
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



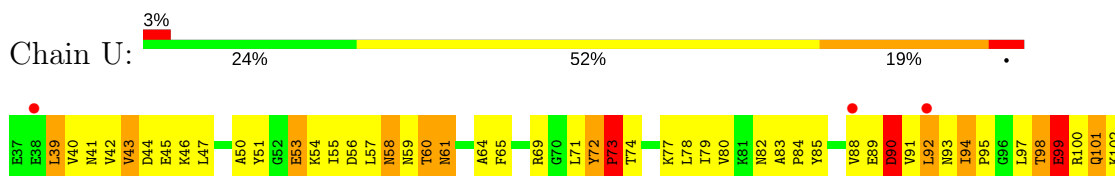
- Molecule 14: Photosystem II reaction center protein T

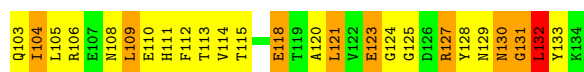


- Molecule 14: Photosystem II reaction center protein T



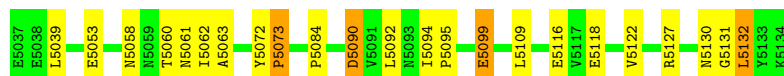
- Molecule 15: Photosystem II 12 kDa extrinsic protein





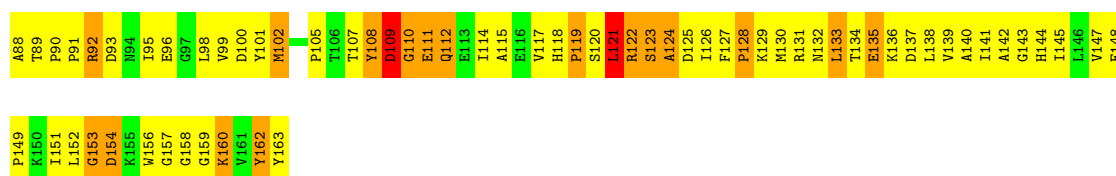
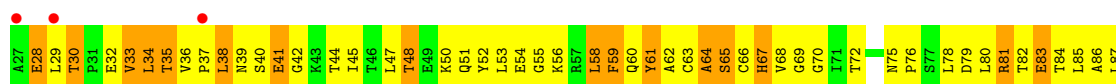
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 77% 19%



- Molecule 16: Cytochrome c-550

Chain V: 2% 15% 59% 24%



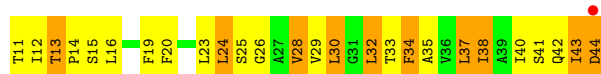
- Molecule 16: Cytochrome c-550

Chain v: 2% 76% 23%



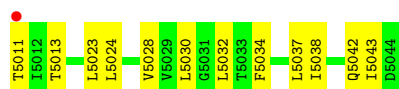
- Molecule 17: Photosystem II reaction center protein X

Chain X: 3% 24% 47% 29%



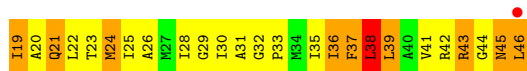
- Molecule 17: Photosystem II reaction center protein X

Chain x: 3% 65% 35%



- Molecule 18: Photosystem II reaction center protein ycf12

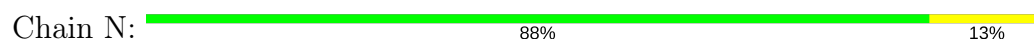
Chain Y: 4% 11% 54% 32%



- Molecule 18: Photosystem II reaction center protein ycf12



- Molecule 19: Photosystem II reaction center protein Y

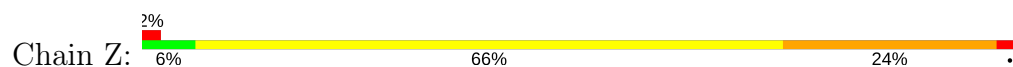


- Molecule 19: Photosystem II reaction center protein Y

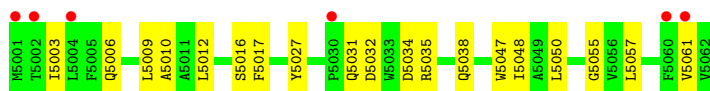


There are no outlier residues recorded for this chain.

- 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	130.59Å 226.39Å 307.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 3.70 34.69 – 3.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.70-3.70) 85.8 (34.69-3.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.302 , 0.358 0.285 , 0.284	Depositor DCC
R_{free} test set	4216 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47988	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, BR, PQ9, OEC, HEM, 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	0.51	0/2714	0.77	1/3699 (0.0%)
1	a	0.51	0/2714	0.77	0/3699
2	B	0.51	0/3951	0.79	3/5383 (0.1%)
2	b	0.51	0/3951	0.79	0/5383
3	C	0.48	0/3568	0.74	0/4858
3	c	0.49	0/3568	0.72	1/4858 (0.0%)
4	D	0.52	0/2801	0.77	1/3818 (0.0%)
4	d	0.52	0/2801	0.78	0/3818
5	E	0.46	0/685	0.74	0/933
5	e	0.50	0/685	0.76	0/933
6	F	0.50	0/291	0.77	0/397
6	f	0.58	0/291	0.69	0/397
7	H	0.52	0/520	0.81	0/708
7	h	0.50	0/520	0.82	1/708 (0.1%)
8	I	0.55	0/294	0.68	0/395
8	i	0.55	0/294	0.64	0/395
9	J	0.48	0/255	0.66	0/346
9	j	0.52	0/255	0.72	0/346
10	K	0.54	0/287	0.79	0/394
10	k	0.53	0/287	0.81	0/394
11	L	0.48	0/311	0.76	0/422
11	l	0.49	0/311	0.73	0/422
12	M	0.58	0/287	0.76	0/388
12	m	0.48	0/287	0.76	0/388
13	O	0.48	0/1872	0.79	0/2539
13	o	0.47	0/1872	0.78	0/2539
14	T	0.67	0/266	0.82	0/359
14	t	0.64	0/266	0.74	1/359 (0.3%)
15	U	0.48	0/794	0.77	0/1076
15	u	0.46	0/794	0.81	0/1076
16	V	0.50	0/1085	0.82	1/1473 (0.1%)
16	v	0.50	0/1085	0.82	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.52	0/249	0.78	0/337
17	x	0.52	0/249	0.71	0/337
18	Y	0.51	0/209	0.88	1/279 (0.4%)
18	y	0.47	0/209	0.83	0/279
20	Z	0.50	0/490	0.75	0/669
20	z	0.51	0/490	0.79	0/669
All	All	0.50	0/41858	0.77	10/56946 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	108	TYR	N-CA-C	-5.84	95.24	111.00
2	B	232	GLY	N-CA-C	-5.64	99.00	113.10
2	B	106	LEU	CB-CG-CD1	-5.42	101.78	111.00
18	Y	38	LEU	CA-CB-CG	5.37	127.65	115.30
14	t	5016	LEU	CA-CB-CG	5.32	127.54	115.30
2	B	466	HIS	N-CA-C	-5.16	97.06	111.00
1	A	69	GLY	N-CA-C	-5.09	100.38	113.10
7	h	5012	ARG	N-CA-C	-5.07	97.32	111.00
4	D	63	LEU	CA-CB-CG	5.05	126.92	115.30
3	c	5150	ASP	N-CA-C	-5.04	97.40	111.00

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	773	0
1	a	2630	0	2528	0	0
2	B	3816	0	3680	965	0
2	b	3816	0	3680	0	0
3	C	3455	0	3376	789	0
3	c	3455	0	3376	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2706	0	2608	774	0
4	d	2706	0	2608	0	0
5	E	666	0	651	140	0
5	e	666	0	651	0	0
6	F	282	0	291	74	0
6	f	282	0	291	0	0
7	H	507	0	529	130	0
7	h	507	0	529	0	0
8	I	287	0	308	77	0
8	i	287	0	305	0	0
9	J	249	0	262	63	0
9	j	249	0	262	0	0
10	K	278	0	289	115	0
10	k	278	0	289	0	0
11	L	304	0	316	100	0
11	l	304	0	313	0	0
12	M	283	0	297	58	0
12	m	283	0	294	0	0
13	O	1841	0	1799	283	0
13	o	1841	0	1799	0	0
14	T	257	0	262	90	0
14	t	257	0	259	0	0
15	U	783	0	779	148	0
15	u	783	0	779	0	0
16	V	1064	0	1072	193	0
16	v	1064	0	1072	0	0
17	X	246	0	269	46	0
17	x	246	0	269	0	0
18	Y	208	0	237	54	0
18	y	208	0	237	0	0
19	N	121	0	26	2	0
19	n	121	0	26	0	0
20	Z	479	0	516	122	0
20	z	479	0	513	0	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	166	0
23	B	975	0	1079	778	0
23	C	845	0	935	534	0
23	D	195	0	216	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	H	65	0	72	60	0
23	a	195	0	216	0	0
23	b	1040	0	1151	0	0
23	c	845	0	935	0	0
23	d	195	0	216	0	0
24	A	128	0	148	116	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	45	0	64	7	0
25	D	45	0	64	32	0
25	a	45	0	64	0	0
25	d	45	0	62	0	0
26	A	40	0	48	25	0
26	B	120	0	141	86	0
26	C	40	0	47	26	0
26	D	40	0	48	62	0
26	H	40	0	47	53	0
26	K	80	0	94	81	0
26	T	40	0	47	18	0
26	Z	40	0	48	41	0
26	a	40	0	48	0	0
26	b	120	0	141	0	0
26	c	40	0	47	0	0
26	d	40	0	48	0	0
26	h	40	0	47	0	0
26	k	80	0	94	0	0
26	t	40	0	47	0	0
26	z	40	0	48	0	0
27	A	49	0	74	58	0
27	a	49	0	74	0	0
28	A	2	0	0	4	0
28	a	1	0	0	0	0
28	d	1	0	0	0	0
29	B	48	0	72	47	0
29	D	48	0	72	23	0
29	J	48	0	72	34	0
29	L	48	0	72	33	0
29	b	48	0	72	0	0
29	d	144	0	216	0	0
30	C	198	0	288	149	0
30	H	66	0	96	32	0
30	c	198	0	288	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	h	66	0	96	0	0
31	E	43	0	30	10	0
31	V	43	0	30	10	0
31	e	43	0	30	0	0
31	v	43	0	30	0	0
All	All	47988	0	48413	6019	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 126.

All (6019) 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)
26:T:6046:BCR:H371	26:T:6046:BCR:C26	1.34	1.51
23:B:1009:CLA:CMB	26:H:1049:BCR:H393	1.41	1.49
23:C:1032:CLA:CED	23:C:1032:CLA:H2A	1.41	1.47
23:A:1003:CLA:H141	24:A:1038:PHO:C9	1.41	1.47
10:K:28:ILE:CG2	10:K:29:PRO:HD3	1.42	1.46
23:B:1012:CLA:HED2	23:B:1012:CLA:CAA	1.44	1.46
23:B:1019:CLA:HED2	23:B:1019:CLA:CAA	1.46	1.45
26:K:1051:BCR:H322	26:K:1052:BCR:C10	1.42	1.45
23:A:1006:CLA:H171	26:D:1050:BCR:C29	1.48	1.44
3:C:63:TRP:CZ3	23:C:1027:CLA:HBC1	1.51	1.43
23:B:1011:CLA:HBB2	23:B:1013:CLA:C20	1.49	1.42
23:B:1022:CLA:H72	23:B:1022:CLA:C14	1.45	1.42
23:C:1031:CLA:CGD	23:C:1033:CLA:H101	1.48	1.41
23:D:1005:CLA:H2A	23:D:1005:CLA:CED	1.48	1.40
26:B:1047:BCR:C34	26:B:1047:BCR:H321	1.50	1.39
24:A:1038:PHO:C19	24:A:1038:PHO:H141	1.52	1.37
29:B:1060:MGE:H251	29:B:1060:MGE:CBB	1.55	1.36
23:B:1012:CLA:HAA2	23:B:1012:CLA:CED	1.55	1.36
23:B:1010:CLA:C12	23:B:1010:CLA:H91	1.51	1.36
2:B:464:PHE:CZ	29:B:1060:MGE:H4B2	1.58	1.36
23:C:1032:CLA:HED3	23:C:1032:CLA:C2A	1.53	1.36
23:C:1034:CLA:H41	23:C:1034:CLA:C8	1.55	1.36
10:K:28:ILE:HD11	26:K:1051:BCR:C8	1.56	1.35
23:B:1014:CLA:C9	23:B:1014:CLA:H122	1.57	1.34
23:B:1019:CLA:CED	23:B:1019:CLA:H2A	1.56	1.33
23:B:1016:CLA:H52	23:H:1017:CLA:C10	1.56	1.33
26:B:1045:BCR:H371	26:B:1045:BCR:C40	1.59	1.33
26:K:1051:BCR:H371	26:K:1051:BCR:C40	1.59	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:1050:BCR:HC8	26:D:1050:BCR:C33	1.52	1.32
26:K:1051:BCR:C39	26:K:1051:BCR:H371	1.59	1.32
23:B:1022:CLA:HHD	23:B:1022:CLA:CBC	1.53	1.32
23:C:1028:CLA:H121	23:C:1028:CLA:C17	1.57	1.32
26:D:1050:BCR:H371	26:D:1050:BCR:C39	1.58	1.31
26:T:6046:BCR:H371	26:T:6046:BCR:C38	1.60	1.31
29:B:1060:MGE:H212	29:B:1060:MGE:CFB	1.50	1.31
26:B:1045:BCR:H371	26:B:1045:BCR:C39	1.59	1.31
10:K:28:ILE:HG22	10:K:29:PRO:CD	1.59	1.31
12:M:1:MET:N	12:M:1:MET:HE2	1.40	1.31
23:A:1003:CLA:CAB	23:A:1006:CLA:HMD2	1.58	1.31
23:C:1033:CLA:C14	23:C:1033:CLA:H18	1.60	1.31
26:A:1044:BCR:C39	26:A:1044:BCR:H371	1.60	1.30
23:B:1020:CLA:H91	23:B:1020:CLA:C12	1.59	1.30
26:A:1044:BCR:C40	26:A:1044:BCR:H371	1.59	1.30
1:A:72:LEU:O	1:A:73:TYR:CD2	1.85	1.30
23:B:1012:CLA:C9	23:B:1012:CLA:H121	1.58	1.30
26:D:1050:BCR:C40	26:D:1050:BCR:H371	1.59	1.30
26:C:1054:BCR:C38	26:C:1054:BCR:H23C	1.58	1.29
23:B:1014:CLA:O1A	23:B:1014:CLA:HMA3	1.33	1.29
23:B:1020:CLA:CMA	23:B:1020:CLA:HBA1	1.57	1.29
23:C:1033:CLA:C15	23:C:1033:CLA:H192	1.60	1.29
26:D:1050:BCR:C37	29:J:1059:MGE:H4A2	1.62	1.28
23:B:1014:CLA:H112	23:B:1014:CLA:C16	1.63	1.27
23:B:1022:CLA:H92	23:B:1022:CLA:C5	1.62	1.27
26:B:1045:BCR:C30	26:B:1045:BCR:H371	1.65	1.27
23:C:1029:CLA:C15	23:C:1029:CLA:H192	1.51	1.27
26:A:1044:BCR:C30	26:A:1044:BCR:H371	1.63	1.26
23:B:1010:CLA:C9	23:B:1010:CLA:H122	1.49	1.26
24:A:1038:PHO:H193	24:A:1038:PHO:C14	1.64	1.26
26:A:1044:BCR:C37	26:A:1044:BCR:H403	1.64	1.26
26:A:1044:BCR:H392	26:A:1044:BCR:C37	1.64	1.26
26:K:1051:BCR:H392	26:K:1051:BCR:C37	1.65	1.25
23:B:1022:CLA:H52	23:B:1022:CLA:C9	1.51	1.25
26:K:1051:BCR:H322	26:K:1052:BCR:C11	1.65	1.25
26:D:1050:BCR:C37	26:D:1050:BCR:H403	1.65	1.25
26:K:1051:BCR:H371	26:K:1051:BCR:C30	1.64	1.25
14:T:1:MET:CE	14:T:1:MET:H1	1.47	1.25
1:A:72:LEU:C	1:A:73:TYR:HD2	1.37	1.25
10:K:32:PHE:CE1	26:K:1052:BCR:H24C	1.72	1.25
26:B:1045:BCR:C37	26:B:1045:BCR:H392	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:1050:BCR:C30	26:D:1050:BCR:H371	1.66	1.24
26:D:1050:BCR:C37	26:D:1050:BCR:H392	1.65	1.24
26:D:1050:BCR:H373	29:J:1059:MGE:C4A	1.66	1.24
26:B:1048:BCR:H23C	26:B:1048:BCR:C38	1.63	1.24
2:B:464:PHE:CZ	29:B:1060:MGE:C4B	2.21	1.24
26:B:1045:BCR:C37	26:B:1045:BCR:H403	1.66	1.24
26:K:1051:BCR:H403	26:K:1051:BCR:C37	1.66	1.24
23:B:1009:CLA:HMB2	26:H:1049:BCR:C39	1.68	1.24
23:C:1029:CLA:C19	23:C:1029:CLA:H152	1.57	1.23
23:C:1034:CLA:C7	23:C:1034:CLA:H41	1.54	1.23
23:B:1010:CLA:OBD	23:B:1010:CLA:HED3	1.36	1.23
23:A:1006:CLA:CMB	24:A:1039:PHO:H161	1.66	1.23
23:B:1021:CLA:C17	29:B:1060:MGE:H132	1.68	1.23
23:C:1033:CLA:C19	23:C:1033:CLA:H151	1.63	1.23
23:C:1026:CLA:H51	23:C:1026:CLA:O1A	1.34	1.23
23:C:1029:CLA:HMA2	23:C:1029:CLA:CBA	1.60	1.23
1:A:72:LEU:C	1:A:73:TYR:CD2	2.12	1.23
23:B:1022:CLA:C17	23:B:1022:CLA:H141	1.67	1.22
14:T:4:ILE:O	14:T:4:ILE:HD12	1.34	1.22
23:B:1020:CLA:CBA	23:B:1020:CLA:HMA2	1.67	1.22
23:D:1008:CLA:H71	23:D:1008:CLA:C4	1.64	1.22
10:K:28:ILE:HA	10:K:31:LEU:CD1	1.70	1.21
23:C:1033:CLA:C12	23:C:1033:CLA:H91	1.66	1.21
23:B:1009:CLA:CGD	23:B:1009:CLA:HBA2	1.69	1.21
23:B:1020:CLA:H12	23:B:1023:CLA:CED	1.69	1.21
23:C:1031:CLA:O2D	23:C:1031:CLA:HAA2	1.36	1.21
26:B:1047:BCR:H343	26:B:1047:BCR:C32	1.72	1.20
23:B:1020:CLA:C13	23:B:1020:CLA:H91	1.70	1.20
23:A:1006:CLA:H111	30:C:1057:DGD:CIB	1.71	1.20
23:B:1022:CLA:HED2	23:B:1022:CLA:OBD	1.39	1.20
23:C:1031:CLA:CED	23:C:1031:CLA:HAA2	1.70	1.20
23:B:1011:CLA:CBB	23:B:1013:CLA:H171	1.71	1.20
23:B:1014:CLA:H91	23:B:1014:CLA:C12	1.71	1.20
23:B:1020:CLA:C8	23:B:1020:CLA:H13	1.54	1.19
26:B:1047:BCR:C9	26:B:1047:BCR:H321	1.71	1.19
23:C:1025:CLA:C16	23:C:1031:CLA:HMB3	1.71	1.19
23:A:1006:CLA:HBC3	23:A:1006:CLA:HHD	1.25	1.19
23:B:1014:CLA:CMA	23:B:1014:CLA:HBA1	1.69	1.19
26:Z:1053:BCR:C38	26:Z:1053:BCR:H23C	1.65	1.19
23:B:1009:CLA:H12	26:H:1049:BCR:C16	1.73	1.18
23:C:1034:CLA:C17	23:C:1034:CLA:H141	1.71	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1009:CLA:HMB1	26:H:1049:BCR:H393	1.21	1.18
30:C:1056:DGD:C3E	30:C:1056:DGD:HD61	1.62	1.18
23:B:1022:CLA:H172	23:B:1022:CLA:C14	1.71	1.18
23:B:1022:CLA:O1D	23:B:1022:CLA:HAA1	1.39	1.18
23:C:1031:CLA:H2	23:C:1031:CLA:CMA	1.70	1.18
23:B:1023:CLA:HAA2	23:B:1023:CLA:CGD	1.74	1.18
23:C:1033:CLA:C18	23:C:1033:CLA:H141	1.72	1.18
23:C:1037:CLA:HAA1	23:C:1037:CLA:O2D	1.43	1.18
23:B:1014:CLA:HHD	23:B:1014:CLA:HBC2	1.24	1.17
10:K:26:PRO:O	10:K:29:PRO:HD2	1.44	1.17
23:C:1025:CLA:CBB	23:C:1025:CLA:H93	1.75	1.17
24:A:1038:PHO:HMB3	23:D:1005:CLA:C9	1.74	1.17
10:K:32:PHE:CE1	26:K:1052:BCR:H392	1.80	1.17
23:B:1012:CLA:H121	23:B:1012:CLA:H91	1.23	1.17
23:B:1011:CLA:C3D	23:B:1013:CLA:H43	1.74	1.17
26:K:1051:BCR:H331	26:K:1051:BCR:C8	1.59	1.17
23:B:1014:CLA:C19	23:B:1014:CLA:H151	1.74	1.17
23:C:1033:CLA:HHD	23:C:1033:CLA:HBC3	1.26	1.16
10:K:39:VAL:HG22	18:Y:36:ILE:CD1	1.75	1.16
23:B:1022:CLA:C8	23:B:1022:CLA:H13	1.75	1.16
23:B:1009:CLA:HAA1	23:B:1009:CLA:O2D	1.45	1.16
23:B:1011:CLA:CBB	23:B:1013:CLA:H203	1.74	1.16
23:D:1005:CLA:H202	23:D:1005:CLA:H151	1.27	1.16
14:T:1:MET:O	14:T:4:ILE:HG22	1.46	1.16
23:C:1033:CLA:CMA	23:C:1033:CLA:HBA1	1.75	1.16
23:A:1003:CLA:H161	24:A:1038:PHO:C9	1.75	1.15
23:B:1022:CLA:CGD	23:B:1022:CLA:HAA1	1.75	1.15
27:A:1063:LHG:H161	27:A:1063:LHG:H121	1.19	1.15
23:A:1006:CLA:C17	26:D:1050:BCR:H291	1.76	1.15
1:A:279:ARG:NH2	24:A:1038:PHO:HAC1	1.62	1.15
23:B:1022:CLA:H8	23:B:1022:CLA:H13	1.23	1.15
23:C:1029:CLA:CMA	23:C:1029:CLA:HBA2	1.70	1.15
1:A:78:ILE:HA	1:A:176:ILE:HD12	1.27	1.15
23:A:1003:CLA:C16	24:A:1038:PHO:H93	1.76	1.15
23:B:1010:CLA:CMD	23:B:1011:CLA:H8	1.74	1.15
23:C:1034:CLA:H172	23:C:1034:CLA:C14	1.73	1.15
23:B:1023:CLA:C12	23:B:1023:CLA:H91	1.74	1.15
2:B:103:LEU:HB2	23:B:1014:CLA:H71	1.25	1.15
2:B:460:LEU:HA	30:H:1058:DGD:HAG1	1.16	1.15
7:H:35:MET:HG2	26:H:1049:BCR:H333	1.28	1.14
24:A:1038:PHO:H193	24:A:1038:PHO:C13	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1036:CLA:H172	26:Z:1053:BCR:H373	1.19	1.14
23:C:1034:CLA:H102	23:C:1034:CLA:C4	1.78	1.14
23:C:1033:CLA:CBA	23:C:1033:CLA:HMA3	1.76	1.14
2:B:257:TRP:CZ3	4:D:291:LEU:HG	1.81	1.14
23:A:1006:CLA:C17	26:D:1050:BCR:H401	1.77	1.14
23:B:1011:CLA:HBB2	23:B:1013:CLA:C18	1.77	1.14
23:A:1006:CLA:H172	26:D:1050:BCR:H401	1.30	1.14
1:A:60:ILE:HG12	1:A:61:ASP:H	1.03	1.13
23:B:1022:CLA:H72	23:B:1022:CLA:H141	1.29	1.13
1:A:54:ALA:HB2	1:A:72:LEU:HD12	1.24	1.13
23:H:1017:CLA:HHD	23:H:1017:CLA:HBC2	1.27	1.13
23:C:1028:CLA:C12	23:C:1028:CLA:H172	1.77	1.12
23:C:1033:CLA:HED3	23:C:1033:CLA:OBD	1.48	1.12
10:K:28:ILE:HD11	26:K:1051:BCR:C9	1.78	1.12
3:C:62:PHE:CE2	10:K:28:ILE:HG21	1.84	1.12
23:B:1023:CLA:H91	23:B:1023:CLA:H121	1.29	1.12
2:B:271:THR:HG23	2:B:274:GLN:HB2	1.18	1.12
23:C:1034:CLA:H41	23:C:1034:CLA:C10	1.79	1.12
3:C:264:PHE:CE1	26:C:1054:BCR:H311	1.83	1.12
1:A:57:PRO:HA	1:A:68:SER:CB	1.79	1.12
23:B:1020:CLA:H12	23:B:1023:CLA:HED1	1.12	1.12
26:C:1054:BCR:H383	26:C:1054:BCR:H23C	1.18	1.12
29:D:1062:MGE:H241	14:T:13:ILE:HG21	1.31	1.12
23:B:1009:CLA:HHC	23:B:1009:CLA:HBB1	1.15	1.12
1:A:150:PRO:HA	23:A:1003:CLA:H42	1.23	1.12
23:B:1012:CLA:H12	23:B:1013:CLA:C1	1.78	1.12
23:C:1036:CLA:C17	23:C:1036:CLA:H142	1.75	1.12
23:B:1009:CLA:HMB2	26:H:1049:BCR:H393	1.13	1.12
23:C:1034:CLA:C9	23:C:1034:CLA:H142	1.79	1.11
23:D:1005:CLA:C20	23:D:1005:CLA:H151	1.81	1.11
10:K:28:ILE:CA	10:K:31:LEU:HD12	1.81	1.11
23:C:1034:CLA:HHD	23:C:1034:CLA:HBC3	1.27	1.11
23:C:1034:CLA:C9	23:C:1034:CLA:H121	1.77	1.11
23:B:1016:CLA:H52	23:H:1017:CLA:H101	1.24	1.11
23:A:1003:CLA:H161	24:A:1038:PHO:H93	1.11	1.10
23:C:1025:CLA:HAA1	23:C:1025:CLA:CGD	1.80	1.10
26:D:1050:BCR:C8	26:D:1050:BCR:H331	1.53	1.10
23:C:1025:CLA:H162	23:C:1031:CLA:HMB3	1.33	1.10
23:B:1019:CLA:HAA2	23:B:1019:CLA:CED	1.79	1.10
23:B:1022:CLA:C7	23:B:1022:CLA:C14	2.30	1.10
23:C:1036:CLA:H171	23:C:1036:CLA:H142	1.24	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB1	1:A:283:VAL:CG2	1.80	1.10
23:C:1034:CLA:H92	23:C:1034:CLA:C14	1.82	1.10
23:B:1009:CLA:CGD	23:B:1009:CLA:CBA	2.30	1.10
23:C:1031:CLA:C14	23:C:1031:CLA:H171	1.81	1.10
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.21	1.10
26:T:6046:BCR:C37	26:T:6046:BCR:C38	2.30	1.10
23:A:1006:CLA:H111	30:C:1057:DGD:HGB3	1.13	1.10
2:B:38:ALA:O	2:B:42:LEU:HB2	1.52	1.10
23:H:1017:CLA:C19	23:H:1017:CLA:H152	1.81	1.09
23:C:1034:CLA:H142	23:C:1034:CLA:H92	1.10	1.09
24:A:1038:PHO:CMB	23:D:1005:CLA:H92	1.80	1.09
23:B:1014:CLA:CGA	23:B:1014:CLA:HMA3	1.81	1.09
13:O:119:LEU:H	13:O:155:THR:HG22	1.14	1.09
1:A:95:PRO:HA	23:A:1007:CLA:HED1	1.12	1.09
27:A:1063:LHG:H322	23:C:1034:CLA:C14	1.82	1.09
1:A:279:ARG:HH22	24:A:1038:PHO:HAC1	1.08	1.09
23:B:1019:CLA:H62	23:B:1021:CLA:HED1	1.34	1.09
26:B:1045:BCR:H353	26:B:1047:BCR:C10	1.82	1.09
23:D:1005:CLA:C2A	23:D:1005:CLA:HED2	1.80	1.09
6:F:37:ILE:HA	6:F:40:MET:HE3	1.30	1.09
23:B:1016:CLA:C5	23:H:1017:CLA:C10	2.29	1.09
24:A:1038:PHO:HED2	24:A:1038:PHO:CAD	1.79	1.09
1:A:95:PRO:HA	23:A:1007:CLA:CED	1.82	1.09
10:K:28:ILE:CD1	26:K:1051:BCR:C8	2.30	1.09
26:T:6046:BCR:C37	26:T:6046:BCR:C26	2.30	1.09
16:V:160:LYS:NZ	16:V:160:LYS:HB2	1.48	1.09
23:A:1007:CLA:CBC	23:A:1007:CLA:HHH	1.81	1.09
2:B:253:ALA:HB2	2:B:455:HIS:HB2	1.10	1.09
23:C:1029:CLA:C20	23:C:1030:CLA:H192	1.83	1.09
23:C:1034:CLA:C4	23:C:1034:CLA:H71	1.78	1.09
29:L:1061:MGE:H1G2	29:L:1061:MGE:O1B	1.53	1.09
23:B:1022:CLA:H171	23:B:1022:CLA:H71	1.31	1.09
10:K:39:VAL:HG22	18:Y:36:ILE:HD11	1.25	1.09
24:A:1038:PHO:CED	24:A:1038:PHO:C3D	2.30	1.08
23:B:1011:CLA:HBB1	23:B:1011:CLA:HHH	1.34	1.08
23:B:1022:CLA:C7	23:B:1022:CLA:H171	1.83	1.08
23:D:1008:CLA:H41	23:D:1008:CLA:H71	1.10	1.08
23:B:1019:CLA:CED	23:B:1019:CLA:CAA	2.30	1.08
26:B:1047:BCR:C8	26:B:1047:BCR:H321	1.66	1.08
24:A:1038:PHO:HED2	24:A:1038:PHO:C3D	1.83	1.08
23:H:1017:CLA:HBB1	26:H:1049:BCR:C32	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1036:CLA:C17	23:C:1036:CLA:C14	2.31	1.08
23:A:1007:CLA:HHD	23:A:1007:CLA:HBC2	1.11	1.08
23:B:1020:CLA:H91	23:B:1020:CLA:H121	1.26	1.08
23:B:1021:CLA:H62	29:B:1060:MGE:H231	1.31	1.08
23:B:1019:CLA:C2A	23:B:1019:CLA:CED	2.31	1.08
26:B:1047:BCR:C8	26:B:1047:BCR:C32	2.30	1.08
23:C:1034:CLA:C12	23:C:1034:CLA:H91	1.83	1.08
30:C:1056:DGD:C6D	30:C:1056:DGD:HE3	1.83	1.08
26:K:1051:BCR:H322	26:K:1052:BCR:H10C	1.08	1.08
23:B:1014:CLA:CMA	23:B:1014:CLA:CBA	2.29	1.08
23:B:1016:CLA:H52	23:H:1017:CLA:H102	1.28	1.08
26:B:1047:BCR:C34	26:B:1047:BCR:C32	2.30	1.08
23:C:1030:CLA:HMC2	23:C:1031:CLA:H101	1.15	1.08
23:B:1009:CLA:C2B	26:H:1049:BCR:H382	1.82	1.07
23:B:1012:CLA:C9	23:B:1012:CLA:C12	2.31	1.07
23:B:1009:CLA:H43	26:H:1049:BCR:H353	1.35	1.07
23:C:1034:CLA:C9	23:C:1034:CLA:C14	2.33	1.07
23:B:1020:CLA:H2	23:B:1023:CLA:HBA1	1.36	1.07
23:B:1022:CLA:CHD	23:B:1022:CLA:CBC	2.30	1.07
23:C:1031:CLA:HMA2	23:C:1031:CLA:C2	1.83	1.07
23:B:1020:CLA:H91	23:B:1020:CLA:C14	1.84	1.07
2:B:64:PRO:HB2	2:B:268:PHE:CE2	1.90	1.07
23:C:1030:CLA:HMC2	23:C:1031:CLA:C10	1.84	1.07
23:C:1034:CLA:C10	23:C:1034:CLA:C4	2.32	1.07
23:B:1016:CLA:C5	23:H:1017:CLA:H102	1.85	1.07
26:K:1052:BCR:H23C	26:K:1052:BCR:H382	1.11	1.07
23:B:1020:CLA:C13	23:B:1020:CLA:C9	2.32	1.07
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.33	1.07
23:H:1017:CLA:H192	23:H:1017:CLA:H152	1.31	1.07
23:B:1021:CLA:H172	29:B:1060:MGE:CDA	1.84	1.06
23:C:1026:CLA:HMB1	23:C:1026:CLA:HBB1	1.31	1.06
26:H:1049:BCR:H403	26:H:1049:BCR:H23C	1.23	1.06
23:B:1020:CLA:C9	23:B:1020:CLA:H142	1.83	1.06
23:B:1021:CLA:H172	29:B:1060:MGE:H132	1.07	1.06
23:C:1032:CLA:H43	23:C:1032:CLA:O1A	1.54	1.06
13:O:127:ILE:HD12	13:O:127:ILE:H	1.15	1.06
23:B:1011:CLA:H42	23:B:1013:CLA:H91	1.07	1.06
23:C:1029:CLA:H201	23:C:1030:CLA:H192	1.35	1.06
3:C:45:LEU:HD22	3:C:140:LEU:H	1.08	1.06
23:B:1020:CLA:H8	23:B:1020:CLA:H13	1.08	1.06
23:C:1033:CLA:C9	23:C:1033:CLA:C12	2.30	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1019:CLA:H193	23:B:1021:CLA:H71	1.24	1.06
23:D:1005:CLA:HED2	23:D:1005:CLA:H2A	1.08	1.06
23:H:1017:CLA:H192	23:H:1017:CLA:C15	1.86	1.06
23:B:1022:CLA:H41	23:B:1022:CLA:H93	1.11	1.06
23:C:1035:CLA:H101	26:K:1052:BCR:H403	1.35	1.06
23:B:1009:CLA:H43	26:H:1049:BCR:C35	1.85	1.06
23:B:1009:CLA:HED3	23:B:1009:CLA:H2A	1.38	1.06
23:C:1033:CLA:H122	23:C:1033:CLA:H91	1.21	1.06
2:B:465:GLY:H	23:B:1019:CLA:CBC	1.68	1.05
23:B:1016:CLA:C14	23:D:1008:CLA:HMB2	1.86	1.05
23:B:1021:CLA:H2A	23:B:1021:CLA:O2A	1.52	1.05
30:C:1056:DGD:C6D	30:C:1056:DGD:HE5	1.86	1.05
23:C:1031:CLA:C17	23:C:1031:CLA:H141	1.86	1.05
2:B:464:PHE:O	2:B:467:ILE:HB	1.56	1.05
30:C:1056:DGD:HAV1	30:C:1057:DGD:HA82	1.31	1.05
1:A:149:ALA:HB1	1:A:283:VAL:HG22	1.33	1.05
13:O:65:ARG:HH22	13:O:66:ILE:HG12	1.18	1.05
14:T:1:MET:HE2	14:T:1:MET:H1	1.17	1.05
23:A:1003:CLA:CBB	23:A:1006:CLA:HMD2	1.86	1.04
23:B:1014:CLA:C15	23:B:1014:CLA:H193	1.84	1.04
23:B:1021:CLA:H193	29:B:1060:MGE:H133	1.39	1.04
23:B:1021:CLA:OBD	23:B:1022:CLA:HHC	1.57	1.04
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.34	1.04
23:C:1034:CLA:C7	23:C:1034:CLA:C4	2.30	1.04
23:B:1012:CLA:H93	23:B:1012:CLA:H121	1.37	1.04
23:B:1014:CLA:C11	23:B:1014:CLA:H161	1.87	1.04
23:B:1016:CLA:HHD	23:B:1016:CLA:CBC	1.86	1.04
23:B:1022:CLA:HHD	23:B:1022:CLA:HBC3	1.10	1.04
10:K:32:PHE:HE1	26:K:1052:BCR:H24C	0.94	1.04
30:C:1056:DGD:HE5	30:C:1056:DGD:HD62	1.10	1.04
23:B:1010:CLA:HMD3	23:B:1011:CLA:C8	1.86	1.04
26:K:1051:BCR:C32	26:K:1052:BCR:C11	2.35	1.04
24:A:1038:PHO:C19	24:A:1038:PHO:C14	2.30	1.04
3:C:62:PHE:CE2	10:K:28:ILE:CG2	2.39	1.04
10:K:28:ILE:CD1	26:K:1051:BCR:C7	2.36	1.04
10:K:33:PHE:O	10:K:33:PHE:HD1	1.38	1.04
23:A:1006:CLA:C17	26:D:1050:BCR:C29	2.35	1.04
23:A:1003:CLA:C14	24:A:1038:PHO:C9	2.34	1.04
2:B:25:MET:HG3	26:B:1045:BCR:H292	1.06	1.04
26:B:1047:BCR:H23C	26:B:1047:BCR:H383	1.05	1.04
23:B:1012:CLA:HHD	23:B:1012:CLA:CBC	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1019:CLA:O2D	23:B:1019:CLA:H2A	1.57	1.04
23:B:1019:CLA:H193	23:B:1021:CLA:H52	1.36	1.03
23:A:1003:CLA:H141	24:A:1038:PHO:H93	1.39	1.03
23:B:1019:CLA:HHC	23:B:1019:CLA:HBB1	1.05	1.03
3:C:107:ASP:OD1	3:C:110:PRO:HD3	1.57	1.03
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.37	1.03
3:C:294:ASN:HB2	30:C:1055:DGD:O3E	1.59	1.03
24:A:1038:PHO:H102	24:A:1038:PHO:H143	1.37	1.03
1:A:193:LEU:HD11	4:D:182:LEU:HD12	1.39	1.03
23:B:1022:CLA:CHD	23:B:1022:CLA:HBC3	1.87	1.03
27:A:1063:LHG:C32	23:C:1034:CLA:C14	2.35	1.03
23:A:1006:CLA:H171	26:D:1050:BCR:H291	1.06	1.03
23:B:1011:CLA:H121	26:H:1049:BCR:H322	1.36	1.03
23:A:1003:CLA:H141	24:A:1038:PHO:H91	1.06	1.03
23:C:1025:CLA:HBB1	23:C:1025:CLA:H93	1.36	1.03
23:B:1024:CLA:HMC1	23:B:1024:CLA:HBC2	1.08	1.03
20:Z:15:LEU:HD22	20:Z:50:LEU:HD12	1.39	1.03
23:B:1022:CLA:C7	23:B:1022:CLA:H13	1.88	1.02
3:C:63:TRP:HZ3	23:C:1027:CLA:CBC	1.72	1.02
18:Y:39:LEU:HD21	20:Z:25:VAL:HG22	1.41	1.02
23:B:1014:CLA:HBA1	23:B:1014:CLA:HMA2	1.07	1.02
23:C:1034:CLA:C12	23:C:1034:CLA:C9	2.35	1.02
23:B:1021:CLA:OBD	23:B:1022:CLA:HMC3	1.57	1.02
26:B:1045:BCR:C37	26:B:1045:BCR:C40	2.30	1.02
3:C:169:GLY:HA3	3:C:245:ILE:HG12	1.41	1.02
10:K:28:ILE:HA	10:K:31:LEU:HD12	1.05	1.02
23:A:1006:CLA:HMB3	24:A:1039:PHO:H161	1.41	1.02
23:B:1022:CLA:C13	23:B:1022:CLA:C8	2.30	1.02
23:C:1028:CLA:H43	30:C:1057:DGD:HA22	1.37	1.02
23:B:1009:CLA:H12	26:H:1049:BCR:C17	1.90	1.02
2:B:465:GLY:H	23:B:1019:CLA:HBC1	1.23	1.02
23:B:1022:CLA:HHH	23:B:1022:CLA:HBC2	1.40	1.02
2:B:254:GLY:O	2:B:258:TYR:HD1	1.40	1.02
26:D:1050:BCR:C37	26:D:1050:BCR:C40	2.30	1.02
23:C:1030:CLA:CMC	23:C:1031:CLA:H101	1.87	1.02
23:A:1006:CLA:C2	23:A:1006:CLA:H72	1.84	1.02
23:B:1009:CLA:CMB	26:H:1049:BCR:C39	2.29	1.02
23:B:1022:CLA:H142	23:B:1022:CLA:H72	1.39	1.02
27:A:1063:LHG:C32	23:C:1034:CLA:H143	1.89	1.02
30:C:1056:DGD:HBN2	10:K:30:VAL:HG21	1.42	1.02
23:A:1006:CLA:H171	26:D:1050:BCR:C40	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1063:LHG:H312	23:C:1034:CLA:C9	1.90	1.02
23:B:1014:CLA:HBB1	23:B:1014:CLA:HMB1	1.04	1.02
23:A:1003:CLA:HBC2	23:A:1003:CLA:HHD	1.39	1.01
6:F:41:GLN:NE2	9:J:27:LEU:HB3	1.74	1.01
2:B:221:PRO:HA	23:H:1017:CLA:HED2	1.39	1.01
3:C:223:TRP:HB3	3:C:224:ILE:HD13	1.41	1.01
10:K:32:PHE:CD1	26:K:1052:BCR:H392	1.95	1.01
23:A:1003:CLA:H172	24:A:1038:PHO:H43	1.42	1.01
23:B:1011:CLA:H192	23:H:1017:CLA:H121	1.39	1.01
23:C:1026:CLA:H203	23:C:1026:CLA:ND	1.75	1.01
27:A:1063:LHG:H322	23:C:1034:CLA:H142	1.40	1.01
1:A:57:PRO:HA	1:A:68:SER:HB2	1.43	1.01
2:B:64:PRO:HB2	2:B:268:PHE:HE2	1.22	1.01
23:B:1019:CLA:HHC	23:B:1019:CLA:CBB	1.86	1.01
23:C:1031:CLA:H171	23:C:1031:CLA:H141	1.42	1.01
23:B:1016:CLA:H142	23:D:1008:CLA:CMB	1.89	1.01
26:B:1047:BCR:H343	26:B:1047:BCR:H321	1.30	1.01
23:D:1005:CLA:C20	23:D:1005:CLA:C15	2.34	1.01
13:O:111:LEU:HD13	13:O:121:PHE:HB2	1.41	1.01
23:A:1006:CLA:H171	26:D:1050:BCR:C30	1.91	1.00
27:A:1063:LHG:O4	27:A:1063:LHG:HC61	1.61	1.00
23:B:1020:CLA:C13	23:B:1020:CLA:C8	2.35	1.00
23:C:1031:CLA:O1D	23:C:1033:CLA:H101	1.60	1.00
10:K:33:PHE:C	10:K:33:PHE:CD1	2.29	1.00
2:B:27:THR:HG21	23:B:1020:CLA:H11	1.40	1.00
30:C:1056:DGD:HB61	30:C:1056:DGD:CAB	1.90	1.00
4:D:209:LEU:HD22	25:D:1042:PQ9:H192	1.41	1.00
1:A:81:ALA:CB	1:A:175:GLY:HA3	1.90	1.00
2:B:460:LEU:CA	30:H:1058:DGD:HAG1	1.90	1.00
24:A:1038:PHO:H193	24:A:1038:PHO:H141	1.12	1.00
23:B:1019:CLA:C19	23:B:1021:CLA:H52	1.90	1.00
2:B:458:PHE:CD2	23:B:1012:CLA:HMC3	1.95	1.00
2:B:456:ALA:HA	30:H:1058:DGD:CIB	1.92	1.00
26:T:6046:BCR:H382	26:T:6046:BCR:C37	1.91	1.00
23:B:1019:CLA:HBB1	23:B:1019:CLA:CHC	1.84	1.00
23:B:1014:CLA:H151	23:B:1014:CLA:H193	1.00	1.00
26:B:1047:BCR:C23	26:B:1047:BCR:H383	1.92	1.00
26:K:1051:BCR:C32	26:K:1052:BCR:C10	2.39	1.00
1:A:278:TRP:HA	1:A:278:TRP:CE3	1.95	0.99
23:C:1025:CLA:HMD2	23:C:1026:CLA:H43	1.44	0.99
23:C:1036:CLA:H172	23:C:1036:CLA:C14	1.90	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:55:GLY:HA2	26:Z:1053:BCR:H311	1.40	0.99
23:D:1008:CLA:C4	23:D:1008:CLA:C7	2.39	0.99
4:D:49:LEU:HD21	29:J:1059:MGE:H7A1	1.44	0.99
24:A:1038:PHO:HBC2	24:A:1038:PHO:CHD	1.90	0.99
23:B:1012:CLA:H101	23:B:1023:CLA:H42	1.43	0.99
26:K:1051:BCR:C40	26:K:1051:BCR:C37	2.30	0.99
26:D:1050:BCR:C37	26:D:1050:BCR:C39	2.30	0.99
26:A:1044:BCR:C40	26:A:1044:BCR:C37	2.30	0.99
23:B:1020:CLA:C9	23:B:1020:CLA:C12	2.37	0.99
26:B:1047:BCR:H23C	26:B:1047:BCR:C38	1.85	0.99
13:O:65:ARG:CZ	13:O:66:ILE:H	1.74	0.99
23:B:1015:CLA:H18	29:B:1060:MGE:H8A1	1.43	0.99
10:K:28:ILE:HD13	26:K:1051:BCR:HC7	1.45	0.99
23:B:1011:CLA:C3D	23:B:1013:CLA:C4	2.39	0.99
30:C:1056:DGD:HBG2	30:C:1056:DGD:HBF1	1.43	0.98
10:K:32:PHE:CD1	26:K:1052:BCR:C39	2.45	0.98
26:A:1044:BCR:C37	26:A:1044:BCR:C39	2.30	0.98
23:B:1011:CLA:CAD	23:B:1013:CLA:H43	1.91	0.98
2:B:223:GLN:HG3	2:B:224:ARG:H	1.27	0.98
14:T:18:PHE:CD1	26:T:6046:BCR:H343	1.97	0.98
26:Z:1053:BCR:H382	26:Z:1053:BCR:C23	1.88	0.98
1:A:203:ALA:HA	23:A:1006:CLA:O1A	1.59	0.98
23:D:1008:CLA:H41	23:D:1008:CLA:C7	1.92	0.98
26:B:1045:BCR:C37	26:B:1045:BCR:C39	2.30	0.98
26:D:1050:BCR:H282	29:J:1059:MGE:H212	1.42	0.98
26:D:1050:BCR:H281	29:J:1059:MGE:H9B2	1.45	0.98
23:B:1024:CLA:HMC1	23:B:1024:CLA:CBC	1.94	0.98
7:H:35:MET:CG	26:H:1049:BCR:H333	1.93	0.98
23:A:1006:CLA:C17	26:D:1050:BCR:C40	2.41	0.98
24:A:1038:PHO:H193	24:A:1038:PHO:C15	1.92	0.98
1:A:97:TRP:HA	8:I:1:MET:SD	2.03	0.98
23:B:1014:CLA:H91	23:B:1014:CLA:H122	0.98	0.98
26:B:1048:BCR:H383	26:B:1048:BCR:C23	1.85	0.98
23:C:1034:CLA:HHD	23:C:1034:CLA:CBC	1.93	0.98
11:L:23:LEU:O	11:L:27:LEU:HB2	1.63	0.98
23:C:1034:CLA:H121	23:C:1034:CLA:H91	1.00	0.98
23:H:1017:CLA:HHD	23:H:1017:CLA:CBC	1.93	0.98
23:B:1022:CLA:H142	23:B:1022:CLA:C10	1.92	0.98
2:B:253:ALA:HB2	2:B:455:HIS:CB	1.93	0.98
24:A:1038:PHO:CED	24:A:1038:PHO:CAD	2.40	0.98
23:B:1012:CLA:HBB1	23:B:1012:CLA:HHC	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1019:CLA:O1A	23:B:1019:CLA:H3A	1.62	0.98
23:H:1017:CLA:HBB1	26:H:1049:BCR:H323	1.44	0.98
2:B:464:PHE:HZ	29:B:1060:MGE:H4B2	1.21	0.97
23:B:1016:CLA:C20	23:D:1008:CLA:HMA2	1.93	0.97
26:K:1052:BCR:C38	26:K:1052:BCR:H23C	1.90	0.97
4:D:17:ILE:HG22	17:X:41:SER:HB3	1.46	0.97
13:O:127:ILE:HD12	13:O:127:ILE:N	1.79	0.97
24:A:1038:PHO:HED3	24:A:1038:PHO:C4D	1.95	0.97
3:C:63:TRP:HZ3	23:C:1027:CLA:HBC1	0.84	0.97
2:B:385:ARG:HD3	15:U:44:ASP:HB3	1.44	0.97
23:C:1033:CLA:H18	23:C:1033:CLA:H141	0.99	0.97
30:C:1056:DGD:HB21	30:C:1056:DGD:HG12	1.47	0.97
6:F:37:ILE:HG21	9:J:28:PHE:CZ	1.99	0.97
23:B:1012:CLA:C1	23:B:1013:CLA:H2	1.95	0.97
3:C:99:VAL:HG11	3:C:196:VAL:HB	1.47	0.97
23:B:1011:CLA:HHD	23:B:1014:CLA:HBB2	1.43	0.97
23:B:1013:CLA:HBB2	23:B:1023:CLA:H41	1.45	0.97
23:C:1027:CLA:HBA1	23:C:1027:CLA:CHA	1.93	0.97
2:B:256:MET:CE	2:B:448:ARG:NH1	2.28	0.97
26:K:1051:BCR:C32	26:K:1052:BCR:H10C	1.93	0.97
2:B:222:PRO:HG2	2:B:225:LEU:HD12	1.47	0.96
3:C:99:VAL:HG21	3:C:196:VAL:HG11	1.43	0.96
26:K:1051:BCR:C39	26:K:1051:BCR:C37	2.30	0.96
23:B:1022:CLA:HBB1	23:B:1022:CLA:HMB1	1.45	0.96
23:B:1011:CLA:H192	23:H:1017:CLA:C12	1.95	0.96
23:B:1020:CLA:H52	23:B:1020:CLA:O2A	1.62	0.96
23:C:1025:CLA:C4	23:C:1025:CLA:C2B	2.43	0.96
10:K:33:PHE:HD1	10:K:33:PHE:C	1.64	0.96
1:A:150:PRO:HA	23:A:1003:CLA:C4	1.95	0.96
1:A:219:VAL:HB	4:D:268:HIS:ND1	1.80	0.96
23:B:1020:CLA:C1	23:B:1023:CLA:HED1	1.95	0.96
2:B:257:TRP:CZ2	4:D:291:LEU:HD12	2.00	0.96
23:C:1033:CLA:HHD	23:C:1033:CLA:CBC	1.95	0.96
30:C:1057:DGD:HAS1	29:J:1059:MGE:CCB	1.94	0.96
23:C:1036:CLA:C17	26:Z:1053:BCR:H373	1.95	0.96
2:B:450:TRP:HB3	23:B:1015:CLA:HMB2	1.44	0.96
13:O:223:ILE:HG12	13:O:224:SER:H	1.27	0.96
27:A:1063:LHG:H271	23:C:1032:CLA:H8	1.48	0.96
23:B:1012:CLA:H11	23:B:1013:CLA:H2	1.45	0.96
2:B:464:PHE:CE2	29:B:1060:MGE:H4B2	2.01	0.96
23:B:1010:CLA:HMB1	23:B:1010:CLA:HBB1	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CBB	23:B:1013:CLA:C17	2.43	0.96
4:D:98:GLN:HE21	5:E:73:LYS:HE3	1.31	0.96
1:A:278:TRP:HE3	1:A:278:TRP:HA	1.30	0.96
23:B:1012:CLA:HED2	23:B:1012:CLA:C2A	1.95	0.96
3:C:51:GLY:HA3	3:C:132:HIS:HB2	1.46	0.96
23:D:1008:CLA:HBB1	23:D:1008:CLA:HMB1	1.47	0.96
2:B:354:LEU:HB3	2:B:370:LEU:HD22	1.47	0.96
23:C:1028:CLA:HBB1	23:C:1028:CLA:HHC	1.48	0.95
23:A:1006:CLA:CED	30:C:1057:DGD:HBH2	1.94	0.95
24:A:1038:PHO:C19	24:A:1038:PHO:H152	1.94	0.95
2:B:380:ASP:OD2	4:D:345:VAL:HG22	1.66	0.95
27:A:1063:LHG:H161	27:A:1063:LHG:C12	1.95	0.95
2:B:25:MET:HG3	26:B:1045:BCR:C29	1.96	0.95
4:D:164:GLN:HG3	4:D:165:SER:H	1.31	0.95
23:B:1012:CLA:H11	23:B:1013:CLA:C2	1.97	0.95
26:K:1051:BCR:C8	26:K:1051:BCR:C33	2.44	0.95
13:O:148:VAL:HG12	13:O:151:LEU:HB2	1.49	0.95
1:A:76:ASN:OD1	11:L:33:SER:HB3	1.66	0.95
23:C:1033:CLA:H93	23:C:1033:CLA:H51	1.48	0.95
4:D:261:PHE:HE2	4:D:266:TRP:HD1	1.10	0.95
14:T:1:MET:CE	14:T:1:MET:N	2.30	0.95
23:C:1034:CLA:H43	23:C:1034:CLA:H102	1.43	0.95
30:C:1055:DGD:HA72	30:C:1055:DGD:HAE1	1.48	0.95
23:B:1022:CLA:H72	23:B:1022:CLA:C17	1.97	0.95
16:V:160:LYS:NZ	16:V:160:LYS:CB	2.30	0.95
24:A:1038:PHO:HBC2	24:A:1038:PHO:HHD	1.45	0.95
23:B:1022:CLA:C7	23:B:1022:CLA:C13	2.44	0.95
6:F:41:GLN:HE22	9:J:27:LEU:C	1.69	0.95
27:A:1063:LHG:H291	23:C:1032:CLA:H8	1.47	0.95
30:C:1056:DGD:CIB	30:C:1056:DGD:CEB	2.44	0.95
3:C:63:TRP:CZ3	23:C:1027:CLA:CBC	2.46	0.95
23:B:1012:CLA:HHD	23:B:1012:CLA:HBC3	1.46	0.94
23:B:1016:CLA:C5	23:H:1017:CLA:H101	1.96	0.94
6:F:40:MET:HB3	29:J:1059:MGE:O5D	1.67	0.94
23:A:1003:CLA:C14	24:A:1038:PHO:H91	1.96	0.94
23:B:1011:CLA:C4	23:B:1013:CLA:H91	1.97	0.94
23:B:1014:CLA:H111	26:B:1048:BCR:H10C	1.49	0.94
2:B:135:LEU:HD12	2:B:135:LEU:H	1.31	0.94
26:H:1049:BCR:H403	26:H:1049:BCR:C23	1.95	0.94
1:A:29:TYR:HE2	1:A:132:GLU:HB3	1.30	0.94
23:B:1014:CLA:H112	23:B:1014:CLA:H161	0.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1052:BCR:C23	26:K:1052:BCR:H382	1.97	0.94
23:B:1019:CLA:HED2	23:B:1019:CLA:HAA2	0.95	0.94
23:C:1031:CLA:CGD	23:C:1033:CLA:C10	2.43	0.94
16:V:120:SER:H	16:V:123:SER:HB2	1.32	0.94
23:A:1003:CLA:CAB	23:A:1006:CLA:CMD	2.45	0.94
23:B:1019:CLA:H193	23:B:1021:CLA:C7	1.97	0.94
23:B:1023:CLA:C4C	23:B:1024:CLA:HBC1	1.96	0.94
23:C:1028:CLA:H121	23:C:1028:CLA:H172	0.94	0.94
23:C:1031:CLA:C17	23:C:1031:CLA:C14	2.36	0.94
11:L:12:LEU:HD12	12:M:26:TYR:HA	1.47	0.94
24:A:1038:PHO:C10	24:A:1038:PHO:H143	1.98	0.94
1:A:140:ARG:HH22	27:A:1063:LHG:HC2	1.30	0.94
26:C:1054:BCR:C23	26:C:1054:BCR:C38	2.37	0.94
26:K:1051:BCR:H392	26:K:1051:BCR:H371	1.31	0.94
23:B:1016:CLA:H142	23:D:1008:CLA:HMB2	0.96	0.94
2:B:99:ALA:HB1	23:B:1014:CLA:H2	1.49	0.94
23:C:1025:CLA:H202	23:C:1025:CLA:H151	1.50	0.94
12:M:1:MET:N	12:M:1:MET:CE	2.30	0.94
1:A:199:GLN:CD	1:A:200:LEU:HG	1.87	0.94
24:A:1038:PHO:C19	24:A:1038:PHO:C15	2.45	0.94
23:B:1011:CLA:C19	23:H:1017:CLA:H13	1.98	0.94
1:A:96:ILE:HA	1:A:105:TRP:CD1	2.02	0.94
23:B:1012:CLA:C1	23:B:1013:CLA:C2	2.44	0.94
2:B:17:GLY:HA2	2:B:123:PHE:HE2	1.32	0.94
30:C:1056:DGD:CIB	30:C:1056:DGD:HB1	1.97	0.93
3:C:139:THR:HG22	3:C:141:GLU:H	1.33	0.93
23:C:1033:CLA:C18	23:C:1033:CLA:C14	2.36	0.93
1:A:279:ARG:HD3	4:D:208:ALA:HB1	1.50	0.93
23:C:1025:CLA:O1D	23:C:1025:CLA:HBA2	1.67	0.93
26:Z:1053:BCR:H382	26:Z:1053:BCR:H23C	0.95	0.93
23:C:1025:CLA:C20	23:C:1031:CLA:H121	1.99	0.93
30:C:1056:DGD:C5E	30:C:1056:DGD:HD62	1.98	0.93
10:K:32:PHE:HE1	26:K:1052:BCR:C24	1.81	0.93
23:B:1023:CLA:CHD	23:B:1024:CLA:HBC1	1.97	0.93
23:C:1037:CLA:CGD	23:C:1037:CLA:CBA	2.47	0.93
30:C:1056:DGD:HBT2	30:C:1056:DGD:HB61	1.48	0.93
20:Z:61:VAL:HG23	20:Z:62:VAL:H	1.33	0.93
23:C:1029:CLA:CMA	23:C:1029:CLA:CBA	2.30	0.93
2:B:464:PHE:HB2	4:D:280:TRP:CZ2	2.04	0.93
4:D:303:ILE:HD12	4:D:304:ARG:N	1.84	0.93
27:A:1063:LHG:H312	23:C:1034:CLA:H91	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:1055:DGD:HAE1	30:C:1055:DGD:C7A	1.99	0.93
3:C:203:THR:HG21	3:C:232:ASP:HA	1.48	0.93
3:C:256:PRO:HB3	3:C:261:ARG:HH21	1.31	0.93
13:O:188:ARG:HD3	13:O:197:ALA:H	1.32	0.93
26:C:1054:BCR:H382	26:C:1054:BCR:H23C	1.51	0.92
3:C:259:TRP:O	3:C:262:ARG:HG2	1.69	0.92
7:H:53:LEU:HG	7:H:55:LEU:HD11	1.50	0.92
8:I:6:ILE:HD13	8:I:6:ILE:H	1.34	0.92
23:A:1003:CLA:HMB1	23:A:1003:CLA:HBB1	1.52	0.92
1:A:188:ALA:HB2	1:A:328:MET:HG3	1.50	0.92
23:B:1013:CLA:CMC	23:B:1023:CLA:H11	1.99	0.92
23:B:1015:CLA:H18	29:B:1060:MGE:C8A	1.99	0.92
23:B:1020:CLA:OBD	23:B:1020:CLA:HED2	1.70	0.92
2:B:325:PHE:CE1	11:L:34:TYR:HB3	2.03	0.92
4:D:43:LEU:H	4:D:43:LEU:HD22	1.35	0.92
23:B:1011:CLA:H172	23:B:1016:CLA:HBC1	1.50	0.92
3:C:184:GLY:HA3	3:C:198:VAL:HA	1.49	0.92
3:C:75:PHE:HE2	3:C:105:VAL:HG11	1.33	0.92
23:B:1020:CLA:C14	23:B:1020:CLA:C9	2.43	0.92
23:B:1022:CLA:C4	23:B:1022:CLA:H93	1.99	0.92
24:A:1038:PHO:H141	24:A:1038:PHO:H191	1.52	0.92
1:A:210:LEU:HD23	23:A:1006:CLA:H41	1.50	0.92
26:C:1054:BCR:H393	26:C:1054:BCR:H271	1.51	0.92
13:O:99:ARG:O	13:O:101:THR:HG23	1.69	0.92
23:B:1022:CLA:H142	23:B:1022:CLA:H101	1.50	0.92
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.05	0.91
23:B:1012:CLA:H12	23:B:1013:CLA:O2A	1.69	0.91
2:B:214:LEU:O	2:B:217:ILE:HG22	1.70	0.91
13:O:46:PRO:HD2	13:O:266:TYR:HD2	1.35	0.91
1:A:57:PRO:HA	1:A:68:SER:HB3	1.52	0.91
23:A:1006:CLA:H122	30:C:1057:DGD:HBB1	1.51	0.91
2:B:419:SER:HA	2:B:422:ARG:HH12	1.35	0.91
2:B:318:ASN:ND2	2:B:320:ALA:H	1.68	0.91
12:M:1:MET:HE2	12:M:1:MET:H1	1.22	0.91
23:C:1028:CLA:HBC2	23:C:1028:CLA:HHD	1.51	0.91
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.52	0.91
23:C:1037:CLA:C2B	26:Z:1053:BCR:H282	2.00	0.91
1:A:60:ILE:CG1	1:A:61:ASP:H	1.83	0.91
23:B:1009:CLA:CHC	23:B:1009:CLA:HBB1	2.00	0.91
23:B:1011:CLA:H93	23:B:1011:CLA:H122	1.52	0.91
23:C:1027:CLA:HED1	23:C:1036:CLA:C20	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1023:CLA:C9	23:B:1023:CLA:C12	2.45	0.91
3:C:322:GLN:HE22	3:C:381:LYS:HA	1.34	0.91
13:O:105:ASP:O	13:O:127:ILE:HD11	1.71	0.91
16:V:160:LYS:HZ2	16:V:160:LYS:HB2	1.12	0.91
23:B:1011:CLA:HBB2	23:B:1013:CLA:H203	0.94	0.91
26:B:1048:BCR:H383	26:B:1048:BCR:H23C	0.92	0.91
23:C:1031:CLA:HED3	23:C:1031:CLA:HAA2	1.52	0.91
23:C:1027:CLA:O1D	23:C:1036:CLA:H11	1.71	0.91
1:A:279:ARG:CD	4:D:208:ALA:HB1	2.01	0.91
23:A:1007:CLA:CHD	23:A:1007:CLA:HBC2	1.99	0.90
23:B:1019:CLA:H62	23:B:1021:CLA:CED	2.00	0.90
3:C:264:PHE:CZ	26:C:1054:BCR:H311	2.06	0.90
4:D:259:ILE:HD11	14:T:21:ILE:HA	1.50	0.90
4:D:51:GLY:HA2	4:D:55:VAL:HG23	1.53	0.90
15:U:46:LYS:HE2	15:U:59:ASN:ND2	1.86	0.90
23:B:1022:CLA:H72	23:B:1022:CLA:H172	1.53	0.90
23:H:1017:CLA:C19	23:H:1017:CLA:C15	2.39	0.90
23:B:1019:CLA:C9	29:L:1061:MGE:H8A1	2.02	0.90
23:B:1009:CLA:C1	26:H:1049:BCR:C17	2.49	0.90
23:B:1012:CLA:H102	23:B:1023:CLA:O2A	1.71	0.90
3:C:113:VAL:O	3:C:117:VAL:HG23	1.71	0.90
4:D:49:LEU:O	4:D:53:THR:HG23	1.70	0.90
10:K:28:ILE:CG2	10:K:29:PRO:CD	2.30	0.90
23:B:1014:CLA:HBB1	23:B:1014:CLA:CMB	1.88	0.90
23:B:1019:CLA:C19	23:B:1021:CLA:H71	2.02	0.90
23:C:1036:CLA:H141	23:C:1036:CLA:H172	1.51	0.90
23:A:1006:CLA:HMB1	24:A:1039:PHO:H161	1.53	0.90
26:A:1044:BCR:H392	26:A:1044:BCR:H373	1.50	0.90
1:A:310:LYS:HA	16:V:29:LEU:HB3	1.51	0.90
1:A:60:ILE:HG12	1:A:61:ASP:N	1.86	0.90
23:C:1035:CLA:C10	26:K:1052:BCR:H403	2.02	0.90
2:B:463:PHE:CE1	23:B:1016:CLA:HBB1	2.06	0.90
23:C:1031:CLA:CGD	23:C:1031:CLA:HAA2	2.02	0.90
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.53	0.90
23:B:1016:CLA:HBC2	23:B:1016:CLA:HHD	1.51	0.90
2:B:12:LEU:HB3	2:B:19:LEU:HD23	1.52	0.90
26:K:1051:BCR:C32	26:K:1052:BCR:C12	2.50	0.90
23:B:1019:CLA:HED1	23:B:1019:CLA:H2A	1.52	0.90
2:B:280:PHE:CE1	2:B:312:TYR:HB3	2.06	0.90
26:A:1044:BCR:H372	26:A:1044:BCR:H403	1.51	0.90
26:D:1050:BCR:H371	26:D:1050:BCR:H392	1.29	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1051:BCR:H392	26:K:1051:BCR:H373	1.54	0.90
1:A:51:ALA:O	1:A:55:ALA:HB2	1.70	0.89
23:B:1010:CLA:O1D	23:B:1010:CLA:H2A	1.71	0.89
23:B:1011:CLA:H42	23:B:1013:CLA:C9	2.00	0.89
23:B:1015:CLA:HBC1	26:B:1045:BCR:H342	1.54	0.89
23:B:1016:CLA:H203	23:D:1008:CLA:HMA2	1.53	0.89
15:U:94:ILE:O	15:U:97:LEU:HD13	1.72	0.89
23:B:1015:CLA:C4A	23:B:1015:CLA:CBA	2.50	0.89
23:B:1021:CLA:H142	23:B:1021:CLA:C20	2.01	0.89
3:C:363:GLY:O	3:C:367:GLU:HG2	1.72	0.89
3:C:75:PHE:HD1	3:C:84:GLN:HE22	1.20	0.89
2:B:464:PHE:CE2	29:B:1060:MGE:H5B1	2.07	0.89
2:B:153:PHE:CA	23:B:1014:CLA:HMC3	2.02	0.89
24:A:1038:PHO:H192	24:A:1038:PHO:H152	1.55	0.89
4:D:246:MET:SD	4:D:264:LYS:HB3	2.12	0.89
23:A:1006:CLA:HED2	30:C:1057:DGD:HBH2	1.51	0.89
24:A:1038:PHO:HED3	24:A:1038:PHO:C3D	2.00	0.89
23:B:1014:CLA:HMB1	23:B:1014:CLA:CBB	1.98	0.89
23:C:1028:CLA:C4	30:C:1057:DGD:HA22	2.03	0.89
13:O:215:ARG:H	13:O:215:ARG:HD2	1.37	0.89
2:B:326:ARG:HB3	2:B:444:ARG:HG3	1.54	0.89
5:E:38:VAL:HG11	6:F:39:ALA:HB3	1.53	0.89
20:Z:53:VAL:O	20:Z:57:LEU:HB2	1.73	0.89
23:A:1006:CLA:C11	30:C:1057:DGD:CIB	2.50	0.89
23:B:1012:CLA:H93	23:B:1012:CLA:C12	1.98	0.89
23:B:1015:CLA:NA	23:B:1015:CLA:HBA2	1.83	0.89
26:C:1054:BCR:H383	26:C:1054:BCR:C23	2.03	0.89
23:D:1005:CLA:O2A	23:D:1005:CLA:H51	1.71	0.89
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.51	0.89
1:A:25:ASP:HA	4:D:251:ARG:NH2	1.87	0.89
23:B:1010:CLA:HMD3	23:B:1011:CLA:H8	0.92	0.89
30:C:1057:DGD:HAS1	29:J:1059:MGE:H221	1.54	0.89
1:A:322:ASN:ND2	3:C:412:THR:HG22	1.88	0.89
4:D:342:PRO:HB2	4:D:345:VAL:HG23	1.54	0.88
3:C:62:PHE:HE2	10:K:28:ILE:CG2	1.85	0.88
23:A:1006:CLA:HBB1	23:A:1006:CLA:HHC	1.54	0.88
23:B:1011:CLA:HED2	23:B:1011:CLA:OBD	1.74	0.88
23:B:1023:CLA:H3A	23:B:1023:CLA:O1A	1.73	0.88
24:A:1039:PHO:HAB	23:D:1004:CLA:H12	1.56	0.88
23:B:1022:CLA:C13	23:B:1022:CLA:H72	2.03	0.88
2:B:223:GLN:HG3	2:B:224:ARG:N	1.84	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1025:CLA:CBB	23:C:1025:CLA:C9	2.51	0.88
30:C:1056:DGD:C6D	30:C:1056:DGD:C5E	2.52	0.88
23:H:1017:CLA:H3A	23:H:1017:CLA:O1A	1.73	0.88
23:A:1006:CLA:H2A	23:A:1006:CLA:CED	2.04	0.88
23:B:1022:CLA:C7	23:B:1022:CLA:C17	2.50	0.88
3:C:350:ILE:HG13	3:C:359:TRP:HB2	1.56	0.88
26:D:1050:BCR:H373	26:D:1050:BCR:H392	1.56	0.88
1:A:331:MET:SD	4:D:348:ARG:HA	2.13	0.88
1:A:195:HIS:ND1	1:A:196:PRO:HD2	1.88	0.88
23:B:1021:CLA:HMB1	23:B:1021:CLA:HBB1	1.54	0.88
4:D:210:LEU:HA	4:D:213:ILE:CG2	2.03	0.88
27:A:1063:LHG:C16	27:A:1063:LHG:H121	2.04	0.88
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.54	0.88
3:C:179:ALA:HB1	3:C:199:ILE:HD13	1.55	0.88
26:D:1050:BCR:H403	26:D:1050:BCR:H371	1.32	0.88
23:B:1009:CLA:C3B	26:H:1049:BCR:H382	2.03	0.88
1:A:219:VAL:HG21	4:D:268:HIS:CG	2.08	0.88
13:O:31:LEU:HD23	13:O:31:LEU:H	1.36	0.88
13:O:46:PRO:HD2	13:O:266:TYR:CD2	2.08	0.88
30:C:1056:DGD:CEB	30:C:1056:DGD:HGB3	2.03	0.88
5:E:27:ILE:HB	5:E:28:PRO:CD	2.03	0.88
14:T:2:GLU:O	14:T:6:TYR:CD2	2.27	0.88
18:Y:24:MET:O	18:Y:28:ILE:HG23	1.74	0.88
1:A:215:HIS:O	1:A:219:VAL:HG22	1.74	0.87
1:A:219:VAL:CG2	4:D:268:HIS:HB3	2.04	0.87
23:B:1009:CLA:C1B	26:H:1049:BCR:H382	2.03	0.87
4:D:213:ILE:O	4:D:217:THR:HB	1.74	0.87
26:B:1045:BCR:C8	26:B:1045:BCR:H331	2.02	0.87
2:B:99:ALA:O	2:B:102:VAL:HG12	1.73	0.87
3:C:135:ARG:HH12	20:Z:33:TRP:CB	1.87	0.87
26:K:1051:BCR:H372	26:K:1051:BCR:H403	1.55	0.87
2:B:454:ALA:C	2:B:456:ALA:H	1.71	0.87
23:C:1037:CLA:H101	23:C:1037:CLA:H143	1.54	0.87
8:I:31:ASN:HB2	8:I:32:PRO:HD2	1.56	0.87
12:M:1:MET:CE	12:M:1:MET:H3	1.84	0.87
3:C:63:TRP:H	23:C:1034:CLA:HED3	1.39	0.87
27:A:1063:LHG:H383	27:A:1063:LHG:H341	1.57	0.87
1:A:76:ASN:HD22	1:A:79:THR:H	1.23	0.87
23:B:1009:CLA:C1	26:H:1049:BCR:C16	2.53	0.87
9:J:21:VAL:O	9:J:25:VAL:HG13	1.75	0.87
1:A:317:TRP:N	4:D:63:LEU:HD21	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1015:CLA:C4A	23:B:1015:CLA:HBA1	2.04	0.87
26:B:1045:BCR:H392	26:B:1045:BCR:H373	1.55	0.87
23:C:1027:CLA:CED	23:C:1036:CLA:H201	2.04	0.87
1:A:237:TYR:HE2	1:A:239:PHE:HA	1.37	0.87
23:B:1013:CLA:CBB	23:B:1023:CLA:H41	2.05	0.87
23:B:1014:CLA:HBC2	23:B:1014:CLA:CHD	2.05	0.87
23:B:1021:CLA:H193	29:B:1060:MGE:CDA	2.04	0.87
2:B:66:MET:HB3	2:B:71:VAL:CG1	2.05	0.87
27:A:1063:LHG:C29	23:C:1032:CLA:H8	2.03	0.87
23:B:1019:CLA:C6	23:B:1021:CLA:HED1	2.03	0.87
2:B:113:TRP:HB2	26:B:1048:BCR:H372	1.54	0.87
26:T:6046:BCR:C27	26:T:6046:BCR:H371	2.05	0.86
23:C:1031:CLA:O2D	23:C:1033:CLA:H101	1.73	0.86
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.54	0.86
24:A:1038:PHO:HBC1	4:D:212:ALA:HB3	1.58	0.86
23:B:1023:CLA:C14	23:B:1024:CLA:H8	2.06	0.86
2:B:253:ALA:CB	2:B:455:HIS:HB2	2.00	0.86
23:A:1006:CLA:H2	23:A:1006:CLA:H72	1.55	0.86
2:B:284:ILE:HG22	2:B:309:LEU:HD22	1.57	0.86
16:V:160:LYS:N	16:V:163:TYR:CE1	2.43	0.86
23:B:1020:CLA:H142	23:B:1020:CLA:H92	1.55	0.86
3:C:284:PHE:HB3	30:C:1055:DGD:HB81	1.57	0.86
3:C:45:LEU:HD22	3:C:140:LEU:N	1.90	0.86
23:D:1005:CLA:H203	23:D:1005:CLA:C15	2.04	0.86
11:L:27:LEU:HD12	12:M:14:PHE:HZ	1.38	0.86
12:M:1:MET:HE2	12:M:1:MET:H3	1.12	0.86
16:V:98:LEU:HD21	16:V:145:ILE:HG21	1.56	0.86
8:I:30:ARG:HA	8:I:30:ARG:NH1	1.90	0.86
11:L:24:ILE:HD11	12:M:18:PRO:HG2	1.57	0.86
23:C:1033:CLA:H91	23:C:1033:CLA:H121	1.55	0.86
3:C:185:LEU:HD13	3:C:230:LEU:HD11	1.57	0.86
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.56	0.86
3:C:97:TRP:HE1	3:C:178:LYS:CE	1.88	0.86
23:B:1019:CLA:H93	29:L:1061:MGE:H8A1	1.57	0.86
1:A:37:MET:HG2	1:A:41:LEU:HD23	1.56	0.86
23:B:1013:CLA:HMC2	23:B:1023:CLA:H11	1.56	0.86
23:B:1019:CLA:HED2	23:B:1019:CLA:C2A	2.02	0.86
23:C:1031:CLA:H142	23:C:1031:CLA:H171	1.56	0.86
23:C:1031:CLA:HED1	23:C:1031:CLA:O1A	1.74	0.86
23:C:1033:CLA:HMA3	23:C:1033:CLA:HBA1	0.90	0.86
3:C:350:ILE:HD13	3:C:351:PHE:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1031:CLA:H2	23:C:1031:CLA:HMA2	0.90	0.86
27:A:1063:LHG:C31	23:C:1034:CLA:H143	2.06	0.86
2:B:152:GLY:HA2	2:B:155:ALA:HB3	1.56	0.85
23:C:1031:CLA:O2D	23:C:1033:CLA:H8	1.76	0.85
3:C:281:MET:O	3:C:285:ILE:HG22	1.75	0.85
3:C:62:PHE:HE2	10:K:28:ILE:HG22	1.39	0.85
2:B:465:GLY:N	23:B:1019:CLA:CBC	2.38	0.85
26:B:1045:BCR:H372	26:B:1045:BCR:H403	1.56	0.85
23:C:1033:CLA:CMA	23:C:1033:CLA:CBA	2.44	0.85
30:C:1056:DGD:CFB	10:K:30:VAL:HG21	2.06	0.85
16:V:64:ALA:O	16:V:68:VAL:HG23	1.76	0.85
23:A:1007:CLA:H2A	23:A:1007:CLA:O1D	1.76	0.85
24:A:1038:PHO:HHD	24:A:1038:PHO:CBC	2.06	0.85
23:B:1011:CLA:C19	23:H:1017:CLA:C13	2.53	0.85
2:B:262:THR:O	2:B:264:PRO:HD3	1.76	0.85
23:C:1031:CLA:HBA2	23:C:1033:CLA:HED2	1.58	0.85
1:A:135:TYR:CZ	3:C:449:ARG:HD2	2.10	0.85
3:C:76:ILE:HG23	3:C:77:PRO:HD2	1.58	0.85
23:B:1016:CLA:HBC3	23:B:1016:CLA:HHD	1.58	0.85
2:B:323:GLY:HA3	2:B:326:ARG:HH11	1.41	0.85
13:O:65:ARG:NH2	13:O:66:ILE:HG12	1.92	0.85
16:V:48:THR:H	16:V:51:GLN:HG2	1.39	0.85
2:B:171:PRO:HG3	7:H:63:LYS:HA	1.58	0.85
23:C:1029:CLA:O2D	23:C:1029:CLA:H2A	1.76	0.85
3:C:250:TRP:HE1	23:C:1030:CLA:CED	1.89	0.85
4:D:269:PHE:CD1	4:D:269:PHE:O	2.30	0.85
20:Z:3:ILE:H	20:Z:3:ILE:HD12	1.41	0.85
23:B:1009:CLA:CGD	23:B:1009:CLA:CAA	2.55	0.85
1:A:328:MET:HB3	4:D:325:ILE:HD11	1.55	0.85
23:A:1006:CLA:CBC	23:A:1006:CLA:HHD	2.06	0.85
1:A:60:ILE:HG22	1:A:83:VAL:HG13	1.58	0.85
23:B:1013:CLA:H141	23:B:1018:CLA:HMA2	1.56	0.85
2:B:284:ILE:HG13	2:B:285:ASN:N	1.90	0.85
30:C:1057:DGD:HB82	29:J:1059:MGE:H8B2	1.58	0.85
23:C:1032:CLA:H2A	23:C:1032:CLA:HED3	0.86	0.85
4:D:251:ARG:HE	4:D:255:GLN:NE2	1.74	0.85
4:D:257:PHE:HA	29:D:1062:MGE:H121	1.57	0.85
4:D:261:PHE:CE2	4:D:267:LEU:HB2	2.11	0.85
30:C:1056:DGD:C6D	30:C:1056:DGD:C3E	2.45	0.85
15:U:39:LEU:H	15:U:39:LEU:HD12	1.40	0.85
2:B:153:PHE:N	23:B:1014:CLA:HMC3	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:447:ARG:HG3	3:C:448:ALA:N	1.90	0.84
9:J:9:PRO:HG2	9:J:12:ILE:HB	1.56	0.84
13:O:184:ASP:HB2	13:O:185:PRO:HD2	1.59	0.84
1:A:173:PRO:HD2	1:A:182:PHE:HB2	1.59	0.84
23:B:1011:CLA:CBB	23:B:1013:CLA:C18	2.54	0.84
3:C:63:TRP:CE3	23:C:1027:CLA:HBC1	2.10	0.84
23:D:1005:CLA:CAA	23:D:1005:CLA:HED2	2.06	0.84
27:A:1063:LHG:C31	23:C:1034:CLA:H93	2.07	0.84
3:C:428:THR:HG23	3:C:429:SER:H	1.40	0.84
23:B:1021:CLA:C14	23:B:1021:CLA:H203	2.07	0.84
26:B:1045:BCR:H353	26:B:1047:BCR:C11	2.06	0.84
26:H:1049:BCR:C40	26:H:1049:BCR:H23C	2.02	0.84
20:Z:13:VAL:HG13	20:Z:14:ILE:N	1.92	0.84
1:A:195:HIS:ND1	1:A:197:PHE:HB2	1.92	0.84
23:B:1020:CLA:HBB1	23:B:1021:CLA:HBA2	1.57	0.84
23:B:1022:CLA:C5	23:B:1022:CLA:C9	2.30	0.84
2:B:256:MET:HE1	2:B:448:ARG:NH1	1.93	0.84
29:D:1062:MGE:O5D	11:L:15:THR:HB	1.77	0.84
23:B:1020:CLA:H91	23:B:1020:CLA:H142	1.47	0.84
2:B:460:LEU:HG	30:H:1058:DGD:CIA	2.08	0.84
23:C:1025:CLA:HMD2	23:C:1026:CLA:C4	2.08	0.84
23:C:1032:CLA:HHC	23:C:1032:CLA:HBB1	1.58	0.84
4:D:68:LEU:HA	6:F:40:MET:HG2	1.60	0.84
14:T:4:ILE:C	14:T:4:ILE:HD12	1.92	0.84
23:B:1024:CLA:CMC	23:B:1024:CLA:HBC2	1.96	0.84
26:D:1050:BCR:H403	26:D:1050:BCR:H372	1.57	0.84
23:C:1037:CLA:HAB	26:Z:1053:BCR:C30	2.08	0.84
23:C:1025:CLA:H161	23:C:1031:CLA:HMB3	1.56	0.84
4:D:110:LEU:O	4:D:113:PHE:HB3	1.76	0.84
4:D:261:PHE:HE2	4:D:266:TRP:CD1	1.94	0.84
10:K:28:ILE:HD13	26:K:1051:BCR:C7	2.04	0.84
13:O:68:ARG:O	13:O:267:ALA:HA	1.77	0.84
23:C:1029:CLA:HMA2	23:C:1029:CLA:HBA2	0.84	0.84
3:C:214:LEU:HD23	3:C:215:LYS:HB2	1.59	0.84
3:C:264:PHE:CE1	26:C:1054:BCR:C31	2.60	0.84
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.59	0.84
26:H:1049:BCR:H361	26:H:1049:BCR:H373	1.59	0.84
14:T:1:MET:HE2	14:T:1:MET:N	1.91	0.84
3:C:304:PRO:HB3	3:C:395:TYR:CD2	2.12	0.84
1:A:219:VAL:HB	4:D:268:HIS:HD1	1.37	0.84
4:D:72:ASN:HD22	4:D:74:LEU:H	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:PHE:HA	23:B:1014:CLA:HMC3	1.59	0.83
2:B:65:PHE:O	2:B:68:ARG:HG2	1.77	0.83
23:C:1031:CLA:CAA	23:C:1031:CLA:HED3	2.08	0.83
1:A:322:ASN:HD21	3:C:412:THR:HG22	1.41	0.83
23:A:1003:CLA:C14	24:A:1038:PHO:H93	2.05	0.83
23:C:1031:CLA:CAA	23:C:1031:CLA:CED	2.55	0.83
6:F:11:VAL:HG12	6:F:12:SER:H	1.43	0.83
18:Y:32:GLY:HA2	18:Y:35:ILE:HG23	1.59	0.83
23:C:1037:CLA:CGD	23:C:1037:CLA:HBA1	2.09	0.83
30:C:1056:DGD:HE3	30:C:1056:DGD:HD61	0.87	0.83
4:D:253:TRP:HA	4:D:256:ILE:CG2	2.08	0.83
23:B:1010:CLA:HAA2	23:B:1010:CLA:O1D	1.77	0.83
23:B:1011:CLA:CBB	23:B:1013:CLA:H192	2.09	0.83
2:B:257:TRP:CZ3	4:D:291:LEU:CG	2.61	0.83
5:E:35:TRP:CE3	6:F:38:ALA:HB3	2.13	0.83
2:B:457:VAL:HG22	4:D:284:ILE:HG23	1.57	0.83
3:C:117:VAL:O	3:C:121:SER:HB2	1.79	0.83
3:C:315:MET:O	3:C:319:ILE:HG13	1.78	0.83
1:A:213:ALA:O	1:A:217:SER:HB2	1.79	0.83
30:C:1056:DGD:HA52	30:C:1056:DGD:O1A	1.78	0.83
16:V:28:GLU:HA	16:V:28:GLU:OE2	1.78	0.83
23:B:1013:CLA:HMA1	23:B:1014:CLA:HMA1	1.59	0.83
23:C:1033:CLA:C17	23:C:1033:CLA:H141	2.08	0.83
3:C:124:VAL:HG23	3:C:125:LEU:H	1.43	0.83
3:C:158:THR:O	3:C:251:HIS:HB3	1.79	0.83
3:C:288:CYS:SG	30:C:1055:DGD:HB21	2.19	0.83
5:E:35:TRP:CZ3	6:F:38:ALA:HB3	2.12	0.83
10:K:32:PHE:HE2	26:K:1051:BCR:H341	1.43	0.83
23:B:1015:CLA:HBC2	23:B:1015:CLA:HHD	1.61	0.83
23:C:1027:CLA:CGD	23:C:1036:CLA:H11	2.08	0.83
23:C:1027:CLA:HED2	23:C:1036:CLA:H201	1.60	0.83
20:Z:55:GLY:HA2	26:Z:1053:BCR:C31	2.06	0.83
1:A:42:LEU:O	1:A:46:ILE:HG23	1.78	0.83
23:C:1033:CLA:C9	23:C:1033:CLA:H121	2.09	0.83
4:D:303:ILE:HD12	4:D:304:ARG:H	1.43	0.83
4:D:48:TRP:HE3	4:D:49:LEU:HG	1.43	0.83
12:M:21:PHE:HA	12:M:24:ILE:HD12	1.59	0.83
23:B:1019:CLA:CMB	23:B:1020:CLA:C1C	2.56	0.82
23:C:1027:CLA:CED	23:C:1036:CLA:C20	2.56	0.82
3:C:184:GLY:H	3:C:198:VAL:HG22	1.44	0.82
10:K:39:VAL:CG2	18:Y:36:ILE:HD11	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:ILE:HD11	3:C:285:ILE:HD11	1.60	0.82
3:C:45:LEU:CD2	3:C:141:GLU:HG2	2.09	0.82
23:C:1034:CLA:HAA1	10:K:29:PRO:HB3	1.60	0.82
1:A:323:ARG:HH11	1:A:323:ARG:HG3	1.42	0.82
1:A:58:VAL:H	1:A:68:SER:HB2	1.43	0.82
2:B:27:THR:CG2	23:B:1020:CLA:H11	2.08	0.82
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.60	0.82
5:E:35:TRP:CZ3	6:F:38:ALA:CB	2.63	0.82
23:B:1016:CLA:H143	23:D:1008:CLA:HHB	1.61	0.82
2:B:27:THR:HG23	23:B:1013:CLA:HAC2	1.59	0.82
3:C:206:PRO:O	3:C:210:PHE:HB2	1.79	0.82
10:K:28:ILE:CD1	26:K:1051:BCR:C9	2.54	0.82
2:B:487:SER:HB3	2:B:488:PRO:HD3	1.61	0.82
1:A:60:ILE:CG2	1:A:83:VAL:HG13	2.09	0.82
23:C:1032:CLA:H92	23:C:1032:CLA:H51	1.62	0.82
4:D:134:ARG:HE	4:D:134:ARG:HA	1.43	0.82
13:O:119:LEU:H	13:O:155:THR:CG2	1.90	0.82
17:X:13:THR:HG22	17:X:15:SER:H	1.43	0.82
23:B:1021:CLA:HMC1	23:B:1021:CLA:HBC2	1.62	0.82
4:D:277:THR:HG22	4:D:278:GLY:N	1.93	0.82
1:A:116:ILE:HD11	1:A:158:PHE:HB3	1.62	0.82
23:B:1021:CLA:OBD	23:B:1022:CLA:CMC	2.26	0.82
23:B:1012:CLA:HHH	23:B:1012:CLA:HBC2	1.62	0.81
23:B:1012:CLA:C1	23:B:1013:CLA:C1	2.58	0.81
23:B:1014:CLA:H93	23:B:1014:CLA:H122	1.59	0.81
23:B:1014:CLA:H102	26:B:1048:BCR:H311	1.62	0.81
23:C:1033:CLA:H18	23:C:1033:CLA:H143	1.62	0.81
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.15	0.81
31:E:1040:HEM:HMA3	31:E:1040:HEM:O1A	1.80	0.81
11:L:20:GLY:O	11:L:24:ILE:HG22	1.79	0.81
1:A:208:GLY:HA3	1:A:279:ARG:HD2	1.62	0.81
23:B:1023:CLA:C4D	23:B:1024:CLA:CMC	2.59	0.81
2:B:110:ALA:CB	23:B:1024:CLA:HMB2	2.09	0.81
2:B:464:PHE:CZ	29:B:1060:MGE:H4B1	2.13	0.81
4:D:207:GLY:HA3	4:D:275:PRO:HG3	1.62	0.81
23:A:1006:CLA:HMB3	24:A:1039:PHO:C16	2.09	0.81
23:B:1020:CLA:CBA	23:B:1020:CLA:CMA	2.34	0.81
2:B:257:TRP:CH2	4:D:291:LEU:CG	2.63	0.81
11:L:26:VAL:HG21	29:L:1061:MGE:H261	1.61	0.81
17:X:26:GLY:O	17:X:29:VAL:HG12	1.80	0.81
1:A:187:GLN:HB2	23:A:1003:CLA:HAC2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1020:CLA:C9	23:B:1020:CLA:H13	2.05	0.81
2:B:138:MET:HB3	23:B:1023:CLA:HBC3	1.61	0.81
23:B:1024:CLA:H2A	23:B:1024:CLA:O2A	1.79	0.81
23:B:1014:CLA:H172	26:B:1048:BCR:H312	1.61	0.81
2:B:391:SER:HB3	2:B:394:GLN:CD	2.01	0.81
29:L:1061:MGE:H7B1	29:L:1061:MGE:C3B	2.10	0.81
15:U:91:VAL:HG12	15:U:105:LEU:HD13	1.61	0.81
23:B:1023:CLA:H72	26:B:1048:BCR:C34	2.09	0.81
3:C:162:GLY:HA3	3:C:248:GLY:HA2	1.60	0.81
6:F:37:ILE:HG21	9:J:28:PHE:CE1	2.15	0.81
13:O:127:ILE:CD1	13:O:127:ILE:H	1.80	0.81
26:B:1048:BCR:H331	26:B:1048:BCR:C8	2.10	0.81
23:C:1029:CLA:H52	23:C:1029:CLA:C1C	2.11	0.81
23:C:1035:CLA:H93	26:K:1052:BCR:H402	1.60	0.81
3:C:261:ARG:HH11	3:C:261:ARG:HG2	1.45	0.81
10:K:35:LEU:O	10:K:38:VAL:HG23	1.79	0.81
1:A:247:ASN:HD22	1:A:250:ALA:H	1.27	0.81
23:B:1019:CLA:HED2	23:B:1019:CLA:CBA	2.10	0.81
3:C:78:GLU:OE1	3:C:104:GLU:HB2	1.81	0.81
12:M:9:ILE:HD12	12:M:9:ILE:H	1.46	0.81
23:A:1006:CLA:H2A	23:A:1006:CLA:O2D	1.80	0.81
6:F:29:PRO:O	6:F:32:PHE:HB3	1.79	0.81
10:K:28:ILE:HD11	26:K:1051:BCR:C7	2.04	0.81
2:B:384:ARG:HA	13:O:192:SER:OG	1.81	0.81
20:Z:13:VAL:HG13	20:Z:14:ILE:H	1.46	0.81
2:B:45:PHE:O	2:B:47:PRO:HD3	1.81	0.81
2:B:464:PHE:HB2	4:D:280:TRP:CH2	2.16	0.81
7:H:53:LEU:HG	7:H:55:LEU:CD1	2.11	0.81
12:M:18:PRO:O	12:M:21:PHE:HB3	1.81	0.81
23:C:1031:CLA:HED3	23:C:1031:CLA:H2A	1.61	0.81
30:C:1055:DGD:HB72	30:C:1055:DGD:HB22	1.61	0.81
30:C:1056:DGD:HA41	30:C:1056:DGD:O1A	1.81	0.81
1:A:223:LEU:HD21	1:A:245:THR:OG1	1.80	0.80
2:B:223:GLN:HB2	2:B:227:LYS:NZ	1.96	0.80
11:L:30:LEU:HD22	11:L:31:PHE:HD1	1.44	0.80
13:O:187:GLY:HA3	13:O:194:TYR:HD1	1.45	0.80
23:B:1012:CLA:C12	23:B:1012:CLA:H91	2.01	0.80
4:D:261:PHE:CE2	4:D:266:TRP:HD1	1.99	0.80
1:A:219:VAL:HG23	4:D:268:HIS:HB3	1.63	0.80
1:A:324:ALA:HB2	4:D:329:MET:SD	2.20	0.80
1:A:84:PRO:HA	1:A:112:TYR:CD2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:MET:CG	23:B:1013:CLA:HED1	2.11	0.80
23:B:1011:CLA:H202	7:H:38:PHE:HE2	1.43	0.80
18:Y:25:ILE:O	18:Y:28:ILE:HG12	1.80	0.80
23:A:1006:CLA:C14	23:D:1004:CLA:H192	2.12	0.80
23:B:1022:CLA:C7	23:B:1022:CLA:H142	2.01	0.80
1:A:184:ILE:HG21	4:D:321:LEU:HD13	1.62	0.80
23:B:1009:CLA:CHA	23:B:1009:CLA:HBA2	2.11	0.80
23:B:1020:CLA:C13	23:B:1020:CLA:H8	2.02	0.80
26:B:1047:BCR:H322	26:B:1047:BCR:H343	1.63	0.80
4:D:195:PRO:HA	4:D:198:MET:CE	2.12	0.80
27:A:1063:LHG:H312	23:C:1034:CLA:H93	1.62	0.80
23:B:1012:CLA:H12	23:B:1013:CLA:C2	2.11	0.80
23:B:1013:CLA:HMA1	23:B:1014:CLA:CMA	2.11	0.80
2:B:110:ALA:HB3	23:B:1024:CLA:HMB2	1.63	0.80
2:B:17:GLY:HA2	2:B:123:PHE:CE2	2.16	0.80
30:C:1056:DGD:C4A	30:C:1056:DGD:O1A	2.30	0.80
30:C:1056:DGD:CHA	30:C:1057:DGD:HA82	2.11	0.80
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.62	0.80
23:B:1010:CLA:H101	23:H:1017:CLA:H203	1.62	0.80
23:C:1031:CLA:CED	23:C:1031:CLA:O1A	2.30	0.80
7:H:33:VAL:O	7:H:37:LEU:HD13	1.82	0.80
23:B:1022:CLA:CHA	23:B:1022:CLA:O1A	2.30	0.80
23:B:1023:CLA:O1A	23:B:1023:CLA:C3A	2.30	0.80
23:B:1022:CLA:HMB2	26:B:1045:BCR:H401	1.62	0.80
2:B:148:LEU:N	2:B:210:ILE:HD11	1.97	0.80
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.17	0.80
2:B:257:TRP:CH2	4:D:291:LEU:CB	2.64	0.80
3:C:75:PHE:CE2	3:C:105:VAL:HG11	2.17	0.80
23:B:1011:CLA:C12	26:H:1049:BCR:H322	2.10	0.80
16:V:160:LYS:HB2	16:V:160:LYS:HZ3	1.42	0.80
24:A:1039:PHO:H18	4:D:48:TRP:NE1	1.96	0.80
23:B:1011:CLA:CED	23:B:1011:CLA:OBD	2.30	0.80
30:C:1055:DGD:C1B	30:C:1055:DGD:HB51	2.10	0.80
23:C:1035:CLA:H101	26:K:1052:BCR:C40	2.11	0.80
16:V:48:THR:N	16:V:51:GLN:HE21	1.79	0.80
23:B:1014:CLA:O2D	23:B:1014:CLA:CAA	2.30	0.79
1:A:142:TRP:H	4:D:220:ASN:HD21	1.30	0.79
31:E:1040:HEM:HBB2	31:E:1040:HEM:HMB2	1.64	0.79
1:A:149:ALA:HB1	1:A:283:VAL:HG21	1.62	0.79
23:B:1014:CLA:C19	23:B:1014:CLA:C15	2.44	0.79
2:B:103:LEU:CB	23:B:1014:CLA:H71	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1021:CLA:C2A	23:B:1021:CLA:O2A	2.30	0.79
1:A:48:PHE:HB2	1:A:115:ILE:HD13	1.62	0.79
1:A:39:PRO:HB2	23:A:1007:CLA:HAB	1.64	0.79
23:B:1019:CLA:O1A	23:B:1019:CLA:C3A	2.30	0.79
23:B:1019:CLA:C19	23:B:1021:CLA:C7	2.60	0.79
23:B:1022:CLA:H41	23:B:1022:CLA:C9	2.05	0.79
2:B:25:MET:CG	26:B:1045:BCR:H292	2.03	0.79
2:B:183:PRO:HB3	2:B:200:ALA:HB2	1.61	0.79
23:C:1032:CLA:O1A	23:C:1032:CLA:C4	2.30	0.79
4:D:274:VAL:CB	4:D:275:PRO:HD3	2.11	0.79
1:A:95:PRO:CA	23:A:1007:CLA:HED1	2.05	0.79
1:A:247:ASN:HB3	1:A:250:ALA:HB3	1.64	0.79
4:D:261:PHE:CE1	25:D:1042:PQ9:H143	2.18	0.79
1:A:307:ILE:HG13	1:A:308:ASP:H	1.47	0.79
26:B:1045:BCR:C35	26:B:1047:BCR:C10	2.60	0.79
3:C:459:ILE:HD12	3:C:459:ILE:N	1.97	0.79
31:E:1040:HEM:O1A	31:E:1040:HEM:CMA	2.30	0.79
1:A:90:GLY:HA3	1:A:167:SER:HB2	1.64	0.79
2:B:133:LEU:HB3	2:B:138:MET:CE	2.13	0.79
23:C:1025:CLA:O1D	23:C:1025:CLA:CBA	2.30	0.79
23:C:1032:CLA:H152	23:C:1032:CLA:H193	1.62	0.79
5:E:38:VAL:CG1	6:F:39:ALA:HB3	2.12	0.79
3:C:347:GLY:HA3	13:O:43:ASN:HB2	1.64	0.79
1:A:206:PHE:CE2	23:D:1004:CLA:HBA2	2.18	0.79
23:B:1014:CLA:C11	23:B:1014:CLA:C16	2.40	0.79
29:D:1062:MGE:H3G1	11:L:15:THR:HG21	1.62	0.79
13:O:121:PHE:HB3	13:O:153:ALA:HB3	1.65	0.79
13:O:145:LEU:HD23	13:O:145:LEU:H	1.47	0.79
13:O:213:VAL:HG11	15:U:39:LEU:HD13	1.62	0.79
15:U:97:LEU:HB3	15:U:102:LYS:HG2	1.62	0.79
23:B:1009:CLA:O2D	23:B:1009:CLA:CAA	2.30	0.79
23:B:1011:CLA:HBC2	23:B:1011:CLA:HMC1	1.64	0.79
23:C:1037:CLA:O1A	23:C:1037:CLA:C4A	2.30	0.79
24:A:1039:PHO:CAB	23:D:1004:CLA:H12	2.13	0.79
27:A:1063:LHG:O4	27:A:1063:LHG:C6	2.30	0.79
1:A:81:ALA:HB1	1:A:175:GLY:HA3	1.64	0.79
2:B:382:PRO:HG2	2:B:391:SER:HB2	1.63	0.79
23:C:1037:CLA:CHA	23:C:1037:CLA:HBA1	2.10	0.79
3:C:384:ILE:O	3:C:384:ILE:HG23	1.83	0.79
3:C:287:THR:HG23	3:C:427:ALA:HA	1.65	0.79
1:A:91:LEU:HD13	1:A:166:GLY:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1019:CLA:H193	23:B:1021:CLA:C5	2.12	0.79
8:I:27:ASP:HB3	8:I:28:PRO:HD3	1.65	0.79
20:Z:16:SER:O	20:Z:20:VAL:HG23	1.82	0.79
24:A:1038:PHO:H102	24:A:1038:PHO:C14	1.94	0.78
3:C:32:GLY:HA2	3:C:41:ARG:HH21	1.48	0.78
3:C:51:GLY:O	3:C:55:ALA:HB2	1.82	0.78
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.64	0.78
1:A:90:GLY:HA2	1:A:167:SER:OG	1.84	0.78
23:B:1010:CLA:CAD	23:B:1010:CLA:HED3	2.08	0.78
3:C:157:MET:HB3	23:C:1031:CLA:HBC1	1.64	0.78
3:C:256:PRO:HB3	3:C:261:ARG:NH2	1.97	0.78
23:C:1034:CLA:HAA1	10:K:29:PRO:CB	2.13	0.78
29:L:1061:MGE:H6A1	12:M:22:LEU:HD21	1.65	0.78
13:O:169:LYS:HB3	13:O:169:LYS:HZ2	1.47	0.78
1:A:279:ARG:NH2	24:A:1038:PHO:CAC	2.44	0.78
23:B:1014:CLA:HMA3	23:B:1014:CLA:CBA	2.03	0.78
23:B:1014:CLA:CGA	23:B:1014:CLA:CMA	2.58	0.78
23:B:1023:CLA:C1D	23:B:1024:CLA:HBC2	2.12	0.78
3:C:346:THR:HG21	13:O:38:GLY:H	1.48	0.78
29:L:1061:MGE:C1G	29:L:1061:MGE:O1B	2.30	0.78
26:T:6046:BCR:H382	26:T:6046:BCR:H373	1.63	0.78
24:A:1038:PHO:CHD	24:A:1038:PHO:CBC	2.62	0.78
23:B:1021:CLA:OBD	23:B:1022:CLA:CHC	2.29	0.78
29:B:1060:MGE:H3A2	29:B:1060:MGE:H261	1.65	0.78
3:C:160:ILE:HA	3:C:163:PHE:HD2	1.48	0.78
23:B:1011:CLA:H202	7:H:38:PHE:CE2	2.19	0.78
16:V:38:LEU:HD22	16:V:45:ILE:HB	1.65	0.78
3:C:78:GLU:OE2	3:C:78:GLU:HA	1.83	0.78
14:T:1:MET:O	14:T:4:ILE:CG2	2.30	0.78
1:A:344:ALA:HB1	3:C:357:ARG:HH22	1.48	0.78
26:B:1048:BCR:C38	26:B:1048:BCR:C23	2.38	0.78
23:C:1029:CLA:H201	23:C:1030:CLA:C19	2.13	0.78
2:B:250:PHE:HZ	30:H:1058:DGD:HAG2	1.47	0.78
23:B:1014:CLA:H2A	23:B:1014:CLA:O2D	1.83	0.78
2:B:91:TRP:HB3	23:B:1014:CLA:HED2	1.64	0.78
23:C:1029:CLA:H111	23:C:1029:CLA:H192	1.64	0.78
23:A:1003:CLA:C2D	23:D:1005:CLA:HBC1	2.14	0.78
1:A:279:ARG:HD3	4:D:208:ALA:CB	2.14	0.78
2:B:156:PHE:N	2:B:156:PHE:HD2	1.81	0.78
2:B:12:LEU:CB	2:B:19:LEU:HD23	2.13	0.78
2:B:460:LEU:HA	30:H:1058:DGD:CIA	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1034:CLA:H172	23:C:1034:CLA:H141	0.84	0.78
1:A:278:TRP:HH2	30:C:1057:DGD:CIA	1.97	0.78
26:D:1050:BCR:C21	29:J:1059:MGE:H3A1	2.13	0.78
2:B:456:ALA:HA	30:H:1058:DGD:HGB2	1.65	0.78
12:M:32:GLN:HA	12:M:32:GLN:HE21	1.48	0.78
23:A:1006:CLA:C2	23:A:1006:CLA:C7	2.62	0.78
23:B:1016:CLA:C4A	23:B:1016:CLA:O1A	2.32	0.78
23:B:1022:CLA:HED2	23:B:1022:CLA:CAD	2.14	0.78
2:B:464:PHE:CB	4:D:280:TRP:CH2	2.67	0.78
6:F:40:MET:HA	6:F:43:ILE:HD11	1.66	0.78
1:A:116:ILE:HG23	1:A:117:PHE:HD2	1.49	0.78
1:A:255:PHE:HB3	1:A:264:SER:OG	1.83	0.78
2:B:102:VAL:HG13	23:B:1014:CLA:H92	1.66	0.78
23:C:1036:CLA:H193	26:Z:1053:BCR:C37	2.14	0.78
23:C:1037:CLA:C10	23:C:1037:CLA:H143	2.14	0.78
3:C:96:GLY:HA2	3:C:99:VAL:HG13	1.66	0.78
3:C:99:VAL:HG21	3:C:196:VAL:CG1	2.14	0.78
4:D:186:GLN:HB2	23:D:1004:CLA:HBC1	1.65	0.78
10:K:39:VAL:HG22	18:Y:36:ILE:HD12	1.63	0.78
23:B:1020:CLA:C9	23:B:1020:CLA:H121	2.10	0.77
2:B:74:SER:HB2	2:B:94:GLU:OE1	1.84	0.77
3:C:48:LYS:HD2	3:C:133:ALA:O	1.84	0.77
4:D:93:TRP:HZ2	23:D:1008:CLA:O1A	1.66	0.77
10:K:32:PHE:CE1	26:K:1052:BCR:C39	2.65	0.77
15:U:58:ASN:N	15:U:58:ASN:HD22	1.82	0.77
23:B:1011:CLA:C1D	23:B:1013:CLA:H51	2.14	0.77
3:C:63:TRP:HB2	23:C:1034:CLA:CED	2.14	0.77
4:D:195:PRO:HA	4:D:198:MET:HE2	1.65	0.77
3:C:357:ARG:HH11	3:C:357:ARG:HB3	1.49	0.77
2:B:152:GLY:C	23:B:1014:CLA:HMC1	2.05	0.77
23:C:1031:CLA:O2D	23:C:1033:CLA:C10	2.33	0.77
3:C:337:LEU:HA	13:O:131:PRO:HG3	1.64	0.77
23:B:1019:CLA:C2A	23:B:1019:CLA:O2D	2.30	0.77
23:C:1029:CLA:C4	23:C:1029:CLA:H191	2.15	0.77
23:H:1017:CLA:H193	23:H:1017:CLA:H152	1.65	0.77
12:M:11:THR:HG22	12:M:12:ALA:N	1.99	0.77
1:A:247:ASN:ND2	1:A:250:ALA:H	1.82	0.77
4:D:281:MET:HA	4:D:281:MET:CE	2.13	0.77
13:O:58:ILE:HG12	13:O:160:THR:O	1.85	0.77
1:A:134:SER:HB3	1:A:141:PRO:HA	1.65	0.77
1:A:215:HIS:O	1:A:219:VAL:HG13	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PRO:HG2	7:H:49:TYR:CE1	2.18	0.77
23:C:1025:CLA:C4	23:C:1025:CLA:C1B	2.62	0.77
3:C:135:ARG:HH12	20:Z:33:TRP:HB3	1.49	0.77
3:C:166:ILE:HA	3:C:245:ILE:HD13	1.64	0.77
20:Z:37:LYS:NZ	20:Z:38:GLN:HG2	1.99	0.77
1:A:37:MET:HG2	1:A:41:LEU:CD2	2.15	0.77
23:B:1022:CLA:CHD	23:B:1022:CLA:HBC2	2.05	0.77
2:B:465:GLY:HA2	2:B:468:TRP:H	1.50	0.77
23:C:1025:CLA:CMD	23:C:1026:CLA:C4	2.62	0.77
10:K:32:PHE:CE1	26:K:1052:BCR:C21	2.68	0.77
13:O:173:ASN:OD1	13:O:220:LYS:HE2	1.84	0.77
20:Z:9:LEU:C	20:Z:11:ALA:H	1.87	0.77
23:B:1012:CLA:CHD	23:B:1012:CLA:CBC	2.63	0.77
2:B:66:MET:HB3	2:B:71:VAL:HG13	1.67	0.77
23:C:1025:CLA:H43	23:C:1025:CLA:C1B	2.14	0.77
23:A:1003:CLA:C3D	23:D:1005:CLA:HBC1	2.14	0.77
23:B:1011:CLA:C4D	23:B:1013:CLA:H41	2.14	0.77
2:B:448:ARG:HH11	2:B:448:ARG:HB2	1.50	0.77
23:C:1028:CLA:O2A	30:C:1056:DGD:HG11	1.85	0.77
26:D:1050:BCR:H373	29:J:1059:MGE:H4A2	0.81	0.77
1:A:90:GLY:CA	1:A:167:SER:HB2	2.14	0.76
23:B:1010:CLA:CMD	23:B:1011:CLA:C8	2.53	0.76
23:C:1025:CLA:CMD	23:C:1026:CLA:H43	2.15	0.76
3:C:88:LEU:HD21	23:C:1027:CLA:CBC	2.14	0.76
26:C:1054:BCR:H393	26:C:1054:BCR:C27	2.14	0.76
30:C:1056:DGD:HBG3	30:C:1056:DGD:HBF2	1.67	0.76
3:C:311:GLN:NE2	3:C:351:PHE:HD2	1.83	0.76
15:U:82:ASN:HB2	15:U:85:TYR:OH	1.86	0.76
16:V:85:LEU:HB3	16:V:92:ARG:O	1.85	0.76
10:K:39:VAL:CG2	18:Y:36:ILE:CD1	2.62	0.76
23:B:1016:CLA:CHA	23:B:1016:CLA:HBA1	2.14	0.76
2:B:120:LEU:O	2:B:123:PHE:HB2	1.84	0.76
2:B:423:LYS:O	2:B:429:ILE:HG13	1.85	0.76
23:C:1032:CLA:C1A	23:C:1032:CLA:HED3	2.14	0.76
3:C:95:LEU:N	3:C:95:LEU:HD22	1.99	0.76
26:K:1052:BCR:H331	26:K:1052:BCR:C8	2.16	0.76
13:O:129:PHE:O	13:O:130:GLN:HG2	1.84	0.76
1:A:196:PRO:HB2	30:C:1057:DGD:HA81	1.66	0.76
1:A:279:ARG:HH22	24:A:1038:PHO:CAC	1.94	0.76
1:A:27:ARG:O	1:A:28:LEU:HD23	1.86	0.76
23:B:1016:CLA:CGA	23:B:1016:CLA:C1A	2.63	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:TRP:O	3:C:243:ILE:HG13	1.85	0.76
3:C:305:THR:CG2	3:C:308:GLU:HB2	2.16	0.76
7:H:22:ALA:HB1	7:H:23:PRO:HD2	1.66	0.76
2:B:426:PHE:HZ	13:O:201:PRO:HB3	1.50	0.76
1:A:210:LEU:CD2	23:A:1006:CLA:H41	2.16	0.76
3:C:343:ARG:HH11	3:C:343:ARG:HG3	1.50	0.76
6:F:41:GLN:HE22	9:J:27:LEU:HB3	1.47	0.76
26:D:1050:BCR:C21	29:J:1059:MGE:C3A	2.64	0.76
13:O:169:LYS:HB3	13:O:169:LYS:NZ	1.99	0.76
14:T:1:MET:C	14:T:4:ILE:HG22	2.05	0.76
23:B:1010:CLA:O1D	23:B:1010:CLA:C2A	2.33	0.76
23:B:1019:CLA:HMB3	23:B:1020:CLA:C1C	2.15	0.76
13:O:178:ARG:HD3	13:O:182:PHE:CD2	2.20	0.76
1:A:200:LEU:HA	1:A:203:ALA:HB3	1.66	0.76
23:B:1023:CLA:C4D	23:B:1024:CLA:HMC1	2.15	0.76
23:C:1033:CLA:CHD	23:C:1033:CLA:HBC3	2.12	0.76
23:C:1034:CLA:H43	23:C:1034:CLA:O1A	1.86	0.76
30:C:1055:DGD:HB72	30:C:1055:DGD:C3B	2.15	0.76
3:C:263:ALA:H	8:I:28:PRO:HG2	1.51	0.76
4:D:236:ASN:HB3	4:D:237:PRO:HA	1.67	0.76
4:D:251:ARG:HE	4:D:255:GLN:HE22	1.29	0.76
4:D:89:LEU:HG	4:D:91:LEU:HD13	1.68	0.76
10:K:32:PHE:HD1	26:K:1052:BCR:H393	1.49	0.76
15:U:41:ASN:HB3	15:U:44:ASP:OD2	1.86	0.76
16:V:82:THR:HA	16:V:85:LEU:HD12	1.67	0.76
4:D:72:ASN:ND2	4:D:74:LEU:H	1.83	0.76
15:U:101:GLN:O	15:U:105:LEU:HG	1.85	0.76
23:B:1012:CLA:H102	23:B:1023:CLA:C1	2.16	0.76
23:B:1023:CLA:H122	23:B:1023:CLA:H91	1.67	0.76
2:B:257:TRP:CH2	4:D:291:LEU:HD12	2.20	0.76
3:C:34:ALA:HB2	4:D:230:SER:OG	1.85	0.76
8:I:33:LYS:HB3	8:I:35:LYS:HE3	1.67	0.76
23:C:1029:CLA:C15	23:C:1029:CLA:C19	2.30	0.76
23:C:1029:CLA:C20	23:C:1030:CLA:C19	2.64	0.76
3:C:34:ALA:O	3:C:38:GLY:HA2	1.86	0.76
7:H:12:ARG:HB3	7:H:12:ARG:HH11	1.49	0.76
1:A:99:ALA:HA	1:A:104:GLU:OE2	1.85	0.76
23:B:1022:CLA:CED	23:B:1022:CLA:OBD	2.30	0.76
2:B:113:TRP:CD1	26:B:1048:BCR:H373	2.20	0.76
23:C:1034:CLA:H41	23:C:1034:CLA:H71	1.39	0.76
5:E:83:LEU:H	5:E:83:LEU:HD13	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:151:LEU:HA	13:O:171:GLU:O	1.86	0.76
14:T:2:GLU:HB2	14:T:6:TYR:HE2	1.51	0.76
23:B:1013:CLA:CBB	23:B:1023:CLA:C4	2.64	0.75
2:B:156:PHE:CD2	2:B:156:PHE:N	2.53	0.75
2:B:464:PHE:CE2	29:B:1060:MGE:C4B	2.63	0.75
23:C:1025:CLA:HMB2	23:C:1025:CLA:H42	1.66	0.75
30:C:1056:DGD:HAV1	30:C:1057:DGD:C8A	2.14	0.75
4:D:148:ALA:HA	4:D:280:TRP:HD1	1.48	0.75
5:E:50:PRO:HB3	5:E:54:SER:O	1.86	0.75
10:K:32:PHE:CZ	26:K:1052:BCR:C20	2.68	0.75
13:O:73:PRO:HA	13:O:263:GLY:HA3	1.67	0.75
4:D:67:TYR:CE1	29:J:1059:MGE:H1G1	2.22	0.75
23:A:1006:CLA:CHD	23:A:1006:CLA:HBC3	2.12	0.75
1:A:82:VAL:HB	1:A:174:LEU:HG	1.68	0.75
2:B:17:GLY:CA	2:B:123:PHE:HE2	2.00	0.75
3:C:322:GLN:NE2	3:C:381:LYS:HD3	2.01	0.75
20:Z:9:LEU:HD13	20:Z:10:ALA:N	2.02	0.75
23:B:1011:CLA:H101	23:B:1011:CLA:H143	1.68	0.75
2:B:326:ARG:HB3	2:B:444:ARG:CG	2.16	0.75
3:C:76:ILE:HG23	3:C:77:PRO:CD	2.16	0.75
12:M:26:TYR:O	12:M:29:THR:HB	1.86	0.75
15:U:44:ASP:HA	15:U:47:LEU:HG	1.69	0.75
17:X:42:GLN:O	17:X:43:ILE:HG13	1.87	0.75
23:B:1011:CLA:HBB2	23:B:1013:CLA:C17	2.13	0.75
2:B:297:THR:HG23	2:B:300:GLU:H	1.51	0.75
4:D:292:ASN:O	4:D:294:ARG:HD3	1.87	0.75
1:A:328:MET:HB3	4:D:325:ILE:CD1	2.16	0.75
2:B:238:LEU:O	2:B:242:ILE:HG13	1.87	0.75
4:D:256:ILE:HG23	4:D:257:PHE:H	1.49	0.75
17:X:43:ILE:HG22	17:X:43:ILE:O	1.86	0.75
1:A:174:LEU:HB3	24:A:1038:PHO:H172	1.68	0.75
27:A:1063:LHG:H322	23:C:1034:CLA:C9	2.17	0.75
1:A:57:PRO:HG2	13:O:141:ARG:NH1	2.02	0.75
23:B:1021:CLA:H141	23:B:1021:CLA:H203	1.68	0.75
23:C:1027:CLA:HED1	23:C:1036:CLA:H203	1.67	0.75
23:C:1037:CLA:CAA	23:C:1037:CLA:O2D	2.30	0.75
2:B:460:LEU:HD23	4:D:280:TRP:CZ3	2.22	0.75
11:L:36:PHE:HD2	14:T:6:TYR:OH	1.70	0.75
24:A:1038:PHO:HHB	23:D:1005:CLA:H93	1.69	0.75
1:A:54:ALA:CB	1:A:72:LEU:HD12	2.13	0.75
23:C:1031:CLA:CGD	23:C:1031:CLA:CAA	2.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:PHE:CG	23:C:1036:CLA:HBB1	2.21	0.75
3:C:236:GLY:HA3	26:C:1054:BCR:H391	1.66	0.75
23:B:1009:CLA:HMB2	26:H:1049:BCR:H392	1.69	0.75
23:C:1025:CLA:C2B	23:C:1025:CLA:H41	2.17	0.75
3:C:179:ALA:HA	3:C:184:GLY:HA2	1.68	0.75
1:A:296:ASN:ND2	3:C:401:LEU:HG	2.02	0.75
4:D:148:ALA:HA	4:D:280:TRP:CD1	2.22	0.75
2:B:224:ARG:HB3	7:H:25:TRP:HB3	1.69	0.75
8:I:10:ILE:O	8:I:13:THR:HG22	1.87	0.75
27:A:1063:LHG:C32	23:C:1034:CLA:H93	2.17	0.74
23:B:1011:CLA:CBB	23:B:1013:CLA:C20	2.45	0.74
2:B:256:MET:HE3	2:B:448:ARG:NH1	2.00	0.74
2:B:66:MET:HG2	23:B:1013:CLA:HED1	1.67	0.74
23:C:1031:CLA:O1D	23:C:1033:CLA:H142	1.86	0.74
23:C:1037:CLA:CGD	23:C:1037:CLA:CAA	2.65	0.74
3:C:449:ARG:CZ	23:C:1029:CLA:HED2	2.16	0.74
23:D:1005:CLA:C16	29:D:1062:MGE:H261	2.16	0.74
4:D:39:PRO:HB2	23:D:1008:CLA:HMC3	1.68	0.74
3:C:262:ARG:HH11	3:C:262:ARG:HB3	1.51	0.74
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.67	0.74
5:E:19:TYR:CD1	5:E:20:TRP:HD1	2.05	0.74
7:H:11:LEU:O	7:H:14:LEU:HD13	1.87	0.74
1:A:90:GLY:C	1:A:92:HIS:H	1.88	0.74
23:B:1011:CLA:C9	23:B:1011:CLA:H122	2.17	0.74
23:B:1019:CLA:HMB2	23:B:1020:CLA:CHC	2.17	0.74
23:B:1022:CLA:O1D	23:B:1022:CLA:CAA	2.30	0.74
3:C:40:ALA:HA	23:C:1033:CLA:HMC3	1.68	0.74
4:D:325:ILE:HG22	4:D:325:ILE:O	1.86	0.74
23:B:1011:CLA:H191	23:H:1017:CLA:C15	2.17	0.74
30:C:1055:DGD:HB72	30:C:1055:DGD:C2B	2.18	0.74
3:C:160:ILE:O	3:C:163:PHE:HB2	1.88	0.74
4:D:92:LEU:HB3	4:D:93:TRP:CE3	2.22	0.74
1:A:89:ILE:HD13	13:O:99:ARG:HD2	1.69	0.74
16:V:91:PRO:O	16:V:92:ARG:HD3	1.87	0.74
23:B:1020:CLA:OBD	23:B:1020:CLA:CED	2.35	0.74
3:C:282:MET:HA	3:C:285:ILE:CG2	2.17	0.74
1:A:142:TRP:N	4:D:220:ASN:HD21	1.85	0.74
4:D:281:MET:CE	4:D:284:ILE:HD12	2.16	0.74
23:B:1009:CLA:H11	26:H:1049:BCR:H351	1.69	0.74
1:A:160:ILE:HG21	1:A:291:SER:HA	1.68	0.74
23:B:1023:CLA:HBB1	23:B:1023:CLA:HHC	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:LEU:HA	17:X:41:SER:OG	1.87	0.74
10:K:33:PHE:O	10:K:33:PHE:CD1	2.30	0.74
16:V:121:LEU:HD23	16:V:138:LEU:HD11	1.70	0.74
16:V:138:LEU:HA	16:V:141:ILE:HD12	1.69	0.74
1:A:142:TRP:N	4:D:220:ASN:ND2	2.36	0.74
1:A:328:MET:HB3	4:D:325:ILE:CG1	2.17	0.74
23:C:1030:CLA:H43	26:C:1054:BCR:H323	1.67	0.74
1:A:202:VAL:HG21	23:A:1006:CLA:OBD	1.87	0.74
1:A:29:TYR:CE2	1:A:132:GLU:HB3	2.19	0.74
23:B:1012:CLA:C10	23:B:1023:CLA:H42	2.15	0.74
2:B:226:TYR:CD2	2:B:231:MET:HG3	2.23	0.74
2:B:231:MET:HA	2:B:236:THR:HG21	1.68	0.74
2:B:257:TRP:CH2	4:D:291:LEU:HB3	2.23	0.74
23:C:1034:CLA:HBC3	23:C:1034:CLA:CHD	2.13	0.74
26:K:1051:BCR:H321	26:K:1052:BCR:C12	2.17	0.74
23:B:1016:CLA:HMA1	4:D:130:PHE:CE1	2.22	0.74
23:B:1016:CLA:HMD1	23:B:1018:CLA:HAB	1.69	0.74
23:B:1012:CLA:C10	23:B:1023:CLA:O2A	2.35	0.74
2:B:106:LEU:HD11	26:B:1048:BCR:C13	2.17	0.74
23:C:1025:CLA:HMB2	23:C:1025:CLA:C4	2.18	0.74
23:C:1034:CLA:C8	23:C:1034:CLA:C4	2.50	0.74
4:D:146:PHE:O	4:D:149:PRO:HG2	1.87	0.74
23:A:1006:CLA:H101	25:A:1043:PQ9:H441	1.70	0.74
1:A:141:PRO:HG3	3:C:447:ARG:HA	1.69	0.74
1:A:219:VAL:CB	4:D:268:HIS:ND1	2.50	0.74
23:B:1021:CLA:O2A	23:B:1021:CLA:HMA2	1.87	0.74
23:B:1022:CLA:C4A	23:B:1022:CLA:HBA2	2.15	0.74
2:B:31:ALA:HB3	2:B:103:LEU:HD12	1.69	0.74
23:C:1025:CLA:O1D	23:C:1025:CLA:HAA1	1.86	0.74
3:C:42:LEU:HG	3:C:46:SER:HB2	1.70	0.74
13:O:215:ARG:H	13:O:215:ARG:CD	2.01	0.74
16:V:105:PRO:HG3	16:V:115:ALA:HA	1.69	0.74
16:V:123:SER:O	16:V:125:ASP:N	2.20	0.74
23:B:1022:CLA:H172	23:B:1022:CLA:H141	0.80	0.73
18:Y:32:GLY:HA2	18:Y:35:ILE:CG2	2.18	0.73
20:Z:50:LEU:O	20:Z:54:VAL:HG23	1.88	0.73
2:B:5:TRP:HE3	23:B:1019:CLA:H42	1.52	0.73
2:B:92:SER:O	2:B:94:GLU:N	2.21	0.73
3:C:286:ALA:HB2	23:C:1026:CLA:HMD3	1.69	0.73
4:D:80:THR:HG22	4:D:111:TRP:NE1	2.03	0.73
7:H:44:ILE:O	7:H:48:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:ALA:HB1	26:K:1052:BCR:H371	1.70	0.73
29:B:1060:MGE:CAA	29:L:1061:MGE:H8A2	2.18	0.73
20:Z:10:ALA:C	20:Z:13:VAL:HG12	2.08	0.73
1:A:118:HIS:O	1:A:121:LEU:HD23	1.88	0.73
23:B:1012:CLA:C11	23:B:1023:CLA:O2A	2.36	0.73
2:B:38:ALA:O	2:B:42:LEU:CB	2.33	0.73
4:D:149:PRO:O	4:D:152:VAL:HG12	1.88	0.73
4:D:98:GLN:HE21	5:E:73:LYS:CE	2.00	0.73
5:E:23:HIS:O	5:E:27:ILE:HG12	1.89	0.73
18:Y:39:LEU:CD2	20:Z:25:VAL:HG22	2.17	0.73
1:A:219:VAL:HG23	1:A:220:THR:H	1.54	0.73
1:A:219:VAL:HG23	1:A:220:THR:N	2.02	0.73
23:C:1031:CLA:O2D	23:C:1033:CLA:C8	2.36	0.73
2:B:251:VAL:HG13	30:H:1058:DGD:HB51	1.69	0.73
23:B:1011:CLA:C20	7:H:38:PHE:HE2	2.01	0.73
27:A:1063:LHG:H322	23:C:1034:CLA:H93	1.70	0.73
16:V:29:LEU:H	16:V:29:LEU:HD23	1.53	0.73
26:A:1044:BCR:H331	26:A:1044:BCR:HC8	1.70	0.73
23:B:1019:CLA:OBD	29:B:1060:MGE:H2G	1.88	0.73
23:B:1021:CLA:C14	23:B:1021:CLA:C20	2.64	0.73
23:B:1023:CLA:H143	23:B:1024:CLA:H8	1.68	0.73
23:C:1032:CLA:CGA	23:C:1032:CLA:C4	2.65	0.73
5:E:38:VAL:CG1	6:F:39:ALA:CB	2.67	0.73
17:X:43:ILE:O	17:X:44:ASP:HB3	1.87	0.73
29:B:1060:MGE:O2D	29:B:1060:MGE:H3G1	1.86	0.73
23:C:1037:CLA:CGD	23:C:1037:CLA:HAA1	2.18	0.73
23:C:1029:CLA:H42	26:C:1054:BCR:H333	1.69	0.73
3:C:185:LEU:HB2	3:C:230:LEU:HD21	1.69	0.73
3:C:303:GLY:C	3:C:423:ARG:HD2	2.09	0.73
3:C:451:ALA:C	3:C:453:ALA:H	1.89	0.73
16:V:30:THR:OG1	16:V:32:GLU:HG2	1.88	0.73
23:A:1006:CLA:H2	23:A:1006:CLA:C7	2.18	0.73
1:A:249:VAL:HG23	4:D:238:THR:HB	1.71	0.73
3:C:236:GLY:HA3	26:C:1054:BCR:C39	2.18	0.73
4:D:267:LEU:O	4:D:271:MET:HG3	1.89	0.73
23:B:1014:CLA:CB	23:B:1014:CLA:HHD	2.12	0.73
23:B:1019:CLA:C19	23:B:1021:CLA:C5	2.67	0.73
1:A:199:GLN:CD	30:C:1057:DGD:HBW2	2.09	0.73
1:A:74:GLY:O	1:A:76:ASN:N	2.21	0.73
23:B:1023:CLA:C1D	23:B:1024:CLA:CB	2.67	0.73
2:B:26:HIS:O	2:B:30:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:LEU:HG	30:H:1058:DGD:HAG3	1.70	0.73
4:D:74:LEU:HA	4:D:175:VAL:HG21	1.71	0.73
10:K:28:ILE:C	10:K:31:LEU:HD12	2.09	0.73
1:A:174:LEU:HD23	1:A:174:LEU:N	2.04	0.72
23:B:1009:CLA:HAA1	23:B:1009:CLA:CGD	2.15	0.72
2:B:456:ALA:HA	30:H:1058:DGD:HAG1	1.68	0.72
26:D:1050:BCR:C22	29:J:1059:MGE:H3A1	2.19	0.72
13:O:73:PRO:HG3	13:O:102:THR:OG1	1.89	0.72
20:Z:35:ARG:HD3	20:Z:36:SER:N	2.04	0.72
20:Z:36:SER:O	20:Z:40:ILE:HG12	1.89	0.72
1:A:322:ASN:O	1:A:326:LEU:HG	1.89	0.72
23:B:1009:CLA:HHC	23:B:1009:CLA:CBB	2.06	0.72
30:C:1056:DGD:HBT2	30:C:1056:DGD:HBF2	1.71	0.72
1:A:157:VAL:HG11	23:D:1005:CLA:HMC3	1.69	0.72
24:A:1038:PHO:HMB3	23:D:1005:CLA:H92	0.83	0.72
23:B:1011:CLA:H121	26:H:1049:BCR:C32	2.15	0.72
23:B:1021:CLA:C17	29:B:1060:MGE:CDA	2.56	0.72
2:B:464:PHE:CE2	29:B:1060:MGE:C5B	2.72	0.72
13:O:94:THR:HB	13:O:134:VAL:HB	1.71	0.72
13:O:179:THR:HG22	13:O:180:ALA:N	2.05	0.72
14:T:2:GLU:HB2	14:T:6:TYR:CE2	2.24	0.72
2:B:241:SER:HB3	23:B:1020:CLA:CED	2.19	0.72
3:C:88:LEU:HD21	23:C:1027:CLA:HBC2	1.69	0.72
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.24	0.72
29:L:1061:MGE:H3B1	29:L:1061:MGE:H7B1	1.69	0.72
13:O:142:ILE:HD12	13:O:142:ILE:N	2.04	0.72
11:L:36:PHE:CE2	14:T:2:GLU:HA	2.24	0.72
23:B:1014:CLA:C12	23:B:1014:CLA:C9	2.30	0.72
3:C:218:PHE:HA	30:C:1055:DGD:HG11	1.72	0.72
10:K:32:PHE:CD1	26:K:1052:BCR:H393	2.22	0.72
2:B:241:SER:HB3	23:B:1020:CLA:HED3	1.72	0.72
1:A:279:ARG:HD3	4:D:208:ALA:CA	2.19	0.72
31:E:1040:HEM:HHA	31:E:1040:HEM:O1D	1.89	0.72
5:E:28:PRO:O	5:E:32:ILE:HG13	1.89	0.72
23:B:1016:CLA:C2	23:H:1017:CLA:H102	2.19	0.72
13:O:119:LEU:N	13:O:155:THR:HG22	1.98	0.72
1:A:279:ARG:O	1:A:283:VAL:CG1	2.37	0.72
23:B:1011:CLA:CGA	23:B:1011:CLA:H3A	2.18	0.72
23:C:1030:CLA:H43	26:C:1054:BCR:C32	2.19	0.72
23:C:1031:CLA:HED3	23:C:1031:CLA:C2A	2.19	0.72
1:A:215:HIS:O	1:A:219:VAL:CG2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:GLN:HB2	2:B:227:LYS:HZ2	1.53	0.72
3:C:282:MET:HG2	23:C:1025:CLA:H71	1.72	0.72
23:C:1034:CLA:CHD	23:C:1034:CLA:CBC	2.67	0.72
23:D:1004:CLA:CAB	23:D:1005:CLA:HMD2	2.20	0.72
4:D:232:PHE:O	4:D:232:PHE:CD2	2.43	0.72
13:O:188:ARG:CD	13:O:197:ALA:H	2.01	0.72
1:A:309:ALA:O	16:V:29:LEU:HD22	1.90	0.72
1:A:13:LEU:HD22	1:A:13:LEU:H	1.54	0.72
23:B:1009:CLA:CBD	23:B:1009:CLA:HBA2	2.18	0.72
27:A:1063:LHG:C31	23:C:1034:CLA:C9	2.63	0.72
4:D:57:SER:OG	4:D:79:SER:HB2	1.88	0.72
5:E:10:PHE:O	5:E:12:ASP:N	2.22	0.72
5:E:83:LEU:HD22	5:E:84:LYS:H	1.55	0.72
12:M:20:VAL:O	12:M:24:ILE:HG13	1.90	0.72
26:T:6046:BCR:HC42	26:T:6046:BCR:H312	1.71	0.72
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.19	0.72
16:V:109:ASP:OD2	16:V:109:ASP:O	2.08	0.72
1:A:33:PHE:HB2	1:A:129:ARG:HB2	1.72	0.72
23:B:1009:CLA:HAA1	23:B:1009:CLA:CED	2.18	0.72
23:C:1031:CLA:H141	23:C:1031:CLA:H172	1.68	0.72
3:C:42:LEU:HD22	3:C:151:TRP:CH2	2.25	0.72
23:H:1017:CLA:HBB1	26:H:1049:BCR:H321	1.71	0.72
23:A:1003:CLA:C17	24:A:1038:PHO:H43	2.17	0.71
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.08	0.71
2:B:440:ASP:OD2	2:B:441:GLY:N	2.23	0.71
3:C:128:GLY:HA3	23:C:1037:CLA:CAC	2.20	0.71
1:A:219:VAL:HG21	4:D:268:HIS:CB	2.19	0.71
6:F:26:LEU:HD13	6:F:26:LEU:H	1.55	0.71
4:D:89:LEU:HD22	7:H:50:ASN:OD1	1.89	0.71
7:H:54:ILE:O	17:X:13:THR:HG21	1.90	0.71
18:Y:39:LEU:HD21	20:Z:25:VAL:CG2	2.18	0.71
1:A:210:LEU:HD12	1:A:210:LEU:O	1.90	0.71
1:A:237:TYR:CE2	1:A:239:PHE:HA	2.25	0.71
23:C:1027:CLA:HED1	23:C:1036:CLA:C19	2.20	0.71
23:C:1029:CLA:HBD	23:C:1029:CLA:HAA1	1.71	0.71
3:C:424:SER:O	3:C:428:THR:HG22	1.89	0.71
3:C:72:LEU:HD11	10:K:12:PRO:HD3	1.72	0.71
4:D:197:HIS:O	4:D:201:VAL:HG23	1.89	0.71
4:D:45:LEU:C	4:D:45:LEU:HD13	2.10	0.71
4:D:65:SER:HB3	4:D:77:ALA:O	1.90	0.71
7:H:40:VAL:O	7:H:44:ILE:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:8:VAL:O	8:I:12:VAL:HG23	1.90	0.71
1:A:116:ILE:HG23	1:A:117:PHE:CD2	2.25	0.71
1:A:43:ALA:HA	26:A:1044:BCR:C16	2.20	0.71
2:B:280:PHE:CZ	2:B:312:TYR:HB3	2.25	0.71
23:C:1029:CLA:HHD	23:C:1029:CLA:HBC3	1.71	0.71
4:D:80:THR:HG23	4:D:172:SER:OG	1.90	0.71
4:D:302:GLU:OE1	13:O:186:LYS:HD2	1.91	0.71
4:D:90:LEU:HA	4:D:96:GLU:HG3	1.70	0.71
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.05	0.71
1:A:279:ARG:O	1:A:283:VAL:HG12	1.90	0.71
23:B:1012:CLA:H2A	23:B:1012:CLA:HED2	1.70	0.71
2:B:230:ARG:NH1	2:B:230:ARG:HA	2.04	0.71
23:C:1025:CLA:CAA	23:C:1025:CLA:CGD	2.65	0.71
3:C:318:LEU:CD2	3:C:328:VAL:HG11	2.20	0.71
3:C:377:LEU:HA	3:C:380:ILE:CG2	2.20	0.71
4:D:274:VAL:HG22	25:D:1042:PQ9:H262	1.72	0.71
16:V:143:GLY:O	16:V:147:VAL:HG23	1.90	0.71
2:B:241:SER:O	2:B:245:VAL:HG23	1.89	0.71
2:B:277:SER:C	2:B:279:TYR:H	1.91	0.71
11:L:24:ILE:CD1	12:M:18:PRO:HG2	2.21	0.71
13:O:108:GLN:O	13:O:123:GLU:HA	1.90	0.71
27:A:1063:LHG:H291	23:C:1032:CLA:C8	2.21	0.71
1:A:21:VAL:HG23	1:A:22:THR:HG23	1.72	0.71
1:A:269:ARG:HE	4:D:243:THR:CG2	2.03	0.71
23:B:1024:CLA:HMB3	26:B:1048:BCR:H351	1.73	0.71
2:B:254:GLY:O	2:B:258:TYR:CD1	2.33	0.71
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.26	0.71
3:C:464:GLU:OE2	3:C:467:LEU:HD12	1.90	0.71
20:Z:15:LEU:HD22	20:Z:50:LEU:CD1	2.19	0.71
3:C:45:LEU:HD21	3:C:141:GLU:HG2	1.70	0.71
23:D:1005:CLA:H203	23:D:1005:CLA:H152	1.71	0.71
4:D:134:ARG:HE	4:D:134:ARG:CA	2.04	0.71
6:F:41:GLN:HE21	9:J:27:LEU:HB3	1.54	0.71
5:E:17:VAL:HG13	9:J:7:ARG:N	2.06	0.71
13:O:105:ASP:O	13:O:106:GLN:HB2	1.91	0.71
13:O:105:ASP:O	13:O:127:ILE:CD1	2.38	0.71
1:A:140:ARG:C	4:D:220:ASN:HD22	1.93	0.71
1:A:72:LEU:O	1:A:73:TYR:CE2	2.43	0.71
23:B:1016:CLA:C20	23:D:1008:CLA:CMA	2.68	0.71
2:B:465:GLY:HA3	23:B:1019:CLA:CBC	2.20	0.71
2:B:173:GLY:HA3	2:B:312:TYR:CE1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASP:OD1	2:B:390:TYR:HB2	1.90	0.71
23:C:1026:CLA:H203	23:C:1026:CLA:C4D	2.21	0.71
23:C:1034:CLA:H41	23:C:1034:CLA:H8	1.67	0.71
3:C:53:HIS:HB2	23:C:1036:CLA:CMD	2.20	0.71
3:C:140:LEU:HB3	3:C:148:GLY:HA2	1.73	0.71
3:C:450:ALA:O	3:C:454:GLY:N	2.24	0.71
23:D:1005:CLA:C2A	23:D:1005:CLA:CED	2.43	0.71
4:D:93:TRP:CZ2	23:D:1008:CLA:O1A	2.43	0.71
11:L:12:LEU:HD12	12:M:26:TYR:CA	2.20	0.71
12:M:29:THR:HG22	12:M:30:GLU:OE1	1.90	0.71
15:U:92:LEU:HD12	15:U:92:LEU:H	1.54	0.71
16:V:135:GLU:O	16:V:139:VAL:HG22	1.89	0.71
1:A:140:ARG:HH22	27:A:1063:LHG:C2	2.03	0.71
1:A:159:LEU:HG	1:A:163:ILE:HD11	1.72	0.71
23:B:1009:CLA:O2A	26:H:1049:BCR:C17	2.38	0.71
2:B:391:SER:HB3	2:B:394:GLN:NE2	2.06	0.71
10:K:28:ILE:CD1	26:K:1051:BCR:HC7	2.11	0.71
1:A:174:LEU:H	1:A:174:LEU:HD23	1.56	0.71
1:A:307:ILE:HD11	1:A:311:GLY:O	1.91	0.71
2:B:157:HIS:ND1	2:B:158:LEU:HD23	2.06	0.71
2:B:391:SER:O	2:B:394:GLN:HG3	1.90	0.71
2:B:441:GLY:O	2:B:442:ILE:HD13	1.91	0.71
23:C:1027:CLA:O2A	23:C:1027:CLA:HMA2	1.91	0.71
3:C:164:HIS:O	3:C:168:LEU:HG	1.90	0.71
1:A:288:LEU:HD11	3:C:435:PHE:CD2	2.25	0.71
4:D:39:PRO:O	4:D:43:LEU:HD22	1.91	0.71
13:O:59:ASP:OD1	13:O:61:SER:HB3	1.91	0.71
16:V:105:PRO:CG	16:V:115:ALA:HA	2.21	0.71
1:A:157:VAL:HG22	1:A:182:PHE:CE2	2.26	0.70
1:A:33:PHE:CD2	1:A:128:GLY:HA3	2.26	0.70
23:B:1021:CLA:H202	23:B:1021:CLA:H142	1.72	0.70
1:A:217:SER:OG	4:D:142:ASN:HA	1.90	0.70
4:D:129:GLN:HB2	4:D:143:ALA:HB2	1.72	0.70
23:H:1017:CLA:CHD	23:H:1017:CLA:CBC	2.68	0.70
13:O:123:GLU:OE1	13:O:150:ASN:N	2.23	0.70
16:V:47:LEU:HA	16:V:51:GLN:NE2	2.04	0.70
1:A:147:TYR:O	1:A:150:PRO:HG2	1.90	0.70
23:B:1011:CLA:HBB1	23:B:1013:CLA:H171	1.70	0.70
2:B:138:MET:SD	23:B:1023:CLA:HBC2	2.30	0.70
2:B:86:ILE:O	2:B:87:ASP:HB3	1.90	0.70
3:C:202:PRO:HB2	3:C:235:GLY:HA2	1.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LYS:HD2	3:C:133:ALA:C	2.12	0.70
4:D:210:LEU:CA	4:D:213:ILE:HG22	2.21	0.70
29:J:1059:MGE:H2A2	29:J:1059:MGE:H5B1	1.72	0.70
13:O:65:ARG:HE	13:O:110:GLU:HA	1.57	0.70
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.74	0.70
23:B:1016:CLA:CHD	23:B:1016:CLA:CBC	2.62	0.70
2:B:288:VAL:O	2:B:292:LEU:HB2	1.91	0.70
3:C:197:ARG:HG2	3:C:198:VAL:N	2.05	0.70
3:C:199:ILE:H	3:C:199:ILE:HD12	1.54	0.70
4:D:209:LEU:HD23	4:D:209:LEU:C	2.11	0.70
6:F:17:THR:O	6:F:20:TRP:HB3	1.91	0.70
23:B:1016:CLA:H2	23:H:1017:CLA:H102	1.74	0.70
1:A:64:ARG:O	13:O:178:ARG:NH2	2.23	0.70
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.70
16:V:48:THR:H	16:V:51:GLN:CG	2.03	0.70
23:A:1006:CLA:HED2	23:A:1006:CLA:HAA2	1.73	0.70
1:A:25:ASP:HA	4:D:251:ARG:HH22	1.54	0.70
23:B:1019:CLA:C5	23:B:1021:CLA:HED1	2.21	0.70
2:B:223:GLN:HG2	7:H:24:GLY:CA	2.21	0.70
3:C:126:GLY:CA	26:K:1052:BCR:H363	2.21	0.70
3:C:162:GLY:HA2	3:C:165:LEU:HD12	1.73	0.70
4:D:258:GLY:O	4:D:259:ILE:HD13	1.91	0.70
15:U:58:ASN:CG	15:U:114:VAL:HG13	2.12	0.70
23:B:1009:CLA:HED3	23:B:1009:CLA:C2A	2.20	0.70
23:B:1011:CLA:H172	23:B:1016:CLA:CBC	2.21	0.70
2:B:193:TYR:O	2:B:195:PRO:HD3	1.92	0.70
2:B:357:ARG:HH11	2:B:357:ARG:HG3	1.56	0.70
2:B:417:VAL:HG12	2:B:418:LYS:N	2.07	0.70
4:D:199:MET:HG2	25:D:1042:PQ9:H351	1.74	0.70
1:A:99:ALA:CB	1:A:105:TRP:HB2	2.22	0.70
1:A:113:GLN:HA	1:A:116:ILE:HG22	1.73	0.70
23:B:1011:CLA:HBB2	23:B:1013:CLA:C19	2.22	0.70
3:C:283:GLY:O	3:C:286:ALA:HB3	1.92	0.70
23:D:1005:CLA:O2D	23:D:1005:CLA:H2A	1.89	0.70
1:A:184:ILE:CG2	4:D:321:LEU:HD13	2.21	0.70
23:B:1012:CLA:HAA2	23:B:1012:CLA:HED2	0.73	0.70
2:B:191:ASN:HD21	2:B:193:TYR:HD2	1.37	0.70
2:B:59:GLY:N	2:B:329:PRO:HB3	2.06	0.70
23:C:1031:CLA:O1D	23:C:1033:CLA:C10	2.39	0.70
3:C:203:THR:N	3:C:235:GLY:HA3	2.07	0.70
3:C:349:ILE:N	3:C:349:ILE:HD12	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:1005:CLA:H72	29:D:1062:MGE:H202	1.72	0.70
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.73	0.70
7:H:43:LEU:O	7:H:43:LEU:HD23	1.91	0.70
15:U:98:THR:HG23	15:U:101:GLN:OE1	1.91	0.70
1:A:128:GLY:C	1:A:130:GLN:H	1.95	0.70
2:B:27:THR:CG2	23:B:1013:CLA:HAC2	2.21	0.70
23:B:1019:CLA:H51	23:B:1021:CLA:HED1	1.74	0.70
23:B:1023:CLA:C9	23:B:1023:CLA:H121	2.08	0.70
2:B:135:LEU:HD12	2:B:135:LEU:N	2.06	0.70
2:B:191:ASN:HD22	2:B:192:PRO:CD	2.05	0.70
3:C:107:ASP:OD1	3:C:109:PHE:HB3	1.90	0.70
4:D:110:LEU:O	4:D:114:ILE:HG13	1.92	0.70
13:O:92:VAL:CG2	13:O:93:PRO:HD2	2.21	0.70
20:Z:37:LYS:O	20:Z:40:ILE:HB	1.92	0.70
23:A:1007:CLA:CHD	23:A:1007:CLA:CBC	2.56	0.70
26:B:1047:BCR:H321	26:B:1047:BCR:H342	1.69	0.70
23:B:1012:CLA:HMB1	23:B:1015:CLA:HMC3	1.74	0.70
2:B:31:ALA:HB2	23:B:1013:CLA:HBC3	1.74	0.70
2:B:7:ARG:HD3	23:B:1019:CLA:HED3	1.74	0.70
3:C:97:TRP:HE1	3:C:178:LYS:HE3	1.56	0.70
8:I:13:THR:CG2	8:I:14:PHE:N	2.54	0.70
11:L:14:ARG:HE	14:T:25:GLU:HB3	1.56	0.70
13:O:123:GLU:HG2	13:O:124:GLU:N	2.07	0.70
15:U:99:GLU:H	15:U:99:GLU:CD	1.95	0.70
1:A:124:SER:O	1:A:127:MET:HB3	1.92	0.69
23:B:1012:CLA:H112	23:B:1023:CLA:CGA	2.22	0.69
23:B:1015:CLA:HBC1	26:B:1045:BCR:C34	2.22	0.69
2:B:362:PHE:HE1	4:D:184:PHE:CZ	2.10	0.69
2:B:417:VAL:CG1	2:B:418:LYS:N	2.55	0.69
2:B:5:TRP:CG	2:B:6:TYR:N	2.59	0.69
2:B:382:PRO:HB3	4:D:344:GLU:HB2	1.74	0.69
13:O:141:ARG:HG3	13:O:141:ARG:HH11	1.57	0.69
16:V:70:GLY:HA3	16:V:156:TRP:O	1.92	0.69
16:V:48:THR:H	16:V:51:GLN:HE21	1.38	0.69
23:B:1009:CLA:HBC2	23:B:1009:CLA:HMC1	1.72	0.69
3:C:203:THR:CG2	3:C:232:ASP:HA	2.22	0.69
23:D:1008:CLA:H71	23:D:1008:CLA:H43	1.71	0.69
1:A:219:VAL:HG11	4:D:268:HIS:CE1	2.27	0.69
12:M:16:LEU:O	12:M:20:VAL:HG12	1.92	0.69
13:O:119:LEU:HG	13:O:155:THR:HG21	1.74	0.69
13:O:223:ILE:HG12	13:O:224:SER:N	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:30:THR:O	16:V:34:LEU:HD13	1.91	0.69
26:Z:1053:BCR:C38	26:Z:1053:BCR:C23	2.41	0.69
1:A:106:LEU:HD21	26:A:1044:BCR:H383	1.74	0.69
23:B:1011:CLA:C4D	23:B:1013:CLA:C4	2.70	0.69
27:A:1063:LHG:C27	23:C:1032:CLA:H8	2.20	0.69
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.27	0.69
23:B:1010:CLA:CAA	23:B:1010:CLA:O1D	2.40	0.69
23:B:1023:CLA:H172	23:B:1023:CLA:H122	1.73	0.69
30:C:1056:DGD:C5A	30:C:1056:DGD:O1A	2.39	0.69
30:C:1056:DGD:C6B	30:C:1056:DGD:CAB	2.63	0.69
16:V:62:ALA:HB1	31:V:1041:HEM:HBB1	1.74	0.69
2:B:158:LEU:HB2	2:B:199:VAL:HG13	1.73	0.69
2:B:38:ALA:O	2:B:42:LEU:N	2.23	0.69
2:B:460:LEU:HG	30:H:1058:DGD:HAG1	1.74	0.69
23:C:1032:CLA:CAB	23:C:1034:CLA:HMC3	2.23	0.69
30:C:1055:DGD:HG32	30:C:1055:DGD:O2D	1.92	0.69
3:C:32:GLY:HA2	3:C:41:ARG:NH2	2.08	0.69
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.27	0.69
1:A:33:PHE:CE2	1:A:128:GLY:HA3	2.26	0.69
1:A:188:ALA:CB	1:A:328:MET:HG3	2.20	0.69
23:B:1012:CLA:O1A	23:B:1013:CLA:C4D	2.40	0.69
2:B:153:PHE:N	23:B:1014:CLA:CMC	2.54	0.69
23:B:1019:CLA:CMB	23:B:1020:CLA:CHC	2.71	0.69
3:C:54:VAL:HG13	23:C:1036:CLA:HED1	1.74	0.69
23:A:1003:CLA:CAD	23:D:1005:CLA:HAC2	2.22	0.69
4:D:256:ILE:HG23	4:D:257:PHE:N	2.08	0.69
15:U:39:LEU:N	15:U:39:LEU:HD12	2.07	0.69
16:V:120:SER:O	16:V:123:SER:N	2.25	0.69
1:A:58:VAL:N	1:A:68:SER:HB2	2.08	0.69
23:B:1011:CLA:CBB	23:B:1013:CLA:C19	2.70	0.69
2:B:26:HIS:HB2	23:B:1020:CLA:HMB2	1.74	0.69
2:B:207:ILE:O	2:B:210:ILE:HB	1.92	0.69
2:B:368:VAL:HG13	2:B:368:VAL:O	1.91	0.69
3:C:63:TRP:N	23:C:1034:CLA:HED3	2.07	0.69
1:A:278:TRP:HH2	30:C:1057:DGD:HAG1	1.58	0.69
3:C:230:LEU:HD12	3:C:233:VAL:HG11	1.74	0.69
11:L:7:ARG:HA	11:L:7:ARG:HE	1.58	0.69
1:A:99:ALA:HB3	1:A:105:TRP:HB2	1.75	0.69
1:A:118:HIS:HA	1:A:121:LEU:CD2	2.23	0.69
2:B:170:ASP:O	2:B:172:TYR:N	2.25	0.69
2:B:487:SER:HB3	2:B:488:PRO:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:THR:HG21	2:B:83:GLU:OE1	1.93	0.69
3:C:305:THR:HG23	3:C:308:GLU:H	1.57	0.69
2:B:362:PHE:CE1	4:D:184:PHE:CZ	2.80	0.69
4:D:302:GLU:HG3	13:O:199:ALA:HB1	1.75	0.69
15:U:85:TYR:O	15:U:114:VAL:HG11	1.91	0.69
16:V:154:ASP:C	16:V:156:TRP:H	1.93	0.69
26:A:1044:BCR:H392	26:A:1044:BCR:H371	1.30	0.69
1:A:54:ALA:HB2	1:A:72:LEU:CD1	2.14	0.69
23:B:1023:CLA:ND	23:B:1024:CLA:HBC2	2.08	0.69
23:B:1011:CLA:H192	23:H:1017:CLA:C13	2.20	0.69
16:V:142:ALA:O	16:V:145:ILE:HB	1.93	0.69
1:A:27:ARG:HB2	1:A:27:ARG:NH1	2.08	0.69
23:B:1016:CLA:H202	23:D:1008:CLA:HMA2	1.75	0.69
2:B:419:SER:HA	2:B:422:ARG:NH1	2.07	0.69
23:C:1027:CLA:HMA2	23:C:1027:CLA:CGA	2.23	0.69
13:O:186:LYS:NZ	13:O:186:LYS:HA	2.07	0.69
23:A:1006:CLA:H172	26:D:1050:BCR:C40	2.13	0.69
27:A:1063:LHG:H341	27:A:1063:LHG:C38	2.19	0.69
2:B:271:THR:HG23	2:B:274:GLN:CB	2.11	0.69
23:A:1006:CLA:HED3	30:C:1057:DGD:HBW1	1.74	0.69
3:C:41:ARG:O	3:C:42:LEU:HB2	1.90	0.69
4:D:123:ILE:HD11	30:H:1058:DGD:HAW2	1.75	0.69
4:D:267:LEU:HD23	4:D:267:LEU:C	2.12	0.69
1:A:178:GLY:HA2	4:D:314:PHE:CD2	2.28	0.69
16:V:125:ASP:OD2	16:V:131:ARG:HG2	1.93	0.69
16:V:128:PRO:HA	16:V:131:ARG:HG3	1.73	0.69
2:B:250:PHE:CD1	2:B:459:ALA:HB1	2.28	0.68
23:C:1029:CLA:H41	23:C:1029:CLA:H191	1.73	0.68
3:C:272:LEU:O	3:C:276:LEU:HB2	1.92	0.68
13:O:202:GLN:OE1	13:O:202:GLN:HA	1.92	0.68
13:O:31:LEU:HD23	13:O:31:LEU:N	2.07	0.68
1:A:321:ILE:O	1:A:325:ASN:ND2	2.27	0.68
1:A:159:LEU:O	1:A:163:ILE:HG13	1.92	0.68
23:B:1014:CLA:H112	23:B:1014:CLA:H162	1.70	0.68
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.58	0.68
2:B:257:TRP:HH2	4:D:291:LEU:HB3	1.57	0.68
1:A:228:THR:HA	2:B:480:SER:HB2	1.73	0.68
3:C:137:PRO:HB2	3:C:143:TYR:CE2	2.28	0.68
1:A:275:LEU:HB3	4:D:211:CYS:O	1.92	0.68
4:D:261:PHE:CE2	4:D:266:TRP:CD1	2.77	0.68
7:H:38:PHE:O	7:H:41:PHE:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HA	2:B:138:MET:HE3	1.76	0.68
2:B:421:ALA:O	2:B:424:ALA:HB3	1.92	0.68
23:C:1025:CLA:CMB	23:C:1025:CLA:C4	2.71	0.68
3:C:137:PRO:HB2	3:C:143:TYR:CD2	2.28	0.68
3:C:186:TYR:HA	3:C:196:VAL:HA	1.76	0.68
1:A:301:ASN:HB3	3:C:407:VAL:HG21	1.76	0.68
4:D:116:LEU:O	4:D:119:ALA:HB3	1.94	0.68
1:A:133:LEU:HD23	4:D:252:PHE:HA	1.76	0.68
1:A:279:ARG:CZ	1:A:279:ARG:HB3	2.23	0.68
1:A:73:TYR:HD2	1:A:73:TYR:N	1.89	0.68
23:B:1022:CLA:HMB2	26:B:1045:BCR:C40	2.24	0.68
2:B:429:ILE:HD12	2:B:429:ILE:N	2.08	0.68
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.59	0.68
3:C:350:ILE:HG13	3:C:359:TRP:CB	2.23	0.68
23:D:1008:CLA:H2A	23:D:1008:CLA:O1D	1.94	0.68
4:D:90:LEU:HD11	4:D:107:LEU:O	1.94	0.68
4:D:42:TYR:CZ	6:F:25:THR:HG22	2.28	0.68
3:C:62:PHE:CE2	10:K:28:ILE:HG22	2.17	0.68
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.28	0.68
18:Y:44:GLY:HA2	20:Z:30:PRO:HD3	1.76	0.68
23:B:1013:CLA:H152	23:B:1018:CLA:HED1	1.76	0.68
2:B:450:TRP:HB3	23:B:1015:CLA:CMB	2.21	0.68
23:C:1032:CLA:H42	23:C:1032:CLA:O2A	1.93	0.68
3:C:59:LEU:O	23:C:1034:CLA:HED3	1.93	0.68
30:C:1055:DGD:O1B	30:C:1055:DGD:HB51	1.93	0.68
3:C:48:LYS:HB2	3:C:48:LYS:HZ3	1.58	0.68
26:D:1050:BCR:HC8	26:D:1050:BCR:H331	0.73	0.68
2:B:258:TYR:O	2:B:259:GLY:O	2.10	0.68
2:B:5:TRP:CD2	2:B:6:TYR:N	2.62	0.68
30:C:1055:DGD:C5B	30:C:1055:DGD:O1B	2.42	0.68
3:C:287:THR:HG23	3:C:427:ALA:CA	2.24	0.68
10:K:32:PHE:CE2	26:K:1051:BCR:H341	2.27	0.68
20:Z:17:PHE:O	20:Z:17:PHE:HD2	1.76	0.68
1:A:261:GLN:C	1:A:263:ALA:H	1.96	0.68
1:A:60:ILE:HD13	1:A:60:ILE:N	2.09	0.68
2:B:465:GLY:CA	23:B:1019:CLA:CBC	2.72	0.68
23:B:1022:CLA:C8	23:B:1022:CLA:C14	2.69	0.68
2:B:106:LEU:C	2:B:106:LEU:HD13	2.14	0.68
2:B:258:TYR:O	2:B:259:GLY:C	2.31	0.68
3:C:45:LEU:HD23	3:C:141:GLU:HG2	1.75	0.68
10:K:24:VAL:HG11	18:Y:25:ILE:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:PRO:HG2	2:B:489:GLU:H	1.59	0.68
3:C:371:GLY:O	13:O:33:TYR:HB2	1.93	0.68
4:D:90:LEU:HD13	4:D:109:GLY:HA2	1.74	0.68
4:D:83:ASN:HA	4:D:166:SER:OG	1.93	0.68
23:B:1018:CLA:C1B	23:H:1017:CLA:HMB2	2.24	0.68
1:A:231:GLU:OE1	11:L:11:GLU:HB3	1.94	0.68
17:X:38:ILE:HA	17:X:41:SER:OG	1.93	0.68
20:Z:15:LEU:CD2	20:Z:50:LEU:HD12	2.21	0.68
2:B:138:MET:HB3	23:B:1023:CLA:CBC	2.24	0.68
2:B:141:ILE:HD12	2:B:142:HIS:N	2.09	0.68
2:B:148:LEU:HB3	2:B:210:ILE:HD11	1.75	0.68
3:C:294:ASN:HB2	30:C:1055:DGD:HO3E	1.59	0.68
4:D:217:THR:HG21	25:D:1042:PQ9:O4	1.94	0.68
5:E:38:VAL:HG11	6:F:39:ALA:CB	2.24	0.68
1:A:243:GLU:HA	4:D:241:GLU:HB3	1.76	0.67
2:B:30:VAL:O	23:B:1013:CLA:HMD3	1.94	0.67
2:B:103:LEU:HB2	23:B:1014:CLA:C7	2.15	0.67
4:D:291:LEU:C	4:D:293:LEU:H	1.95	0.67
4:D:32:TRP:O	4:D:35:ILE:HG13	1.94	0.67
5:E:68:ASP:HB2	5:E:69:ARG:HH21	1.59	0.67
8:I:7:THR:O	8:I:11:VAL:HG23	1.93	0.67
8:I:6:ILE:HD13	8:I:6:ILE:N	2.08	0.67
10:K:39:VAL:HA	18:Y:36:ILE:CD1	2.24	0.67
23:B:1012:CLA:H2A	23:B:1012:CLA:CED	2.24	0.67
23:B:1024:CLA:O2A	23:B:1024:CLA:C2A	2.42	0.67
2:B:456:ALA:CA	30:H:1058:DGD:CIB	2.70	0.67
13:O:97:VAL:HG13	13:O:98:THR:N	2.09	0.67
23:A:1007:CLA:OBD	23:A:1007:CLA:HED3	1.94	0.67
23:B:1009:CLA:H43	26:H:1049:BCR:H351	1.73	0.67
23:C:1028:CLA:H12	30:C:1056:DGD:O1A	1.94	0.67
3:C:35:TRP:O	3:C:38:GLY:N	2.27	0.67
3:C:89:ILE:HG23	3:C:111:PHE:CE2	2.29	0.67
4:D:24:ARG:HG2	4:D:24:ARG:HH21	1.57	0.67
23:B:1011:CLA:H193	23:H:1017:CLA:H13	1.76	0.67
9:J:40:LEU:N	9:J:40:LEU:HD22	2.08	0.67
10:K:19:ASP:HA	10:K:22:VAL:HG12	1.76	0.67
12:M:8:PHE:O	12:M:9:ILE:C	2.32	0.67
24:A:1038:PHO:HED3	24:A:1038:PHO:CHA	2.24	0.67
1:A:199:GLN:NE2	1:A:200:LEU:HG	2.08	0.67
23:B:1010:CLA:C12	23:B:1010:CLA:C9	2.30	0.67
2:B:18:ARG:HD2	11:L:4:ASN:HD21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:SER:CB	2:B:488:PRO:CD	2.72	0.67
2:B:5:TRP:HA	2:B:8:VAL:HB	1.76	0.67
23:C:1025:CLA:O1D	23:C:1025:CLA:CAA	2.42	0.67
3:C:124:VAL:HG23	3:C:125:LEU:N	2.10	0.67
3:C:270:ALA:HB1	3:C:274:TYR:CE1	2.29	0.67
3:C:473:ASP:HB3	14:T:26:PRO:HG3	1.76	0.67
2:B:367:PRO:HB2	4:D:345:VAL:CG1	2.25	0.67
4:D:89:LEU:CD2	7:H:52:THR:HG21	2.24	0.67
13:O:111:LEU:CD1	13:O:121:PHE:HB2	2.21	0.67
13:O:187:GLY:HA3	13:O:194:TYR:CD1	2.27	0.67
20:Z:48:ILE:O	20:Z:52:LEU:HG	1.94	0.67
1:A:268:SER:H	4:D:236:ASN:ND2	1.92	0.67
23:D:1005:CLA:H2A	23:D:1005:CLA:HED1	1.71	0.67
23:D:1005:CLA:HED3	25:D:1042:PQ9:H391	1.77	0.67
4:D:180:ARG:HD2	4:D:181:PHE:N	2.08	0.67
8:I:13:THR:HG22	8:I:14:PHE:H	1.60	0.67
20:Z:49:ALA:O	20:Z:53:VAL:HG23	1.94	0.67
23:B:1016:CLA:H202	23:D:1008:CLA:CMA	2.24	0.67
2:B:422:ARG:HD2	2:B:423:LYS:NZ	2.09	0.67
3:C:128:GLY:HA3	23:C:1037:CLA:HAC1	1.76	0.67
4:D:155:SER:HA	4:D:159:ILE:CD1	2.24	0.67
1:A:73:TYR:CD2	1:A:73:TYR:N	2.58	0.67
2:B:454:ALA:C	2:B:456:ALA:N	2.47	0.67
23:C:1034:CLA:O1A	23:C:1034:CLA:C4	2.43	0.67
3:C:346:THR:HG21	3:C:348:GLU:OE1	1.94	0.67
26:D:1050:BCR:C37	29:J:1059:MGE:C4A	2.47	0.67
4:D:251:ARG:HA	4:D:254:SER:OG	1.93	0.67
13:O:144:LEU:HD11	13:O:261:ILE:HD11	1.77	0.67
16:V:98:LEU:HD21	16:V:145:ILE:CG2	2.24	0.67
20:Z:23:VAL:HB	20:Z:24:PRO:HD3	1.75	0.67
23:B:1010:CLA:CMD	23:B:1011:CLA:H102	2.25	0.67
23:B:1023:CLA:CHD	23:B:1024:CLA:CBC	2.72	0.67
2:B:219:VAL:HG12	2:B:220:ARG:N	2.10	0.67
2:B:30:VAL:HG11	23:B:1020:CLA:H111	1.75	0.67
23:C:1027:CLA:O2D	23:C:1036:CLA:H11	1.95	0.67
3:C:380:ILE:O	3:C:380:ILE:HG12	1.95	0.67
23:H:1017:CLA:CHD	23:H:1017:CLA:HBC2	2.13	0.67
10:K:22:VAL:HG23	10:K:25:LEU:HD22	1.77	0.67
23:A:1006:CLA:C2B	24:A:1039:PHO:H161	2.25	0.67
23:B:1014:CLA:O2D	23:B:1014:CLA:C2A	2.42	0.67
3:C:289:PHE:HB3	3:C:297:TYR:HE2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:299:ILE:O	4:D:303:ILE:HG13	1.95	0.67
10:K:32:PHE:CE1	26:K:1052:BCR:C20	2.78	0.67
1:A:193:LEU:HD22	4:D:179:PHE:CD2	2.29	0.67
1:A:202:VAL:O	1:A:206:PHE:HB2	1.95	0.67
30:C:1056:DGD:HBG2	30:C:1056:DGD:HB41	1.74	0.67
4:D:164:GLN:HG3	4:D:165:SER:N	2.04	0.67
4:D:164:GLN:CG	4:D:165:SER:H	2.03	0.67
4:D:323:GLU:HG2	13:O:194:TYR:OH	1.95	0.67
16:V:133:LEU:H	16:V:133:LEU:HD12	1.59	0.67
1:A:307:ILE:HG13	1:A:308:ASP:N	2.10	0.66
23:C:1032:CLA:H43	23:C:1032:CLA:CGA	2.23	0.66
23:D:1005:CLA:H172	29:D:1062:MGE:H261	1.77	0.66
4:D:125:PHE:O	4:D:128:ARG:HB3	1.96	0.66
4:D:156:VAL:HG12	4:D:156:VAL:O	1.94	0.66
5:E:83:LEU:HD13	5:E:83:LEU:N	2.11	0.66
23:H:1017:CLA:H3A	23:H:1017:CLA:CGA	2.23	0.66
1:A:140:ARG:HD3	4:D:219:GLU:O	1.95	0.66
23:C:1026:CLA:H51	23:C:1026:CLA:CGA	2.22	0.66
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.25	0.66
3:C:290:VAL:HG21	3:C:426:LEU:HB2	1.78	0.66
4:D:261:PHE:HE1	25:D:1042:PQ9:H143	1.59	0.66
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.25	0.66
26:D:1050:BCR:C28	29:J:1059:MGE:H9B2	2.21	0.66
26:K:1051:BCR:H403	26:K:1051:BCR:H371	1.32	0.66
15:U:103:GLN:O	15:U:106:ARG:N	2.28	0.66
16:V:111:GLU:O	16:V:112:GLN:HB2	1.95	0.66
1:A:71:LEU:C	1:A:73:TYR:H	1.97	0.66
4:D:299:ILE:HG22	4:D:300:SER:N	2.09	0.66
25:D:1042:PQ9:H392	11:L:30:LEU:HD12	1.76	0.66
13:O:186:LYS:HZ3	13:O:186:LYS:HA	1.60	0.66
16:V:154:ASP:C	16:V:156:TRP:N	2.47	0.66
1:A:102:LEU:O	1:A:106:LEU:HG	1.96	0.66
23:B:1013:CLA:CMC	23:B:1023:CLA:C1	2.72	0.66
2:B:165:GLY:HA3	2:B:180:PRO:HA	1.78	0.66
23:C:1032:CLA:O2A	23:C:1032:CLA:C4	2.42	0.66
3:C:36:TRP:CD1	3:C:37:ALA:N	2.64	0.66
3:C:39:ASN:O	3:C:40:ALA:CB	2.41	0.66
3:C:48:LYS:NZ	3:C:48:LYS:HB2	2.10	0.66
4:D:347:PRO:O	4:D:348:ARG:HB3	1.94	0.66
4:D:92:LEU:HD13	4:D:99:GLY:HA2	1.78	0.66
11:L:32:SER:O	11:L:35:PHE:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:176:SER:HB3	13:O:216:PHE:CE2	2.30	0.66
23:A:1006:CLA:H122	30:C:1057:DGD:CIB	2.23	0.66
1:A:90:GLY:O	1:A:92:HIS:N	2.28	0.66
23:B:1010:CLA:CMD	23:B:1011:CLA:C10	2.74	0.66
23:B:1010:CLA:OBD	23:B:1010:CLA:CED	2.30	0.66
4:D:269:PHE:O	4:D:269:PHE:CG	2.49	0.66
5:E:17:VAL:CG1	9:J:7:ARG:HG2	2.25	0.66
23:A:1003:CLA:H141	24:A:1038:PHO:C8	2.24	0.66
1:A:191:ASN:O	1:A:299:GLY:HA3	1.96	0.66
23:B:1011:CLA:CMD	23:B:1014:CLA:CBB	2.72	0.66
2:B:463:PHE:HE1	23:B:1016:CLA:HBB1	1.59	0.66
3:C:203:THR:H	3:C:235:GLY:HA3	1.61	0.66
3:C:224:ILE:HD11	3:C:285:ILE:CD1	2.26	0.66
3:C:315:MET:HE2	3:C:366:LEU:CD1	2.25	0.66
23:D:1005:CLA:O2A	23:D:1005:CLA:C5	2.42	0.66
13:O:216:PHE:HB3	15:U:120:ALA:HB2	1.76	0.66
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.77	0.66
16:V:81:ARG:HD3	16:V:157:GLY:HA3	1.78	0.66
20:Z:37:LYS:HD3	20:Z:38:GLN:N	2.10	0.66
1:A:157:VAL:HG22	1:A:182:PHE:HE2	1.59	0.66
2:B:451:PHE:O	2:B:455:HIS:ND1	2.27	0.66
2:B:250:PHE:CE1	2:B:459:ALA:HB1	2.31	0.66
2:B:460:LEU:CB	30:H:1058:DGD:HAG1	2.25	0.66
23:C:1025:CLA:H151	23:C:1025:CLA:C20	2.13	0.66
4:D:134:ARG:HA	4:D:134:ARG:NE	2.11	0.66
4:D:24:ARG:NH2	4:D:24:ARG:HG2	2.09	0.66
13:O:237:ILE:HG13	13:O:237:ILE:O	1.94	0.66
23:A:1003:CLA:HAB	23:A:1006:CLA:HMD2	1.70	0.66
1:A:116:ILE:HG23	1:A:117:PHE:N	2.11	0.66
23:B:1014:CLA:CBA	23:B:1014:CLA:HMA2	1.95	0.66
23:B:1014:CLA:C17	26:B:1048:BCR:H312	2.25	0.66
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.77	0.66
23:C:1030:CLA:CMB	23:C:1031:CLA:NB	2.59	0.66
3:C:159:THR:HG22	3:C:163:PHE:CE2	2.31	0.66
3:C:59:LEU:O	23:C:1034:CLA:CED	2.44	0.66
4:D:209:LEU:HD23	4:D:209:LEU:O	1.96	0.66
20:Z:10:ALA:O	20:Z:13:VAL:HG12	1.96	0.66
1:A:95:PRO:O	1:A:97:TRP:N	2.28	0.66
2:B:133:LEU:HD23	7:H:15:ASN:ND2	2.11	0.66
2:B:141:ILE:HD12	2:B:142:HIS:H	1.61	0.66
2:B:360:PRO:HD2	2:B:363:PHE:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:TRP:CG	2:B:94:GLU:HG3	2.31	0.66
26:D:1050:BCR:H373	29:J:1059:MGE:C3A	2.26	0.66
4:D:90:LEU:HD23	4:D:96:GLU:HG3	1.77	0.66
9:J:19:MET:HA	9:J:22:ILE:HG22	1.78	0.66
15:U:57:LEU:HD11	15:U:112:PHE:HB3	1.78	0.66
16:V:158:GLY:O	16:V:162:TYR:HD2	1.78	0.66
18:Y:19:ILE:HG23	18:Y:20:ALA:N	2.11	0.66
1:A:279:ARG:NE	4:D:208:ALA:HB1	2.09	0.66
23:B:1009:CLA:C4	26:H:1049:BCR:C35	2.68	0.66
23:B:1022:CLA:H52	23:B:1022:CLA:H92	0.70	0.66
29:B:1060:MGE:H2A2	29:L:1061:MGE:H2B1	1.76	0.66
3:C:162:GLY:O	3:C:166:ILE:HG12	1.96	0.66
4:D:209:LEU:HD13	25:D:1042:PQ9:C19	2.26	0.66
6:F:18:VAL:HA	6:F:21:VAL:HG23	1.78	0.66
23:B:1016:CLA:C3	23:H:1017:CLA:H102	2.25	0.66
23:C:1037:CLA:C3B	26:Z:1053:BCR:H282	2.26	0.66
20:Z:13:VAL:CG1	20:Z:14:ILE:H	2.09	0.66
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.78	0.65
3:C:334:PRO:HD2	3:C:335:THR:HG23	1.78	0.65
4:D:72:ASN:HD22	4:D:74:LEU:N	1.93	0.65
1:A:127:MET:HG3	23:C:1029:CLA:HMB1	1.77	0.65
23:C:1032:CLA:O2D	23:C:1032:CLA:H2A	1.96	0.65
3:C:288:CYS:SG	30:C:1055:DGD:C2B	2.85	0.65
1:A:301:ASN:ND2	3:C:407:VAL:HG11	2.11	0.65
4:D:72:ASN:O	4:D:76:VAL:HG23	1.96	0.65
6:F:28:VAL:HA	6:F:31:ILE:HG22	1.77	0.65
2:B:222:PRO:HD2	23:H:1017:CLA:HED2	1.77	0.65
14:T:1:MET:O	14:T:4:ILE:N	2.29	0.65
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.31	0.65
23:B:1021:CLA:C17	23:B:1021:CLA:H142	2.25	0.65
2:B:133:LEU:HD23	7:H:15:ASN:HD21	1.60	0.65
23:C:1028:CLA:C12	23:C:1028:CLA:C17	2.41	0.65
27:A:1063:LHG:H321	23:C:1034:CLA:C14	2.25	0.65
3:C:437:PHE:CZ	23:C:1032:CLA:HBB2	2.30	0.65
3:C:95:LEU:H	3:C:95:LEU:HD22	1.61	0.65
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.27	0.65
1:A:244:GLU:HG3	4:D:264:LYS:NZ	2.11	0.65
23:A:1003:CLA:H162	24:A:1038:PHO:H93	1.77	0.65
23:C:1032:CLA:CED	23:C:1032:CLA:C2A	2.33	0.65
3:C:261:ARG:NH1	3:C:261:ARG:HG2	2.12	0.65
3:C:35:TRP:C	3:C:38:GLY:H	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:141:ARG:HG3	13:O:141:ARG:NH1	2.11	0.65
13:O:136:MET:HB2	13:O:142:ILE:HD13	1.77	0.65
16:V:111:GLU:HG3	16:V:112:GLN:H	1.61	0.65
17:X:13:THR:HG23	17:X:14:PRO:HD2	1.77	0.65
2:B:390:TYR:CD1	2:B:390:TYR:N	2.64	0.65
3:C:60:ILE:HG12	23:C:1027:CLA:HMD3	1.77	0.65
3:C:420:VAL:HB	3:C:425:TRP:HE1	1.62	0.65
4:D:57:SER:CB	4:D:79:SER:HB2	2.27	0.65
2:B:5:TRP:CZ2	29:L:1061:MGE:H3A1	2.32	0.65
14:T:7:VAL:HG12	14:T:8:PHE:N	2.11	0.65
17:X:38:ILE:HA	17:X:41:SER:CB	2.26	0.65
2:B:103:LEU:O	2:B:106:LEU:HB3	1.97	0.65
23:C:1031:CLA:CBA	23:C:1033:CLA:HED2	2.26	0.65
4:D:102:THR:O	4:D:105:CYS:HB3	1.97	0.65
26:H:1049:BCR:C40	26:H:1049:BCR:C23	2.64	0.65
13:O:215:ARG:HH11	13:O:215:ARG:HG2	1.60	0.65
15:U:73:PRO:HG2	16:V:108:TYR:O	1.96	0.65
20:Z:46:LEU:O	20:Z:50:LEU:N	2.29	0.65
23:B:1016:CLA:C3A	23:B:1016:CLA:O1A	2.45	0.65
2:B:81:THR:HB	2:B:83:GLU:HG3	1.78	0.65
3:C:212:TYR:HE1	3:C:227:VAL:HG12	1.61	0.65
3:C:154:LYS:HE2	3:C:256:PRO:HG2	1.77	0.65
3:C:39:ASN:O	3:C:40:ALA:HB3	1.96	0.65
4:D:259:ILE:HD11	14:T:21:ILE:CA	2.26	0.65
23:C:1027:CLA:H152	26:Z:1053:BCR:C33	2.27	0.65
1:A:300:PHE:HB3	1:A:302:PHE:HE1	1.61	0.65
2:B:162:PHE:C	23:B:1014:CLA:HMD3	2.17	0.65
2:B:91:TRP:CE3	2:B:91:TRP:HA	2.32	0.65
23:C:1033:CLA:O1D	23:C:1033:CLA:H2A	1.96	0.65
1:A:284:TRP:CZ2	3:C:439:VAL:HG21	2.32	0.65
1:A:223:LEU:HG	4:D:265:ARG:CZ	2.26	0.65
4:D:304:ARG:NH1	4:D:311:PHE:HD2	1.94	0.65
4:D:89:LEU:HD22	4:D:89:LEU:H	1.60	0.65
6:F:18:VAL:C	6:F:20:TRP:H	1.99	0.65
30:C:1057:DGD:HAS1	29:J:1059:MGE:H222	1.79	0.65
14:T:1:MET:O	14:T:3:THR:N	2.29	0.65
20:Z:25:VAL:HG12	20:Z:29:SER:OG	1.96	0.65
1:A:96:ILE:HG13	1:A:105:TRP:CD2	2.31	0.65
23:B:1020:CLA:HMA2	23:B:1020:CLA:HBA1	0.73	0.65
23:B:1022:CLA:C8	23:B:1022:CLA:H142	2.27	0.65
2:B:64:PRO:HB2	2:B:268:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1028:CLA:C4	30:C:1057:DGD:HA42	2.26	0.65
23:C:1033:CLA:CHD	23:C:1033:CLA:CBC	2.69	0.65
3:C:86:LEU:O	3:C:90:PRO:HG2	1.97	0.65
4:D:102:THR:O	4:D:106:GLN:HG3	1.96	0.65
2:B:364:GLU:HG3	4:D:296:TYR:CD2	2.31	0.65
4:D:259:ILE:CD1	14:T:21:ILE:HA	2.26	0.65
1:A:126:TYR:O	1:A:130:GLN:HB2	1.97	0.65
1:A:296:ASN:HB3	3:C:401:LEU:HA	1.78	0.65
23:B:1010:CLA:C3D	23:B:1011:CLA:HMB2	2.27	0.65
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.79	0.65
2:B:318:ASN:HD22	2:B:318:ASN:C	2.00	0.65
23:C:1028:CLA:HBB1	23:C:1028:CLA:CHC	2.25	0.65
4:D:24:ARG:CG	4:D:24:ARG:HH21	2.10	0.65
6:F:11:VAL:HG12	6:F:12:SER:N	2.10	0.65
8:I:20:VAL:O	8:I:24:LEU:HD23	1.96	0.65
15:U:88:VAL:HG12	15:U:109:LEU:CD1	2.27	0.65
15:U:127:ARG:HG2	15:U:127:ARG:HH11	1.61	0.65
15:U:98:THR:H	15:U:101:GLN:HG3	1.61	0.65
1:A:50:ILE:HB	26:A:1044:BCR:H391	1.79	0.64
1:A:128:GLY:O	1:A:130:GLN:N	2.30	0.64
1:A:63:ILE:HG13	1:A:65:GLU:HG2	1.78	0.64
23:B:1020:CLA:H52	23:B:1020:CLA:CGA	2.26	0.64
23:B:1021:CLA:H172	23:B:1021:CLA:H142	1.79	0.64
2:B:105:GLY:C	26:B:1047:BCR:H282	2.17	0.64
2:B:59:GLY:N	2:B:329:PRO:CB	2.61	0.64
23:C:1025:CLA:H201	23:C:1031:CLA:H121	1.77	0.64
3:C:285:ILE:HG23	23:C:1025:CLA:H52	1.79	0.64
3:C:96:GLY:HA2	3:C:99:VAL:CG1	2.27	0.64
4:D:328:TRP:CD1	4:D:346:LEU:HD11	2.32	0.64
2:B:121:GLU:OE1	7:H:4:ARG:HA	1.98	0.64
9:J:10:LEU:HA	9:J:13:VAL:CG2	2.27	0.64
6:F:41:GLN:NE2	9:J:27:LEU:C	2.47	0.64
15:U:129:ASN:C	15:U:131:GLY:H	2.00	0.64
17:X:30:LEU:O	17:X:34:PHE:HB2	1.97	0.64
18:Y:31:ALA:O	18:Y:35:ILE:HG23	1.96	0.64
26:B:1045:BCR:C8	26:B:1045:BCR:C33	2.76	0.64
2:B:106:LEU:HD11	26:B:1048:BCR:C35	2.27	0.64
2:B:223:GLN:O	2:B:225:LEU:N	2.29	0.64
2:B:7:ARG:HA	23:B:1019:CLA:HBA1	1.79	0.64
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.78	0.64
2:B:257:TRP:NE1	4:D:163:GLY:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:461:ARG:NH2	4:D:223:PHE:HD2	1.95	0.64
2:B:362:PHE:CE2	4:D:164:GLN:NE2	2.65	0.64
4:D:222:LEU:HA	4:D:243:THR:O	1.98	0.64
2:B:388:SER:HA	4:D:344:GLU:OE1	1.97	0.64
7:H:37:LEU:O	7:H:40:VAL:HG12	1.98	0.64
13:O:205:GLU:O	13:O:207:GLU:N	2.30	0.64
15:U:39:LEU:CD1	15:U:39:LEU:H	2.03	0.64
23:A:1003:CLA:CBD	23:D:1005:CLA:HAC2	2.26	0.64
23:B:1011:CLA:HHH	23:B:1014:CLA:CBB	2.22	0.64
2:B:66:MET:SD	23:B:1013:CLA:HED1	2.38	0.64
23:B:1023:CLA:H141	23:B:1024:CLA:H61	1.79	0.64
2:B:223:GLN:O	2:B:227:LYS:HG2	1.98	0.64
2:B:31:ALA:CB	23:B:1013:CLA:HBC3	2.27	0.64
4:D:130:PHE:HE2	4:D:140:PRO:HB2	1.62	0.64
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.79	0.64
4:D:89:LEU:H	4:D:89:LEU:CD2	2.10	0.64
5:E:19:TYR:HD1	5:E:20:TRP:HD1	1.46	0.64
29:L:1061:MGE:H9A2	12:M:18:PRO:HB3	1.80	0.64
24:A:1039:PHO:HBC3	24:A:1039:PHO:HMC1	1.78	0.64
2:B:464:PHE:HB3	4:D:280:TRP:CH2	2.31	0.64
9:J:40:LEU:HD12	16:V:56:LYS:HD3	1.79	0.64
18:Y:20:ALA:HB1	18:Y:22:LEU:HG	1.78	0.64
24:A:1039:PHO:O2D	24:A:1039:PHO:H2A	1.98	0.64
1:A:288:LEU:CD2	3:C:432:VAL:HG13	2.28	0.64
1:A:228:THR:HA	2:B:480:SER:CB	2.28	0.64
23:C:1026:CLA:H203	23:C:1026:CLA:C1D	2.26	0.64
3:C:441:HIS:C	3:C:441:HIS:CD2	2.70	0.64
29:D:1062:MGE:H2A2	14:T:20:ALA:HB1	1.79	0.64
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.66	0.64
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.27	0.64
16:V:102:MET:HE1	16:V:141:ILE:HB	1.80	0.64
20:Z:13:VAL:CG1	20:Z:14:ILE:N	2.61	0.64
1:A:177:SER:HA	1:A:180:PHE:CD2	2.32	0.64
23:B:1015:CLA:NA	23:B:1015:CLA:CBA	2.46	0.64
23:B:1023:CLA:H72	26:B:1048:BCR:H341	1.79	0.64
2:B:15:ASP:OD1	2:B:15:ASP:O	2.15	0.64
2:B:253:ALA:O	30:H:1058:DGD:HBW2	1.97	0.64
2:B:289:GLN:HA	2:B:289:GLN:NE2	2.11	0.64
29:D:1062:MGE:H2A2	14:T:20:ALA:CB	2.28	0.64
9:J:19:MET:HA	9:J:22:ILE:CG2	2.27	0.64
20:Z:43:GLY:O	20:Z:47:TRP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1006:CLA:HBB1	23:D:1004:CLA:H42	1.79	0.64
24:A:1039:PHO:HBC1	4:D:275:PRO:HB3	1.79	0.64
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.32	0.64
23:B:1012:CLA:HBB1	23:B:1012:CLA:CHC	2.22	0.64
23:B:1015:CLA:HBC2	23:B:1015:CLA:CHD	2.27	0.64
2:B:10:THR:O	2:B:13:ILE:HG13	1.97	0.64
2:B:257:TRP:CE3	2:B:452:THR:HG21	2.32	0.64
2:B:68:ARG:HG3	2:B:69:LEU:N	2.12	0.64
23:A:1003:CLA:CHD	23:A:1003:CLA:HBC2	2.20	0.64
1:A:197:PHE:HE1	1:A:285:PHE:CD2	2.15	0.64
1:A:253:GLY:O	1:A:257:ARG:HD2	1.98	0.64
2:B:399:VAL:HG13	2:B:417:VAL:HG22	1.79	0.64
3:C:473:ASP:OXT	14:T:27:PRO:HD2	1.96	0.64
23:D:1005:CLA:H161	29:D:1062:MGE:CGB	2.28	0.64
23:A:1006:CLA:C16	26:D:1050:BCR:H291	2.28	0.64
1:A:221:SER:HA	4:D:139:ARG:HB2	1.80	0.64
1:A:24:THR:O	4:D:251:ARG:NH2	2.31	0.64
4:D:55:VAL:O	4:D:65:SER:HB2	1.97	0.64
12:M:18:PRO:HG2	12:M:19:SER:H	1.63	0.64
1:A:159:LEU:CG	1:A:163:ILE:HD11	2.28	0.64
1:A:76:ASN:ND2	1:A:78:ILE:H	1.95	0.64
23:B:1012:CLA:CBB	23:B:1012:CLA:HHC	2.24	0.64
3:C:222:GLY:O	3:C:223:TRP:C	2.36	0.64
3:C:303:GLY:O	3:C:423:ARG:HD2	1.98	0.64
3:C:53:HIS:HB2	23:C:1036:CLA:HMD1	1.80	0.64
16:V:90:PRO:HD2	16:V:92:ARG:NH2	2.12	0.64
17:X:33:THR:HG23	17:X:34:PHE:N	2.13	0.64
23:B:1011:CLA:CAD	23:B:1013:CLA:C4	2.72	0.63
23:B:1012:CLA:H12	23:B:1013:CLA:H11	1.74	0.63
2:B:159:THR:O	2:B:180:PRO:HB3	1.98	0.63
2:B:354:LEU:HD23	2:B:370:LEU:HB3	1.80	0.63
2:B:373:LYS:C	2:B:375:GLY:H	2.01	0.63
2:B:456:ALA:CA	30:H:1058:DGD:HGB2	2.27	0.63
2:B:6:TYR:CD2	2:B:6:TYR:N	2.65	0.63
23:C:1025:CLA:H201	23:C:1031:CLA:C12	2.28	0.63
4:D:300:SER:O	4:D:303:ILE:HD11	1.98	0.63
13:O:205:GLU:C	13:O:207:GLU:H	2.01	0.63
20:Z:39:LEU:O	20:Z:42:LEU:HB3	1.99	0.63
1:A:278:TRP:CH2	30:C:1057:DGD:HAG1	2.32	0.63
2:B:183:PRO:HB3	2:B:200:ALA:CB	2.28	0.63
2:B:257:TRP:CH2	4:D:291:LEU:CD1	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:ILE:HD12	2:B:429:ILE:H	1.62	0.63
2:B:58:GLN:O	2:B:59:GLY:C	2.37	0.63
3:C:161:LEU:HD11	23:C:1030:CLA:HBB1	1.80	0.63
3:C:41:ARG:HG2	23:C:1035:CLA:HED2	1.79	0.63
3:C:439:VAL:HG13	23:C:1032:CLA:CBC	2.28	0.63
3:C:59:LEU:O	3:C:62:PHE:HB3	1.99	0.63
4:D:148:ALA:HB2	4:D:276:VAL:HA	1.81	0.63
1:A:219:VAL:HG21	4:D:268:HIS:HB3	1.76	0.63
13:O:133:THR:HG22	13:O:134:VAL:N	2.13	0.63
16:V:111:GLU:CG	16:V:112:GLN:H	2.11	0.63
20:Z:9:LEU:C	20:Z:11:ALA:N	2.50	0.63
3:C:41:ARG:CG	23:C:1035:CLA:HED2	2.28	0.63
23:A:1006:CLA:HAA2	30:C:1057:DGD:HBN2	1.80	0.63
4:D:67:TYR:HE1	4:D:73:PHE:HA	1.63	0.63
4:D:91:LEU:HA	23:D:1008:CLA:HED3	1.80	0.63
23:B:1011:CLA:H191	23:H:1017:CLA:H151	1.80	0.63
11:L:22:LEU:HD21	29:L:1061:MGE:H263	1.78	0.63
13:O:65:ARG:NH1	13:O:108:GLN:HB2	2.13	0.63
23:A:1006:CLA:HAB	24:A:1039:PHO:H142	1.78	0.63
1:A:153:SER:O	1:A:156:ALA:N	2.32	0.63
1:A:215:HIS:O	1:A:219:VAL:CG1	2.45	0.63
26:B:1048:BCR:C8	26:B:1048:BCR:C33	2.73	0.63
2:B:214:LEU:O	2:B:218:LEU:HG	1.97	0.63
2:B:288:VAL:HG21	2:B:302:TRP:CE2	2.34	0.63
2:B:66:MET:HG2	23:B:1013:CLA:CED	2.28	0.63
1:A:288:LEU:HD23	3:C:432:VAL:HG22	1.80	0.63
4:D:209:LEU:O	4:D:213:ILE:HG22	1.98	0.63
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.80	0.63
4:D:261:PHE:CD2	4:D:267:LEU:HB2	2.32	0.63
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.32	0.63
14:T:1:MET:HE3	14:T:1:MET:H1	1.56	0.63
12:M:3:VAL:HG11	14:T:2:GLU:OE1	1.97	0.63
1:A:278:TRP:O	1:A:281:VAL:HG12	1.98	0.63
1:A:87:ASN:O	1:A:88:ALA:C	2.37	0.63
23:B:1010:CLA:C1D	23:B:1011:CLA:HMB1	2.28	0.63
2:B:159:THR:CG2	2:B:161:LEU:HD22	2.28	0.63
2:B:346:PHE:HD2	2:B:346:PHE:N	1.96	0.63
23:C:1031:CLA:O2D	23:C:1031:CLA:CAA	2.30	0.63
4:D:53:THR:HG22	4:D:67:TYR:CE2	2.33	0.63
23:B:1016:CLA:H92	23:H:1017:CLA:H101	1.80	0.63
7:H:3:ARG:HH22	11:L:1:MET:N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:THR:O	8:I:7:THR:HG23	1.99	0.63
13:O:215:ARG:NH1	13:O:215:ARG:HG2	2.13	0.63
1:A:147:TYR:HA	1:A:150:PRO:CG	2.28	0.63
1:A:316:THR:O	1:A:319:ASP:HB2	1.99	0.63
23:B:1018:CLA:H151	23:B:1018:CLA:OBD	1.97	0.63
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.34	0.63
2:B:318:ASN:C	2:B:318:ASN:ND2	2.50	0.63
4:D:221:THR:HG23	4:D:244:TYR:HB3	1.80	0.63
1:A:193:LEU:HD22	4:D:179:PHE:CG	2.33	0.63
1:A:196:PRO:HA	1:A:199:GLN:HG2	1.80	0.63
23:B:1014:CLA:C11	23:B:1014:CLA:H162	2.27	0.63
2:B:148:LEU:CB	2:B:210:ILE:HD11	2.28	0.63
2:B:465:GLY:CA	23:B:1019:CLA:HBC2	2.29	0.63
23:C:1033:CLA:C5	23:C:1033:CLA:H93	2.26	0.63
1:A:188:ALA:HB2	1:A:328:MET:HE3	1.79	0.63
1:A:316:THR:C	4:D:63:LEU:HD21	2.18	0.63
2:B:257:TRP:HD1	2:B:273:TYR:HH	1.41	0.63
2:B:417:VAL:HG12	2:B:418:LYS:H	1.62	0.63
23:C:1032:CLA:H42	23:C:1032:CLA:CGA	2.27	0.63
3:C:135:ARG:HB2	20:Z:27:TYR:CD1	2.34	0.63
26:D:1050:BCR:H372	29:J:1059:MGE:H6A1	1.80	0.63
23:B:1016:CLA:HMB3	4:D:126:MET:HE2	1.79	0.63
4:D:150:ILE:O	4:D:154:VAL:HG23	1.98	0.63
4:D:83:ASN:H	4:D:168:PHE:HD1	1.46	0.63
6:F:41:GLN:OE1	9:J:28:PHE:HA	1.99	0.63
23:H:1017:CLA:CBB	26:H:1049:BCR:C32	2.71	0.63
13:O:228:ALA:O	13:O:229:LYS:HG3	1.99	0.63
20:Z:9:LEU:HD13	20:Z:10:ALA:H	1.62	0.63
24:A:1038:PHO:C2B	23:D:1005:CLA:H52	2.29	0.63
1:A:219:VAL:CG2	4:D:268:HIS:CB	2.76	0.63
1:A:245:THR:HG22	4:D:264:LYS:HD2	1.81	0.63
23:C:1025:CLA:H203	23:C:1031:CLA:H121	1.78	0.63
30:C:1055:DGD:HB72	30:C:1055:DGD:HB32	1.79	0.63
4:D:103:ARG:O	4:D:106:GLN:N	2.32	0.63
4:D:101:PHE:O	4:D:105:CYS:HB2	1.98	0.63
4:D:218:VAL:O	4:D:221:THR:HG22	1.99	0.63
11:L:22:LEU:HD23	11:L:23:LEU:N	2.14	0.63
15:U:113:THR:HG22	15:U:114:VAL:N	2.14	0.63
20:Z:30:PRO:O	20:Z:32:ASP:N	2.31	0.63
27:A:1063:LHG:H351	3:C:436:PHE:CE1	2.34	0.62
1:A:37:MET:HB2	1:A:125:CYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1013:CLA:H102	23:B:1018:CLA:H42	1.81	0.62
23:B:1021:CLA:HMA3	23:B:1021:CLA:H42	1.79	0.62
23:C:1028:CLA:CBB	23:C:1028:CLA:HHC	2.27	0.62
23:C:1034:CLA:C13	23:C:1034:CLA:H92	2.29	0.62
3:C:429:SER:HA	30:C:1056:DGD:HA91	1.81	0.62
30:C:1057:DGD:CAA	30:C:1057:DGD:HA62	2.29	0.62
4:D:209:LEU:CD2	25:D:1042:PQ9:H192	2.23	0.62
5:E:35:TRP:CZ3	6:F:38:ALA:HB1	2.33	0.62
4:D:68:LEU:HA	6:F:40:MET:CG	2.29	0.62
14:T:10:PHE:C	14:T:12:CYS:H	2.02	0.62
1:A:159:LEU:HD23	30:C:1055:DGD:HBW1	1.81	0.62
3:C:207:ARG:HG3	3:C:208:VAL:N	2.13	0.62
3:C:203:THR:HG22	3:C:231:GLU:O	1.99	0.62
2:B:364:GLU:HG3	4:D:296:TYR:HD2	1.64	0.62
11:L:30:LEU:HD23	11:L:31:PHE:N	2.13	0.62
23:C:1027:CLA:H172	26:Z:1053:BCR:H10C	1.79	0.62
1:A:235:TYR:C	1:A:237:TYR:H	2.02	0.62
1:A:279:ARG:C	1:A:283:VAL:CG1	2.68	0.62
2:B:63:LEU:N	2:B:64:PRO:HD2	2.14	0.62
3:C:50:LEU:HD22	3:C:132:HIS:CD2	2.34	0.62
3:C:207:ARG:O	3:C:211:GLY:N	2.31	0.62
3:C:95:LEU:H	3:C:95:LEU:CD2	2.12	0.62
3:C:461:ARG:NH2	4:D:223:PHE:CD2	2.68	0.62
13:O:167:ASP:N	13:O:167:ASP:OD2	2.30	0.62
15:U:69:ARG:HH11	15:U:69:ARG:HG3	1.64	0.62
20:Z:5:PHE:O	20:Z:8:ALA:N	2.27	0.62
27:A:1063:LHG:P	27:A:1063:LHG:C6	2.88	0.62
1:A:142:TRP:H	4:D:220:ASN:ND2	1.95	0.62
1:A:206:PHE:CD1	24:A:1039:PHO:HBB2	2.33	0.62
1:A:223:LEU:HD13	1:A:224:ILE:HG12	1.80	0.62
2:B:144:PHE:CE1	2:B:210:ILE:HD12	2.34	0.62
2:B:346:PHE:CD2	2:B:346:PHE:N	2.67	0.62
2:B:368:VAL:HG11	2:B:381:ILE:CD1	2.25	0.62
2:B:58:GLN:O	2:B:58:GLN:HG3	2.00	0.62
3:C:29:GLU:HG3	10:K:45:PHE:O	1.99	0.62
3:C:377:LEU:HA	3:C:380:ILE:HG22	1.80	0.62
3:C:461:ARG:O	3:C:461:ARG:HG3	1.98	0.62
4:D:281:MET:HE3	4:D:284:ILE:HD12	1.80	0.62
9:J:17:ALA:O	9:J:20:GLY:N	2.33	0.62
10:K:19:ASP:N	10:K:20:PRO:CD	2.63	0.62
13:O:188:ARG:HD3	13:O:197:ALA:N	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:37:LYS:HZ3	20:Z:38:GLN:HG2	1.64	0.62
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.35	0.62
1:A:52:PHE:O	1:A:52:PHE:CD2	2.53	0.62
1:A:90:GLY:C	1:A:92:HIS:N	2.53	0.62
2:B:388:SER:C	2:B:394:GLN:HE22	2.03	0.62
2:B:45:PHE:HB2	2:B:60:MET:SD	2.39	0.62
2:B:6:TYR:HD2	2:B:6:TYR:N	1.97	0.62
2:B:6:TYR:OH	11:L:11:GLU:HG3	1.99	0.62
23:C:1029:CLA:H202	23:C:1030:CLA:C17	2.29	0.62
3:C:264:PHE:CZ	26:C:1054:BCR:C31	2.81	0.62
30:C:1055:DGD:O1B	30:C:1055:DGD:C4B	2.47	0.62
30:C:1055:DGD:CBA	30:C:1055:DGD:HA72	2.26	0.62
3:C:284:PHE:C	3:C:286:ALA:H	2.01	0.62
29:D:1062:MGE:H212	14:T:17:PHE:HZ	1.64	0.62
4:D:218:VAL:HG12	4:D:219:GLU:N	2.13	0.62
5:E:34:GLY:CA	6:F:32:PHE:CE2	2.81	0.62
9:J:11:TRP:CD1	9:J:11:TRP:C	2.71	0.62
16:V:72:THR:HG22	16:V:75:ASN:H	1.65	0.62
23:B:1009:CLA:H2A	23:B:1009:CLA:CED	2.23	0.62
3:C:40:ALA:HA	23:C:1033:CLA:CMC	2.30	0.62
4:D:103:ARG:HH22	5:E:80:LEU:HD12	1.65	0.62
4:D:48:TRP:CE3	4:D:49:LEU:HG	2.29	0.62
9:J:15:THR:O	9:J:19:MET:HG2	1.99	0.62
14:T:18:PHE:O	14:T:22:PHE:HD2	1.82	0.62
1:A:136:ARG:O	1:A:137:LEU:HD23	1.99	0.62
1:A:183:MET:HB3	23:A:1003:CLA:HBC3	1.82	0.62
23:B:1022:CLA:C13	23:B:1022:CLA:H8	1.81	0.62
23:B:1022:CLA:HMB1	23:B:1022:CLA:CBB	2.23	0.62
23:B:1023:CLA:CAA	23:B:1023:CLA:CGD	2.65	0.62
3:C:120:ILE:HG13	26:Z:1053:BCR:H343	1.81	0.62
3:C:348:GLU:OE2	3:C:359:TRP:HZ3	1.82	0.62
3:C:357:ARG:HH11	3:C:357:ARG:CB	2.12	0.62
4:D:277:THR:CG2	4:D:278:GLY:N	2.63	0.62
12:M:8:PHE:O	12:M:11:THR:N	2.32	0.62
15:U:57:LEU:C	15:U:58:ASN:HD22	2.02	0.62
23:A:1006:CLA:CMB	24:A:1039:PHO:C16	2.58	0.62
1:A:184:ILE:O	1:A:328:MET:HE3	2.00	0.62
23:B:1021:CLA:C1	23:B:1021:CLA:HMA2	2.30	0.62
23:B:1015:CLA:C18	29:B:1060:MGE:H8A1	2.26	0.62
2:B:277:SER:C	2:B:279:TYR:N	2.51	0.62
2:B:319:PRO:HG3	2:B:446:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1037:CLA:O1A	23:C:1037:CLA:C3A	2.47	0.62
1:A:135:TYR:CD1	3:C:449:ARG:HG3	2.34	0.62
11:L:36:PHE:HD2	14:T:6:TYR:HH	1.46	0.62
23:A:1003:CLA:C3D	23:D:1005:CLA:CBC	2.78	0.62
1:A:272:HIS:HB2	4:D:218:VAL:HG11	1.82	0.62
23:B:1021:CLA:C19	29:B:1060:MGE:CDA	2.78	0.62
2:B:125:ASP:OD2	2:B:128:THR:HG22	2.00	0.62
23:A:1006:CLA:H141	23:D:1004:CLA:H192	1.81	0.62
4:D:201:VAL:HG21	23:D:1005:CLA:OBD	1.99	0.62
4:D:218:VAL:HG22	4:D:244:TYR:CD1	2.34	0.62
23:H:1017:CLA:H192	23:H:1017:CLA:H151	1.80	0.62
13:O:100:GLU:O	13:O:100:GLU:HG2	2.00	0.62
23:A:1006:CLA:CHC	23:A:1006:CLA:HBB1	2.29	0.62
1:A:219:VAL:CG2	4:D:268:HIS:CG	2.80	0.62
23:B:1011:CLA:H193	23:B:1016:CLA:HAC1	1.82	0.62
23:B:1023:CLA:ND	23:B:1024:CLA:HMC1	2.14	0.62
2:B:380:ASP:OD2	4:D:345:VAL:CG2	2.46	0.62
3:C:85:GLY:N	30:C:1056:DGD:HE4	2.15	0.62
4:D:299:ILE:O	4:D:301:GLN:N	2.33	0.62
7:H:41:PHE:CE2	7:H:45:ILE:HD11	2.35	0.62
7:H:48:ILE:HG12	7:H:53:LEU:HD23	1.81	0.62
10:K:18:PHE:CE2	20:Z:9:LEU:HD11	2.35	0.62
13:O:177:TYR:C	13:O:178:ARG:HG2	2.20	0.62
15:U:55:ILE:HG21	15:U:65:PHE:HE2	1.65	0.62
16:V:120:SER:H	16:V:123:SER:CB	2.11	0.62
1:A:157:VAL:HG13	1:A:157:VAL:O	2.00	0.61
1:A:58:VAL:O	1:A:67:VAL:N	2.33	0.61
2:B:99:ALA:CB	23:B:1014:CLA:H2	2.26	0.61
2:B:152:GLY:C	23:B:1014:CLA:CMC	2.68	0.61
2:B:336:ILE:HG22	2:B:336:ILE:O	1.99	0.61
2:B:71:VAL:O	2:B:71:VAL:HG13	1.99	0.61
23:A:1006:CLA:C12	30:C:1057:DGD:CIB	2.78	0.61
3:C:230:LEU:O	3:C:234:VAL:HG23	2.00	0.61
3:C:269:GLU:O	3:C:272:LEU:HB3	2.00	0.61
3:C:297:TYR:HA	3:C:302:TYR:CE2	2.35	0.61
2:B:457:VAL:CG2	4:D:284:ILE:HG23	2.30	0.61
5:E:34:GLY:O	5:E:37:PHE:N	2.33	0.61
15:U:88:VAL:O	15:U:91:VAL:HG23	2.00	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.82	0.61
1:A:164:GLY:HA3	1:A:294:ALA:O	2.00	0.61
2:B:457:VAL:O	2:B:461:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TRP:HH2	30:C:1057:DGD:HAG3	1.65	0.61
3:C:126:GLY:HA2	26:K:1052:BCR:H363	1.80	0.61
3:C:82:TYR:CD2	3:C:302:TYR:O	2.53	0.61
2:B:222:PRO:HA	7:H:22:ALA:HB3	1.82	0.61
13:O:265:PHE:CD1	13:O:266:TYR:N	2.68	0.61
14:T:4:ILE:CD1	14:T:4:ILE:C	2.64	0.61
23:C:1036:CLA:H193	26:Z:1053:BCR:H372	1.82	0.61
1:A:326:LEU:HD21	3:C:412:THR:HB	1.82	0.61
1:A:65:GLU:O	1:A:65:GLU:HG3	1.99	0.61
2:B:91:TRP:HB3	23:B:1014:CLA:CED	2.31	0.61
23:B:1019:CLA:CMB	23:B:1020:CLA:NC	2.62	0.61
2:B:193:TYR:HA	2:B:261:ALA:HB2	1.81	0.61
2:B:288:VAL:HG22	2:B:301:ALA:HB1	1.81	0.61
3:C:45:LEU:CD1	3:C:139:THR:HG23	2.31	0.61
3:C:311:GLN:HE22	3:C:351:PHE:HD2	1.47	0.61
3:C:53:HIS:CB	23:C:1036:CLA:HMD1	2.30	0.61
23:D:1005:CLA:CED	25:D:1042:PQ9:H412	2.30	0.61
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.82	0.61
4:D:17:ILE:HG21	17:X:42:GLN:HB2	1.81	0.61
1:A:223:LEU:CD2	4:D:265:ARG:HD3	2.29	0.61
10:K:35:LEU:HD12	10:K:38:VAL:HG21	1.82	0.61
13:O:65:ARG:NH1	13:O:66:ILE:H	1.97	0.61
1:A:95:PRO:CA	23:A:1007:CLA:CED	2.71	0.61
27:A:1063:LHG:H271	23:C:1032:CLA:C8	2.28	0.61
1:A:223:LEU:HD23	4:D:265:ARG:HH11	1.65	0.61
23:B:1016:CLA:CMD	23:B:1018:CLA:HAB	2.30	0.61
3:C:253:LEU:HD23	3:C:253:LEU:O	2.01	0.61
23:D:1005:CLA:C17	29:D:1062:MGE:H261	2.30	0.61
4:D:108:GLY:O	4:D:110:LEU:N	2.33	0.61
4:D:83:ASN:HA	4:D:166:SER:CB	2.30	0.61
11:L:15:THR:HG22	11:L:15:THR:O	2.01	0.61
14:T:12:CYS:O	14:T:15:ALA:N	2.33	0.61
24:A:1039:PHO:H42	4:D:41:ALA:HB1	1.81	0.61
24:A:1039:PHO:HBC1	4:D:275:PRO:CB	2.30	0.61
1:A:58:VAL:HG11	1:A:83:VAL:HG12	1.82	0.61
23:B:1016:CLA:C14	23:D:1008:CLA:HHB	2.30	0.61
2:B:141:ILE:N	2:B:217:ILE:HD13	2.16	0.61
2:B:465:GLY:C	2:B:467:ILE:N	2.49	0.61
23:C:1028:CLA:HMA2	23:C:1028:CLA:CBA	2.29	0.61
3:C:443:TRP:HD1	3:C:444:HIS:CE1	2.18	0.61
29:L:1061:MGE:H9A2	12:M:18:PRO:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:92:VAL:HG23	13:O:93:PRO:HD2	1.82	0.61
23:A:1006:CLA:HMB3	24:A:1039:PHO:H172	1.82	0.61
23:B:1011:CLA:C12	23:B:1011:CLA:C9	2.77	0.61
23:B:1011:CLA:C17	23:B:1016:CLA:CBC	2.79	0.61
2:B:173:GLY:HA3	2:B:312:TYR:HE1	1.63	0.61
2:B:68:ARG:NH2	2:B:262:THR:HB	2.16	0.61
3:C:405:ASN:O	3:C:407:VAL:HG23	2.01	0.61
23:B:1011:CLA:C19	23:H:1017:CLA:H121	2.24	0.61
13:O:114:ASN:O	13:O:116:ASP:N	2.33	0.61
1:A:57:PRO:CA	1:A:68:SER:HB2	2.27	0.61
2:B:100:HIS:O	2:B:103:LEU:HB3	2.01	0.61
2:B:121:GLU:O	2:B:123:PHE:N	2.33	0.61
2:B:58:GLN:HA	2:B:329:PRO:HB2	1.83	0.61
4:D:149:PRO:HA	4:D:152:VAL:HG12	1.81	0.61
5:E:34:GLY:HA2	6:F:32:PHE:CE2	2.35	0.61
4:D:91:LEU:HD21	7:H:47:GLU:OE1	2.00	0.61
23:B:1019:CLA:H91	29:L:1061:MGE:H8A1	1.83	0.61
3:C:120:ILE:HG21	26:Z:1053:BCR:H341	1.82	0.61
23:A:1006:CLA:H202	26:D:1050:BCR:H402	1.81	0.61
2:B:465:GLY:N	23:B:1019:CLA:HBC1	2.05	0.61
23:B:1021:CLA:CMA	23:B:1021:CLA:O2A	2.48	0.61
3:C:157:MET:HB3	23:C:1031:CLA:CBC	2.30	0.61
23:C:1032:CLA:CAB	23:C:1034:CLA:CMC	2.79	0.61
3:C:89:ILE:HG23	3:C:111:PHE:HE2	1.66	0.61
1:A:297:LEU:HD21	3:C:404:LEU:HA	1.83	0.61
3:C:459:ILE:HB	4:D:223:PHE:CD1	2.36	0.61
10:K:18:PHE:CE2	20:Z:9:LEU:HD21	2.36	0.61
17:X:13:THR:HG22	17:X:15:SER:N	2.13	0.61
26:Z:1053:BCR:C33	26:Z:1053:BCR:HC8	2.31	0.61
23:A:1006:CLA:HMB3	24:A:1039:PHO:C17	2.30	0.61
27:A:1063:LHG:C34	27:A:1063:LHG:H383	2.29	0.61
2:B:134:ASP:OD1	2:B:137:LYS:HD2	2.00	0.61
2:B:141:ILE:O	2:B:145:LEU:HG	2.01	0.61
2:B:193:TYR:OH	2:B:259:GLY:HA3	2.01	0.61
2:B:5:TRP:CZ2	2:B:6:TYR:HB3	2.35	0.61
3:C:97:TRP:HZ3	3:C:113:VAL:HG21	1.66	0.61
3:C:266:TRP:HE3	3:C:271:TYR:HH	1.46	0.61
3:C:285:ILE:CG2	23:C:1025:CLA:H52	2.30	0.61
4:D:119:ALA:O	4:D:123:ILE:HG12	2.00	0.61
10:K:43:VAL:HG12	10:K:43:VAL:O	2.00	0.61
15:U:123:GLU:O	15:U:125:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:13:THR:CG2	17:X:15:SER:H	2.10	0.61
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.64	0.61
2:B:360:PRO:HD2	2:B:363:PHE:CD2	2.36	0.61
23:C:1035:CLA:C10	26:K:1052:BCR:C40	2.75	0.61
4:D:152:VAL:HG11	23:D:1004:CLA:H51	1.82	0.61
4:D:201:VAL:HA	23:D:1004:CLA:HMB3	1.83	0.61
4:D:101:PHE:C	4:D:101:PHE:CD1	2.73	0.61
10:K:11:LEU:HD23	10:K:12:PRO:HD2	1.81	0.61
1:A:223:LEU:HD23	4:D:265:ARG:NH1	2.16	0.60
2:B:13:ILE:HD12	2:B:14:ASN:OD1	2.01	0.60
2:B:209:GLY:HA3	23:B:1013:CLA:H191	1.82	0.60
2:B:25:MET:O	2:B:26:HIS:C	2.39	0.60
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.30	0.60
23:C:1025:CLA:C20	23:C:1031:CLA:C12	2.79	0.60
3:C:132:HIS:HA	3:C:136:GLY:HA3	1.83	0.60
3:C:237:HIS:O	3:C:240:ILE:HG22	2.00	0.60
4:D:253:TRP:HB2	4:D:260:ALA:HB2	1.82	0.60
1:A:140:ARG:NH2	27:A:1063:LHG:HC2	2.11	0.60
2:B:272:ARG:HD3	2:B:276:ASP:OD2	2.00	0.60
3:C:207:ARG:HG3	3:C:208:VAL:H	1.67	0.60
3:C:262:ARG:NH1	3:C:262:ARG:HB3	2.14	0.60
3:C:451:ALA:HA	3:C:456:GLU:HG2	1.83	0.60
3:C:82:TYR:HD2	3:C:302:TYR:O	1.84	0.60
25:D:1042:PQ9:H441	11:L:29:LEU:HD23	1.82	0.60
1:A:90:GLY:HA2	1:A:167:SER:CB	2.30	0.60
23:B:1020:CLA:H142	23:B:1021:CLA:HAB	1.82	0.60
2:B:260:SER:O	2:B:263:THR:N	2.33	0.60
2:B:33:TRP:HB2	26:B:1047:BCR:H14C	1.83	0.60
2:B:390:TYR:HD1	2:B:390:TYR:N	1.99	0.60
23:C:1032:CLA:H171	23:C:1034:CLA:H191	1.81	0.60
3:C:196:VAL:O	3:C:196:VAL:HG13	1.99	0.60
3:C:36:TRP:CG	3:C:37:ALA:N	2.69	0.60
3:C:42:LEU:HD12	3:C:49:LEU:HG	1.83	0.60
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.36	0.60
9:J:17:ALA:C	9:J:19:MET:H	2.04	0.60
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.82	0.60
2:B:150:CYS:HB2	23:B:1011:CLA:HMC3	1.82	0.60
23:C:1030:CLA:C2C	23:C:1031:CLA:H101	2.31	0.60
23:C:1032:CLA:HHC	23:C:1032:CLA:CBB	2.31	0.60
3:C:197:ARG:HG2	3:C:198:VAL:H	1.66	0.60
3:C:282:MET:HA	3:C:285:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.36	0.60
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.29	0.60
4:D:74:LEU:HA	4:D:175:VAL:CG2	2.31	0.60
7:H:16:SER:O	7:H:18:TYR:N	2.32	0.60
8:I:15:PHE:O	8:I:18:LEU:N	2.34	0.60
13:O:120:THR:HA	13:O:153:ALA:O	2.01	0.60
15:U:46:LYS:HE2	15:U:59:ASN:HD21	1.65	0.60
23:B:1016:CLA:H203	23:D:1008:CLA:CMA	2.31	0.60
2:B:36:SER:N	2:B:101:ILE:HD11	2.16	0.60
23:B:1021:CLA:C18	29:B:1060:MGE:H132	2.30	0.60
2:B:135:LEU:HA	2:B:138:MET:CE	2.30	0.60
2:B:156:PHE:HA	2:B:161:LEU:HB2	1.84	0.60
2:B:20:ILE:O	2:B:24:LEU:HB2	2.01	0.60
2:B:284:ILE:CG1	2:B:285:ASN:N	2.62	0.60
3:C:135:ARG:HG3	3:C:135:ARG:HH21	1.65	0.60
3:C:184:GLY:N	3:C:198:VAL:HG22	2.15	0.60
3:C:199:ILE:N	3:C:199:ILE:HD12	2.16	0.60
4:D:157:PHE:HE2	4:D:173:PHE:CE1	2.19	0.60
1:A:223:LEU:HG	4:D:265:ARG:NE	2.17	0.60
16:V:90:PRO:HD2	16:V:92:ARG:HH21	1.65	0.60
23:A:1007:CLA:O1D	23:A:1007:CLA:C2A	2.49	0.60
23:B:1012:CLA:CHD	23:B:1012:CLA:HBC3	2.25	0.60
23:B:1015:CLA:C18	29:B:1060:MGE:C8A	2.78	0.60
23:C:1034:CLA:C14	23:C:1034:CLA:H91	2.24	0.60
3:C:52:ALA:HB2	23:C:1035:CLA:HMA1	1.84	0.60
30:C:1056:DGD:HBT1	30:C:1056:DGD:HB61	1.82	0.60
3:C:199:ILE:HG12	3:C:234:VAL:HG21	1.84	0.60
3:C:88:LEU:CD2	23:C:1027:CLA:HBC3	2.32	0.60
1:A:206:PHE:CZ	23:D:1004:CLA:HBA2	2.36	0.60
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.31	0.60
7:H:31:MET:SD	23:H:1017:CLA:HAA1	2.42	0.60
16:V:111:GLU:HG3	16:V:112:GLN:N	2.15	0.60
23:A:1006:CLA:HMD3	4:D:182:LEU:HD11	1.82	0.60
2:B:51:VAL:CG1	2:B:52:LEU:HG	2.31	0.60
4:D:28:VAL:HG13	4:D:28:VAL:O	2.01	0.60
4:D:73:PHE:CD2	4:D:74:LEU:HD23	2.36	0.60
8:I:6:ILE:CD1	8:I:6:ILE:H	2.10	0.60
8:I:6:ILE:HG12	8:I:7:THR:H	1.65	0.60
1:A:279:ARG:HB3	1:A:279:ARG:NH2	2.16	0.60
2:B:241:SER:CB	23:B:1020:CLA:HED3	2.31	0.60
23:C:1034:CLA:O2A	23:C:1034:CLA:H42	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HB2	30:C:1057:DGD:C8A	2.32	0.60
3:C:123:ALA:O	3:C:127:PHE:N	2.33	0.60
3:C:162:GLY:HA2	3:C:165:LEU:HB2	1.83	0.60
3:C:99:VAL:HG11	3:C:196:VAL:CB	2.26	0.60
4:D:202:ALA:HA	23:D:1005:CLA:O1A	2.01	0.60
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.37	0.60
7:H:38:PHE:CD1	26:H:1049:BCR:H10C	2.36	0.60
14:T:18:PHE:HB2	26:T:6046:BCR:C8	2.31	0.60
17:X:38:ILE:HA	17:X:41:SER:HB2	1.83	0.60
1:A:188:ALA:HB2	1:A:328:MET:CE	2.32	0.60
1:A:202:VAL:HG13	23:A:1003:CLA:HMB3	1.84	0.60
23:B:1014:CLA:C10	26:B:1048:BCR:H311	2.29	0.60
23:B:1013:CLA:HHB	23:B:1014:CLA:HMA1	1.84	0.60
23:B:1023:CLA:ND	23:B:1024:CLA:CBC	2.65	0.60
23:C:1028:CLA:HBC2	23:C:1028:CLA:CHD	2.28	0.60
3:C:377:LEU:CA	3:C:380:ILE:HG22	2.32	0.60
3:C:95:LEU:CD2	3:C:95:LEU:N	2.65	0.60
3:C:95:LEU:O	3:C:185:LEU:HA	2.01	0.60
8:I:31:ASN:HB2	8:I:32:PRO:CD	2.30	0.60
23:A:1006:CLA:CED	30:C:1057:DGD:CDB	2.78	0.60
1:A:161:TYR:HA	1:A:294:ALA:CB	2.32	0.60
2:B:229:LEU:O	2:B:231:MET:N	2.35	0.60
2:B:343:HIS:HE1	2:B:345:VAL:HG13	1.66	0.60
2:B:407:ASN:OD1	2:B:408:GLY:N	2.35	0.60
2:B:7:ARG:CA	23:B:1019:CLA:HBA1	2.31	0.60
3:C:439:VAL:HG13	23:C:1032:CLA:HBC2	1.84	0.60
23:C:1036:CLA:C17	26:Z:1053:BCR:C37	2.77	0.60
4:D:186:GLN:O	4:D:186:GLN:NE2	2.34	0.60
6:F:41:GLN:HE22	9:J:27:LEU:CB	2.15	0.60
29:L:1061:MGE:C7B	29:L:1061:MGE:C3B	2.80	0.60
1:A:310:LYS:HB2	16:V:28:GLU:HG3	1.84	0.60
23:A:1003:CLA:CBC	23:A:1003:CLA:HHD	2.25	0.59
1:A:298:ASN:OD1	1:A:298:ASN:N	2.35	0.59
2:B:30:VAL:HG12	23:B:1013:CLA:HMD2	1.83	0.59
23:C:1029:CLA:O2D	23:C:1029:CLA:C2A	2.50	0.59
27:A:1063:LHG:H321	23:C:1034:CLA:H143	1.81	0.59
27:A:1063:LHG:O1	3:C:447:ARG:NH2	2.35	0.59
23:H:1017:CLA:CBB	26:H:1049:BCR:H323	2.26	0.59
8:I:13:THR:O	8:I:17:LEU:HG	2.02	0.59
15:U:56:ASP:OD1	15:U:58:ASN:N	2.33	0.59
10:K:20:PRO:O	18:Y:21:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:O	1:A:21:VAL:HG13	2.02	0.59
1:A:79:THR:OG1	1:A:80:GLY:N	2.35	0.59
26:B:1047:BCR:C23	26:B:1047:BCR:C38	2.55	0.59
23:B:1024:CLA:H172	26:B:1048:BCR:H343	1.83	0.59
2:B:230:ARG:HA	2:B:230:ARG:HH11	1.65	0.59
2:B:237:VAL:HG22	23:B:1020:CLA:HMD1	1.84	0.59
3:C:304:PRO:HG3	3:C:398:HIS:O	2.02	0.59
3:C:455:PHE:HZ	8:I:31:ASN:HB2	1.67	0.59
4:D:92:LEU:HB3	4:D:93:TRP:HE3	1.66	0.59
5:E:19:TYR:C	5:E:21:VAL:H	2.05	0.59
7:H:12:ARG:HB3	7:H:12:ARG:NH1	2.17	0.59
12:M:17:VAL:N	12:M:18:PRO:HD2	2.16	0.59
11:L:36:PHE:HD2	14:T:6:TYR:CZ	2.19	0.59
15:U:98:THR:H	15:U:101:GLN:CG	2.14	0.59
15:U:73:PRO:HD2	16:V:109:ASP:OD1	2.02	0.59
2:B:148:LEU:HG	2:B:149:LEU:N	2.16	0.59
2:B:143:LEU:HD12	2:B:213:GLY:CA	2.32	0.59
27:A:1063:LHG:C29	23:C:1032:CLA:C8	2.79	0.59
23:C:1033:CLA:H172	23:C:1033:CLA:H141	1.84	0.59
23:C:1034:CLA:C9	23:C:1034:CLA:C13	2.80	0.59
3:C:367:GLU:O	3:C:370:ARG:HB3	2.01	0.59
4:D:39:PRO:O	4:D:42:TYR:HB3	2.01	0.59
9:J:19:MET:O	9:J:23:VAL:N	2.34	0.59
20:Z:37:LYS:HZ2	20:Z:38:GLN:HG2	1.66	0.59
1:A:160:ILE:HD11	30:C:1055:DGD:HBH2	1.82	0.59
2:B:138:MET:SD	23:B:1023:CLA:CBC	2.89	0.59
2:B:39:LEU:O	2:B:43:ALA:N	2.29	0.59
23:C:1026:CLA:CBA	23:C:1027:CLA:HAC1	2.32	0.59
3:C:449:ARG:NH2	23:C:1029:CLA:HED2	2.17	0.59
3:C:61:VAL:HG21	3:C:125:LEU:HD12	1.84	0.59
3:C:140:LEU:CB	3:C:148:GLY:HA2	2.32	0.59
2:B:320:ALA:O	4:D:292:ASN:HB2	2.03	0.59
5:E:37:PHE:CZ	5:E:46:VAL:HG21	2.37	0.59
9:J:10:LEU:C	9:J:13:VAL:HG23	2.21	0.59
11:L:22:LEU:HD22	29:L:1061:MGE:H201	1.84	0.59
12:M:14:PHE:O	12:M:18:PRO:HG3	2.02	0.59
16:V:148:GLU:O	16:V:151:ILE:HB	2.02	0.59
1:A:132:GLU:O	1:A:136:ARG:HB2	2.02	0.59
1:A:14:TRP:NE1	1:A:18:CYS:SG	2.76	0.59
1:A:341:LEU:HD12	3:C:313:GLN:HE22	1.68	0.59
1:A:37:MET:O	1:A:41:LEU:HD23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1012:CLA:HED3	23:B:1013:CLA:H11	1.84	0.59
23:B:1011:CLA:HMD3	23:B:1014:CLA:CBB	2.32	0.59
23:B:1016:CLA:CBD	23:B:1016:CLA:HBA1	2.31	0.59
23:B:1011:CLA:C17	23:B:1016:CLA:HBC1	2.29	0.59
2:B:226:TYR:HD2	2:B:226:TYR:O	1.85	0.59
2:B:460:LEU:CG	30:H:1058:DGD:CIA	2.80	0.59
23:A:1006:CLA:CBA	30:C:1057:DGD:HBN2	2.32	0.59
3:C:276:LEU:C	3:C:278:ALA:H	2.06	0.59
23:D:1005:CLA:C4	25:D:1042:PQ9:H191	2.32	0.59
4:D:235:PHE:CZ	4:D:243:THR:HG22	2.38	0.59
1:A:237:TYR:CE1	4:D:264:LYS:HG2	2.38	0.59
5:E:58:GLN:OE1	5:E:58:GLN:O	2.20	0.59
7:H:53:LEU:O	7:H:55:LEU:HD13	2.02	0.59
13:O:184:ASP:HB2	13:O:185:PRO:CD	2.32	0.59
15:U:72:TYR:CB	15:U:73:PRO:CD	2.80	0.59
16:V:48:THR:N	16:V:51:GLN:HG2	2.16	0.59
18:Y:39:LEU:CD2	20:Z:25:VAL:HG13	2.32	0.59
2:B:24:LEU:HD13	2:B:111:ALA:CA	2.22	0.59
3:C:436:PHE:O	3:C:439:VAL:CG1	2.50	0.59
3:C:453:ALA:HB1	3:C:455:PHE:CZ	2.37	0.59
23:D:1005:CLA:HMB1	23:D:1005:CLA:HBB1	1.84	0.59
5:E:13:ILE:O	5:E:13:ILE:HG23	2.02	0.59
13:O:136:MET:HB2	13:O:142:ILE:CD1	2.33	0.59
16:V:63:CYS:O	16:V:64:ALA:C	2.40	0.59
23:A:1006:CLA:H171	26:D:1050:BCR:H292	1.71	0.59
23:B:1013:CLA:C15	23:B:1018:CLA:HED1	2.32	0.59
2:B:465:GLY:HA3	23:B:1019:CLA:HBC3	1.83	0.59
2:B:113:TRP:CD1	26:B:1048:BCR:C37	2.85	0.59
23:C:1026:CLA:HMB1	23:C:1026:CLA:CBB	2.20	0.59
3:C:410:VAL:O	3:C:412:THR:N	2.36	0.59
4:D:249:ALA:O	4:D:252:PHE:HB3	2.02	0.59
4:D:73:PHE:HD2	4:D:74:LEU:HD23	1.68	0.59
10:K:35:LEU:C	10:K:37:PHE:H	2.06	0.59
11:L:32:SER:OG	11:L:33:SER:N	2.33	0.59
3:C:346:THR:HG21	13:O:38:GLY:N	2.16	0.59
1:A:219:VAL:CG1	4:D:268:HIS:CE1	2.86	0.59
23:B:1011:CLA:CAB	23:B:1013:CLA:H203	2.30	0.59
2:B:9:HIS:HD1	23:B:1019:CLA:H11	1.67	0.59
2:B:148:LEU:CA	2:B:210:ILE:HD11	2.32	0.59
2:B:143:LEU:HD12	2:B:213:GLY:N	2.17	0.59
3:C:167:VAL:HG11	23:C:1036:CLA:H3A	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:399:ALA:O	3:C:401:LEU:N	2.33	0.59
4:D:291:LEU:C	4:D:293:LEU:N	2.56	0.59
23:B:1009:CLA:C4B	26:H:1049:BCR:H382	2.33	0.59
7:H:14:LEU:HD12	7:H:14:LEU:H	1.66	0.59
16:V:35:THR:O	16:V:35:THR:HG22	2.02	0.59
1:A:154:ALA:HB2	23:A:1003:CLA:H61	1.85	0.59
1:A:116:ILE:HG23	1:A:117:PHE:H	1.67	0.59
1:A:147:TYR:C	1:A:150:PRO:HG2	2.23	0.59
23:B:1009:CLA:CHA	23:B:1009:CLA:CBA	2.79	0.59
2:B:156:PHE:HB2	23:B:1014:CLA:HAC2	1.84	0.59
2:B:133:LEU:HD22	23:B:1023:CLA:HBC1	1.85	0.59
1:A:322:ASN:ND2	3:C:412:THR:CG2	2.65	0.59
24:A:1039:PHO:H71	4:D:122:LEU:HD13	1.84	0.59
4:D:123:ILE:O	4:D:127:LEU:HD23	2.02	0.59
2:B:357:ARG:HH22	4:D:337:GLU:HG2	1.67	0.59
4:D:89:LEU:HD23	7:H:52:THR:HG21	1.82	0.59
5:E:10:PHE:HD2	6:F:19:ARG:HH21	1.50	0.59
10:K:28:ILE:N	10:K:29:PRO:HD2	2.17	0.59
13:O:69:LEU:HD22	13:O:121:PHE:CZ	2.38	0.59
14:T:1:MET:N	14:T:1:MET:HE3	2.12	0.59
15:U:89:GLU:O	15:U:91:VAL:N	2.36	0.59
15:U:92:LEU:CD1	15:U:92:LEU:H	2.16	0.59
15:U:93:ASN:O	15:U:94:ILE:C	2.42	0.59
16:V:62:ALA:CB	31:V:1041:HEM:HBB1	2.33	0.59
16:V:98:LEU:CD2	16:V:145:ILE:HG21	2.30	0.59
2:B:260:SER:HB3	2:B:263:THR:OG1	2.03	0.59
2:B:297:THR:O	2:B:300:GLU:N	2.36	0.59
2:B:304:ALA:O	2:B:306:PRO:HD3	2.03	0.59
2:B:478:VAL:O	2:B:480:SER:N	2.36	0.59
2:B:79:SER:C	2:B:81:THR:H	2.05	0.59
23:C:1033:CLA:CED	23:C:1033:CLA:OBD	2.38	0.59
3:C:175:LEU:HD12	3:C:237:HIS:CD2	2.37	0.59
3:C:464:GLU:HG3	3:C:467:LEU:HB2	1.85	0.59
3:C:88:LEU:HD21	23:C:1027:CLA:HBC3	1.84	0.59
5:E:30:LEU:HG	6:F:28:VAL:HG23	1.83	0.59
26:H:1049:BCR:H341	26:H:1049:BCR:C12	2.33	0.59
8:I:3:THR:HA	8:I:6:ILE:HD11	1.84	0.59
5:E:40:THR:HG21	19:N:3:UNK:CB	2.33	0.59
13:O:66:ILE:HD11	13:O:121:PHE:CE2	2.38	0.59
23:B:1010:CLA:C4	7:H:46:LEU:HA	2.32	0.58
23:B:1019:CLA:H192	23:B:1021:CLA:H52	1.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PHE:CE2	23:B:1010:CLA:H202	2.38	0.58
3:C:460:ASP:O	3:C:462:GLU:N	2.36	0.58
3:C:56:HIS:O	3:C:59:LEU:HB2	2.02	0.58
8:I:17:LEU:O	8:I:21:PHE:HB2	2.03	0.58
10:K:18:PHE:C	10:K:20:PRO:HD2	2.24	0.58
18:Y:32:GLY:CA	18:Y:35:ILE:HG23	2.31	0.58
1:A:127:MET:HB2	1:A:151:LEU:HD22	1.84	0.58
29:B:1060:MGE:H101	29:L:1061:MGE:H8A2	1.85	0.58
2:B:16:PRO:O	2:B:20:ILE:HG13	2.02	0.58
2:B:47:PRO:O	2:B:49:ASP:N	2.36	0.58
23:C:1028:CLA:H51	30:C:1056:DGD:HA52	1.85	0.58
3:C:428:THR:HG23	3:C:429:SER:N	2.14	0.58
1:A:24:THR:HB	3:C:469:MET:HE1	1.84	0.58
4:D:311:PHE:CD1	4:D:311:PHE:C	2.76	0.58
15:U:46:LYS:HE2	15:U:59:ASN:HD22	1.65	0.58
16:V:124:ALA:C	16:V:126:ILE:H	2.05	0.58
1:A:289:GLY:O	1:A:292:THR:HG22	2.03	0.58
1:A:293:MET:C	1:A:295:PHE:H	2.04	0.58
23:B:1010:CLA:CAD	23:B:1010:CLA:CED	2.79	0.58
23:B:1020:CLA:H142	23:B:1021:CLA:CAB	2.33	0.58
23:B:1022:CLA:CED	23:B:1022:CLA:CAD	2.80	0.58
26:B:1045:BCR:H353	26:B:1047:BCR:H10C	1.77	0.58
23:C:1029:CLA:H43	23:C:1029:CLA:H191	1.84	0.58
23:C:1033:CLA:CAD	23:C:1033:CLA:HED3	2.31	0.58
3:C:171:GLY:HA2	3:C:174:LEU:HG	1.83	0.58
3:C:297:TYR:HA	3:C:302:TYR:HE2	1.67	0.58
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.83	0.58
4:D:210:LEU:O	4:D:212:ALA:N	2.36	0.58
5:E:42:LEU:O	5:E:46:VAL:HG23	2.03	0.58
4:D:195:PRO:HB3	11:L:30:LEU:HD21	1.84	0.58
18:Y:29:GLY:O	18:Y:33:PRO:CD	2.52	0.58
1:A:223:LEU:HB2	4:D:265:ARG:NH1	2.18	0.58
1:A:86:SER:O	1:A:87:ASN:C	2.41	0.58
23:B:1010:CLA:C3D	23:B:1011:CLA:CMB	2.81	0.58
2:B:297:THR:HG23	2:B:300:GLU:N	2.19	0.58
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.38	0.58
2:B:478:VAL:HG12	4:D:139:ARG:HD2	1.86	0.58
3:C:166:ILE:HG23	3:C:245:ILE:CD1	2.33	0.58
3:C:249:ILE:O	3:C:249:ILE:HG22	2.02	0.58
26:D:1050:BCR:C22	26:D:1050:BCR:H403	2.32	0.58
4:D:24:ARG:O	4:D:26:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:17:VAL:HG11	9:J:7:ARG:HG2	1.84	0.58
13:O:65:ARG:NE	13:O:110:GLU:HA	2.18	0.58
13:O:76:PHE:C	13:O:77:LEU:HD12	2.23	0.58
16:V:122:ARG:O	16:V:123:SER:C	2.41	0.58
16:V:85:LEU:HB3	16:V:92:ARG:C	2.23	0.58
17:X:35:ALA:HA	17:X:38:ILE:HD11	1.86	0.58
24:A:1038:PHO:HBC1	4:D:212:ALA:CB	2.32	0.58
1:A:187:GLN:OE1	1:A:193:LEU:HB2	2.04	0.58
1:A:214:MET:O	1:A:217:SER:N	2.37	0.58
1:A:269:ARG:HE	4:D:243:THR:HG21	1.67	0.58
2:B:464:PHE:CD1	23:B:1019:CLA:HBC1	2.38	0.58
3:C:45:LEU:HD21	3:C:141:GLU:CG	2.32	0.58
3:C:436:PHE:O	3:C:439:VAL:HG13	2.02	0.58
4:D:253:TRP:CA	4:D:256:ILE:HG22	2.23	0.58
23:B:1016:CLA:H51	23:H:1017:CLA:C10	2.29	0.58
2:B:5:TRP:CH2	29:L:1061:MGE:H3A1	2.39	0.58
16:V:48:THR:H	16:V:51:GLN:NE2	2.01	0.58
18:Y:39:LEU:HD21	20:Z:25:VAL:HG13	1.86	0.58
24:A:1039:PHO:H203	24:A:1039:PHO:H141	1.86	0.58
1:A:60:ILE:CD1	1:A:60:ILE:N	2.66	0.58
23:B:1010:CLA:C2D	23:B:1011:CLA:CMB	2.81	0.58
23:B:1022:CLA:HBB1	23:B:1022:CLA:CMB	2.21	0.58
2:B:113:TRP:HB2	26:B:1048:BCR:C37	2.29	0.58
2:B:460:LEU:CG	30:H:1058:DGD:HAG1	2.33	0.58
2:B:80:ILE:O	2:B:80:ILE:HG13	2.04	0.58
23:C:1025:CLA:H202	23:C:1025:CLA:C15	2.27	0.58
3:C:282:MET:O	3:C:286:ALA:HB2	2.04	0.58
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.85	0.58
24:A:1038:PHO:H92	23:D:1005:CLA:H192	1.85	0.58
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.69	0.58
4:D:20:ASP:HA	4:D:23:LYS:NZ	2.19	0.58
4:D:273:PHE:O	4:D:277:THR:HB	2.04	0.58
4:D:291:LEU:HD13	4:D:291:LEU:N	2.19	0.58
13:O:66:ILE:HD12	13:O:267:ALA:HB1	1.84	0.58
23:A:1003:CLA:CMD	23:D:1005:CLA:HBC1	2.34	0.58
1:A:190:HIS:O	1:A:192:ILE:N	2.36	0.58
1:A:248:ILE:O	1:A:251:ALA:HB3	2.04	0.58
1:A:304:HIS:O	1:A:305:SER:C	2.41	0.58
23:B:1023:CLA:H101	23:B:1024:CLA:H13	1.86	0.58
23:C:1030:CLA:HMB2	23:C:1031:CLA:NB	2.19	0.58
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:451:ALA:C	3:C:453:ALA:N	2.57	0.58
3:C:463:SER:O	3:C:465:PRO:HD3	2.03	0.58
3:C:70:PHE:O	3:C:74:HIS:ND1	2.37	0.58
4:D:103:ARG:HH11	4:D:103:ARG:HG3	1.68	0.58
4:D:235:PHE:HZ	4:D:242:GLU:C	2.07	0.58
10:K:24:VAL:O	10:K:27:VAL:HG12	2.03	0.58
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	0.58
2:B:263:THR:HB	2:B:448:ARG:HH22	1.69	0.58
2:B:5:TRP:CE2	2:B:6:TYR:HB3	2.39	0.58
1:A:131:TRP:CH2	23:C:1029:CLA:HMA3	2.39	0.58
24:A:1039:PHO:H93	4:D:118:GLY:HA3	1.86	0.58
4:D:52:THR:HG22	4:D:67:TYR:CE2	2.39	0.58
4:D:96:GLU:OE2	7:H:52:THR:HG22	2.03	0.58
26:T:6046:BCR:C4	26:T:6046:BCR:H312	2.30	0.58
16:V:64:ALA:O	16:V:65:SER:C	2.42	0.58
16:V:98:LEU:HD12	16:V:98:LEU:H	1.69	0.58
1:A:307:ILE:CG1	1:A:308:ASP:H	2.13	0.58
23:B:1016:CLA:O1D	23:B:1016:CLA:H2A	2.03	0.58
23:C:1026:CLA:HBA2	23:C:1027:CLA:HAC1	1.84	0.58
23:C:1028:CLA:HMA2	23:C:1028:CLA:HBA1	1.86	0.58
23:C:1033:CLA:C15	23:C:1036:CLA:HMD2	2.34	0.58
30:C:1056:DGD:HB51	9:J:29:PHE:HE1	1.68	0.58
23:B:1018:CLA:C1B	23:H:1017:CLA:CMB	2.81	0.58
1:A:157:VAL:CG2	1:A:182:PHE:HE2	2.16	0.58
1:A:60:ILE:O	1:A:86:SER:HA	2.04	0.58
2:B:234:ILE:HD12	2:B:237:VAL:CG1	2.34	0.58
2:B:256:MET:CE	2:B:448:ARG:HH12	2.14	0.58
2:B:272:ARG:HG2	2:B:320:ALA:HB2	1.86	0.58
23:C:1025:CLA:CMB	23:C:1025:CLA:H42	2.31	0.58
23:C:1032:CLA:CHC	23:C:1032:CLA:HBB1	2.32	0.58
3:C:260:ALA:HB3	3:C:261:ARG:HH22	1.69	0.58
3:C:377:LEU:C	3:C:380:ILE:HG22	2.23	0.58
7:H:12:ARG:HD3	7:H:16:SER:HB2	1.86	0.58
13:O:218:LEU:HD23	13:O:218:LEU:C	2.23	0.58
16:V:148:GLU:HA	16:V:148:GLU:OE2	2.03	0.58
23:C:1036:CLA:H141	26:Z:1053:BCR:H373	1.85	0.58
1:A:121:LEU:HD11	23:A:1007:CLA:HMB3	1.86	0.57
2:B:273:TYR:HA	2:B:276:ASP:OD2	2.03	0.57
23:C:1025:CLA:CMB	23:C:1025:CLA:H41	2.33	0.57
3:C:270:ALA:HB1	3:C:274:TYR:HE1	1.67	0.57
3:C:391:ARG:HG3	3:C:391:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:262:SER:O	4:D:263:ASN:HB3	2.03	0.57
5:E:10:PHE:C	5:E:12:ASP:H	2.07	0.57
5:E:34:GLY:HA3	6:F:32:PHE:CE2	2.38	0.57
5:E:53:ASP:C	5:E:53:ASP:OD2	2.43	0.57
5:E:34:GLY:HA2	6:F:32:PHE:CZ	2.39	0.57
10:K:28:ILE:HD11	26:K:1051:BCR:C10	2.32	0.57
18:Y:21:GLN:C	18:Y:23:THR:H	2.06	0.57
1:A:275:LEU:O	4:D:211:CYS:O	2.21	0.57
1:A:45:THR:O	1:A:49:VAL:HG23	2.04	0.57
1:A:58:VAL:HB	1:A:83:VAL:HG11	1.86	0.57
1:A:85:SER:OG	1:A:168:PHE:HB2	2.04	0.57
23:B:1012:CLA:C11	23:B:1023:CLA:CGA	2.82	0.57
2:B:154:GLY:HA2	2:B:199:VAL:HG13	1.85	0.57
3:C:61:VAL:HA	23:C:1027:CLA:HMD2	1.85	0.57
23:C:1028:CLA:H41	30:C:1057:DGD:HA42	1.85	0.57
23:C:1037:CLA:H101	23:C:1037:CLA:C14	2.31	0.57
3:C:126:GLY:HA3	26:K:1052:BCR:H363	1.86	0.57
3:C:328:VAL:HG12	3:C:340:TYR:CG	2.38	0.57
23:A:1006:CLA:C18	26:D:1050:BCR:H292	2.34	0.57
1:A:239:PHE:HE2	4:D:246:MET:O	1.88	0.57
4:D:261:PHE:CZ	4:D:267:LEU:HA	2.39	0.57
26:K:1052:BCR:C33	26:K:1052:BCR:C8	2.82	0.57
10:K:18:PHE:HE2	20:Z:9:LEU:HD11	1.68	0.57
14:T:18:PHE:CG	26:T:6046:BCR:H343	2.37	0.57
16:V:59:PHE:CD2	16:V:63:CYS:SG	2.96	0.57
20:Z:16:SER:HB3	20:Z:47:TRP:HE1	1.69	0.57
20:Z:33:TRP:O	20:Z:37:LYS:HB3	2.04	0.57
1:A:46:ILE:O	1:A:50:ILE:HG13	2.03	0.57
23:B:1024:CLA:C2	23:B:1024:CLA:HMA2	2.34	0.57
2:B:27:THR:O	2:B:107:LEU:HD12	2.03	0.57
2:B:117:TYR:HB3	2:B:120:LEU:HD21	1.86	0.57
2:B:368:VAL:CG1	2:B:381:ILE:HB	2.34	0.57
3:C:346:THR:O	3:C:346:THR:HG22	2.03	0.57
4:D:147:SER:C	4:D:280:TRP:HE1	2.08	0.57
5:E:38:VAL:CG2	6:F:36:ALA:HB1	2.34	0.57
8:I:27:ASP:C	8:I:29:ALA:H	2.07	0.57
11:L:17:LEU:O	11:L:21:LEU:N	2.31	0.57
1:A:304:HIS:NE2	16:V:163:TYR:O	2.37	0.57
2:B:234:ILE:HD12	2:B:237:VAL:HG11	1.86	0.57
2:B:31:ALA:HA	2:B:34:ALA:HB2	1.86	0.57
2:B:392:PHE:O	2:B:393:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1033:CLA:C9	23:C:1033:CLA:H51	2.29	0.57
3:C:113:VAL:CG2	3:C:114:VAL:N	2.67	0.57
3:C:190:ALA:HB3	3:C:193:GLY:O	2.04	0.57
3:C:209:ILE:N	3:C:209:ILE:HD12	2.20	0.57
1:A:223:LEU:HD21	4:D:265:ARG:HD3	1.85	0.57
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.86	0.57
7:H:18:TYR:O	7:H:20:LYS:N	2.32	0.57
11:L:26:VAL:HG13	11:L:27:LEU:N	2.20	0.57
13:O:187:GLY:HA3	13:O:194:TYR:HB2	1.87	0.57
13:O:59:ASP:O	13:O:60:SER:HB3	2.05	0.57
16:V:151:ILE:HG22	16:V:152:LEU:HD23	1.86	0.57
17:X:43:ILE:CG2	17:X:43:ILE:O	2.53	0.57
18:Y:21:GLN:C	18:Y:23:THR:N	2.56	0.57
1:A:273:PHE:CD2	27:A:1063:LHG:HC42	2.39	0.57
1:A:27:ARG:HB2	1:A:27:ARG:HH11	1.67	0.57
1:A:330:VAL:HB	4:D:348:ARG:HB2	1.86	0.57
1:A:331:MET:SD	4:D:348:ARG:CA	2.90	0.57
23:C:1037:CLA:HAB	26:Z:1053:BCR:C39	2.35	0.57
3:C:56:HIS:C	3:C:56:HIS:ND1	2.58	0.57
4:D:106:GLN:HE21	5:E:48:GLY:HA3	1.68	0.57
4:D:214:HIS:O	4:D:217:THR:HG22	2.04	0.57
4:D:36:LEU:O	4:D:39:PRO:HD2	2.04	0.57
12:M:32:GLN:NE2	12:M:32:GLN:HA	2.17	0.57
15:U:59:ASN:N	15:U:127:ARG:NH2	2.53	0.57
3:C:243:ILE:HG22	23:C:1030:CLA:HMC1	1.87	0.57
3:C:249:ILE:O	3:C:249:ILE:CG2	2.53	0.57
11:L:15:THR:HA	11:L:18:TYR:HB2	1.86	0.57
13:O:156:GLN:HG2	13:O:167:ASP:OD2	2.05	0.57
2:B:442:ILE:HD11	13:O:200:LEU:HD23	1.87	0.57
15:U:82:ASN:HD21	15:U:94:ILE:HG23	1.68	0.57
16:V:130:MET:HA	16:V:133:LEU:HD13	1.87	0.57
16:V:61:TYR:CD1	16:V:61:TYR:C	2.78	0.57
23:A:1003:CLA:C16	24:A:1038:PHO:C9	2.57	0.57
1:A:166:GLY:HA3	3:C:357:ARG:NH1	2.19	0.57
2:B:454:ALA:O	2:B:458:PHE:HB2	2.05	0.57
23:C:1026:CLA:C7	23:C:1026:CLA:C4	2.80	0.57
23:C:1035:CLA:H151	20:Z:20:VAL:HG13	1.87	0.57
3:C:315:MET:SD	3:C:319:ILE:HD11	2.45	0.57
4:D:183:LEU:HD23	4:D:183:LEU:N	2.19	0.57
2:B:323:GLY:C	4:D:293:LEU:HD22	2.24	0.57
5:E:22:ILE:HA	5:E:25:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:30:ARG:HA	8:I:30:ARG:CZ	2.34	0.57
13:O:148:VAL:HG11	13:O:151:LEU:HD22	1.87	0.57
15:U:98:THR:O	15:U:101:GLN:N	2.38	0.57
17:X:24:LEU:HD12	17:X:24:LEU:C	2.25	0.57
23:A:1006:CLA:HHC	23:A:1006:CLA:CBB	2.29	0.57
24:A:1038:PHO:HAC2	4:D:209:LEU:HA	1.85	0.57
1:A:113:GLN:O	1:A:114:LEU:C	2.40	0.57
1:A:113:GLN:O	1:A:116:ILE:HG22	2.05	0.57
1:A:149:ALA:HB2	1:A:280:VAL:HG13	1.86	0.57
1:A:161:TYR:HA	1:A:294:ALA:HB1	1.85	0.57
2:B:106:LEU:HD11	26:B:1048:BCR:H352	1.86	0.57
2:B:398:THR:HA	2:B:417:VAL:HG21	1.87	0.57
2:B:472:ARG:HG2	2:B:479:PHE:CZ	2.39	0.57
2:B:66:MET:SD	23:B:1013:CLA:CED	2.93	0.57
30:C:1056:DGD:HBT2	30:C:1056:DGD:CEB	2.35	0.57
3:C:261:ARG:CZ	3:C:261:ARG:N	2.68	0.57
4:D:235:PHE:CZ	4:D:243:THR:CG2	2.87	0.57
4:D:246:MET:HE1	4:D:264:LYS:N	2.20	0.57
5:E:19:TYR:O	5:E:21:VAL:N	2.38	0.57
2:B:122:LEU:HB2	7:H:12:ARG:HB2	1.87	0.57
4:D:88:SER:HA	7:H:50:ASN:ND2	2.20	0.57
11:L:30:LEU:CD2	11:L:31:PHE:N	2.68	0.57
3:C:336:GLY:O	13:O:131:PRO:HG3	2.05	0.57
15:U:58:ASN:C	15:U:127:ARG:HH21	2.08	0.57
1:A:340:PRO:HD3	15:U:133:TYR:CE2	2.40	0.57
17:X:12:ILE:O	17:X:12:ILE:HG13	2.05	0.57
1:A:81:ALA:HB1	1:A:174:LEU:O	2.05	0.57
1:A:324:ALA:O	4:D:325:ILE:HG23	2.05	0.57
23:B:1016:CLA:H202	23:D:1008:CLA:C3A	2.35	0.57
2:B:135:LEU:CD1	2:B:135:LEU:H	2.05	0.57
2:B:223:GLN:HG2	7:H:24:GLY:C	2.25	0.57
23:C:1026:CLA:CMB	23:C:1026:CLA:HBB1	2.13	0.57
23:A:1006:CLA:C12	30:C:1057:DGD:HGB1	2.29	0.57
23:A:1006:CLA:CAA	30:C:1057:DGD:HBN2	2.34	0.57
3:C:164:HIS:ND1	23:C:1031:CLA:OBD	2.37	0.57
3:C:213:LEU:HG	3:C:214:LEU:N	2.19	0.57
3:C:189:TRP:CD1	3:C:295:THR:HG22	2.39	0.57
3:C:61:VAL:HG21	3:C:125:LEU:CD1	2.35	0.57
4:D:92:LEU:HD22	4:D:104:TRP:CG	2.40	0.57
4:D:152:VAL:HG13	4:D:153:PHE:N	2.19	0.57
13:O:225:LEU:HD23	13:O:265:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:10:PHE:O	14:T:12:CYS:N	2.37	0.57
31:V:1041:HEM:HBC2	31:V:1041:HEM:HHD	1.87	0.57
1:A:162:PRO:O	1:A:165:GLN:O	2.22	0.57
23:B:1011:CLA:HBB1	23:B:1013:CLA:H192	1.85	0.57
23:C:1034:CLA:H42	23:C:1034:CLA:CGA	2.34	0.57
4:D:36:LEU:HD11	4:D:120:PHE:HB3	1.87	0.57
1:A:314:ILE:HD12	4:D:58:TRP:CZ3	2.39	0.57
5:E:44:TYR:CD2	5:E:51:ARG:NE	2.73	0.57
23:B:1009:CLA:C1	26:H:1049:BCR:H351	2.34	0.57
2:B:426:PHE:CZ	13:O:201:PRO:HB3	2.36	0.57
16:V:81:ARG:HD3	16:V:157:GLY:CA	2.34	0.57
16:V:95:ILE:O	16:V:99:VAL:HG23	2.04	0.57
1:A:31:GLY:O	1:A:34:GLY:N	2.39	0.56
1:A:33:PHE:CE1	8:I:23:PHE:HE2	2.23	0.56
2:B:219:VAL:CG1	2:B:220:ARG:N	2.67	0.56
2:B:368:VAL:HG21	2:B:421:ALA:HB1	1.87	0.56
2:B:448:ARG:HH11	2:B:448:ARG:CB	2.17	0.56
2:B:92:SER:C	2:B:94:GLU:N	2.59	0.56
3:C:204:LEU:N	3:C:204:LEU:HD22	2.20	0.56
3:C:284:PHE:C	3:C:286:ALA:N	2.57	0.56
3:C:311:GLN:NE2	3:C:351:PHE:CD2	2.69	0.56
3:C:354:GLU:HA	3:C:356:MET:HE2	1.85	0.56
4:D:23:LYS:HA	4:D:29:PHE:HE1	1.69	0.56
31:E:1040:HEM:CBC	6:F:19:ARG:HH12	2.17	0.56
4:D:105:CYS:SG	5:E:47:PHE:HB3	2.45	0.56
1:A:140:ARG:NH2	27:A:1063:LHG:C1	2.68	0.56
1:A:90:GLY:CA	1:A:167:SER:CB	2.81	0.56
2:B:190:PHE:CZ	23:B:1009:CLA:HMA3	2.41	0.56
2:B:105:GLY:HA3	26:B:1047:BCR:H282	1.85	0.56
2:B:223:GLN:C	2:B:225:LEU:H	2.08	0.56
2:B:174:LEU:N	2:B:266:GLU:OE1	2.38	0.56
3:C:224:ILE:N	3:C:224:ILE:HD13	2.20	0.56
3:C:97:TRP:HE1	3:C:178:LYS:HE2	1.70	0.56
7:H:48:ILE:CG1	7:H:53:LEU:HD23	2.35	0.56
13:O:147:THR:OG1	13:O:148:VAL:N	2.38	0.56
15:U:71:LEU:HD11	15:U:108:ASN:ND2	2.21	0.56
16:V:159:GLY:HA2	16:V:163:TYR:HE1	1.71	0.56
1:A:41:LEU:HD12	24:A:1038:PHO:C5	2.35	0.56
1:A:106:LEU:HD21	26:A:1044:BCR:C38	2.36	0.56
1:A:104:GLU:OE2	13:O:99:ARG:NH1	2.38	0.56
1:A:116:ILE:HD11	1:A:158:PHE:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TRP:O	1:A:287:ALA:HB3	2.05	0.56
23:B:1011:CLA:HBD	23:B:1011:CLA:HAA1	1.88	0.56
23:B:1013:CLA:HMC3	23:B:1023:CLA:H11	1.87	0.56
29:B:1060:MGE:CBB	29:B:1060:MGE:CFB	2.36	0.56
29:B:1060:MGE:O2D	29:B:1060:MGE:C3G	2.53	0.56
2:B:206:GLY:O	2:B:210:ILE:HG12	2.05	0.56
2:B:259:GLY:HA2	7:H:62:TRP:CZ2	2.40	0.56
23:C:1029:CLA:HBC3	23:C:1029:CLA:CHD	2.35	0.56
3:C:250:TRP:O	3:C:254:THR:HB	2.05	0.56
4:D:199:MET:O	4:D:200:GLY:C	2.42	0.56
12:M:8:PHE:O	12:M:10:ALA:N	2.38	0.56
13:O:65:ARG:HE	13:O:110:GLU:CA	2.17	0.56
14:T:14:ILE:HG23	26:T:6046:BCR:H10C	1.87	0.56
15:U:80:VAL:HG13	15:U:127:ARG:HD3	1.87	0.56
16:V:85:LEU:HD22	16:V:92:ARG:O	2.05	0.56
17:X:24:LEU:HD12	17:X:25:SER:N	2.20	0.56
1:A:269:ARG:HH11	4:D:231:THR:HG23	1.70	0.56
23:B:1020:CLA:HBD	23:B:1020:CLA:HAA1	1.86	0.56
2:B:257:TRP:CZ2	4:D:291:LEU:HA	2.40	0.56
2:B:321:LYS:HB3	2:B:321:LYS:NZ	2.21	0.56
23:C:1033:CLA:H152	23:C:1036:CLA:HMD2	1.88	0.56
3:C:297:TYR:OH	23:C:1026:CLA:O1D	2.23	0.56
3:C:343:ARG:NH1	3:C:343:ARG:HG3	2.20	0.56
4:D:324:GLY:C	4:D:326:ARG:H	2.08	0.56
13:O:133:THR:HG22	13:O:134:VAL:H	1.70	0.56
13:O:36:ILE:HD12	13:O:36:ILE:H	1.70	0.56
14:T:2:GLU:HA	14:T:5:THR:HB	1.87	0.56
14:T:2:GLU:O	14:T:6:TYR:HD2	1.86	0.56
16:V:162:TYR:O	16:V:163:TYR:HB2	2.05	0.56
23:A:1006:CLA:HAA2	30:C:1057:DGD:CFB	2.36	0.56
24:A:1038:PHO:HMA2	4:D:257:PHE:HE2	1.70	0.56
2:B:31:ALA:CB	2:B:103:LEU:HD12	2.34	0.56
2:B:105:GLY:CA	26:B:1047:BCR:H282	2.36	0.56
2:B:159:THR:HG21	2:B:161:LEU:CD2	2.35	0.56
3:C:261:ARG:NH1	3:C:261:ARG:H	2.04	0.56
4:D:103:ARG:HG3	4:D:103:ARG:NH1	2.20	0.56
4:D:199:MET:SD	4:D:281:MET:HG2	2.45	0.56
4:D:92:LEU:CD1	4:D:99:GLY:HA2	2.34	0.56
4:D:93:TRP:N	4:D:93:TRP:CE3	2.71	0.56
8:I:26:GLY:O	8:I:30:ARG:HG2	2.05	0.56
6:F:37:ILE:CG2	9:J:28:PHE:CE1	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:SER:O	1:A:104:GLU:N	2.38	0.56
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.88	0.56
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.88	0.56
2:B:454:ALA:CB	23:B:1015:CLA:CBB	2.83	0.56
2:B:23:HIS:HE1	23:B:1018:CLA:H193	1.70	0.56
23:B:1021:CLA:HBD	23:B:1021:CLA:HAA2	1.87	0.56
2:B:117:TYR:O	2:B:120:LEU:HD21	2.05	0.56
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.88	0.56
2:B:18:ARG:NH1	11:L:4:ASN:ND2	2.53	0.56
23:C:1033:CLA:H151	23:C:1033:CLA:H192	0.71	0.56
23:C:1036:CLA:H172	26:Z:1053:BCR:C37	2.13	0.56
3:C:304:PRO:HB3	3:C:395:TYR:HD2	1.66	0.56
4:D:139:ARG:HH11	4:D:139:ARG:HG3	1.68	0.56
11:L:30:LEU:C	11:L:30:LEU:HD23	2.26	0.56
13:O:178:ARG:HD3	13:O:182:PHE:CG	2.41	0.56
15:U:100:ARG:O	15:U:103:GLN:HB3	2.04	0.56
23:B:1014:CLA:CBC	23:B:1014:CLA:CHD	2.78	0.56
2:B:108:PHE:HD2	2:B:109:LEU:HD23	1.71	0.56
2:B:121:GLU:C	2:B:123:PHE:H	2.07	0.56
30:C:1057:DGD:HBV1	30:C:1057:DGD:HAG2	1.87	0.56
3:C:265:ILE:HG13	3:C:449:ARG:HE	1.69	0.56
3:C:318:LEU:CG	3:C:328:VAL:HG11	2.36	0.56
4:D:274:VAL:HG13	25:D:1042:PQ9:C27	2.35	0.56
7:H:12:ARG:HG3	7:H:15:ASN:HB3	1.88	0.56
13:O:66:ILE:HG13	13:O:66:ILE:O	2.04	0.56
15:U:103:GLN:O	15:U:104:ILE:C	2.44	0.56
23:A:1003:CLA:H193	24:A:1038:PHO:CMA	2.35	0.56
1:A:273:PHE:CE2	1:A:277:ALA:HB2	2.41	0.56
1:A:60:ILE:CD1	1:A:60:ILE:H	2.19	0.56
1:A:91:LEU:HD21	1:A:163:ILE:HA	1.87	0.56
23:B:1012:CLA:O1A	23:B:1013:CLA:CHA	2.53	0.56
23:B:1023:CLA:H122	23:B:1023:CLA:C17	2.25	0.56
2:B:166:MET:HE3	2:B:181:VAL:HG21	1.87	0.56
23:C:1034:CLA:O2A	23:C:1034:CLA:C4	2.53	0.56
23:C:1035:CLA:H172	20:Z:20:VAL:HA	1.88	0.56
3:C:379:LYS:HA	3:C:383:ASP:HB2	1.87	0.56
3:C:441:HIS:HD2	3:C:442:LEU:HD23	1.69	0.56
8:I:6:ILE:HG12	8:I:7:THR:N	2.21	0.56
13:O:37:VAL:O	13:O:37:VAL:HG13	2.06	0.56
13:O:85:LYS:HG3	13:O:86:ARG:H	1.71	0.56
16:V:90:PRO:HG2	16:V:92:ARG:CZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:43:ARG:O	20:Z:30:PRO:HD2	2.06	0.56
23:A:1003:CLA:H172	24:A:1038:PHO:C4	2.28	0.56
1:A:183:MET:HB3	23:A:1003:CLA:CBC	2.34	0.56
1:A:94:TYR:CE2	13:O:99:ARG:NH1	2.74	0.56
2:B:113:TRP:HD1	26:B:1048:BCR:H373	1.67	0.56
2:B:141:ILE:HG23	2:B:217:ILE:CD1	2.35	0.56
23:C:1029:CLA:HAA1	23:C:1029:CLA:CBD	2.36	0.56
23:C:1030:CLA:HMC2	23:C:1031:CLA:C8	2.35	0.56
3:C:459:ILE:HB	4:D:223:PHE:CE1	2.41	0.56
3:C:94:THR:HG22	3:C:298:PRO:HG3	1.88	0.56
24:A:1038:PHO:HHB	23:D:1005:CLA:C9	2.34	0.56
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.05	0.56
4:D:168:PHE:CD2	4:D:168:PHE:C	2.79	0.56
31:E:1040:HEM:CBB	31:E:1040:HEM:HMB2	2.34	0.56
5:E:8:ARG:HA	5:E:8:ARG:HE	1.71	0.56
8:I:4:LEU:O	8:I:4:LEU:HD12	2.06	0.56
15:U:58:ASN:C	15:U:127:ARG:NH2	2.60	0.56
16:V:36:VAL:HG23	16:V:37:PRO:N	2.21	0.56
17:X:13:THR:HG23	17:X:14:PRO:CD	2.36	0.56
1:A:239:PHE:CZ	4:D:247:VAL:HG13	2.41	0.56
1:A:22:THR:HA	1:A:29:TYR:HE1	1.70	0.56
23:B:1022:CLA:C4D	23:B:1022:CLA:O1A	2.53	0.56
23:B:1012:CLA:H102	23:B:1023:CLA:H11	1.86	0.56
2:B:12:LEU:HD13	2:B:19:LEU:HA	1.86	0.56
2:B:279:TYR:O	2:B:280:PHE:C	2.43	0.56
2:B:443:PHE:O	2:B:443:PHE:HD2	1.88	0.56
3:C:244:CYS:HA	23:C:1030:CLA:HMC3	1.88	0.56
23:C:1034:CLA:H143	23:C:1034:CLA:C9	2.32	0.56
30:C:1057:DGD:CEA	29:J:1059:MGE:H222	2.36	0.56
4:D:284:ILE:O	4:D:287:VAL:HG13	2.06	0.56
13:O:205:GLU:C	13:O:207:GLU:N	2.59	0.56
13:O:41:LEU:C	13:O:43:ASN:H	2.10	0.56
23:B:1013:CLA:H152	23:B:1018:CLA:CED	2.36	0.56
2:B:464:PHE:HD1	23:B:1019:CLA:HBC1	1.70	0.56
2:B:13:ILE:HD12	2:B:14:ASN:N	2.21	0.56
3:C:123:ALA:HA	26:K:1052:BCR:H351	1.88	0.56
13:O:145:LEU:HD23	13:O:145:LEU:N	2.18	0.56
11:L:18:TYR:HE2	14:T:20:ALA:HA	1.71	0.56
15:U:118:GLU:C	15:U:118:GLU:OE2	2.44	0.56
16:V:105:PRO:HD2	16:V:115:ALA:HB2	1.86	0.56
18:Y:19:ILE:C	18:Y:19:ILE:HD13	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:O	1:A:115:ILE:N	2.39	0.55
1:A:194:MET:CE	1:A:300:PHE:HB2	2.35	0.55
23:B:1010:CLA:C4D	23:B:1011:CLA:CMB	2.84	0.55
2:B:158:LEU:CD1	2:B:199:VAL:HG22	2.36	0.55
2:B:362:PHE:H	2:B:362:PHE:HD2	1.53	0.55
3:C:250:TRP:NE1	23:C:1030:CLA:CED	2.65	0.55
23:A:1003:CLA:CAD	23:D:1005:CLA:CBC	2.85	0.55
5:E:37:PHE:HE2	5:E:43:ALA:HA	1.71	0.55
7:H:6:TRP:CD1	7:H:10:ILE:HD11	2.41	0.55
26:T:6046:BCR:C38	26:T:6046:BCR:H373	2.25	0.55
15:U:109:LEU:O	15:U:111:HIS:N	2.39	0.55
16:V:89:THR:OG1	16:V:109:ASP:HA	2.05	0.55
1:A:273:PHE:CZ	1:A:277:ALA:HB2	2.41	0.55
1:A:313:VAL:HG13	1:A:313:VAL:O	2.07	0.55
23:B:1023:CLA:CBB	23:B:1023:CLA:HHC	2.34	0.55
2:B:191:ASN:HD22	2:B:192:PRO:N	2.03	0.55
2:B:371:THR:HG23	2:B:371:THR:O	2.05	0.55
23:C:1035:CLA:HAA1	23:C:1035:CLA:HBD	1.87	0.55
3:C:274:TYR:H	3:C:274:TYR:HD1	1.53	0.55
1:A:296:ASN:CG	3:C:401:LEU:HG	2.27	0.55
4:D:311:PHE:HD1	4:D:311:PHE:C	2.08	0.55
5:E:23:HIS:HA	5:E:26:THR:OG1	2.06	0.55
7:H:11:LEU:O	7:H:14:LEU:HB2	2.06	0.55
12:M:4:ASN:OD1	12:M:6:LEU:HG	2.06	0.55
15:U:88:VAL:HG12	15:U:109:LEU:HD13	1.88	0.55
23:C:1036:CLA:H151	26:Z:1053:BCR:C36	2.36	0.55
1:A:149:ALA:HA	1:A:284:TRP:CD1	2.40	0.55
1:A:288:LEU:HD23	3:C:432:VAL:HG13	1.88	0.55
23:B:1016:CLA:HBC2	23:B:1016:CLA:CHD	2.28	0.55
23:B:1018:CLA:HBD	23:B:1018:CLA:HAA2	1.87	0.55
23:B:1022:CLA:C17	23:B:1022:CLA:C14	2.39	0.55
23:B:1014:CLA:H143	26:B:1048:BCR:H10C	1.88	0.55
2:B:15:ASP:C	2:B:17:GLY:H	2.09	0.55
2:B:256:MET:HG3	2:B:451:PHE:CD2	2.42	0.55
3:C:459:ILE:CD1	3:C:459:ILE:N	2.68	0.55
4:D:261:PHE:CE2	4:D:267:LEU:CB	2.88	0.55
4:D:91:LEU:HA	23:D:1008:CLA:CED	2.36	0.55
13:O:162:ILE:HD12	13:O:162:ILE:H	1.71	0.55
1:A:231:GLU:HG2	1:A:235:TYR:HE1	1.72	0.55
1:A:288:LEU:O	1:A:292:THR:N	2.39	0.55
1:A:33:PHE:CB	1:A:129:ARG:HB2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:PHE:CD1	23:B:1014:CLA:HBC1	2.41	0.55
2:B:165:GLY:CA	2:B:180:PRO:HA	2.36	0.55
2:B:246:PHE:C	2:B:246:PHE:CD1	2.79	0.55
2:B:262:THR:C	2:B:264:PRO:HD3	2.27	0.55
2:B:315:ILE:HG23	2:B:316:GLY:N	2.21	0.55
2:B:354:LEU:HD22	2:B:370:LEU:HD13	1.87	0.55
23:C:1028:CLA:H42	30:C:1056:DGD:HB32	1.88	0.55
23:C:1034:CLA:C12	23:C:1034:CLA:H92	2.27	0.55
3:C:262:ARG:O	3:C:263:ALA:HB3	2.07	0.55
2:B:384:ARG:NH1	4:D:348:ARG:HD3	2.21	0.55
7:H:3:ARG:HH22	11:L:1:MET:H1	1.55	0.55
10:K:35:LEU:O	10:K:37:PHE:N	2.40	0.55
13:O:120:THR:O	13:O:120:THR:HG22	2.06	0.55
16:V:64:ALA:O	16:V:66:CYS:O	2.24	0.55
1:A:128:GLY:C	1:A:130:GLN:N	2.60	0.55
2:B:155:ALA:O	2:B:161:LEU:HD23	2.07	0.55
23:A:1006:CLA:C11	30:C:1057:DGD:HBG3	2.07	0.55
3:C:295:THR:O	3:C:298:PRO:HD3	2.05	0.55
4:D:286:VAL:HG21	23:D:1004:CLA:HED2	1.88	0.55
4:D:80:THR:HB	4:D:81:PRO:HD2	1.89	0.55
7:H:40:VAL:CG1	7:H:41:PHE:N	2.70	0.55
10:K:32:PHE:HE2	26:K:1051:BCR:C34	2.15	0.55
1:A:57:PRO:HG2	13:O:141:ARG:HH12	1.69	0.55
13:O:179:THR:HG22	13:O:180:ALA:H	1.69	0.55
13:O:266:TYR:CD1	13:O:267:ALA:N	2.75	0.55
16:V:114:ILE:HG23	16:V:114:ILE:O	2.06	0.55
18:Y:19:ILE:O	18:Y:19:ILE:HD13	2.06	0.55
1:A:192:ILE:HD13	1:A:198:HIS:CD2	2.42	0.55
1:A:309:ALA:HB3	16:V:28:GLU:HG2	1.89	0.55
1:A:339:PHE:HD2	28:A:1065:BR:BR	2.45	0.55
23:B:1019:CLA:H91	29:L:1061:MGE:C8A	2.37	0.55
2:B:25:MET:CE	2:B:108:PHE:CD1	2.89	0.55
2:B:152:GLY:HA2	2:B:155:ALA:CB	2.34	0.55
2:B:326:ARG:CB	2:B:444:ARG:HG3	2.32	0.55
2:B:434:THR:OG1	13:O:204:LYS:HE3	2.06	0.55
14:T:25:GLU:O	14:T:25:GLU:HG3	2.07	0.55
16:V:61:TYR:HD1	16:V:61:TYR:C	2.09	0.55
16:V:68:VAL:C	16:V:70:GLY:H	2.08	0.55
1:A:126:TYR:CE2	24:A:1038:PHO:O1A	2.59	0.55
1:A:53:ILE:HG22	1:A:54:ALA:N	2.21	0.55
1:A:76:ASN:ND2	1:A:79:THR:HG23	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1016:CLA:HBD	23:B:1016:CLA:HBA1	1.88	0.55
2:B:142:HIS:HA	2:B:145:LEU:HD12	1.88	0.55
2:B:226:TYR:O	2:B:226:TYR:CD2	2.60	0.55
2:B:422:ARG:HD2	2:B:423:LYS:HZ1	1.70	0.55
4:D:213:ILE:HG23	4:D:214:HIS:H	1.72	0.55
4:D:89:LEU:HG	4:D:91:LEU:CD1	2.35	0.55
5:E:42:LEU:O	5:E:43:ALA:C	2.44	0.55
5:E:68:ASP:CA	5:E:69:ARG:HE	2.19	0.55
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.37	0.55
15:U:98:THR:N	15:U:101:GLN:HG3	2.22	0.55
17:X:34:PHE:O	17:X:38:ILE:HD11	2.06	0.55
1:A:210:LEU:HD23	23:A:1006:CLA:H51	1.88	0.55
23:B:1016:CLA:H202	23:D:1008:CLA:H3A	1.87	0.55
23:B:1024:CLA:C1	23:B:1024:CLA:HMA2	2.36	0.55
2:B:144:PHE:O	2:B:210:ILE:HD13	2.06	0.55
2:B:348:ASN:HD21	2:B:350:GLU:HB2	1.71	0.55
23:C:1026:CLA:C3B	23:C:1028:CLA:HBB2	2.36	0.55
1:A:155:PHE:CD1	30:C:1055:DGD:HBF2	2.42	0.55
3:C:162:GLY:O	3:C:165:LEU:HB2	2.07	0.55
3:C:248:GLY:C	3:C:250:TRP:H	2.09	0.55
4:D:155:SER:HA	4:D:159:ILE:HD11	1.88	0.55
4:D:65:SER:O	4:D:76:VAL:HG22	2.07	0.55
6:F:18:VAL:C	6:F:20:TRP:N	2.59	0.55
10:K:39:VAL:CG2	18:Y:36:ILE:HD12	2.33	0.55
13:O:150:ASN:O	13:O:151:LEU:O	2.24	0.55
16:V:120:SER:N	16:V:123:SER:HB2	2.13	0.55
26:A:1044:BCR:H371	26:A:1044:BCR:H403	1.30	0.55
1:A:199:GLN:HG3	1:A:200:LEU:H	1.72	0.55
23:B:1010:CLA:C1D	23:B:1011:CLA:CMB	2.85	0.55
23:B:1020:CLA:C1	23:B:1023:CLA:CED	2.63	0.55
23:B:1023:CLA:CMA	23:B:1023:CLA:O1A	2.55	0.55
2:B:185:TRP:CD1	2:B:185:TRP:N	2.74	0.55
2:B:226:TYR:HE2	2:B:231:MET:O	1.90	0.55
2:B:229:LEU:HD21	2:B:236:THR:OG1	2.06	0.55
2:B:250:PHE:CE2	23:B:1010:CLA:C20	2.90	0.55
2:B:277:SER:O	2:B:278:SER:HB2	2.07	0.55
2:B:74:SER:HA	2:B:92:SER:HB2	1.88	0.55
3:C:85:GLY:H	30:C:1056:DGD:HE4	1.71	0.55
3:C:254:THR:HG22	3:C:255:THR:O	2.06	0.55
23:A:1006:CLA:C18	26:D:1050:BCR:C29	2.85	0.55
4:D:168:PHE:HD2	4:D:168:PHE:C	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:331:PRO:HA	4:D:339:PHE:HB2	1.88	0.55
1:A:97:TRP:HB2	8:I:1:MET:HG3	1.88	0.55
1:A:57:PRO:HG2	13:O:141:ARG:CZ	2.37	0.55
13:O:154:SER:O	13:O:168:PHE:HA	2.07	0.55
17:X:33:THR:CG2	17:X:34:PHE:N	2.70	0.55
23:C:1027:CLA:C17	26:Z:1053:BCR:H10C	2.35	0.55
20:Z:62:VAL:O	20:Z:62:VAL:HG22	2.06	0.55
2:B:249:ALA:HB2	23:B:1012:CLA:CBC	2.37	0.55
2:B:456:ALA:CB	30:H:1058:DGD:HBG2	2.36	0.55
3:C:63:TRP:N	23:C:1034:CLA:CED	2.69	0.55
23:C:1036:CLA:C18	26:Z:1053:BCR:C37	2.85	0.55
30:C:1056:DGD:HBN2	10:K:30:VAL:CG2	2.28	0.55
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.07	0.55
3:C:56:HIS:ND1	3:C:57:ALA:N	2.54	0.55
1:A:244:GLU:HG3	4:D:264:LYS:HZ1	1.71	0.55
11:L:16:SER:HA	11:L:19:LEU:HD12	1.88	0.55
13:O:71:LEU:HD22	13:O:148:VAL:HG21	1.89	0.55
1:A:94:TYR:HE2	13:O:99:ARG:NH1	2.04	0.55
11:L:21:LEU:HB3	14:T:16:LEU:HD21	1.89	0.55
17:X:11:THR:O	17:X:12:ILE:HG22	2.07	0.55
23:B:1016:CLA:CHA	23:B:1016:CLA:CBA	2.80	0.54
23:B:1021:CLA:C18	29:B:1060:MGE:CDA	2.85	0.54
2:B:221:PRO:HA	23:H:1017:CLA:CED	2.26	0.54
2:B:248:ALA:O	2:B:252:VAL:HG23	2.07	0.54
2:B:73:GLY:HA3	2:B:88:PRO:HD2	1.89	0.54
4:D:227:GLU:O	4:D:228:GLY:O	2.24	0.54
5:E:32:ILE:O	5:E:36:LEU:HG	2.07	0.54
7:H:38:PHE:HD1	26:H:1049:BCR:H10C	1.72	0.54
11:L:18:TYR:HE2	14:T:19:PHE:O	1.90	0.54
2:B:325:PHE:CD1	11:L:34:TYR:HB3	2.42	0.54
13:O:31:LEU:CD2	13:O:31:LEU:N	2.70	0.54
15:U:42:VAL:HG23	15:U:43:VAL:N	2.22	0.54
2:B:159:THR:HG21	2:B:161:LEU:HD22	1.89	0.54
2:B:165:GLY:HA3	2:B:180:PRO:CA	2.37	0.54
2:B:397:VAL:HG22	2:B:417:VAL:HG11	1.88	0.54
3:C:276:LEU:HD22	3:C:441:HIS:HB2	1.89	0.54
1:A:234:ASN:O	4:D:263:ASN:ND2	2.39	0.54
4:D:72:ASN:ND2	4:D:74:LEU:HG	2.21	0.54
4:D:76:VAL:O	4:D:77:ALA:HB2	2.06	0.54
8:I:13:THR:CG2	8:I:14:PHE:H	2.18	0.54
8:I:3:THR:O	8:I:6:ILE:HD11	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:8:ILE:HG22	9:J:9:PRO:HD2	1.89	0.54
20:Z:12:LEU:HD11	20:Z:51:VAL:HB	1.89	0.54
1:A:119:PHE:CZ	23:A:1003:CLA:H91	2.43	0.54
1:A:160:ILE:HG21	1:A:291:SER:CA	2.36	0.54
1:A:76:ASN:HD22	1:A:79:THR:HG23	1.71	0.54
2:B:458:PHE:CG	23:B:1012:CLA:HMC3	2.41	0.54
2:B:150:CYS:O	2:B:153:PHE:N	2.25	0.54
2:B:223:GLN:HB2	2:B:227:LYS:HZ3	1.72	0.54
2:B:326:ARG:HE	2:B:442:ILE:HG22	1.71	0.54
2:B:414:PRO:O	2:B:415:PRO:C	2.44	0.54
2:B:91:TRP:HE3	2:B:91:TRP:HA	1.72	0.54
23:C:1025:CLA:C2B	23:C:1025:CLA:H42	2.34	0.54
3:C:314:ALA:O	3:C:315:MET:C	2.46	0.54
3:C:405:ASN:CG	3:C:405:ASN:O	2.45	0.54
1:A:130:GLN:HA	4:D:256:ILE:HD12	1.89	0.54
4:D:43:LEU:N	4:D:43:LEU:HD13	2.22	0.54
13:O:56:TYR:HH	13:O:64:TYR:HE2	1.56	0.54
15:U:59:ASN:O	15:U:60:THR:O	2.25	0.54
23:C:1037:CLA:C1B	26:Z:1053:BCR:H282	2.37	0.54
20:Z:49:ALA:C	20:Z:53:VAL:HG23	2.28	0.54
1:A:197:PHE:O	1:A:200:LEU:N	2.39	0.54
2:B:13:ILE:O	2:B:234:ILE:HG21	2.08	0.54
2:B:277:SER:HB3	2:B:279:TYR:HB2	1.89	0.54
2:B:288:VAL:HG21	2:B:302:TRP:CD2	2.42	0.54
2:B:461:LEU:HA	4:D:280:TRP:HZ3	1.72	0.54
2:B:9:HIS:HB2	23:B:1019:CLA:CGA	2.38	0.54
3:C:116:VAL:C	3:C:118:HIS:H	2.09	0.54
3:C:211:GLY:O	3:C:214:LEU:HB3	2.07	0.54
3:C:336:GLY:HA3	13:O:177:TYR:O	2.07	0.54
4:D:350:ASN:O	4:D:351:ALA:HB3	2.08	0.54
4:D:44:ALA:O	4:D:45:LEU:C	2.45	0.54
4:D:52:THR:O	4:D:66:SER:HA	2.07	0.54
4:D:54:PHE:HB3	5:E:47:PHE:CE1	2.43	0.54
9:J:10:LEU:CA	9:J:13:VAL:HG23	2.38	0.54
15:U:43:VAL:HG12	15:U:44:ASP:N	2.21	0.54
1:A:149:ALA:CB	1:A:283:VAL:HG22	2.23	0.54
1:A:30:VAL:O	1:A:30:VAL:HG12	2.07	0.54
2:B:281:GLN:HA	2:B:284:ILE:HG12	1.90	0.54
3:C:100:GLY:O	3:C:103:GLY:N	2.38	0.54
23:C:1034:CLA:C4	23:C:1034:CLA:CGA	2.85	0.54
3:C:211:GLY:O	3:C:212:TYR:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:C	3:C:72:LEU:HD13	2.28	0.54
23:D:1008:CLA:HAA1	23:D:1008:CLA:HBD	1.89	0.54
23:A:1006:CLA:H171	26:D:1050:BCR:H401	1.55	0.54
4:D:27:PHE:HB3	6:F:19:ARG:HB2	1.90	0.54
4:D:58:TRP:O	4:D:62:GLY:HA2	2.07	0.54
2:B:212:ALA:HB2	23:H:1017:CLA:HMC3	1.88	0.54
7:H:35:MET:HG3	26:H:1049:BCR:H333	1.85	0.54
10:K:28:ILE:HG22	10:K:29:PRO:HD3	0.62	0.54
2:B:6:TYR:CE2	11:L:11:GLU:HG3	2.43	0.54
16:V:130:MET:HA	16:V:133:LEU:CD1	2.37	0.54
20:Z:17:PHE:O	20:Z:21:ILE:HG13	2.07	0.54
23:A:1006:CLA:CBC	23:A:1006:CLA:CHD	2.77	0.54
23:A:1006:CLA:H142	23:D:1004:CLA:H192	1.88	0.54
1:A:200:LEU:O	1:A:282:GLY:HA3	2.08	0.54
1:A:261:GLN:O	1:A:263:ALA:N	2.38	0.54
23:B:1009:CLA:C3B	26:H:1049:BCR:C38	2.82	0.54
30:C:1057:DGD:HB92	30:C:1057:DGD:HA92	1.90	0.54
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.20	0.54
4:D:313:THR:H	4:D:316:THR:HG23	1.73	0.54
7:H:41:PHE:HD2	7:H:42:LEU:HD23	1.72	0.54
7:H:61:SER:OG	7:H:63:LYS:HB2	2.08	0.54
9:J:21:VAL:HG13	9:J:22:ILE:H	1.73	0.54
10:K:28:ILE:O	10:K:31:LEU:HD12	2.06	0.54
26:Z:1053:BCR:C27	26:Z:1053:BCR:H403	2.38	0.54
23:B:1010:CLA:H12	7:H:49:TYR:HD2	1.73	0.54
29:B:1060:MGE:O1B	29:B:1060:MGE:H1G1	2.07	0.54
2:B:449:GLY:O	2:B:452:THR:HB	2.07	0.54
3:C:163:PHE:CD2	23:C:1036:CLA:HBB1	2.43	0.54
3:C:42:LEU:HB3	3:C:151:TRP:HH2	1.71	0.54
23:A:1003:CLA:CHA	23:D:1005:CLA:HAC2	2.37	0.54
4:D:281:MET:HA	4:D:281:MET:HE2	1.90	0.54
4:D:21:TRP:CD1	17:X:40:ILE:HG22	2.43	0.54
1:A:223:LEU:O	1:A:224:ILE:O	2.26	0.54
2:B:9:HIS:CE1	23:B:1020:CLA:HBB2	2.42	0.54
2:B:153:PHE:HD2	2:B:202:HIS:ND1	2.06	0.54
2:B:217:ILE:HG23	2:B:218:LEU:CD2	2.38	0.54
2:B:462:PHE:CE1	23:B:1012:CLA:HAC1	2.43	0.54
2:B:51:VAL:HG13	2:B:52:LEU:HG	1.89	0.54
3:C:324:LEU:O	15:U:77:LYS:HG3	2.08	0.54
23:D:1005:CLA:H72	29:D:1062:MGE:CAB	2.36	0.54
4:D:26:ARG:NH1	6:F:17:THR:OG1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:TYR:O	5:E:46:VAL:N	2.40	0.54
14:T:2:GLU:HG3	14:T:3:THR:N	2.22	0.54
16:V:55:GLY:O	16:V:59:PHE:HB2	2.07	0.54
23:C:1036:CLA:C18	26:Z:1053:BCR:H373	2.37	0.54
20:Z:3:ILE:CD1	20:Z:3:ILE:H	2.05	0.54
23:B:1015:CLA:H13	23:B:1021:CLA:H121	1.89	0.54
2:B:16:PRO:HA	2:B:19:LEU:HB3	1.89	0.54
2:B:235:GLU:OE2	2:B:472:ARG:HB2	2.07	0.54
2:B:27:THR:HG23	23:B:1013:CLA:CAC	2.36	0.54
2:B:309:LEU:O	2:B:309:LEU:HD23	2.08	0.54
3:C:60:ILE:HG12	23:C:1027:CLA:CMD	2.38	0.54
3:C:171:GLY:C	3:C:173:LEU:H	2.11	0.54
3:C:349:ILE:N	3:C:349:ILE:CD1	2.71	0.54
4:D:213:ILE:HG23	4:D:214:HIS:N	2.21	0.54
4:D:256:ILE:CG2	4:D:257:PHE:H	2.19	0.54
5:E:75:GLN:HG3	5:E:79:PHE:HE1	1.72	0.54
26:K:1051:BCR:H331	26:K:1051:BCR:C9	2.24	0.54
13:O:179:THR:CG2	13:O:180:ALA:N	2.71	0.54
13:O:65:ARG:CZ	13:O:66:ILE:N	2.59	0.54
11:L:25:LEU:HD22	14:T:13:ILE:HD13	1.89	0.54
3:C:325:GLY:C	15:U:128:TYR:CE2	2.82	0.54
16:V:108:TYR:O	16:V:109:ASP:O	2.26	0.54
16:V:54:GLU:O	16:V:58:LEU:HB2	2.08	0.54
1:A:59:ASP:OD1	1:A:64:ARG:HA	2.08	0.54
1:A:95:PRO:O	1:A:96:ILE:C	2.45	0.54
23:B:1013:CLA:HMC2	23:B:1023:CLA:C1	2.33	0.54
23:B:1016:CLA:HBC3	23:B:1016:CLA:CHD	2.32	0.54
23:B:1024:CLA:CMB	26:B:1048:BCR:H351	2.38	0.54
2:B:160:GLY:O	2:B:162:PHE:N	2.41	0.54
2:B:280:PHE:CZ	2:B:312:TYR:CD1	2.96	0.54
2:B:315:ILE:HG12	2:B:321:LYS:HG3	1.90	0.54
2:B:373:LYS:CG	2:B:374:ASN:H	2.21	0.54
3:C:240:ILE:HD13	26:C:1054:BCR:C37	2.37	0.54
26:C:1054:BCR:C23	26:C:1054:BCR:H382	2.23	0.54
3:C:116:VAL:C	3:C:118:HIS:N	2.60	0.54
3:C:160:ILE:HB	23:C:1031:CLA:HMD1	1.90	0.54
3:C:162:GLY:CA	3:C:165:LEU:HB2	2.38	0.54
23:D:1005:CLA:HMA1	23:D:1005:CLA:H142	1.90	0.54
4:D:344:GLU:HG3	4:D:345:VAL:H	1.73	0.54
13:O:227:VAL:HG12	13:O:228:ALA:N	2.23	0.54
2:B:297:THR:HG22	2:B:300:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:HIS:CG	23:B:1020:CLA:HBB2	2.43	0.53
23:C:1032:CLA:H92	23:C:1032:CLA:C5	2.36	0.53
3:C:116:VAL:HG11	26:Z:1053:BCR:HC31	1.90	0.53
1:A:296:ASN:HB2	3:C:400:PRO:O	2.07	0.53
3:C:435:PHE:O	3:C:438:LEU:N	2.40	0.53
3:C:88:LEU:O	3:C:92:ILE:HG23	2.07	0.53
4:D:270:PHE:O	4:D:274:VAL:HG23	2.07	0.53
24:A:1039:PHO:H18	4:D:48:TRP:CE2	2.42	0.53
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.89	0.53
8:I:1:MET:CE	8:I:4:LEU:HD23	2.37	0.53
13:O:247:SER:OG	13:O:257:HIS:N	2.37	0.53
20:Z:16:SER:HA	20:Z:19:MET:HB2	1.90	0.53
23:B:1014:CLA:HAA1	23:B:1014:CLA:HBD	1.89	0.53
23:B:1024:CLA:CMC	23:B:1024:CLA:CBC	2.66	0.53
26:B:1045:BCR:H403	26:B:1045:BCR:C22	2.34	0.53
2:B:272:ARG:CG	2:B:320:ALA:HB2	2.38	0.53
2:B:75:TRP:HB2	2:B:94:GLU:HG3	1.90	0.53
27:A:1063:LHG:C32	23:C:1034:CLA:C9	2.79	0.53
3:C:54:VAL:O	3:C:54:VAL:HG12	2.09	0.53
4:D:129:GLN:CB	4:D:143:ALA:HB2	2.37	0.53
4:D:218:VAL:HA	4:D:221:THR:CG2	2.38	0.53
1:A:323:ARG:NH1	4:D:328:TRP:O	2.41	0.53
9:J:21:VAL:HG13	9:J:22:ILE:N	2.23	0.53
3:C:116:VAL:HG23	26:K:1052:BCR:HC41	1.90	0.53
15:U:80:VAL:HG22	15:U:127:ARG:CZ	2.39	0.53
20:Z:42:LEU:HD13	20:Z:43:GLY:N	2.23	0.53
1:A:337:HIS:CB	28:A:1065:BR:BR	3.12	0.53
1:A:150:PRO:O	1:A:151:LEU:C	2.46	0.53
23:B:1020:CLA:H12	23:B:1023:CLA:O2D	2.08	0.53
2:B:370:LEU:HB2	2:B:379:ALA:O	2.07	0.53
2:B:465:GLY:N	23:B:1019:CLA:HBC2	2.19	0.53
3:C:60:ILE:CG1	23:C:1027:CLA:HMD3	2.37	0.53
23:C:1029:CLA:H111	23:C:1029:CLA:C19	2.35	0.53
23:C:1037:CLA:H191	23:C:1037:CLA:HMD2	1.91	0.53
3:C:117:VAL:HG12	3:C:117:VAL:O	2.08	0.53
3:C:46:SER:H	3:C:140:LEU:CD2	2.21	0.53
3:C:233:VAL:HG13	3:C:234:VAL:H	1.72	0.53
3:C:273:SER:O	3:C:276:LEU:N	2.38	0.53
4:D:158:LEU:O	4:D:162:LEU:HG	2.08	0.53
4:D:45:LEU:HD13	4:D:46:GLY:N	2.24	0.53
5:E:15:THR:OG1	9:J:10:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:183:LEU:H	13:O:183:LEU:HD12	1.73	0.53
15:U:73:PRO:HD2	16:V:109:ASP:CG	2.28	0.53
15:U:80:VAL:CG1	15:U:127:ARG:HD3	2.38	0.53
23:A:1003:CLA:C3D	23:D:1005:CLA:HAC2	2.38	0.53
1:A:60:ILE:CG2	1:A:83:VAL:CG1	2.85	0.53
2:B:247:PHE:HE1	23:B:1010:CLA:H8	1.72	0.53
23:B:1013:CLA:H71	23:B:1018:CLA:H42	1.91	0.53
23:B:1014:CLA:C11	26:B:1048:BCR:H10C	2.32	0.53
2:B:11:VAL:O	2:B:12:LEU:HD23	2.09	0.53
2:B:457:VAL:CG1	4:D:284:ILE:HD13	2.38	0.53
3:C:155:ASN:O	3:C:156:LYS:C	2.47	0.53
1:A:130:GLN:HA	4:D:256:ILE:HD11	1.90	0.53
4:D:284:ILE:O	4:D:287:VAL:N	2.40	0.53
4:D:29:PHE:CE2	4:D:132:ILE:HG12	2.43	0.53
4:D:53:THR:HG22	4:D:67:TYR:HE2	1.72	0.53
2:B:250:PHE:CZ	30:H:1058:DGD:HAG2	2.35	0.53
10:K:32:PHE:CD1	26:K:1052:BCR:H24C	2.36	0.53
11:L:25:LEU:O	11:L:28:ALA:HB3	2.09	0.53
16:V:33:VAL:HG12	16:V:34:LEU:HD12	1.90	0.53
1:A:133:LEU:HG	1:A:137:LEU:CD1	2.39	0.53
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.57	0.53
1:A:237:TYR:C	1:A:237:TYR:CD2	2.81	0.53
2:B:233:ASN:O	2:B:236:THR:HG22	2.08	0.53
2:B:444:ARG:HG2	2:B:444:ARG:NH1	2.23	0.53
2:B:65:PHE:O	2:B:68:ARG:CG	2.54	0.53
23:C:1028:CLA:O1D	23:C:1028:CLA:H2A	2.07	0.53
23:C:1033:CLA:H92	23:C:1033:CLA:H121	1.91	0.53
3:C:418:ASN:H	3:C:418:ASN:HD22	1.57	0.53
3:C:472:LEU:O	3:C:473:ASP:HB2	2.08	0.53
4:D:175:VAL:O	4:D:178:ILE:HG12	2.08	0.53
4:D:237:PRO:O	4:D:238:THR:HG22	2.08	0.53
6:F:41:GLN:HB2	9:J:31:GLY:HA3	1.90	0.53
14:T:10:PHE:C	14:T:12:CYS:N	2.61	0.53
15:U:40:VAL:HG12	15:U:41:ASN:N	2.22	0.53
23:A:1003:CLA:C17	24:A:1038:PHO:C4	2.85	0.53
1:A:223:LEU:HD13	1:A:224:ILE:CG1	2.38	0.53
2:B:68:ARG:NE	23:B:1011:CLA:HED1	2.24	0.53
23:B:1022:CLA:O1D	23:B:1022:CLA:CGA	2.57	0.53
2:B:103:LEU:HD13	2:B:103:LEU:C	2.28	0.53
2:B:355:PHE:HB2	2:B:371:THR:O	2.09	0.53
2:B:456:ALA:CB	30:H:1058:DGD:CIB	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:PHE:O	2:B:463:PHE:C	2.47	0.53
23:C:1025:CLA:H162	23:C:1031:CLA:CMB	2.23	0.53
3:C:282:MET:CG	23:C:1025:CLA:H71	2.39	0.53
23:C:1034:CLA:C17	23:C:1034:CLA:C14	2.49	0.53
3:C:429:SER:HA	30:C:1056:DGD:C9A	2.39	0.53
3:C:245:ILE:C	3:C:247:GLY:H	2.12	0.53
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.44	0.53
23:D:1005:CLA:H161	29:D:1062:MGE:H251	1.91	0.53
4:D:134:ARG:HH21	4:D:137:GLY:HA2	1.73	0.53
9:J:10:LEU:HA	9:J:13:VAL:HG21	1.91	0.53
27:A:1063:LHG:H312	23:C:1034:CLA:H143	1.86	0.53
1:A:78:ILE:CA	1:A:176:ILE:HD12	2.18	0.53
2:B:145:LEU:O	2:B:146:ALA:C	2.47	0.53
2:B:17:GLY:CA	2:B:123:PHE:CE2	2.85	0.53
3:C:276:LEU:O	3:C:278:ALA:N	2.41	0.53
3:C:289:PHE:HB3	3:C:297:TYR:CE2	2.43	0.53
3:C:369:LEU:HD13	3:C:369:LEU:O	2.09	0.53
5:E:21:VAL:C	5:E:23:HIS:H	2.12	0.53
10:K:28:ILE:CB	10:K:29:PRO:HD3	2.29	0.53
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.09	0.53
1:A:292:THR:CG2	1:A:293:MET:N	2.72	0.53
1:A:41:LEU:HD12	24:A:1038:PHO:H51	1.89	0.53
23:B:1011:CLA:HBB1	23:B:1011:CLA:CHC	2.16	0.53
2:B:25:MET:HG2	2:B:111:ALA:CB	2.39	0.53
2:B:283:GLU:O	2:B:284:ILE:C	2.47	0.53
2:B:453:PHE:O	2:B:456:ALA:HB3	2.08	0.53
2:B:476:ARG:HG3	2:B:477:ASP:N	2.24	0.53
3:C:285:ILE:HG21	23:C:1025:CLA:H72	1.91	0.53
3:C:124:VAL:HG23	3:C:125:LEU:HG	1.90	0.53
3:C:429:SER:CA	30:C:1056:DGD:HA91	2.39	0.53
3:C:84:GLN:HB2	3:C:86:LEU:HD13	1.91	0.53
4:D:122:LEU:HB3	4:D:150:ILE:HD11	1.89	0.53
5:E:37:PHE:CE2	5:E:43:ALA:HA	2.44	0.53
5:E:30:LEU:CD1	6:F:32:PHE:HB2	2.38	0.53
9:J:30:TYR:C	9:J:32:ALA:H	2.12	0.53
11:L:27:LEU:CD1	12:M:14:PHE:HZ	2.15	0.53
13:O:92:VAL:HG22	13:O:93:PRO:HD2	1.89	0.53
16:V:105:PRO:HD3	16:V:120:SER:CB	2.39	0.53
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.44	0.53
1:A:131:TRP:CE3	1:A:132:GLU:N	2.77	0.53
1:A:268:SER:CB	4:D:236:ASN:HD21	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1010:CLA:HMD2	23:B:1011:CLA:C10	2.39	0.53
2:B:258:TYR:OH	4:D:162:LEU:HB3	2.09	0.53
23:C:1026:CLA:HBA1	23:C:1027:CLA:CMC	2.39	0.53
23:C:1034:CLA:H43	23:C:1034:CLA:H71	1.83	0.53
3:C:72:LEU:HD23	3:C:108:THR:HB	1.90	0.53
3:C:441:HIS:CD2	3:C:442:LEU:HD23	2.43	0.53
4:D:291:LEU:O	4:D:293:LEU:N	2.41	0.53
8:I:13:THR:HG23	8:I:14:PHE:N	2.24	0.53
10:K:35:LEU:HD12	10:K:38:VAL:CG2	2.38	0.53
15:U:97:LEU:HB3	15:U:102:LYS:CG	2.36	0.53
18:Y:19:ILE:CG2	18:Y:20:ALA:N	2.72	0.53
20:Z:15:LEU:O	20:Z:18:VAL:HB	2.07	0.53
3:C:135:ARG:NH1	20:Z:33:TRP:CG	2.77	0.53
20:Z:39:LEU:HD12	20:Z:42:LEU:HB2	1.91	0.53
1:A:265:PHE:CZ	27:A:1063:LHG:H152	2.44	0.53
1:A:121:LEU:O	1:A:124:SER:HB2	2.08	0.53
1:A:193:LEU:O	4:D:179:PHE:CE2	2.62	0.53
2:B:465:GLY:HA3	23:B:1019:CLA:HBC2	1.88	0.53
2:B:72:THR:C	2:B:93:PHE:HE2	2.13	0.53
4:D:166:SER:OG	4:D:167:TRP:N	2.42	0.53
5:E:38:VAL:HG12	6:F:39:ALA:HB1	1.91	0.53
13:O:188:ARG:HA	13:O:194:TYR:O	2.09	0.53
14:T:8:PHE:O	14:T:10:PHE:N	2.42	0.53
15:U:113:THR:HG22	15:U:114:VAL:H	1.73	0.53
23:C:1036:CLA:H151	26:Z:1053:BCR:H361	1.91	0.53
20:Z:12:LEU:CD1	20:Z:51:VAL:HB	2.39	0.53
1:A:219:VAL:CG2	1:A:220:THR:H	2.20	0.52
1:A:219:VAL:CG2	1:A:220:THR:N	2.71	0.52
2:B:149:LEU:CG	23:B:1011:CLA:HBC1	2.39	0.52
2:B:346:PHE:CG	2:B:399:VAL:HG12	2.45	0.52
2:B:367:PRO:HB2	4:D:345:VAL:HG12	1.90	0.52
2:B:75:TRP:CB	2:B:94:GLU:HG3	2.38	0.52
23:C:1028:CLA:H71	30:C:1056:DGD:HA71	1.92	0.52
23:C:1029:CLA:H202	23:C:1030:CLA:H172	1.90	0.52
30:C:1056:DGD:CIB	30:C:1056:DGD:HB41	2.39	0.52
3:C:311:GLN:OE1	3:C:355:THR:HG22	2.09	0.52
4:D:180:ARG:C	4:D:180:ARG:CD	2.77	0.52
2:B:362:PHE:HE1	4:D:184:PHE:CE1	2.27	0.52
5:E:82:GLN:O	5:E:84:LYS:N	2.41	0.52
7:H:37:LEU:N	7:H:37:LEU:HD12	2.24	0.52
26:K:1052:BCR:C38	26:K:1052:BCR:C23	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:24:VAL:O	10:K:24:VAL:HG12	2.08	0.52
13:O:208:LEU:HD12	13:O:208:LEU:N	2.23	0.52
23:B:1011:CLA:HMD2	23:B:1014:CLA:HMB1	1.91	0.52
23:B:1022:CLA:H62	26:B:1045:BCR:C20	2.38	0.52
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.43	0.52
3:C:162:GLY:C	3:C:165:LEU:HB2	2.29	0.52
1:A:328:MET:SD	4:D:325:ILE:CD1	2.97	0.52
31:E:1040:HEM:NC	6:F:24:HIS:CE1	2.76	0.52
23:H:1017:CLA:HAA1	23:H:1017:CLA:HBD	1.92	0.52
7:H:40:VAL:HG13	7:H:41:PHE:N	2.24	0.52
9:J:11:TRP:HH2	18:Y:37:PHE:HA	1.73	0.52
11:L:23:LEU:HB2	29:L:1061:MGE:H202	1.91	0.52
1:A:204:GLY:O	1:A:207:GLY:N	2.38	0.52
2:B:454:ALA:HB3	23:B:1015:CLA:CBB	2.39	0.52
2:B:9:HIS:CD2	23:B:1020:CLA:HBB2	2.44	0.52
2:B:44:THR:O	2:B:44:THR:HG22	2.09	0.52
30:C:1055:DGD:C3B	30:C:1055:DGD:C7B	2.86	0.52
4:D:314:PHE:O	4:D:317:LYS:N	2.43	0.52
1:A:33:PHE:HE1	8:I:23:PHE:HE2	1.57	0.52
2:B:26:HIS:CG	23:B:1020:CLA:HMA1	2.45	0.52
2:B:468:TRP:CD1	2:B:469:HIS:ND1	2.76	0.52
23:C:1027:CLA:HED1	23:C:1036:CLA:H192	1.91	0.52
3:C:255:THR:OG1	3:C:256:PRO:HD2	2.08	0.52
4:D:199:MET:O	4:D:202:ALA:N	2.43	0.52
8:I:4:LEU:HD12	8:I:7:THR:HG1	1.75	0.52
30:C:1057:DGD:HAF2	29:J:1059:MGE:H242	1.92	0.52
1:A:99:ALA:HB1	1:A:105:TRP:N	2.25	0.52
1:A:207:GLY:O	1:A:210:LEU:N	2.43	0.52
23:B:1023:CLA:H52	26:B:1048:BCR:H342	1.91	0.52
2:B:456:ALA:HB1	4:D:287:VAL:HG21	1.90	0.52
3:C:223:TRP:CB	3:C:224:ILE:HD13	2.27	0.52
3:C:350:ILE:HD12	3:C:356:MET:HA	1.90	0.52
4:D:175:VAL:C	4:D:177:ALA:N	2.63	0.52
5:E:43:ALA:O	5:E:46:VAL:HB	2.10	0.52
8:I:15:PHE:O	8:I:16:VAL:C	2.47	0.52
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.16	0.52
23:B:1009:CLA:CGD	23:B:1009:CLA:CGA	2.86	0.52
23:B:1014:CLA:O2D	23:B:1014:CLA:HAA1	2.08	0.52
23:B:1019:CLA:HHD	23:B:1019:CLA:HBC3	1.92	0.52
2:B:106:LEU:CD1	2:B:106:LEU:C	2.78	0.52
2:B:25:MET:HG2	2:B:111:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.45	0.52
2:B:454:ALA:HB3	23:B:1015:CLA:HBB2	1.92	0.52
2:B:99:ALA:O	2:B:102:VAL:CG1	2.54	0.52
3:C:203:THR:HG23	3:C:203:THR:O	2.08	0.52
3:C:268:GLY:O	23:C:1033:CLA:HBC1	2.09	0.52
3:C:354:GLU:HA	3:C:356:MET:CE	2.39	0.52
4:D:87:HIS:O	4:D:167:TRP:NE1	2.43	0.52
8:I:5:LYS:O	8:I:8:VAL:HB	2.10	0.52
26:K:1051:BCR:H392	26:K:1051:BCR:C22	2.36	0.52
13:O:128:ASP:O	13:O:147:THR:HA	2.09	0.52
18:Y:39:LEU:HD11	20:Z:28:ALA:HB3	1.91	0.52
20:Z:35:ARG:CD	20:Z:36:SER:N	2.73	0.52
23:A:1006:CLA:H18	26:D:1050:BCR:H292	1.90	0.52
1:A:25:ASP:HA	4:D:251:ARG:HH21	1.74	0.52
1:A:281:VAL:HG13	1:A:282:GLY:N	2.25	0.52
23:B:1010:CLA:H41	7:H:46:LEU:HA	1.92	0.52
2:B:5:TRP:HB2	23:B:1019:CLA:H42	1.91	0.52
2:B:11:VAL:HG11	11:L:7:ARG:HH11	1.74	0.52
2:B:217:ILE:HG23	2:B:218:LEU:HD23	1.90	0.52
2:B:453:PHE:O	2:B:456:ALA:CB	2.58	0.52
23:C:1032:CLA:H2	23:C:1035:CLA:C3C	2.40	0.52
3:C:199:ILE:CD1	3:C:199:ILE:H	2.23	0.52
23:A:1003:CLA:C3D	23:D:1005:CLA:CAC	2.88	0.52
4:D:128:ARG:HG3	4:D:128:ARG:HH11	1.75	0.52
2:B:475:PHE:CE2	4:D:134:ARG:HD2	2.45	0.52
4:D:144:ILE:CG2	4:D:145:ALA:N	2.73	0.52
4:D:52:THR:O	4:D:76:VAL:HG11	2.09	0.52
5:E:22:ILE:O	5:E:22:ILE:HG23	2.10	0.52
13:O:242:GLU:HA	13:O:261:ILE:O	2.10	0.52
16:V:34:LEU:HB3	16:V:47:LEU:HB2	1.92	0.52
1:A:260:PHE:O	1:A:263:ALA:HB3	2.10	0.52
23:B:1021:CLA:CMA	23:B:1021:CLA:H42	2.40	0.52
2:B:158:LEU:HD13	2:B:199:VAL:HG22	1.92	0.52
2:B:465:GLY:HA2	2:B:468:TRP:HB3	1.91	0.52
2:B:471:ALA:HB1	4:D:140:PRO:HG3	1.91	0.52
3:C:39:ASN:HD21	23:C:1033:CLA:HBB2	1.75	0.52
4:D:181:PHE:O	4:D:184:PHE:HB3	2.09	0.52
4:D:90:LEU:HD13	4:D:109:GLY:CA	2.40	0.52
7:H:13:PRO:O	7:H:16:SER:N	2.43	0.52
10:K:26:PRO:O	10:K:29:PRO:CD	2.37	0.52
14:T:1:MET:O	14:T:2:GLU:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:1:MET:HA	14:T:4:ILE:CG2	2.40	0.52
26:T:6046:BCR:C32	26:T:6046:BCR:C8	2.87	0.52
16:V:105:PRO:HD3	16:V:120:SER:HB2	1.90	0.52
7:H:44:ILE:HG22	17:X:19:PHE:HZ	1.75	0.52
23:A:1006:CLA:HBA1	30:C:1057:DGD:CFB	2.40	0.52
1:A:131:TRP:CD2	1:A:131:TRP:C	2.83	0.52
1:A:280:VAL:HA	1:A:283:VAL:HG13	1.91	0.52
23:B:1012:CLA:CED	23:B:1012:CLA:C2A	2.77	0.52
26:B:1045:BCR:C22	26:B:1045:BCR:H392	2.35	0.52
3:C:64:ALA:HA	23:C:1027:CLA:HBC2	1.92	0.52
3:C:140:LEU:HB3	3:C:148:GLY:CA	2.39	0.52
3:C:156:LYS:O	3:C:160:ILE:HG13	2.10	0.52
3:C:456:GLU:O	3:C:457:LYS:CB	2.57	0.52
9:J:18:GLY:O	9:J:22:ILE:HB	2.10	0.52
15:U:114:VAL:HG12	15:U:115:THR:N	2.25	0.52
23:A:1003:CLA:C16	24:A:1038:PHO:H62	2.40	0.52
1:A:196:PRO:C	1:A:199:GLN:HG2	2.31	0.52
1:A:92:HIS:HD2	3:C:220:GLY:N	2.08	0.52
2:B:106:LEU:CD1	26:B:1048:BCR:H352	2.39	0.52
2:B:144:PHE:HB2	2:B:213:GLY:HA3	1.92	0.52
2:B:468:TRP:HA	4:D:144:ILE:HD11	1.91	0.52
30:C:1056:DGD:C6D	30:C:1056:DGD:C4E	2.87	0.52
3:C:35:TRP:CG	3:C:36:TRP:N	2.77	0.52
10:K:28:ILE:HA	10:K:31:LEU:HD11	1.79	0.52
20:Z:39:LEU:HG	20:Z:39:LEU:O	2.10	0.52
27:A:1063:LHG:H292	23:C:1032:CLA:H62	1.91	0.51
1:A:91:LEU:HD13	1:A:167:SER:HA	1.92	0.51
23:B:1010:CLA:CMD	23:B:1011:CLA:H51	2.40	0.51
23:B:1020:CLA:H2	23:B:1023:CLA:CBA	2.25	0.51
23:B:1023:CLA:CHA	23:B:1024:CLA:CMC	2.88	0.51
2:B:458:PHE:HB3	23:B:1012:CLA:CMC	2.40	0.51
2:B:478:VAL:HG13	2:B:482:ILE:HG22	1.92	0.51
2:B:55:MET:HG3	2:B:56:TRP:N	2.24	0.51
23:C:1032:CLA:H2	23:C:1035:CLA:CAC	2.40	0.51
4:D:277:THR:HG22	4:D:278:GLY:H	1.72	0.51
1:A:83:VAL:CG2	4:D:314:PHE:HE1	2.22	0.51
4:D:68:LEU:HD23	4:D:68:LEU:O	2.10	0.51
5:E:35:TRP:HZ3	6:F:38:ALA:CB	2.20	0.51
30:C:1057:DGD:HAF2	29:J:1059:MGE:H222	1.93	0.51
10:K:35:LEU:HA	10:K:38:VAL:HG23	1.91	0.51
13:O:216:PHE:C	13:O:216:PHE:CD1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:59:ASP:O	13:O:60:SER:CB	2.57	0.51
18:Y:35:ILE:C	18:Y:35:ILE:HD12	2.30	0.51
1:A:223:LEU:HD22	1:A:245:THR:O	2.10	0.51
23:B:1019:CLA:HMB1	23:B:1020:CLA:NC	2.25	0.51
2:B:144:PHE:CA	2:B:213:GLY:HA3	2.40	0.51
2:B:373:LYS:HD3	2:B:374:ASN:H	1.75	0.51
2:B:460:LEU:CD2	4:D:280:TRP:CZ3	2.92	0.51
2:B:59:GLY:H	2:B:329:PRO:CB	2.22	0.51
3:C:70:PHE:O	3:C:74:HIS:CE1	2.63	0.51
4:D:148:ALA:CB	4:D:276:VAL:HA	2.40	0.51
1:A:143:ILE:HD13	4:D:216:ALA:O	2.10	0.51
5:E:8:ARG:HG3	5:E:9:PRO:HD2	1.92	0.51
9:J:10:LEU:O	9:J:13:VAL:HG23	2.10	0.51
15:U:133:TYR:CD1	16:V:76:PRO:HG3	2.44	0.51
1:A:214:MET:HE1	24:A:1039:PHO:CGD	2.40	0.51
1:A:205:VAL:HG22	1:A:279:ARG:NH1	2.25	0.51
2:B:27:THR:O	2:B:27:THR:HG22	2.11	0.51
2:B:92:SER:C	2:B:94:GLU:H	2.13	0.51
23:C:1030:CLA:CBB	23:C:1031:CLA:HMA3	2.40	0.51
23:C:1027:CLA:CED	23:C:1036:CLA:C19	2.87	0.51
3:C:250:TRP:NE1	23:C:1030:CLA:HED1	2.25	0.51
4:D:204:VAL:HG12	4:D:204:VAL:O	2.11	0.51
5:E:32:ILE:HD12	5:E:33:ALA:N	2.25	0.51
8:I:16:VAL:O	8:I:19:PHE:N	2.44	0.51
8:I:27:ASP:HA	8:I:30:ARG:HG2	1.93	0.51
11:L:27:LEU:HD12	12:M:14:PHE:CZ	2.30	0.51
15:U:69:ARG:O	15:U:71:LEU:HD12	2.10	0.51
16:V:107:THR:C	16:V:108:TYR:O	2.43	0.51
23:A:1003:CLA:HAB	23:A:1006:CLA:CMD	2.31	0.51
1:A:168:PHE:O	1:A:170:ASP:N	2.44	0.51
1:A:317:TRP:O	1:A:319:ASP:N	2.43	0.51
23:B:1011:CLA:HHC	23:B:1011:CLA:CBB	2.22	0.51
23:B:1010:CLA:C2D	23:B:1011:CLA:HMB1	2.40	0.51
2:B:193:TYR:CE1	2:B:259:GLY:HA3	2.44	0.51
2:B:357:ARG:HG3	2:B:357:ARG:NH1	2.19	0.51
1:A:258:LEU:HD12	4:D:128:ARG:NH1	2.26	0.51
4:D:233:ARG:HD2	4:D:233:ARG:O	2.10	0.51
7:H:31:MET:SD	23:H:1017:CLA:HBA2	2.49	0.51
14:T:29:ILE:N	14:T:29:ILE:HD13	2.26	0.51
15:U:88:VAL:HG12	15:U:109:LEU:HD11	1.92	0.51
15:U:69:ARG:HG3	15:U:69:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1007:CLA:H72	8:I:13:THR:HB	1.93	0.51
2:B:389:LYS:HD2	2:B:390:TYR:CE1	2.46	0.51
2:B:340:TRP:HA	2:B:430:PHE:CD2	2.46	0.51
23:C:1032:CLA:HAA1	23:C:1032:CLA:HBD	1.92	0.51
3:C:233:VAL:HG13	3:C:234:VAL:N	2.26	0.51
4:D:168:PHE:O	4:D:170:ALA:N	2.44	0.51
6:F:28:VAL:N	6:F:29:PRO:HD2	2.25	0.51
13:O:65:ARG:NH2	13:O:66:ILE:H	2.07	0.51
24:A:1038:PHO:H143	23:D:1005:CLA:H201	1.92	0.51
1:A:76:ASN:HB3	1:A:79:THR:OG1	2.11	0.51
2:B:152:GLY:CA	2:B:155:ALA:HB3	2.36	0.51
23:C:1033:CLA:C19	23:C:1033:CLA:C14	2.89	0.51
3:C:47:GLY:O	3:C:132:HIS:HB3	2.11	0.51
3:C:259:TRP:CZ3	3:C:260:ALA:HB2	2.45	0.51
4:D:267:LEU:HD23	4:D:267:LEU:O	2.11	0.51
4:D:270:PHE:CZ	25:D:1042:PQ9:H243	2.46	0.51
5:E:38:VAL:CG1	6:F:39:ALA:HB1	2.40	0.51
5:E:68:ASP:HB2	5:E:69:ARG:NH2	2.25	0.51
9:J:10:LEU:HA	9:J:13:VAL:HG23	1.92	0.51
3:C:62:PHE:CZ	10:K:28:ILE:HG21	2.42	0.51
10:K:35:LEU:C	10:K:37:PHE:N	2.63	0.51
29:B:1060:MGE:H102	29:L:1061:MGE:H8A2	1.91	0.51
13:O:97:VAL:CG1	13:O:98:THR:N	2.74	0.51
24:A:1038:PHO:CED	24:A:1038:PHO:CHA	2.86	0.51
1:A:147:TYR:CA	1:A:150:PRO:HG2	2.41	0.51
1:A:273:PHE:CG	1:A:274:PHE:N	2.79	0.51
1:A:36:ILE:HG22	1:A:125:CYS:SG	2.51	0.51
23:B:1010:CLA:HMD2	23:B:1011:CLA:H102	1.92	0.51
23:B:1023:CLA:HBB1	23:B:1023:CLA:CHC	2.38	0.51
23:B:1023:CLA:H142	23:B:1024:CLA:H8	1.88	0.51
2:B:397:VAL:HG23	2:B:398:THR:N	2.24	0.51
2:B:80:ILE:O	2:B:80:ILE:CG1	2.59	0.51
23:C:1026:CLA:O1A	23:C:1026:CLA:C5	2.29	0.51
23:C:1033:CLA:C19	23:C:1036:CLA:CHD	2.89	0.51
3:C:267:SER:O	3:C:271:TYR:CD2	2.64	0.51
3:C:366:LEU:O	3:C:369:LEU:N	2.44	0.51
3:C:451:ALA:O	3:C:453:ALA:N	2.44	0.51
4:D:293:LEU:O	4:D:293:LEU:HD13	2.11	0.51
1:A:200:LEU:HA	1:A:203:ALA:CB	2.37	0.51
1:A:309:ALA:HB3	16:V:28:GLU:CB	2.41	0.51
1:A:45:THR:HG23	23:D:1005:CLA:H191	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:PHE:CZ	23:B:1021:CLA:HMB3	2.46	0.51
2:B:256:MET:SD	2:B:268:PHE:CD1	3.04	0.51
3:C:161:LEU:CD1	23:C:1030:CLA:HBB1	2.40	0.51
23:C:1036:CLA:C19	26:Z:1053:BCR:C37	2.86	0.51
3:C:214:LEU:HD23	3:C:214:LEU:C	2.31	0.51
3:C:229:ASN:OD1	3:C:231:GLU:HG2	2.11	0.51
1:A:339:PHE:HB3	3:C:313:GLN:OE1	2.11	0.51
3:C:55:ALA:C	26:K:1052:BCR:H372	2.31	0.51
3:C:76:ILE:O	3:C:77:PRO:C	2.49	0.51
3:C:79:LYS:HE2	3:C:83:GLU:HB3	1.92	0.51
3:C:87:ILE:C	3:C:90:PRO:HD2	2.30	0.51
2:B:362:PHE:CZ	4:D:169:PHE:CD1	2.99	0.51
4:D:218:VAL:HA	4:D:221:THR:HG22	1.92	0.51
5:E:71:GLU:HG3	5:E:74:GLN:HB3	1.93	0.51
14:T:1:MET:CA	14:T:4:ILE:HG22	2.40	0.51
15:U:112:PHE:N	15:U:112:PHE:CD2	2.76	0.51
16:V:125:ASP:HB3	16:V:131:ARG:HE	1.75	0.51
1:A:337:HIS:HB2	28:A:1065:BR:BR	2.66	0.51
1:A:227:THR:HG21	1:A:232:SER:O	2.11	0.51
1:A:320:ILE:O	1:A:322:ASN:N	2.44	0.51
1:A:341:LEU:O	1:A:343:LEU:HD22	2.11	0.51
23:B:1021:CLA:H202	29:B:1060:MGE:CDA	2.40	0.51
23:B:1023:CLA:O2D	23:B:1023:CLA:HAA2	2.11	0.51
2:B:184:GLU:O	2:B:189:GLY:HA3	2.11	0.51
3:C:240:ILE:HD13	26:C:1054:BCR:H372	1.92	0.51
3:C:307:PRO:HG3	3:C:358:PHE:CE1	2.46	0.51
3:C:43:ILE:HG23	3:C:44:ASN:H	1.74	0.51
23:D:1005:CLA:HED3	25:D:1042:PQ9:H412	1.93	0.51
26:D:1050:BCR:H372	29:J:1059:MGE:C6A	2.40	0.51
4:D:189:HIS:CD2	4:D:289:LEU:HD12	2.46	0.51
9:J:11:TRP:CD1	9:J:12:ILE:N	2.79	0.51
15:U:61:ASN:HB2	15:U:130:ASN:HB3	1.92	0.51
20:Z:27:TYR:CD2	20:Z:27:TYR:N	2.78	0.51
1:A:140:ARG:NH2	27:A:1063:LHG:C2	2.73	0.51
23:B:1011:CLA:CED	23:B:1011:CLA:CAD	2.88	0.51
23:B:1021:CLA:C17	23:B:1021:CLA:C14	2.88	0.51
23:B:1019:CLA:HMD1	29:B:1060:MGE:O2G	2.10	0.51
2:B:298:LEU:HG	2:B:402:TYR:CD1	2.46	0.51
23:C:1026:CLA:C2B	23:C:1028:CLA:CBB	2.89	0.51
3:C:305:THR:O	3:C:306:GLY:C	2.50	0.51
3:C:472:LEU:O	3:C:473:ASP:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:ASN:O	4:D:198:MET:HG3	2.09	0.51
29:L:1061:MGE:H2A2	29:L:1061:MGE:H2G	1.92	0.51
4:D:300:SER:HB3	11:L:37:ASN:O	2.11	0.51
13:O:164:THR:O	13:O:165:SER:HB2	2.10	0.51
13:O:205:GLU:HA	13:O:208:LEU:HD13	1.92	0.51
13:O:215:ARG:O	13:O:251:MET:HA	2.11	0.51
20:Z:51:VAL:HG13	20:Z:52:LEU:N	2.26	0.51
1:A:117:PHE:CD2	1:A:117:PHE:N	2.78	0.50
1:A:71:LEU:O	1:A:73:TYR:N	2.44	0.50
23:B:1014:CLA:H101	26:B:1048:BCR:C7	2.41	0.50
2:B:241:SER:HB3	23:B:1020:CLA:HED1	1.94	0.50
2:B:443:PHE:N	2:B:443:PHE:CD2	2.77	0.50
3:C:72:LEU:HD22	3:C:72:LEU:O	2.11	0.50
7:H:41:PHE:HB2	26:H:1049:BCR:H14C	1.92	0.50
13:O:34:ASP:O	13:O:35:ASP:C	2.49	0.50
17:X:35:ALA:HA	17:X:38:ILE:CD1	2.41	0.50
20:Z:46:LEU:HB3	20:Z:50:LEU:CD1	2.41	0.50
1:A:210:LEU:HD13	24:A:1039:PHO:NC	2.26	0.50
1:A:131:TRP:O	1:A:134:SER:HB2	2.12	0.50
1:A:228:THR:HG22	1:A:228:THR:O	2.11	0.50
1:A:194:MET:HE2	1:A:300:PHE:HB2	1.92	0.50
1:A:323:ARG:C	1:A:325:ASN:H	2.14	0.50
2:B:192:PRO:HG2	7:H:49:TYR:CD1	2.46	0.50
3:C:456:GLU:O	3:C:457:LYS:HG3	2.11	0.50
4:D:188:PHE:CD1	4:D:188:PHE:N	2.80	0.50
4:D:188:PHE:O	4:D:294:ARG:NH2	2.44	0.50
7:H:31:MET:HB2	23:H:1017:CLA:CAD	2.40	0.50
26:H:1049:BCR:H361	26:H:1049:BCR:C37	2.36	0.50
8:I:16:VAL:HG23	8:I:17:LEU:N	2.26	0.50
10:K:17:ILE:HD12	10:K:17:ILE:H	1.76	0.50
16:V:83:GLU:O	16:V:87:LEU:HD13	2.10	0.50
2:B:389:LYS:HB3	2:B:390:TYR:CD1	2.46	0.50
2:B:467:ILE:HG22	4:D:144:ILE:HD12	1.92	0.50
23:C:1030:CLA:CAB	23:C:1031:CLA:HMA3	2.41	0.50
23:C:1032:CLA:HMC1	23:C:1032:CLA:HBC2	1.93	0.50
23:C:1036:CLA:H193	26:Z:1053:BCR:H371	1.93	0.50
3:C:230:LEU:HD12	3:C:233:VAL:CG1	2.40	0.50
3:C:265:ILE:N	3:C:274:TYR:OH	2.44	0.50
3:C:286:ALA:O	3:C:288:CYS:N	2.44	0.50
3:C:55:ALA:O	26:K:1052:BCR:H372	2.12	0.50
4:D:299:ILE:C	4:D:301:GLN:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:342:PRO:HB2	4:D:345:VAL:CG2	2.32	0.50
4:D:40:CYS:C	4:D:42:TYR:H	2.13	0.50
4:D:92:LEU:O	4:D:99:GLY:HA2	2.09	0.50
23:B:1016:CLA:H2	23:H:1017:CLA:C7	2.40	0.50
13:O:208:LEU:HD12	13:O:208:LEU:H	1.77	0.50
16:V:140:ALA:O	16:V:141:ILE:C	2.50	0.50
16:V:52:TYR:O	16:V:53:LEU:C	2.49	0.50
1:A:281:VAL:HG23	27:A:1063:LHG:H372	1.93	0.50
1:A:196:PRO:CA	1:A:199:GLN:HG2	2.41	0.50
3:C:175:LEU:HD11	23:C:1025:CLA:C2D	2.40	0.50
23:C:1027:CLA:CED	23:C:1036:CLA:H191	2.41	0.50
23:C:1033:CLA:HAA2	23:C:1033:CLA:HBD	1.94	0.50
1:A:163:ILE:HG12	30:C:1055:DGD:O1A	2.10	0.50
3:C:110:PRO:O	3:C:113:VAL:HG22	2.11	0.50
3:C:284:PHE:O	3:C:286:ALA:N	2.45	0.50
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.46	0.50
3:C:382:ASN:C	3:C:384:ILE:H	2.15	0.50
26:D:1050:BCR:C22	26:D:1050:BCR:H392	2.36	0.50
4:D:145:ALA:HB2	4:D:272:LEU:CD1	2.42	0.50
8:I:6:ILE:O	8:I:10:ILE:HG13	2.10	0.50
13:O:180:ALA:HB2	15:U:120:ALA:O	2.12	0.50
20:Z:27:TYR:HD2	20:Z:27:TYR:N	2.08	0.50
1:A:63:ILE:CD1	1:A:65:GLU:HG2	2.42	0.50
1:A:53:ILE:HA	1:A:71:LEU:HD12	1.93	0.50
2:B:172:TYR:O	2:B:173:GLY:C	2.50	0.50
2:B:284:ILE:HG13	2:B:285:ASN:H	1.71	0.50
2:B:291:SER:O	2:B:296:ALA:HB3	2.11	0.50
2:B:392:PHE:CE2	2:B:397:VAL:HG21	2.46	0.50
2:B:391:SER:C	2:B:392:PHE:O	2.47	0.50
23:C:1037:CLA:CGD	23:C:1037:CLA:HBA2	2.41	0.50
3:C:116:VAL:O	3:C:118:HIS:N	2.45	0.50
3:C:346:THR:HB	3:C:348:GLU:HG3	1.92	0.50
3:C:414:ILE:HG12	3:C:415:ASN:N	2.26	0.50
3:C:418:ASN:ND2	3:C:418:ASN:C	2.65	0.50
4:D:98:GLN:NE2	5:E:73:LYS:CE	2.72	0.50
7:H:30:LEU:HG	23:H:1017:CLA:HMD2	1.92	0.50
7:H:12:ARG:CD	7:H:16:SER:HB2	2.41	0.50
9:J:24:ILE:HG23	9:J:28:PHE:CE1	2.46	0.50
13:O:166:THR:HG22	13:O:167:ASP:N	2.26	0.50
13:O:250:ASP:O	13:O:250:ASP:OD1	2.29	0.50
13:O:97:VAL:HG13	13:O:98:THR:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:92:LEU:HD23	15:U:106:ARG:HH11	1.76	0.50
24:A:1039:PHO:H18	4:D:48:TRP:HE1	1.77	0.50
1:A:110:GLY:N	1:A:111:PRO:HD2	2.27	0.50
1:A:151:LEU:HD11	1:A:155:PHE:CE2	2.47	0.50
1:A:152:ALA:O	1:A:155:PHE:HB2	2.12	0.50
23:B:1011:CLA:HMD2	23:B:1014:CLA:CBB	2.41	0.50
23:B:1020:CLA:HBB1	23:B:1021:CLA:CBA	2.37	0.50
23:B:1024:CLA:H18	26:B:1048:BCR:HC41	1.94	0.50
30:C:1057:DGD:HA62	30:C:1057:DGD:HAT2	1.93	0.50
3:C:167:VAL:HG12	23:C:1036:CLA:H52	1.94	0.50
3:C:200:THR:O	3:C:202:PRO:HD2	2.11	0.50
3:C:203:THR:OG1	3:C:209:ILE:HD11	2.10	0.50
3:C:212:TYR:CE1	3:C:227:VAL:HG12	2.44	0.50
3:C:250:TRP:HE1	23:C:1030:CLA:HED2	1.74	0.50
3:C:75:PHE:CZ	3:C:77:PRO:O	2.64	0.50
3:C:78:GLU:OE1	3:C:104:GLU:CB	2.58	0.50
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.46	0.50
1:A:314:ILE:HG23	4:D:58:TRP:HZ3	1.77	0.50
10:K:39:VAL:HA	18:Y:36:ILE:HD13	1.93	0.50
15:U:50:ALA:CB	15:U:113:THR:HG21	2.40	0.50
15:U:58:ASN:O	15:U:59:ASN:OD1	2.30	0.50
15:U:59:ASN:O	15:U:60:THR:C	2.49	0.50
15:U:74:THR:O	15:U:77:LYS:N	2.44	0.50
16:V:111:GLU:CG	16:V:112:GLN:N	2.71	0.50
1:A:127:MET:O	1:A:130:GLN:HB3	2.11	0.50
1:A:31:GLY:HA3	1:A:132:GLU:OE1	2.11	0.50
23:B:1010:CLA:C4D	23:B:1011:CLA:HMB3	2.42	0.50
23:C:1025:CLA:HBB2	23:C:1025:CLA:C9	2.42	0.50
30:C:1057:DGD:HB92	30:C:1057:DGD:C9A	2.42	0.50
3:C:113:VAL:O	3:C:117:VAL:CG2	2.55	0.50
3:C:276:LEU:C	3:C:278:ALA:N	2.65	0.50
5:E:36:LEU:C	5:E:38:VAL:N	2.65	0.50
31:E:1040:HEM:CHD	6:F:20:TRP:HE1	2.25	0.50
10:K:37:PHE:HB3	26:K:1051:BCR:C40	2.42	0.50
15:U:128:TYR:CD1	15:U:128:TYR:N	2.79	0.50
15:U:89:GLU:C	15:U:91:VAL:H	2.15	0.50
16:V:105:PRO:HB3	16:V:120:SER:OG	2.12	0.50
3:C:78:GLU:HB3	16:V:128:PRO:HB2	1.93	0.50
7:H:40:VAL:HG21	17:X:23:LEU:HD21	1.93	0.50
20:Z:52:LEU:O	20:Z:55:GLY:HA3	2.12	0.50
27:A:1063:LHG:C16	27:A:1063:LHG:C12	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:O	1:A:202:VAL:HG23	2.12	0.50
1:A:210:LEU:CD1	24:A:1039:PHO:ND	2.75	0.50
1:A:235:TYR:O	1:A:237:TYR:N	2.40	0.50
1:A:161:TYR:CD1	1:A:294:ALA:HA	2.47	0.50
23:B:1019:CLA:OBD	29:B:1060:MGE:C2G	2.58	0.50
2:B:279:TYR:O	2:B:281:GLN:N	2.45	0.50
2:B:450:TRP:O	2:B:451:PHE:C	2.50	0.50
23:C:1034:CLA:CED	10:K:29:PRO:HG3	2.42	0.50
3:C:137:PRO:O	3:C:138:GLU:O	2.29	0.50
3:C:72:LEU:CD2	3:C:108:THR:HB	2.42	0.50
2:B:482:ILE:HG21	4:D:138:VAL:HA	1.92	0.50
23:B:1010:CLA:H203	4:D:159:ILE:HG23	1.94	0.50
3:C:33:PHE:HB3	4:D:229:ALA:HB3	1.93	0.50
4:D:83:ASN:N	4:D:168:PHE:HD1	2.09	0.50
5:E:17:VAL:O	5:E:21:VAL:HG23	2.11	0.50
13:O:230:VAL:HG22	13:O:237:ILE:HG22	1.93	0.50
15:U:51:TYR:HB2	15:U:56:ASP:HB2	1.93	0.50
2:B:27:THR:C	23:B:1013:CLA:HBC1	2.32	0.50
23:B:1022:CLA:O1D	23:B:1022:CLA:O1A	2.29	0.50
2:B:284:ILE:HG22	2:B:309:LEU:CD2	2.35	0.50
2:B:37:MET:HG2	2:B:62:VAL:HG21	1.94	0.50
2:B:68:ARG:CG	2:B:69:LEU:N	2.75	0.50
23:C:1029:CLA:C5	23:C:1029:CLA:CHC	2.90	0.50
3:C:163:PHE:O	3:C:167:VAL:HG23	2.12	0.50
3:C:278:ALA:O	3:C:281:MET:HB3	2.11	0.50
6:F:22:ALA:O	6:F:25:THR:OG1	2.24	0.50
7:H:54:ILE:O	7:H:54:ILE:CG2	2.59	0.50
2:B:6:TYR:HE2	11:L:11:GLU:CG	2.25	0.50
13:O:144:LEU:HD23	13:O:144:LEU:H	1.77	0.50
15:U:56:ASP:HA	15:U:113:THR:O	2.11	0.50
16:V:102:MET:HB3	16:V:138:LEU:HD13	1.94	0.50
1:A:71:LEU:C	1:A:73:TYR:N	2.63	0.49
2:B:173:GLY:O	2:B:174:LEU:HD12	2.12	0.49
2:B:373:LYS:CD	2:B:374:ASN:H	2.25	0.49
2:B:478:VAL:HG13	2:B:482:ILE:CG2	2.42	0.49
23:C:1032:CLA:H193	23:C:1032:CLA:C15	2.33	0.49
26:C:1054:BCR:C39	26:C:1054:BCR:C27	2.80	0.49
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.94	0.49
3:C:276:LEU:C	3:C:276:LEU:HD23	2.33	0.49
1:A:297:LEU:CD2	3:C:404:LEU:HA	2.42	0.49
9:J:30:TYR:O	9:J:32:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1051:BCR:H403	26:K:1051:BCR:C22	2.36	0.49
13:O:148:VAL:CG1	13:O:151:LEU:HD22	2.42	0.49
13:O:183:LEU:N	13:O:183:LEU:HD12	2.27	0.49
15:U:89:GLU:C	15:U:91:VAL:N	2.65	0.49
1:A:293:MET:C	1:A:295:PHE:N	2.64	0.49
1:A:48:PHE:CD2	1:A:82:VAL:HG21	2.47	0.49
23:B:1021:CLA:HMA2	23:B:1021:CLA:H11	1.94	0.49
23:C:1032:CLA:C17	23:C:1034:CLA:C19	2.90	0.49
3:C:341:LEU:HD22	3:C:375:LEU:HD12	1.95	0.49
3:C:377:LEU:HA	3:C:380:ILE:HG21	1.92	0.49
3:C:37:ALA:O	3:C:39:ASN:O	2.30	0.49
3:C:290:VAL:CG2	3:C:423:ARG:HA	2.41	0.49
23:D:1005:CLA:C15	23:D:1005:CLA:H202	2.01	0.49
4:D:257:PHE:CG	4:D:257:PHE:O	2.64	0.49
4:D:80:THR:HA	4:D:111:TRP:CD1	2.47	0.49
5:E:58:GLN:CD	5:E:58:GLN:O	2.51	0.49
5:E:83:LEU:HD22	5:E:84:LYS:N	2.24	0.49
14:T:8:PHE:C	14:T:10:PHE:N	2.66	0.49
15:U:73:PRO:HB2	16:V:109:ASP:OD1	2.12	0.49
16:V:81:ARG:HD3	16:V:157:GLY:N	2.27	0.49
20:Z:44:SER:O	20:Z:48:ILE:HG13	2.11	0.49
1:A:130:GLN:NE2	24:A:1038:PHO:OBD	2.45	0.49
1:A:180:PHE:CD1	1:A:180:PHE:N	2.79	0.49
1:A:267:ASN:HB3	1:A:270:SER:OG	2.12	0.49
1:A:303:ASN:HD21	3:C:412:THR:HA	1.76	0.49
1:A:314:ILE:HG23	4:D:58:TRP:CZ3	2.47	0.49
2:B:150:CYS:N	23:B:1011:CLA:HBC3	2.27	0.49
2:B:59:GLY:O	23:B:1015:CLA:CED	2.61	0.49
2:B:255:THR:O	2:B:258:TYR:O	2.30	0.49
2:B:464:PHE:CD1	2:B:465:GLY:N	2.81	0.49
3:C:275:SER:HB3	23:C:1033:CLA:HED1	1.94	0.49
3:C:172:ALA:HB3	3:C:241:GLY:HA2	1.94	0.49
1:A:258:LEU:HA	4:D:132:ILE:CD1	2.42	0.49
4:D:45:LEU:O	4:D:45:LEU:HD22	2.12	0.49
4:D:66:SER:O	4:D:71:CYS:HB2	2.12	0.49
23:B:1016:CLA:H2	23:H:1017:CLA:H71	1.94	0.49
3:C:326:ALA:HB2	15:U:128:TYR:CD2	2.48	0.49
3:C:326:ALA:HB2	15:U:128:TYR:CG	2.47	0.49
16:V:63:CYS:HB3	31:V:1041:HEM:CAB	2.42	0.49
20:Z:7:LEU:O	20:Z:11:ALA:HB2	2.12	0.49
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1019:CLA:C6	23:B:1021:CLA:CED	2.77	0.49
2:B:160:GLY:C	2:B:162:PHE:N	2.63	0.49
3:C:171:GLY:C	3:C:173:LEU:N	2.66	0.49
3:C:269:GLU:OE1	3:C:447:ARG:CG	2.60	0.49
23:D:1005:CLA:C16	29:D:1062:MGE:CGB	2.85	0.49
4:D:113:PHE:HE2	23:D:1008:CLA:HMD3	1.77	0.49
4:D:82:ALA:O	4:D:85:MET:HB2	2.12	0.49
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.77	0.49
7:H:54:ILE:O	7:H:54:ILE:HG23	2.10	0.49
9:J:17:ALA:O	9:J:19:MET:N	2.46	0.49
10:K:10:LYS:HG3	10:K:10:LYS:O	2.11	0.49
13:O:206:GLU:N	13:O:206:GLU:OE1	2.40	0.49
13:O:223:ILE:CG1	13:O:224:SER:H	2.11	0.49
13:O:66:ILE:HG22	13:O:269:ILE:HA	1.94	0.49
23:A:1006:CLA:C17	26:D:1050:BCR:H292	2.35	0.49
1:A:91:LEU:CD1	1:A:167:SER:HA	2.43	0.49
1:A:261:GLN:C	1:A:263:ALA:N	2.65	0.49
2:B:121:GLU:HB2	7:H:3:ARG:O	2.12	0.49
2:B:222:PRO:HB2	7:H:25:TRP:O	2.12	0.49
2:B:49:ASP:OD1	2:B:51:VAL:N	2.45	0.49
23:C:1031:CLA:HED3	23:C:1031:CLA:O1A	2.10	0.49
3:C:179:ALA:O	3:C:198:VAL:HG13	2.12	0.49
3:C:394:GLU:OE1	16:V:127:PHE:HE2	1.95	0.49
3:C:418:ASN:N	3:C:418:ASN:HD22	2.10	0.49
4:D:157:PHE:O	4:D:158:LEU:HD23	2.12	0.49
23:A:1006:CLA:O1D	4:D:179:PHE:HZ	1.95	0.49
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.45	0.49
5:E:19:TYR:CE1	5:E:20:TRP:HD1	2.28	0.49
5:E:57:ALA:CB	5:E:83:LEU:HA	2.42	0.49
8:I:33:LYS:HB3	8:I:35:LYS:CE	2.40	0.49
8:I:4:LEU:HD12	8:I:7:THR:OG1	2.12	0.49
1:A:166:GLY:HA3	3:C:357:ARG:HH11	1.77	0.49
1:A:32:TRP:HA	1:A:32:TRP:CE3	2.47	0.49
23:B:1009:CLA:H62	23:B:1009:CLA:H13	1.95	0.49
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.13	0.49
3:C:376:ASP:O	3:C:380:ILE:HG22	2.12	0.49
3:C:399:ALA:C	3:C:401:LEU:H	2.14	0.49
25:D:1042:PQ9:H142	29:D:1062:MGE:H3B2	1.93	0.49
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.48	0.49
4:D:196:PHE:H	4:D:196:PHE:HD1	1.61	0.49
1:A:269:ARG:HD3	4:D:231:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:304:ARG:HG3	4:D:304:ARG:O	2.12	0.49
26:H:1049:BCR:H392	26:H:1049:BCR:H23C	1.94	0.49
2:B:223:GLN:HG2	7:H:24:GLY:O	2.12	0.49
9:J:11:TRP:CG	9:J:12:ILE:N	2.80	0.49
10:K:26:PRO:C	10:K:28:ILE:H	2.16	0.49
14:T:7:VAL:O	14:T:10:PHE:HB3	2.13	0.49
2:B:394:GLN:OE1	15:U:47:LEU:HD13	2.12	0.49
16:V:102:MET:O	16:V:121:LEU:HB2	2.12	0.49
16:V:55:GLY:HA3	16:V:144:HIS:HB2	1.95	0.49
16:V:39:ASN:ND2	16:V:41:GLU:HG2	2.28	0.49
16:V:85:LEU:O	16:V:88:ALA:HB3	2.12	0.49
1:A:140:ARG:NH2	27:A:1063:LHG:HC11	2.27	0.49
1:A:189:GLU:O	3:C:411:ALA:HB2	2.13	0.49
2:B:368:VAL:HG11	2:B:381:ILE:CG1	2.43	0.49
2:B:68:ARG:HG3	2:B:69:LEU:H	1.76	0.49
23:C:1026:CLA:C20	23:C:1026:CLA:C4D	2.85	0.49
27:A:1063:LHG:H292	23:C:1032:CLA:C7	2.42	0.49
23:C:1034:CLA:HED1	10:K:29:PRO:HG3	1.95	0.49
26:D:1050:BCR:H282	29:J:1059:MGE:CBB	2.30	0.49
4:D:235:PHE:CE2	4:D:243:THR:HG22	2.48	0.49
4:D:196:PHE:CD2	4:D:284:ILE:HB	2.47	0.49
1:A:173:PRO:HG3	4:D:314:PHE:CE2	2.47	0.49
11:L:24:ILE:HG23	11:L:25:LEU:N	2.28	0.49
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.94	0.49
1:A:190:HIS:ND1	1:A:298:ASN:CG	2.66	0.49
1:A:195:HIS:CG	1:A:196:PRO:HD2	2.47	0.49
1:A:21:VAL:CG2	1:A:22:THR:HG23	2.41	0.49
23:B:1019:CLA:H193	23:B:1021:CLA:C6	2.41	0.49
23:B:1020:CLA:C5	23:B:1020:CLA:CGA	2.90	0.49
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.94	0.49
2:B:37:MET:HG2	2:B:62:VAL:CG2	2.42	0.49
3:C:418:ASN:OD1	30:C:1057:DGD:HE61	2.13	0.49
23:D:1005:CLA:HBD	23:D:1005:CLA:HAA1	1.94	0.49
7:H:41:PHE:CD2	7:H:42:LEU:HD23	2.48	0.49
8:I:3:THR:CA	8:I:6:ILE:HD11	2.42	0.49
30:C:1056:DGD:HB51	9:J:29:PHE:CE1	2.46	0.49
1:A:78:ILE:HD11	11:L:34:TYR:HE2	1.78	0.49
1:A:273:PHE:O	1:A:275:LEU:N	2.46	0.49
1:A:322:ASN:HD21	3:C:412:THR:CG2	2.20	0.49
26:B:1045:BCR:H341	26:B:1047:BCR:H10C	1.94	0.49
2:B:118:TRP:HD1	2:B:118:TRP:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HA	2:B:148:LEU:HD23	1.95	0.49
2:B:149:LEU:HB3	23:B:1011:CLA:HBC1	1.95	0.49
2:B:150:CYS:O	2:B:151:PHE:C	2.51	0.49
2:B:367:PRO:HG2	2:B:367:PRO:O	2.13	0.49
2:B:390:TYR:O	2:B:391:SER:C	2.51	0.49
3:C:60:ILE:CD1	23:C:1027:CLA:HMD3	2.42	0.49
3:C:174:LEU:O	3:C:178:LYS:N	2.46	0.49
3:C:56:HIS:O	3:C:59:LEU:N	2.46	0.49
3:C:76:ILE:HD13	3:C:77:PRO:HD2	1.93	0.49
4:D:129:GLN:CD	4:D:143:ALA:HA	2.33	0.49
4:D:180:ARG:O	4:D:181:PHE:C	2.51	0.49
10:K:26:PRO:O	10:K:28:ILE:N	2.45	0.49
13:O:149:LYS:O	13:O:150:ASN:CB	2.61	0.49
13:O:36:ILE:N	13:O:36:ILE:HD12	2.27	0.49
15:U:58:ASN:N	15:U:58:ASN:ND2	2.54	0.49
20:Z:5:PHE:O	20:Z:7:LEU:N	2.46	0.49
1:A:199:GLN:CG	1:A:200:LEU:N	2.76	0.49
1:A:50:ILE:CB	26:A:1044:BCR:H391	2.43	0.49
23:B:1024:CLA:HBD	23:B:1024:CLA:HBA2	1.95	0.49
2:B:31:ALA:O	2:B:34:ALA:HB3	2.13	0.49
2:B:252:VAL:HG12	2:B:451:PHE:CE2	2.48	0.49
2:B:483:ASP:O	2:B:485:GLU:N	2.46	0.49
23:C:1028:CLA:H43	30:C:1057:DGD:C2A	2.26	0.49
23:C:1032:CLA:C19	23:C:1032:CLA:C15	2.90	0.49
23:C:1033:CLA:C12	23:C:1033:CLA:H92	2.36	0.49
3:C:173:LEU:O	3:C:176:VAL:HB	2.12	0.49
5:E:59:GLU:OE2	5:E:59:GLU:HA	2.12	0.49
2:B:222:PRO:HG3	7:H:27:THR:HG23	1.95	0.49
13:O:90:GLU:HG3	13:O:91:PHE:N	2.27	0.49
15:U:72:TYR:CD2	15:U:73:PRO:N	2.80	0.49
18:Y:21:GLN:C	18:Y:21:GLN:OE1	2.52	0.49
3:C:120:ILE:HG21	26:Z:1053:BCR:C34	2.43	0.49
1:A:214:MET:HG3	25:A:1043:PQ9:H142	1.95	0.48
1:A:279:ARG:O	1:A:283:VAL:HG13	2.13	0.48
1:A:280:VAL:CA	1:A:283:VAL:HG13	2.43	0.48
1:A:340:PRO:HB3	15:U:133:TYR:CD2	2.48	0.48
1:A:95:PRO:O	1:A:98:GLU:N	2.45	0.48
23:B:1023:CLA:HMA2	23:B:1023:CLA:O1A	2.13	0.48
29:B:1060:MGE:H263	29:B:1060:MGE:H5A2	1.95	0.48
2:B:156:PHE:CB	2:B:162:PHE:HB3	2.42	0.48
2:B:201:HIS:O	2:B:204:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1029:CLA:C7	23:C:1029:CLA:C4	2.89	0.48
3:C:124:VAL:CG2	3:C:125:LEU:H	2.21	0.48
3:C:201:ASN:OD1	3:C:201:ASN:O	2.31	0.48
3:C:230:LEU:C	3:C:233:VAL:HG12	2.33	0.48
3:C:455:PHE:O	3:C:458:GLY:N	2.46	0.48
1:A:139:MET:HA	3:C:459:ILE:HD11	1.94	0.48
1:A:314:ILE:HD12	4:D:58:TRP:CH2	2.48	0.48
4:D:76:VAL:HG12	4:D:77:ALA:N	2.27	0.48
4:D:71:CYS:HB3	4:D:76:VAL:HG22	1.94	0.48
9:J:17:ALA:C	9:J:19:MET:N	2.66	0.48
10:K:33:PHE:CD1	10:K:34:ALA:N	2.79	0.48
11:L:22:LEU:C	11:L:22:LEU:HD23	2.33	0.48
3:C:330:SER:HB2	13:O:149:LYS:NZ	2.28	0.48
16:V:129:LYS:O	16:V:133:LEU:HD11	2.13	0.48
18:Y:31:ALA:O	18:Y:35:ILE:CG2	2.60	0.48
23:B:1019:CLA:H162	23:B:1021:CLA:H52	1.95	0.48
23:B:1023:CLA:CHA	23:B:1024:CLA:HMC3	2.43	0.48
2:B:192:PRO:HG2	7:H:49:TYR:CZ	2.48	0.48
23:C:1029:CLA:H192	23:C:1029:CLA:H152	0.62	0.48
3:C:160:ILE:HB	23:C:1031:CLA:CMD	2.42	0.48
3:C:418:ASN:HB3	30:C:1057:DGD:HE2	1.95	0.48
3:C:155:ASN:O	3:C:159:THR:N	2.46	0.48
3:C:171:GLY:O	3:C:173:LEU:N	2.46	0.48
3:C:240:ILE:O	3:C:244:CYS:SG	2.71	0.48
1:A:279:ARG:HD3	4:D:208:ALA:C	2.33	0.48
6:F:32:PHE:C	6:F:32:PHE:CD2	2.86	0.48
23:B:1023:CLA:H193	7:H:7:LEU:HD11	1.93	0.48
15:U:99:GLU:CD	15:U:99:GLU:N	2.65	0.48
16:V:34:LEU:N	16:V:34:LEU:CD1	2.75	0.48
23:A:1006:CLA:CGA	30:C:1057:DGD:HBN2	2.43	0.48
2:B:121:GLU:C	2:B:123:PHE:N	2.67	0.48
2:B:173:GLY:O	2:B:174:LEU:CD1	2.61	0.48
2:B:380:ASP:O	2:B:382:PRO:HD3	2.13	0.48
29:D:1062:MGE:H222	29:L:1061:MGE:H262	1.96	0.48
4:D:37:LEU:HD13	4:D:125:PHE:HB2	1.95	0.48
4:D:37:LEU:HD22	4:D:128:ARG:HB2	1.95	0.48
4:D:191:TRP:CE2	4:D:197:HIS:HB2	2.48	0.48
4:D:21:TRP:C	4:D:21:TRP:CE3	2.86	0.48
5:E:51:ARG:O	5:E:53:ASP:N	2.45	0.48
7:H:13:PRO:O	7:H:14:LEU:C	2.52	0.48
11:L:37:ASN:OD1	11:L:37:ASN:OXT	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:11:THR:CG2	12:M:12:ALA:N	2.67	0.48
12:M:6:LEU:HA	12:M:9:ILE:HD13	1.95	0.48
15:U:129:ASN:O	15:U:131:GLY:N	2.45	0.48
15:U:82:ASN:ND2	15:U:94:ILE:HG23	2.28	0.48
16:V:124:ALA:C	16:V:126:ILE:N	2.67	0.48
16:V:40:SER:O	16:V:42:GLY:N	2.46	0.48
23:A:1006:CLA:HBA1	30:C:1057:DGD:HBN1	1.95	0.48
1:A:11:ALA:HB1	1:A:15:GLU:HB3	1.95	0.48
1:A:199:GLN:OE1	1:A:200:LEU:N	2.47	0.48
1:A:223:LEU:HB2	4:D:265:ARG:CZ	2.43	0.48
1:A:319:ASP:O	1:A:322:ASN:HB2	2.13	0.48
1:A:323:ARG:C	1:A:325:ASN:N	2.67	0.48
23:B:1012:CLA:CHD	23:B:1012:CLA:HBC2	2.35	0.48
23:B:1019:CLA:HMB3	23:B:1020:CLA:NC	2.27	0.48
23:B:1020:CLA:CAD	23:B:1020:CLA:CED	2.92	0.48
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.95	0.48
2:B:211:ILE:HG22	2:B:212:ALA:N	2.27	0.48
2:B:222:PRO:HD2	23:H:1017:CLA:CED	2.44	0.48
2:B:52:LEU:CD1	2:B:339:ALA:HA	2.44	0.48
2:B:389:LYS:HD2	2:B:390:TYR:HE1	1.77	0.48
2:B:311:PHE:CA	2:B:430:PHE:CZ	2.97	0.48
3:C:449:ARG:NE	23:C:1029:CLA:CED	2.76	0.48
3:C:179:ALA:O	3:C:198:VAL:CG1	2.61	0.48
3:C:172:ALA:CB	3:C:241:GLY:HA2	2.43	0.48
3:C:95:LEU:HD21	23:C:1027:CLA:HBB2	1.96	0.48
4:D:273:PHE:O	4:D:274:VAL:C	2.52	0.48
4:D:210:LEU:HD11	4:D:274:VAL:HG21	1.95	0.48
4:D:281:MET:HE3	4:D:284:ILE:CD1	2.43	0.48
1:A:328:MET:SD	4:D:325:ILE:HD11	2.54	0.48
4:D:90:LEU:HD23	4:D:96:GLU:CG	2.43	0.48
4:D:92:LEU:HB3	4:D:93:TRP:CZ3	2.48	0.48
1:A:97:TRP:CZ2	8:I:9:TYR:HE2	2.31	0.48
16:V:118:HIS:O	16:V:119:PRO:C	2.47	0.48
16:V:82:THR:O	16:V:83:GLU:C	2.52	0.48
26:Z:1053:BCR:H271	26:Z:1053:BCR:H403	1.96	0.48
1:A:191:ASN:HB3	1:A:194:MET:HB2	1.95	0.48
1:A:288:LEU:HD11	3:C:435:PHE:HD2	1.77	0.48
23:B:1011:CLA:C2D	23:B:1013:CLA:C4	2.92	0.48
23:B:1013:CLA:H72	23:B:1020:CLA:H18	1.96	0.48
2:B:5:TRP:CE3	23:B:1019:CLA:H42	2.40	0.48
23:B:1019:CLA:H51	23:B:1021:CLA:CED	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:1026:CLA:HBA1	23:C:1027:CLA:C2C	2.44	0.48
23:C:1028:CLA:H121	23:C:1028:CLA:H171	1.77	0.48
3:C:406:SER:CB	30:C:1056:DGD:HE1	2.44	0.48
3:C:51:GLY:CA	3:C:132:HIS:HB2	2.33	0.48
3:C:71:GLU:HB3	3:C:89:ILE:HD12	1.96	0.48
26:D:1050:BCR:C20	29:J:1059:MGE:H5A1	2.43	0.48
1:A:223:LEU:CG	4:D:265:ARG:CZ	2.91	0.48
4:D:261:PHE:CZ	4:D:267:LEU:HB2	2.47	0.48
4:D:318:ASN:O	4:D:321:LEU:HB2	2.14	0.48
4:D:43:LEU:HD12	26:D:1050:BCR:HC7	1.95	0.48
5:E:34:GLY:HA3	6:F:32:PHE:CD2	2.47	0.48
10:K:19:ASP:N	10:K:20:PRO:HD2	2.28	0.48
13:O:105:ASP:O	13:O:106:GLN:CB	2.62	0.48
18:Y:46:LEU:H	18:Y:46:LEU:HD12	1.77	0.48
1:A:344:ALA:O	3:C:357:ARG:NH2	2.47	0.48
1:A:63:ILE:CG1	1:A:65:GLU:HG2	2.43	0.48
23:B:1009:CLA:H12	26:H:1049:BCR:C15	2.29	0.48
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.14	0.48
2:B:416:THR:O	2:B:419:SER:HB3	2.13	0.48
2:B:326:ARG:HE	2:B:442:ILE:CG2	2.26	0.48
2:B:5:TRP:O	23:B:1019:CLA:H2	2.13	0.48
3:C:268:GLY:C	23:C:1033:CLA:HBC1	2.34	0.48
3:C:118:HIS:O	3:C:122:SER:N	2.43	0.48
3:C:299:SER:HA	3:C:303:GLY:O	2.14	0.48
3:C:354:GLU:O	3:C:356:MET:N	2.46	0.48
3:C:76:ILE:CD1	3:C:77:PRO:HD2	2.44	0.48
4:D:134:ARG:CA	4:D:134:ARG:NE	2.74	0.48
1:A:272:HIS:CG	4:D:218:VAL:HG21	2.49	0.48
4:D:321:LEU:O	4:D:324:GLY:N	2.47	0.48
4:D:72:ASN:HD21	4:D:74:LEU:HG	1.79	0.48
13:O:239:GLY:O	13:O:264:VAL:HG13	2.13	0.48
14:T:7:VAL:CG1	14:T:8:PHE:N	2.70	0.48
16:V:128:PRO:C	16:V:130:MET:N	2.66	0.48
16:V:96:GLU:O	16:V:99:VAL:HB	2.13	0.48
27:A:1063:LHG:HC82	27:A:1063:LHG:O10	2.13	0.48
1:A:122:GLY:O	1:A:125:CYS:HB2	2.12	0.48
1:A:126:TYR:CZ	24:A:1038:PHO:O1A	2.67	0.48
1:A:159:LEU:CD1	1:A:163:ILE:HD11	2.43	0.48
1:A:279:ARG:CZ	4:D:208:ALA:HB1	2.44	0.48
23:B:1009:CLA:O1D	23:B:1009:CLA:O1A	2.30	0.48
23:B:1023:CLA:C4C	23:B:1024:CLA:CB	2.83	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:GLU:O	2:B:286:ARG:N	2.46	0.48
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.48	0.48
2:B:357:ARG:O	2:B:425:ILE:HD12	2.13	0.48
2:B:457:VAL:O	2:B:461:LEU:CG	2.60	0.48
3:C:288:CYS:CB	30:C:1055:DGD:HB21	2.43	0.48
3:C:286:ALA:O	3:C:289:PHE:N	2.47	0.48
3:C:295:THR:C	3:C:297:TYR:H	2.17	0.48
23:D:1005:CLA:CED	25:D:1042:PQ9:H391	2.43	0.48
4:D:97:ALA:CB	4:D:104:TRP:HB2	2.44	0.48
5:E:12:ASP:O	5:E:14:ILE:N	2.47	0.48
7:H:31:MET:HB2	23:H:1017:CLA:C3D	2.44	0.48
15:U:118:GLU:HB3	15:U:121:LEU:HB2	1.95	0.48
16:V:60:GLN:HA	16:V:64:ALA:HB2	1.95	0.48
1:A:142:TRP:HH2	27:A:1063:LHG:HC11	1.79	0.48
1:A:265:PHE:CD1	1:A:271:LEU:HD13	2.47	0.48
2:B:318:ASN:HD22	2:B:319:PRO:N	2.10	0.48
23:C:1029:CLA:H52	23:C:1029:CLA:CHC	2.44	0.48
3:C:244:CYS:HA	23:C:1030:CLA:CMC	2.43	0.48
4:D:270:PHE:HZ	25:D:1042:PQ9:H243	1.78	0.48
1:A:315:ASN:O	4:D:63:LEU:HD23	2.13	0.48
5:E:19:TYR:HD1	5:E:20:TRP:CD1	2.29	0.48
7:H:50:ASN:O	7:H:50:ASN:ND2	2.45	0.48
8:I:30:ARG:HA	8:I:30:ARG:HH11	1.74	0.48
10:K:28:ILE:N	10:K:29:PRO:CD	2.76	0.48
13:O:184:ASP:CB	13:O:185:PRO:HD2	2.37	0.48
13:O:208:LEU:O	13:O:209:ALA:C	2.52	0.48
7:H:44:ILE:HG22	17:X:19:PHE:CZ	2.48	0.48
20:Z:9:LEU:HD22	20:Z:9:LEU:C	2.34	0.48
1:A:147:TYR:HA	1:A:150:PRO:HG2	1.94	0.48
1:A:195:HIS:ND1	1:A:196:PRO:CD	2.68	0.48
1:A:244:GLU:HG3	4:D:264:LYS:HZ2	1.79	0.48
1:A:316:THR:O	1:A:317:TRP:C	2.51	0.48
2:B:113:TRP:HD1	26:B:1048:BCR:C37	2.26	0.48
2:B:150:CYS:O	2:B:152:GLY:N	2.47	0.48
2:B:27:THR:CB	23:B:1020:CLA:H11	2.44	0.48
2:B:444:ARG:HD2	2:B:444:ARG:N	2.29	0.48
2:B:92:SER:OG	2:B:94:GLU:HG2	2.14	0.48
30:C:1056:DGD:HB2	30:C:1056:DGD:CAB	2.34	0.48
1:A:278:TRP:CH2	30:C:1057:DGD:CIA	2.86	0.48
1:A:199:GLN:NE2	30:C:1057:DGD:HBW2	2.29	0.48
3:C:213:LEU:H	3:C:213:LEU:HD23	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:CE2	3:C:449:ARG:NH1	2.82	0.48
4:D:196:PHE:O	4:D:197:HIS:C	2.52	0.48
4:D:267:LEU:HD23	4:D:268:HIS:CD2	2.49	0.48
4:D:189:HIS:CG	4:D:289:LEU:HD12	2.48	0.48
4:D:298:PHE:O	4:D:299:ILE:C	2.52	0.48
11:L:15:THR:O	11:L:15:THR:CG2	2.60	0.48
11:L:30:LEU:HD22	11:L:31:PHE:CD1	2.36	0.48
12:M:15:VAL:O	12:M:15:VAL:HG12	2.14	0.48
14:T:1:MET:C	14:T:4:ILE:CG2	2.80	0.48
16:V:152:LEU:O	16:V:153:GLY:C	2.52	0.48
20:Z:3:ILE:N	20:Z:3:ILE:HD12	2.19	0.48
20:Z:46:LEU:HB3	20:Z:50:LEU:HD12	1.94	0.48
23:A:1003:CLA:H161	24:A:1038:PHO:H62	1.95	0.48
1:A:196:PRO:C	1:A:199:GLN:CG	2.82	0.48
1:A:201:GLY:O	1:A:205:VAL:HG23	2.14	0.48
1:A:202:VAL:HG11	23:A:1006:CLA:CAD	2.44	0.48
1:A:245:THR:OG1	4:D:265:ARG:HD3	2.13	0.48
2:B:458:PHE:HD2	23:B:1012:CLA:HMC3	1.70	0.48
23:B:1016:CLA:H92	23:B:1016:CLA:C5	2.43	0.48
23:B:1011:CLA:H171	23:B:1016:CLA:HBC3	1.95	0.48
2:B:7:ARG:HA	23:B:1019:CLA:CBA	2.42	0.48
2:B:256:MET:HE3	2:B:448:ARG:HH12	1.75	0.48
3:C:449:ARG:CZ	23:C:1029:CLA:CED	2.90	0.48
26:C:1054:BCR:H331	26:C:1054:BCR:C8	2.43	0.48
3:C:218:PHE:O	3:C:221:GLU:O	2.32	0.48
4:D:158:LEU:C	4:D:161:PRO:HD2	2.34	0.48
24:A:1038:PHO:ND	4:D:209:LEU:HD11	2.29	0.48
4:D:222:LEU:HA	4:D:244:TYR:HA	1.96	0.48
6:F:44:GLN:O	6:F:45:ARG:HB3	2.14	0.48
6:F:45:ARG:HH11	6:F:45:ARG:HG3	1.79	0.48
16:V:121:LEU:CD2	16:V:138:LEU:HD11	2.43	0.48
20:Z:37:LYS:C	20:Z:37:LYS:HD3	2.34	0.48
20:Z:50:LEU:HA	20:Z:53:VAL:CG2	2.44	0.48
24:A:1038:PHO:H3A	24:A:1038:PHO:HBA2	1.36	0.47
23:B:1010:CLA:HBB1	23:B:1010:CLA:CMB	2.29	0.47
2:B:434:THR:CG2	13:O:204:LYS:HE2	2.44	0.47
3:C:367:GLU:HB2	3:C:368:PRO:CD	2.38	0.47
3:C:280:SER:OG	3:C:438:LEU:HB2	2.13	0.47
23:A:1003:CLA:CAD	23:D:1005:CLA:CAC	2.91	0.47
23:D:1005:CLA:H161	29:D:1062:MGE:CFB	2.45	0.47
23:A:1006:CLA:CBC	4:D:182:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:GLN:O	5:E:77:GLU:HB3	2.14	0.47
7:H:49:TYR:CG	30:H:1058:DGD:O1B	2.67	0.47
7:H:58:VAL:HG12	7:H:58:VAL:O	2.14	0.47
9:J:40:LEU:N	9:J:40:LEU:CD2	2.77	0.47
10:K:35:LEU:HA	10:K:38:VAL:CG2	2.44	0.47
3:C:334:PRO:HA	13:O:179:THR:HB	1.94	0.47
15:U:57:LEU:CD1	15:U:112:PHE:HB3	2.44	0.47
15:U:46:LYS:HE3	15:U:115:THR:OG1	2.13	0.47
31:V:1041:HEM:HMA2	31:V:1041:HEM:HBA2	1.95	0.47
16:V:48:THR:C	16:V:50:LYS:N	2.63	0.47
20:Z:46:LEU:O	20:Z:50:LEU:HB2	2.14	0.47
23:A:1006:CLA:HED2	23:A:1006:CLA:CAA	2.44	0.47
1:A:199:GLN:OE1	1:A:200:LEU:HG	2.12	0.47
1:A:273:PHE:CD1	1:A:274:PHE:N	2.81	0.47
1:A:323:ARG:HG3	1:A:323:ARG:NH1	2.19	0.47
1:A:59:ASP:O	1:A:86:SER:HB2	2.14	0.47
1:A:76:ASN:ND2	1:A:78:ILE:N	2.62	0.47
23:B:1015:CLA:H93	11:L:31:PHE:HE2	1.78	0.47
23:B:1022:CLA:CAA	23:B:1022:CLA:CGD	2.68	0.47
2:B:103:LEU:HD22	2:B:107:LEU:HG	1.95	0.47
2:B:148:LEU:N	2:B:210:ILE:CD1	2.75	0.47
2:B:33:TRP:HE1	23:B:1015:CLA:CAC	2.28	0.47
2:B:373:LYS:C	2:B:375:GLY:N	2.66	0.47
2:B:445:THR:HG23	2:B:450:TRP:NE1	2.29	0.47
3:C:295:THR:O	3:C:297:TYR:N	2.47	0.47
4:D:139:ARG:NH1	4:D:139:ARG:HG3	2.29	0.47
4:D:212:ALA:O	4:D:213:ILE:C	2.52	0.47
4:D:281:MET:O	4:D:282:SER:C	2.52	0.47
4:D:68:LEU:CD2	5:E:44:TYR:HE1	2.26	0.47
4:D:89:LEU:N	4:D:89:LEU:CD2	2.75	0.47
2:B:460:LEU:CG	30:H:1058:DGD:HAG3	2.43	0.47
7:H:13:PRO:O	7:H:15:ASN:N	2.47	0.47
7:H:38:PHE:CZ	7:H:42:LEU:HG	2.49	0.47
13:O:136:MET:HG3	13:O:137:ALA:H	1.78	0.47
2:B:383:PHE:CE1	13:O:194:TYR:N	2.82	0.47
13:O:71:LEU:N	13:O:71:LEU:HD12	2.29	0.47
14:T:16:LEU:O	14:T:16:LEU:HD13	2.14	0.47
20:Z:22:GLY:O	20:Z:24:PRO:N	2.47	0.47
20:Z:61:VAL:HG23	20:Z:62:VAL:N	2.14	0.47
23:A:1006:CLA:CBA	30:C:1057:DGD:CFB	2.92	0.47
1:A:116:ILE:CG2	1:A:117:PHE:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:O	2:B:107:LEU:CD1	2.62	0.47
2:B:108:PHE:CD2	2:B:109:LEU:HD23	2.49	0.47
2:B:191:ASN:ND2	2:B:192:PRO:HD2	2.28	0.47
2:B:222:PRO:HG2	2:B:225:LEU:CD1	2.31	0.47
2:B:272:ARG:HD2	2:B:273:TYR:CE1	2.49	0.47
23:C:1032:CLA:H141	23:C:1032:CLA:H162	1.71	0.47
3:C:275:SER:HB3	23:C:1033:CLA:CED	2.45	0.47
23:C:1034:CLA:C4D	23:C:1034:CLA:H12	2.43	0.47
3:C:114:VAL:HG12	3:C:118:HIS:HD2	1.78	0.47
3:C:45:LEU:HD13	3:C:139:THR:HG23	1.96	0.47
3:C:236:GLY:HA3	26:C:1054:BCR:H392	1.96	0.47
3:C:263:ALA:H	8:I:28:PRO:CG	2.22	0.47
3:C:327:ASN:HB3	13:O:125:ASP:OD1	2.13	0.47
3:C:466:VAL:CG2	4:D:248:THR:HG22	2.45	0.47
3:C:57:ALA:C	3:C:60:ILE:HG22	2.35	0.47
3:C:63:TRP:HB2	23:C:1034:CLA:O2D	2.14	0.47
26:D:1050:BCR:H14C	6:F:33:PHE:CE2	2.50	0.47
4:D:209:LEU:CD2	4:D:209:LEU:C	2.83	0.47
1:A:28:LEU:HA	4:D:255:GLN:HA	1.96	0.47
4:D:76:VAL:CG1	4:D:77:ALA:N	2.77	0.47
8:I:14:PHE:O	8:I:18:LEU:HG	2.15	0.47
11:L:26:VAL:CG1	11:L:27:LEU:N	2.77	0.47
12:M:4:ASN:O	12:M:6:LEU:N	2.47	0.47
13:O:187:GLY:C	13:O:194:TYR:HB2	2.34	0.47
13:O:41:LEU:C	13:O:43:ASN:N	2.66	0.47
15:U:72:TYR:CD2	15:U:73:PRO:HD3	2.49	0.47
20:Z:51:VAL:O	20:Z:55:GLY:N	2.47	0.47
23:A:1003:CLA:H161	24:A:1038:PHO:H92	1.85	0.47
23:A:1007:CLA:H11	8:I:9:TYR:CE2	2.50	0.47
24:A:1039:PHO:H162	24:A:1039:PHO:H203	1.58	0.47
1:A:179:THR:HG22	1:A:183:MET:SD	2.53	0.47
1:A:246:TYR:HE1	4:D:264:LYS:NZ	2.12	0.47
2:B:143:LEU:O	2:B:144:PHE:C	2.52	0.47
2:B:338:GLN:OE1	2:B:338:GLN:HA	2.14	0.47
2:B:402:TYR:CD2	2:B:402:TYR:N	2.82	0.47
2:B:450:TRP:CH2	23:B:1015:CLA:H2	2.50	0.47
23:C:1025:CLA:HMB2	23:C:1025:CLA:H41	1.95	0.47
3:C:437:PHE:CZ	23:C:1026:CLA:HMC1	2.49	0.47
23:C:1034:CLA:H12	23:C:1034:CLA:CHA	2.44	0.47
3:C:245:ILE:C	3:C:247:GLY:N	2.68	0.47
3:C:33:PHE:CD2	3:C:33:PHE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:THR:CG2	3:C:348:GLU:OE1	2.59	0.47
3:C:450:ALA:HA	3:C:453:ALA:HB3	1.96	0.47
3:C:75:PHE:CE2	3:C:105:VAL:CG1	2.95	0.47
4:D:175:VAL:O	4:D:177:ALA:N	2.47	0.47
4:D:180:ARG:HD2	4:D:180:ARG:C	2.35	0.47
4:D:252:PHE:O	4:D:256:ILE:HG22	2.14	0.47
4:D:261:PHE:CE2	4:D:267:LEU:CA	2.97	0.47
31:E:1040:HEM:NC	6:F:24:HIS:HE1	2.10	0.47
7:H:41:PHE:O	7:H:42:LEU:C	2.52	0.47
13:O:167:ASP:HA	13:O:225:LEU:O	2.14	0.47
13:O:37:VAL:CG1	13:O:37:VAL:O	2.62	0.47
1:A:48:PHE:N	1:A:115:ILE:HD11	2.29	0.47
23:B:1022:CLA:H61	23:B:1022:CLA:H11	1.95	0.47
2:B:447:PRO:HA	2:B:450:TRP:HB2	1.96	0.47
2:B:45:PHE:O	2:B:47:PRO:CD	2.59	0.47
23:C:1028:CLA:C5	30:C:1056:DGD:HA52	2.44	0.47
3:C:335:THR:OG1	3:C:337:LEU:HB2	2.14	0.47
4:D:141:TYR:O	4:D:144:ILE:HG22	2.13	0.47
4:D:236:ASN:CB	4:D:237:PRO:HA	2.37	0.47
4:D:324:GLY:O	4:D:326:ARG:N	2.46	0.47
5:E:19:TYR:CD1	5:E:20:TRP:CD1	2.95	0.47
6:F:18:VAL:O	6:F:20:TRP:N	2.47	0.47
13:O:57:PRO:HA	13:O:161:SER:OG	2.14	0.47
16:V:86:ALA:N	16:V:93:ASP:HB3	2.29	0.47
17:X:34:PHE:O	17:X:38:ILE:CD1	2.63	0.47
1:A:279:ARG:CB	1:A:279:ARG:CZ	2.91	0.47
23:B:1019:CLA:C9	29:L:1061:MGE:C8A	2.83	0.47
23:B:1013:CLA:H72	23:B:1020:CLA:H172	1.97	0.47
2:B:443:PHE:O	2:B:443:PHE:CD2	2.68	0.47
23:C:1029:CLA:H71	23:C:1029:CLA:H191	1.95	0.47
23:D:1005:CLA:H43	25:D:1042:PQ9:H212	1.96	0.47
4:D:111:TRP:O	4:D:112:THR:C	2.51	0.47
4:D:267:LEU:CD2	4:D:268:HIS:CD2	2.97	0.47
4:D:91:LEU:HG	4:D:93:TRP:CZ2	2.49	0.47
13:O:169:LYS:CB	13:O:169:LYS:NZ	2.73	0.47
1:A:107:TYR:HB2	13:O:97:VAL:CG2	2.43	0.47
14:T:18:PHE:HB2	26:T:6046:BCR:C9	2.44	0.47
27:A:1063:LHG:H292	23:C:1032:CLA:C6	2.44	0.47
1:A:36:ILE:CD1	8:I:19:PHE:HB2	2.44	0.47
23:B:1019:CLA:HMB2	23:B:1020:CLA:C4B	2.44	0.47
23:B:1020:CLA:C14	23:B:1021:CLA:HAB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ILE:O	2:B:142:HIS:C	2.53	0.47
2:B:18:ARG:HG2	2:B:115:TRP:CD1	2.49	0.47
2:B:246:PHE:HB3	2:B:462:PHE:HB3	1.96	0.47
2:B:343:HIS:CE1	2:B:345:VAL:HG13	2.48	0.47
2:B:46:ASP:OD2	2:B:48:SER:OG	2.32	0.47
4:D:201:VAL:HG11	23:D:1005:CLA:CAD	2.45	0.47
4:D:72:ASN:ND2	4:D:73:PHE:N	2.62	0.47
8:I:27:ASP:C	8:I:29:ALA:N	2.67	0.47
29:L:1061:MGE:H3B1	29:L:1061:MGE:C7B	2.34	0.47
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.48	0.47
13:O:145:LEU:HG	13:O:145:LEU:O	2.14	0.47
1:A:13:LEU:HD22	1:A:13:LEU:N	2.28	0.47
1:A:140:ARG:HH21	27:A:1063:LHG:HC11	1.80	0.47
1:A:141:PRO:HG3	3:C:447:ARG:CA	2.40	0.47
1:A:258:LEU:O	4:D:128:ARG:NH1	2.44	0.47
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.49	0.47
1:A:320:ILE:C	1:A:322:ASN:N	2.67	0.47
1:A:93:PHE:O	1:A:95:PRO:HD3	2.15	0.47
23:B:1014:CLA:O2D	23:B:1014:CLA:HAA2	2.12	0.47
2:B:143:LEU:CD1	2:B:209:GLY:O	2.63	0.47
2:B:158:LEU:HD12	2:B:199:VAL:HA	1.96	0.47
2:B:465:GLY:H	23:B:1019:CLA:HBC2	1.65	0.47
2:B:66:MET:CG	23:B:1013:CLA:CED	2.90	0.47
23:C:1034:CLA:H3A	23:C:1034:CLA:HBA1	1.34	0.47
3:C:166:ILE:HD11	3:C:248:GLY:HA3	1.97	0.47
3:C:248:GLY:O	3:C:252:ILE:HB	2.14	0.47
3:C:443:TRP:CD1	3:C:444:HIS:CE1	3.02	0.47
4:D:27:PHE:CD2	6:F:19:ARG:HG3	2.50	0.47
2:B:384:ARG:HH12	4:D:348:ARG:CZ	2.28	0.47
4:D:42:TYR:HD2	4:D:43:LEU:HD13	1.80	0.47
11:L:23:LEU:HD12	11:L:23:LEU:O	2.15	0.47
13:O:108:GLN:O	13:O:124:GLU:N	2.46	0.47
13:O:74:THR:OG1	13:O:263:GLY:HA2	2.15	0.47
11:L:36:PHE:CD2	14:T:6:TYR:OH	2.56	0.47
15:U:72:TYR:O	15:U:73:PRO:C	2.53	0.47
15:U:80:VAL:C	15:U:82:ASN:N	2.68	0.47
15:U:94:ILE:HA	15:U:95:PRO:HD3	1.75	0.47
16:V:75:ASN:HA	16:V:76:PRO:HD2	1.74	0.47
16:V:81:ARG:HG3	16:V:81:ARG:HH11	1.80	0.47
26:A:1044:BCR:H403	26:A:1044:BCR:C22	2.40	0.47
27:A:1063:LHG:H202	27:A:1063:LHG:H171	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:O	1:A:53:ILE:HB	2.14	0.47
2:B:483:ASP:C	2:B:485:GLU:H	2.18	0.47
23:C:1034:CLA:O1A	23:C:1034:CLA:H102	2.14	0.47
3:C:383:ASP:O	3:C:385:GLN:N	2.47	0.47
2:B:463:PHE:CD2	30:H:1058:DGD:HAV1	2.50	0.47
13:O:109:GLY:HA3	13:O:123:GLU:HA	1.97	0.47
14:T:18:PHE:CD1	26:T:6046:BCR:C34	2.85	0.47
15:U:127:ARG:HG2	15:U:127:ARG:NH1	2.28	0.47
15:U:129:ASN:C	15:U:131:GLY:N	2.67	0.47
15:U:58:ASN:C	15:U:59:ASN:OD1	2.54	0.47
16:V:102:MET:HE1	16:V:141:ILE:CG2	2.45	0.47
20:Z:49:ALA:O	20:Z:52:LEU:N	2.48	0.47
24:A:1039:PHO:HAC1	24:A:1039:PHO:HMC3	1.67	0.47
1:A:246:TYR:HE1	4:D:264:LYS:HZ2	1.63	0.47
1:A:278:TRP:CA	1:A:278:TRP:CE3	2.84	0.47
23:B:1016:CLA:CGA	23:B:1016:CLA:NA	2.78	0.47
2:B:12:LEU:HB2	23:B:1020:CLA:HMC2	1.97	0.47
2:B:141:ILE:HG23	2:B:217:ILE:HD13	1.97	0.47
2:B:468:TRP:HD1	2:B:469:HIS:ND1	2.13	0.47
2:B:478:VAL:HG12	2:B:479:PHE:N	2.30	0.47
2:B:83:GLU:HG3	2:B:83:GLU:H	1.50	0.47
23:C:1025:CLA:HED3	23:C:1025:CLA:OBD	2.15	0.47
23:C:1031:CLA:CBA	23:C:1033:CLA:CED	2.93	0.47
1:A:333:GLU:OE1	3:C:354:GLU:OE2	2.32	0.47
3:C:374:GLY:HA2	13:O:33:TYR:CE1	2.50	0.47
3:C:62:PHE:HB2	3:C:122:SER:OG	2.15	0.47
23:D:1005:CLA:H203	23:D:1005:CLA:H151	1.70	0.47
4:D:102:THR:HG22	4:D:103:ARG:N	2.30	0.47
4:D:253:TRP:CD1	25:D:1042:PQ9:H93	2.50	0.47
4:D:252:PHE:CD1	4:D:252:PHE:C	2.88	0.47
4:D:257:PHE:CD1	4:D:257:PHE:O	2.68	0.47
7:H:39:LEU:HD13	7:H:39:LEU:O	2.15	0.47
13:O:184:ASP:OD1	13:O:188:ARG:O	2.33	0.47
2:B:384:ARG:HA	13:O:192:SER:CB	2.45	0.47
4:D:302:GLU:CG	13:O:199:ALA:HB1	2.44	0.47
16:V:52:TYR:O	16:V:55:GLY:N	2.48	0.47
16:V:98:LEU:HD12	16:V:98:LEU:N	2.30	0.47
20:Z:31:GLN:O	20:Z:32:ASP:O	2.33	0.47
1:A:174:LEU:H	1:A:174:LEU:CD2	2.20	0.47
1:A:50:ILE:HB	26:A:1044:BCR:C39	2.44	0.47
1:A:92:HIS:CD2	3:C:220:GLY:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1011:CLA:CHD	23:B:1013:CLA:H51	2.44	0.47
2:B:25:MET:HE3	2:B:108:PHE:CD1	2.50	0.47
2:B:135:LEU:HD13	2:B:136:PRO:HD3	1.96	0.47
2:B:256:MET:HA	2:B:256:MET:HE3	1.97	0.47
2:B:266:GLU:HG3	2:B:312:TYR:OH	2.15	0.47
2:B:450:TRP:CZ3	23:B:1015:CLA:H2	2.49	0.47
2:B:53:ASN:ND2	2:B:53:ASN:O	2.48	0.47
23:C:1028:CLA:HHD	23:C:1028:CLA:CBC	2.36	0.47
3:C:131:TYR:C	3:C:133:ALA:N	2.68	0.47
3:C:48:LYS:HZ1	3:C:138:GLU:CD	2.17	0.47
3:C:318:LEU:HD21	3:C:328:VAL:HG11	1.94	0.47
4:D:103:ARG:C	4:D:105:CYS:N	2.67	0.47
7:H:21:VAL:HG12	7:H:22:ALA:H	1.79	0.47
11:L:30:LEU:CD2	11:L:31:PHE:HD1	2.22	0.47
13:O:116:ASP:OD2	13:O:157:PRO:O	2.33	0.47
13:O:208:LEU:O	13:O:210:ARG:N	2.48	0.47
13:O:239:GLY:O	13:O:264:VAL:HA	2.15	0.47
13:O:65:ARG:NH1	13:O:66:ILE:O	2.48	0.47
16:V:88:ALA:HA	16:V:108:TYR:CE1	2.49	0.47
16:V:64:ALA:O	16:V:66:CYS:N	2.47	0.47
16:V:45:ILE:HG21	16:V:95:ILE:HD12	1.97	0.47
23:A:1003:CLA:H18	23:A:1003:CLA:H152	1.74	0.46
1:A:97:TRP:O	8:I:1:MET:HG2	2.15	0.46
23:B:1010:CLA:HAA2	23:B:1010:CLA:CGD	2.43	0.46
2:B:98:LEU:O	2:B:101:ILE:HB	2.15	0.46
2:B:273:TYR:O	2:B:277:SER:HB2	2.14	0.46
2:B:41:GLU:CD	2:B:62:VAL:H	2.19	0.46
2:B:465:GLY:C	2:B:467:ILE:H	2.14	0.46
3:C:222:GLY:H	3:C:226:SER:HB3	1.80	0.46
3:C:269:GLU:OE2	3:C:447:ARG:HD2	2.16	0.46
1:A:135:TYR:CE1	3:C:449:ARG:HD2	2.50	0.46
3:C:456:GLU:O	3:C:457:LYS:HB2	2.15	0.46
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.46
4:D:328:TRP:NE1	4:D:346:LEU:HD11	2.30	0.46
4:D:330:ALA:O	4:D:334:GLN:N	2.42	0.46
5:E:38:VAL:CB	6:F:39:ALA:HB3	2.45	0.46
26:H:1049:BCR:C8	26:H:1049:BCR:H311	2.45	0.46
8:I:16:VAL:O	8:I:20:VAL:HG23	2.14	0.46
23:A:1007:CLA:HAC2	26:A:1044:BCR:H351	1.96	0.46
1:A:226:GLU:HG3	1:A:236:GLY:HA2	1.97	0.46
1:A:334:ARG:O	1:A:336:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HG2	1:A:98:GLU:CG	2.43	0.46
1:A:96:ILE:HA	1:A:105:TRP:NE1	2.29	0.46
23:B:1018:CLA:O2D	23:B:1018:CLA:H2A	2.16	0.46
29:B:1060:MGE:H3A2	29:B:1060:MGE:CGB	2.39	0.46
2:B:256:MET:HE2	2:B:448:ARG:HG3	1.96	0.46
23:C:1032:CLA:C19	23:C:1032:CLA:H152	2.39	0.46
3:C:39:ASN:HA	23:C:1035:CLA:CED	2.44	0.46
4:D:196:PHE:CE2	4:D:284:ILE:HB	2.49	0.46
4:D:213:ILE:HD12	4:D:213:ILE:O	2.15	0.46
4:D:253:TRP:CD1	4:D:253:TRP:N	2.82	0.46
4:D:284:ILE:O	4:D:285:GLY:C	2.52	0.46
1:A:184:ILE:CB	4:D:321:LEU:HD13	2.45	0.46
2:B:369:ILE:HD13	4:D:340:VAL:O	2.14	0.46
26:D:1050:BCR:C19	29:J:1059:MGE:H5A1	2.46	0.46
9:J:23:VAL:CG1	9:J:24:ILE:N	2.78	0.46
25:D:1042:PQ9:H361	29:L:1061:MGE:H231	1.96	0.46
11:L:25:LEU:HD11	14:T:12:CYS:HB3	1.98	0.46
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.72	0.46
13:O:70:CYS:HA	13:O:104:LEU:O	2.15	0.46
20:Z:38:GLN:C	20:Z:40:ILE:N	2.67	0.46
20:Z:59:PHE:HD1	20:Z:59:PHE:H	1.62	0.46
1:A:286:ALA:HB1	23:A:1003:CLA:O1D	2.14	0.46
24:A:1038:PHO:C10	24:A:1038:PHO:C14	2.67	0.46
1:A:113:GLN:O	1:A:116:ILE:N	2.48	0.46
1:A:116:ILE:CG2	1:A:117:PHE:H	2.27	0.46
1:A:117:PHE:HD2	1:A:117:PHE:N	2.12	0.46
1:A:224:ILE:O	2:B:481:GLY:C	2.53	0.46
2:B:92:SER:O	2:B:93:PHE:C	2.53	0.46
2:B:71:VAL:HG21	2:B:96:VAL:CG2	2.43	0.46
23:C:1025:CLA:CHB	23:C:1025:CLA:H42	2.45	0.46
23:C:1026:CLA:C4	23:C:1026:CLA:H71	2.45	0.46
23:C:1033:CLA:H111	23:C:1033:CLA:H143	1.60	0.46
1:A:155:PHE:HE1	30:C:1055:DGD:HAT2	1.80	0.46
4:D:190:ASN:HD21	4:D:193:LEU:CD2	2.29	0.46
4:D:235:PHE:O	4:D:236:ASN:CB	2.63	0.46
4:D:298:PHE:O	4:D:301:GLN:HB2	2.15	0.46
5:E:21:VAL:O	5:E:25:ILE:HG13	2.15	0.46
5:E:68:ASP:HA	5:E:69:ARG:HE	1.79	0.46
10:K:19:ASP:OD2	10:K:20:PRO:HD3	2.15	0.46
20:Z:43:GLY:O	20:Z:47:TRP:N	2.35	0.46
1:A:22:THR:HA	1:A:29:TYR:CE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1009:CLA:CAA	23:B:1009:CLA:CED	2.91	0.46
23:B:1012:CLA:C10	23:B:1023:CLA:C1	2.90	0.46
23:B:1023:CLA:H112	23:B:1023:CLA:H142	1.59	0.46
23:B:1024:CLA:H92	23:B:1024:CLA:H62	1.67	0.46
29:B:1060:MGE:O1B	29:B:1060:MGE:C1G	2.62	0.46
2:B:257:TRP:CZ3	4:D:291:LEU:CD1	2.98	0.46
2:B:297:THR:CG2	2:B:300:GLU:HG3	2.46	0.46
2:B:280:PHE:CZ	2:B:312:TYR:HD1	2.33	0.46
2:B:450:TRP:O	2:B:453:PHE:N	2.42	0.46
2:B:474:LEU:C	2:B:475:PHE:HD2	2.19	0.46
3:C:404:LEU:HD12	30:C:1057:DGD:HA21	1.98	0.46
3:C:108:THR:HG21	10:K:10:LYS:HD2	1.96	0.46
3:C:92:ILE:HD12	3:C:97:TRP:HB2	1.98	0.46
4:D:113:PHE:O	4:D:114:ILE:C	2.53	0.46
2:B:258:TYR:HH	4:D:162:LEU:C	2.18	0.46
4:D:196:PHE:HA	4:D:199:MET:HE3	1.97	0.46
3:C:457:LYS:HB3	4:D:224:GLN:HG3	1.96	0.46
5:E:69:ARG:N	5:E:69:ARG:HE	2.13	0.46
13:O:254:HIS:O	13:O:255:GLU:C	2.54	0.46
16:V:102:MET:CE	16:V:141:ILE:HB	2.45	0.46
16:V:144:HIS:O	16:V:148:GLU:HG2	2.15	0.46
18:Y:26:ALA:O	18:Y:30:ILE:HG22	2.15	0.46
18:Y:28:ILE:CG1	18:Y:29:GLY:N	2.78	0.46
20:Z:59:PHE:CD1	20:Z:59:PHE:N	2.82	0.46
1:A:94:TYR:OH	1:A:104:GLU:HG2	2.16	0.46
23:B:1012:CLA:HED3	23:B:1013:CLA:C1	2.45	0.46
2:B:191:ASN:HD22	2:B:191:ASN:C	2.18	0.46
2:B:55:MET:SD	2:B:64:PRO:HA	2.56	0.46
2:B:86:ILE:HG13	2:B:87:ASP:N	2.30	0.46
23:C:1026:CLA:OBD	23:C:1026:CLA:C9	2.63	0.46
23:C:1027:CLA:CBA	23:C:1027:CLA:CHA	2.76	0.46
1:A:131:TRP:CZ3	23:C:1029:CLA:HMA3	2.50	0.46
23:C:1037:CLA:HMC1	23:C:1037:CLA:HBC3	1.97	0.46
3:C:306:GLY:O	3:C:309:ALA:HB3	2.15	0.46
4:D:175:VAL:O	4:D:178:ILE:N	2.49	0.46
3:C:469:MET:HE2	4:D:251:ARG:CZ	2.46	0.46
7:H:28:THR:O	7:H:31:MET:HB3	2.16	0.46
12:M:9:ILE:N	12:M:9:ILE:HD12	2.23	0.46
15:U:106:ARG:O	15:U:109:LEU:HB2	2.16	0.46
16:V:120:SER:O	16:V:123:SER:CB	2.63	0.46
16:V:63:CYS:O	16:V:66:CYS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:68:VAL:C	16:V:70:GLY:N	2.68	0.46
20:Z:39:LEU:O	20:Z:42:LEU:CB	2.63	0.46
26:A:1044:BCR:H392	26:A:1044:BCR:C22	2.41	0.46
23:B:1010:CLA:H161	30:H:1058:DGD:HA82	1.98	0.46
23:C:1032:CLA:C17	23:C:1034:CLA:H191	2.44	0.46
3:C:334:PRO:CD	3:C:335:THR:H	2.28	0.46
3:C:34:ALA:O	3:C:38:GLY:CA	2.61	0.46
1:A:269:ARG:HH11	4:D:231:THR:CG2	2.29	0.46
4:D:336:HIS:CD2	4:D:336:HIS:H	2.33	0.46
13:O:65:ARG:HA	13:O:65:ARG:NE	2.31	0.46
26:Z:1053:BCR:H24C	26:Z:1053:BCR:H371	1.64	0.46
23:B:1011:CLA:HMD2	23:B:1014:CLA:HBB1	1.96	0.46
23:B:1019:CLA:H191	23:B:1021:CLA:C7	2.44	0.46
2:B:223:GLN:CD	7:H:24:GLY:HA2	2.35	0.46
2:B:229:LEU:HD23	2:B:231:MET:N	2.31	0.46
3:C:255:THR:O	3:C:256:PRO:O	2.33	0.46
23:D:1004:CLA:H61	23:D:1004:CLA:H41	1.71	0.46
4:D:209:LEU:HD13	25:D:1042:PQ9:H193	1.97	0.46
6:F:37:ILE:CA	6:F:40:MET:HE3	2.22	0.46
13:O:114:ASN:OD1	13:O:114:ASN:N	2.48	0.46
14:T:2:GLU:HG3	14:T:3:THR:H	1.80	0.46
16:V:120:SER:O	16:V:121:LEU:C	2.54	0.46
23:C:1037:CLA:CHC	26:Z:1053:BCR:H383	2.45	0.46
1:A:279:ARG:HH22	24:A:1038:PHO:HMC1	1.80	0.46
1:A:227:THR:O	1:A:230:THR:HG23	2.16	0.46
1:A:260:PHE:O	1:A:261:GLN:O	2.33	0.46
1:A:279:ARG:HA	1:A:279:ARG:NE	2.31	0.46
23:B:1010:CLA:CBD	23:B:1010:CLA:CAA	2.94	0.46
2:B:249:ALA:HB2	23:B:1012:CLA:HBC1	1.96	0.46
23:B:1019:CLA:H193	23:B:1019:CLA:H162	1.55	0.46
2:B:178:VAL:O	2:B:179:GLN:HG2	2.16	0.46
2:B:19:LEU:O	2:B:19:LEU:HD13	2.16	0.46
2:B:215:PHE:CE1	2:B:219:VAL:HG21	2.51	0.46
2:B:224:ARG:HB3	7:H:25:TRP:CB	2.42	0.46
2:B:406:LEU:HD23	2:B:409:GLN:NE2	2.31	0.46
3:C:128:GLY:HA3	23:C:1037:CLA:HAC2	1.95	0.46
26:C:1054:BCR:C8	26:C:1054:BCR:C33	2.90	0.46
3:C:234:VAL:O	3:C:238:ILE:HG13	2.15	0.46
3:C:237:HIS:O	3:C:240:ILE:CG2	2.64	0.46
3:C:250:TRP:CD1	3:C:250:TRP:C	2.88	0.46
3:C:271:TYR:C	23:C:1033:CLA:HMD3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:CG	3:C:443:TRP:CZ3	3.04	0.46
3:C:67:MET:O	3:C:70:PHE:HB3	2.15	0.46
4:D:152:VAL:HG23	23:D:1004:CLA:O2D	2.15	0.46
23:A:1003:CLA:C4D	23:D:1005:CLA:HAC2	2.46	0.46
26:D:1050:BCR:C8	26:D:1050:BCR:C33	2.36	0.46
26:D:1050:BCR:H281	29:J:1059:MGE:C9B	2.33	0.46
4:D:126:MET:HG3	4:D:146:PHE:HB3	1.97	0.46
4:D:236:ASN:HB3	4:D:237:PRO:CA	2.39	0.46
4:D:263:ASN:O	4:D:263:ASN:OD1	2.34	0.46
4:D:298:PHE:O	4:D:301:GLN:N	2.29	0.46
4:D:39:PRO:O	4:D:43:LEU:CD2	2.62	0.46
4:D:67:TYR:CD1	4:D:76:VAL:HG21	2.51	0.46
6:F:32:PHE:C	6:F:32:PHE:HD2	2.19	0.46
23:B:1009:CLA:C4	26:H:1049:BCR:H353	2.24	0.46
7:H:53:LEU:CG	7:H:55:LEU:HD11	2.36	0.46
15:U:40:VAL:CG1	15:U:41:ASN:N	2.78	0.46
1:A:325:ASN:O	1:A:328:MET:HG2	2.16	0.46
23:B:1013:CLA:H93	23:B:1013:CLA:H62	1.71	0.46
23:B:1023:CLA:C7	26:B:1048:BCR:H341	2.46	0.46
2:B:284:ILE:CG1	2:B:285:ASN:H	2.27	0.46
2:B:422:ARG:HD2	2:B:423:LYS:HZ2	1.77	0.46
2:B:429:ILE:CD1	2:B:429:ILE:N	2.78	0.46
3:C:100:GLY:O	3:C:102:GLY:N	2.49	0.46
23:C:1027:CLA:CED	23:C:1036:CLA:H203	2.37	0.46
3:C:234:VAL:C	3:C:236:GLY:H	2.18	0.46
3:C:453:ALA:HB1	3:C:455:PHE:CE2	2.50	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.98	0.46
2:B:457:VAL:HG13	4:D:284:ILE:HD13	1.98	0.46
4:D:61:HIS:O	4:D:63:LEU:N	2.49	0.46
7:H:32:ALA:HA	7:H:35:MET:HE2	1.97	0.46
11:L:32:SER:O	11:L:35:PHE:N	2.38	0.46
13:O:117:GLY:HA3	13:O:158:ASN:ND2	2.31	0.46
13:O:153:ALA:HB1	13:O:168:PHE:CD2	2.51	0.46
15:U:72:TYR:HD2	15:U:73:PRO:HD3	1.81	0.46
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.30	0.46
16:V:99:VAL:O	16:V:100:ASP:C	2.55	0.46
20:Z:1:MET:SD	20:Z:60:PHE:HD2	2.39	0.46
1:A:41:LEU:HD12	24:A:1038:PHO:H52	1.98	0.46
27:A:1063:LHG:HC62	27:A:1063:LHG:P	2.54	0.46
1:A:223:LEU:CD2	1:A:245:THR:O	2.64	0.46
1:A:243:GLU:N	1:A:243:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:SER:HB3	4:D:236:ASN:HD21	1.81	0.46
2:B:156:PHE:HB3	2:B:162:PHE:CB	2.45	0.46
2:B:252:VAL:C	2:B:254:GLY:H	2.19	0.46
2:B:422:ARG:HH11	2:B:422:ARG:HB3	1.80	0.46
23:C:1029:CLA:H51	23:C:1029:CLA:C4B	2.46	0.46
3:C:228:ASN:O	3:C:295:THR:HG21	2.16	0.46
3:C:72:LEU:C	3:C:74:HIS:H	2.19	0.46
3:C:94:THR:HG22	3:C:298:PRO:CG	2.45	0.46
24:A:1038:PHO:H92	23:D:1005:CLA:C19	2.45	0.46
25:D:1042:PQ9:H292	25:D:1042:PQ9:H261	1.27	0.46
4:D:161:PRO:HG3	4:D:170:ALA:CB	2.45	0.46
4:D:18:LEU:O	4:D:22:LEU:HG	2.16	0.46
4:D:263:ASN:OD1	4:D:266:TRP:N	2.48	0.46
4:D:299:ILE:O	4:D:300:SER:C	2.55	0.46
4:D:55:VAL:CG1	4:D:105:CYS:SG	3.04	0.46
4:D:70:GLY:O	9:J:37:GLY:HA3	2.16	0.46
5:E:45:ASP:OD1	5:E:51:ARG:NH2	2.49	0.46
23:B:1010:CLA:H41	7:H:46:LEU:CA	2.46	0.46
14:T:15:ALA:O	14:T:17:PHE:N	2.49	0.46
31:V:1041:HEM:CBC	31:V:1041:HEM:HHH	2.45	0.46
16:V:120:SER:O	16:V:122:ARG:N	2.48	0.46
16:V:68:VAL:O	16:V:70:GLY:N	2.49	0.46
20:Z:10:ALA:O	20:Z:13:VAL:CG1	2.63	0.46
1:A:150:PRO:CA	23:A:1003:CLA:C4	2.82	0.45
2:B:193:TYR:O	2:B:261:ALA:HB2	2.16	0.45
2:B:223:GLN:CG	7:H:24:GLY:HA2	2.45	0.45
2:B:224:ARG:HG2	7:H:25:TRP:CD1	2.52	0.45
2:B:324:LEU:O	2:B:325:PHE:CD2	2.69	0.45
2:B:463:PHE:O	2:B:466:HIS:HB3	2.16	0.45
23:C:1028:CLA:H71	30:C:1056:DGD:C7A	2.46	0.45
3:C:384:ILE:O	3:C:384:ILE:CG2	2.54	0.45
3:C:418:ASN:HD22	3:C:418:ASN:C	2.19	0.45
4:D:198:MET:HE2	4:D:198:MET:HB2	1.67	0.45
1:A:126:TYR:OH	4:D:257:PHE:HB2	2.16	0.45
1:A:69:GLY:HA2	4:D:313:THR:HG22	1.98	0.45
4:D:314:PHE:O	4:D:315:TYR:C	2.55	0.45
29:J:1059:MGE:H1D	29:J:1059:MGE:H6D2	1.78	0.45
10:K:10:LYS:O	10:K:10:LYS:CG	2.65	0.45
13:O:142:ILE:N	13:O:142:ILE:CD1	2.75	0.45
13:O:218:LEU:HD23	13:O:219:THR:N	2.31	0.45
13:O:269:ILE:O	13:O:270:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:24:ARG:O	14:T:26:PRO:HD3	2.16	0.45
16:V:67:HIS:ND1	16:V:80:LEU:HD11	2.30	0.45
1:A:243:GLU:HA	4:D:241:GLU:CB	2.45	0.45
1:A:322:ASN:HA	1:A:322:ASN:HD22	1.53	0.45
2:B:454:ALA:CB	23:B:1015:CLA:HBB2	2.46	0.45
2:B:18:ARG:HB3	2:B:115:TRP:CD1	2.51	0.45
2:B:256:MET:HE3	2:B:448:ARG:CZ	2.46	0.45
2:B:355:PHE:C	2:B:370:LEU:HD23	2.36	0.45
2:B:416:THR:O	2:B:417:VAL:C	2.53	0.45
23:C:1033:CLA:C2	23:C:1033:CLA:O1A	2.64	0.45
3:C:151:TRP:CD2	3:C:268:GLY:HA3	2.51	0.45
3:C:39:ASN:HB3	23:C:1032:CLA:HBA1	1.98	0.45
3:C:449:ARG:NE	23:C:1029:CLA:HED2	2.30	0.45
4:D:103:ARG:HD3	5:E:73:LYS:HD2	1.98	0.45
24:A:1039:PHO:H71	4:D:122:LEU:CD1	2.44	0.45
4:D:68:LEU:HD21	5:E:44:TYR:CE1	2.51	0.45
13:O:148:VAL:HG12	13:O:151:LEU:CB	2.33	0.45
1:A:75:ASN:ND2	14:T:3:THR:OG1	2.49	0.45
15:U:78:LEU:O	15:U:79:ILE:C	2.53	0.45
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.37	0.45
18:Y:29:GLY:O	18:Y:33:PRO:HD2	2.16	0.45
18:Y:29:GLY:O	18:Y:33:PRO:HD3	2.16	0.45
1:A:119:PHE:HZ	23:A:1003:CLA:H91	1.80	0.45
26:A:1044:BCR:H373	26:A:1044:BCR:C39	2.26	0.45
1:A:160:ILE:CG2	1:A:291:SER:HA	2.44	0.45
23:B:1022:CLA:C1A	23:B:1022:CLA:O1A	2.65	0.45
2:B:120:LEU:O	2:B:121:GLU:O	2.35	0.45
2:B:149:LEU:HG	23:B:1011:CLA:HBC1	1.98	0.45
2:B:315:ILE:CG2	2:B:316:GLY:N	2.79	0.45
2:B:342:GLY:CA	2:B:404:GLY:HA3	2.46	0.45
2:B:429:ILE:CD1	2:B:429:ILE:H	2.28	0.45
2:B:467:ILE:O	2:B:471:ALA:HB2	2.16	0.45
2:B:86:ILE:O	2:B:87:ASP:CB	2.60	0.45
23:C:1027:CLA:HMA3	23:C:1027:CLA:HAA2	1.68	0.45
30:C:1055:DGD:HB61	30:C:1055:DGD:HB91	1.54	0.45
23:A:1006:CLA:CED	30:C:1057:DGD:HBW1	2.44	0.45
3:C:369:LEU:O	3:C:369:LEU:CD1	2.65	0.45
3:C:322:GLN:NE2	3:C:381:LYS:HA	2.17	0.45
4:D:123:ILE:O	4:D:127:LEU:CD2	2.65	0.45
4:D:146:PHE:C	4:D:149:PRO:HD2	2.36	0.45
4:D:74:LEU:O	4:D:175:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:ASP:OD2	5:E:54:SER:N	2.49	0.45
3:C:329:GLY:O	13:O:127:ILE:HG23	2.16	0.45
13:O:172:PHE:CD1	13:O:172:PHE:C	2.90	0.45
13:O:215:ARG:N	13:O:215:ARG:CD	2.73	0.45
11:L:36:PHE:CD2	14:T:6:TYR:CZ	3.04	0.45
16:V:105:PRO:HG2	16:V:115:ALA:HA	1.97	0.45
20:Z:54:VAL:O	26:Z:1053:BCR:H313	2.16	0.45
24:A:1038:PHO:H101	24:A:1038:PHO:H143	1.93	0.45
1:A:259:ILE:O	1:A:260:PHE:C	2.54	0.45
1:A:306:VAL:CG2	1:A:316:THR:HG23	2.46	0.45
2:B:486:LEU:HD12	2:B:489:GLU:OE1	2.16	0.45
3:C:158:THR:O	3:C:158:THR:HG22	2.16	0.45
3:C:249:ILE:HD12	3:C:249:ILE:N	2.31	0.45
3:C:270:ALA:O	3:C:274:TYR:HD1	1.98	0.45
3:C:391:ARG:HB2	3:C:391:ARG:CZ	2.45	0.45
3:C:464:GLU:CG	3:C:467:LEU:HB2	2.45	0.45
3:C:61:VAL:O	3:C:64:ALA:HB3	2.16	0.45
3:C:84:GLN:CB	3:C:86:LEU:HD13	2.46	0.45
23:D:1004:CLA:H3A	23:D:1004:CLA:HBA1	1.60	0.45
7:H:6:TRP:C	7:H:6:TRP:CD1	2.90	0.45
11:L:24:ILE:HG23	11:L:25:LEU:H	1.80	0.45
13:O:239:GLY:O	13:O:264:VAL:CG1	2.65	0.45
13:O:237:ILE:HD13	13:O:269:ILE:HD11	1.99	0.45
16:V:141:ILE:O	16:V:142:ALA:C	2.54	0.45
16:V:66:CYS:O	16:V:68:VAL:N	2.50	0.45
10:K:18:PHE:CZ	20:Z:9:LEU:HD21	2.52	0.45
23:A:1006:CLA:H111	30:C:1057:DGD:HBG2	1.86	0.45
25:A:1043:PQ9:H292	25:A:1043:PQ9:H261	1.50	0.45
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.51	0.45
23:B:1016:CLA:H143	23:B:1016:CLA:H162	1.62	0.45
2:B:373:LYS:HG3	2:B:374:ASN:H	1.80	0.45
2:B:389:LYS:HB3	2:B:390:TYR:HD1	1.81	0.45
23:C:1027:CLA:HBA1	23:C:1027:CLA:CB	2.45	0.45
30:C:1056:DGD:C2B	30:C:1056:DGD:HG12	2.01	0.45
3:C:341:LEU:HD23	3:C:351:PHE:HA	1.99	0.45
4:D:110:LEU:C	4:D:113:PHE:HB3	2.37	0.45
4:D:156:VAL:O	4:D:157:PHE:CD1	2.69	0.45
4:D:198:MET:O	25:D:1042:PQ9:H393	2.17	0.45
4:D:221:THR:HG23	4:D:244:TYR:CB	2.47	0.45
24:A:1038:PHO:HMA2	4:D:257:PHE:CE2	2.51	0.45
4:D:68:LEU:HD22	5:E:44:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:GLN:HG3	5:E:79:PHE:CE1	2.52	0.45
8:I:3:THR:C	8:I:6:ILE:HD11	2.36	0.45
2:B:441:GLY:O	13:O:201:PRO:HD2	2.17	0.45
13:O:36:ILE:O	13:O:36:ILE:HG22	2.14	0.45
15:U:60:THR:O	15:U:127:ARG:NH1	2.50	0.45
18:Y:42:ARG:HG2	18:Y:42:ARG:HH11	1.81	0.45
23:A:1003:CLA:HAA2	23:A:1003:CLA:HBD	1.99	0.45
24:A:1038:PHO:H92	23:D:1005:CLA:H203	1.98	0.45
1:A:176:ILE:O	1:A:179:THR:HB	2.17	0.45
23:B:1012:CLA:HBA2	23:B:1012:CLA:H3A	1.42	0.45
23:B:1022:CLA:C17	23:B:1022:CLA:H71	2.19	0.45
2:B:219:VAL:CG1	2:B:220:ARG:H	2.29	0.45
2:B:442:ILE:O	2:B:443:PHE:O	2.35	0.45
2:B:68:ARG:CG	2:B:69:LEU:H	2.30	0.45
23:C:1028:CLA:H92	30:C:1056:DGD:HBW1	1.98	0.45
23:C:1036:CLA:HBC2	23:C:1036:CLA:HMC1	1.99	0.45
3:C:166:ILE:HD13	3:C:245:ILE:HA	1.98	0.45
3:C:297:TYR:O	3:C:298:PRO:C	2.55	0.45
3:C:391:ARG:HH11	3:C:391:ARG:CG	2.29	0.45
1:A:160:ILE:HG13	3:C:431:PHE:HE1	1.81	0.45
1:A:258:LEU:HA	4:D:132:ILE:HD12	1.99	0.45
4:D:147:SER:O	4:D:148:ALA:C	2.55	0.45
7:H:30:LEU:O	7:H:33:VAL:HG12	2.17	0.45
4:D:18:LEU:HD13	17:X:37:LEU:HB3	1.98	0.45
23:A:1003:CLA:CHD	23:A:1003:CLA:CBC	2.91	0.45
1:A:140:ARG:HB2	4:D:220:ASN:CA	2.47	0.45
1:A:159:LEU:HG	1:A:163:ILE:CD1	2.45	0.45
1:A:329:GLU:OE1	3:C:412:THR:OG1	2.35	0.45
2:B:280:PHE:O	2:B:284:ILE:HG23	2.16	0.45
2:B:95:GLY:O	2:B:99:ALA:N	2.23	0.45
3:C:131:TYR:C	3:C:133:ALA:H	2.20	0.45
3:C:320:ARG:O	3:C:324:LEU:HD13	2.16	0.45
3:C:435:PHE:O	3:C:436:PHE:C	2.54	0.45
3:C:95:LEU:HA	3:C:185:LEU:HD23	1.99	0.45
23:A:1006:CLA:H162	26:D:1050:BCR:H291	1.98	0.45
24:A:1038:PHO:HED1	4:D:213:ILE:HB	1.98	0.45
4:D:337:GLU:O	4:D:338:ASN:C	2.55	0.45
4:D:68:LEU:CD2	5:E:44:TYR:CE1	2.99	0.45
5:E:30:LEU:HD12	6:F:31:ILE:HG23	1.98	0.45
7:H:7:LEU:HD23	7:H:7:LEU:O	2.17	0.45
8:I:13:THR:O	8:I:16:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1051:BCR:C39	26:K:1051:BCR:H373	2.29	0.45
11:L:26:VAL:HG21	29:L:1061:MGE:CGB	2.39	0.45
13:O:121:PHE:HE1	13:O:151:LEU:HD23	1.82	0.45
3:C:334:PRO:HA	13:O:179:THR:CB	2.47	0.45
13:O:65:ARG:HH11	13:O:108:GLN:HB2	1.82	0.45
13:O:91:PHE:CE1	13:O:260:LYS:HE3	2.52	0.45
15:U:98:THR:O	15:U:100:ARG:N	2.49	0.45
16:V:159:GLY:O	16:V:160:LYS:HB3	2.17	0.45
23:A:1003:CLA:H112	23:A:1003:CLA:H91	1.64	0.45
1:A:151:LEU:O	1:A:152:ALA:C	2.54	0.45
23:B:1011:CLA:C2D	23:B:1013:CLA:C3	2.94	0.45
23:B:1023:CLA:H72	26:B:1048:BCR:H343	1.96	0.45
2:B:230:ARG:O	2:B:230:ARG:HG3	2.16	0.45
2:B:280:PHE:CE2	2:B:312:TYR:HD1	2.35	0.45
2:B:334:ASP:O	2:B:432:PHE:CD2	2.70	0.45
2:B:399:VAL:HG13	2:B:417:VAL:CG2	2.46	0.45
3:C:118:HIS:NE2	23:C:1027:CLA:O1A	2.49	0.45
23:C:1025:CLA:H201	23:C:1031:CLA:H122	1.98	0.45
3:C:248:GLY:C	3:C:250:TRP:N	2.69	0.45
3:C:297:TYR:HD1	3:C:302:TYR:CE2	2.34	0.45
3:C:458:GLY:C	3:C:459:ILE:HD12	2.37	0.45
1:A:328:MET:HB2	4:D:321:LEU:HD22	1.98	0.45
7:H:12:ARG:CB	7:H:12:ARG:NH1	2.80	0.45
13:O:234:THR:HG21	13:O:236:GLU:HG3	1.98	0.45
18:Y:44:GLY:O	18:Y:45:ASN:C	2.55	0.45
1:A:135:TYR:C	1:A:137:LEU:H	2.19	0.45
1:A:279:ARG:C	1:A:283:VAL:HG12	2.37	0.45
23:B:1011:CLA:C2D	23:B:1013:CLA:H43	2.41	0.45
23:B:1019:CLA:H3A	23:B:1019:CLA:CGA	2.30	0.45
23:B:1019:CLA:H41	23:B:1019:CLA:H61	1.34	0.45
23:B:1024:CLA:H102	23:B:1024:CLA:H143	1.99	0.45
2:B:122:LEU:HD22	2:B:122:LEU:C	2.37	0.45
2:B:18:ARG:HG2	2:B:18:ARG:HH11	1.81	0.45
2:B:188:ASP:C	2:B:190:PHE:H	2.18	0.45
2:B:201:HIS:CD2	2:B:202:HIS:N	2.85	0.45
2:B:223:GLN:C	2:B:225:LEU:N	2.69	0.45
2:B:385:ARG:HA	2:B:388:SER:OG	2.17	0.45
2:B:6:TYR:O	23:B:1019:CLA:HAA2	2.17	0.45
2:B:5:TRP:O	2:B:7:ARG:N	2.49	0.45
23:C:1026:CLA:HAA1	23:C:1026:CLA:HBD	1.97	0.45
23:C:1031:CLA:HBA1	23:C:1031:CLA:H3A	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD11	30:C:1055:DGD:HA22	1.99	0.45
23:C:1034:CLA:H193	30:C:1057:DGD:HAF1	1.99	0.45
3:C:249:ILE:CD1	3:C:249:ILE:N	2.80	0.45
3:C:287:THR:HG23	3:C:427:ALA:O	2.16	0.45
3:C:431:PHE:CD2	3:C:431:PHE:C	2.90	0.45
1:A:288:LEU:HD11	3:C:435:PHE:CE2	2.52	0.45
1:A:257:ARG:HB3	4:D:132:ILE:CG2	2.46	0.45
1:A:260:PHE:HB3	4:D:28:VAL:HB	1.99	0.45
23:H:1017:CLA:H92	23:H:1017:CLA:H62	1.81	0.45
8:I:3:THR:O	8:I:6:ILE:CD1	2.64	0.45
10:K:22:VAL:HA	10:K:25:LEU:HB2	1.98	0.45
30:C:1056:DGD:HBN1	10:K:30:VAL:HG21	1.94	0.45
13:O:145:LEU:CD2	13:O:145:LEU:N	2.79	0.45
14:T:2:GLU:C	14:T:6:TYR:CD2	2.90	0.45
15:U:56:ASP:C	15:U:58:ASN:H	2.20	0.45
31:V:1041:HEM:HHC	31:V:1041:HEM:HBB2	1.98	0.45
16:V:88:ALA:O	16:V:89:THR:HG23	2.16	0.45
1:A:93:PHE:CE1	30:C:1055:DGD:HAG2	2.52	0.45
23:B:1011:CLA:C19	23:H:1017:CLA:C15	2.85	0.45
23:B:1020:CLA:C14	23:B:1021:CLA:CAB	2.95	0.45
23:B:1021:CLA:H61	23:B:1021:CLA:H41	1.53	0.45
2:B:113:TRP:O	2:B:117:TYR:HB2	2.17	0.45
2:B:156:PHE:CB	23:B:1014:CLA:HAC2	2.47	0.45
2:B:191:ASN:ND2	2:B:193:TYR:HD2	2.09	0.45
2:B:307:GLU:O	2:B:308:LYS:C	2.55	0.45
23:C:1029:CLA:H51	23:C:1029:CLA:CHC	2.47	0.45
3:C:41:ARG:H	23:C:1035:CLA:HED1	1.81	0.45
3:C:110:PRO:HA	3:C:113:VAL:HG13	1.99	0.45
1:A:135:TYR:CD1	3:C:455:PHE:HE1	2.35	0.45
3:C:85:GLY:C	3:C:86:LEU:HD12	2.37	0.45
4:D:195:PRO:O	4:D:199:MET:HG3	2.17	0.45
4:D:235:PHE:O	4:D:236:ASN:OD1	2.35	0.45
4:D:300:SER:O	4:D:303:ILE:CD1	2.65	0.45
4:D:57:SER:HB3	4:D:79:SER:HB2	1.97	0.45
5:E:35:TRP:HA	6:F:36:ALA:HA	1.98	0.45
13:O:51:THR:O	13:O:52:ALA:HB2	2.17	0.45
5:E:61:ARG:NH1	16:V:153:GLY:HA2	2.32	0.45
23:A:1006:CLA:H92	23:A:1006:CLA:H61	1.78	0.44
1:A:180:PHE:O	1:A:184:ILE:HG13	2.17	0.44
1:A:202:VAL:O	1:A:206:PHE:N	2.34	0.44
1:A:324:ALA:CA	4:D:325:ILE:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1012:CLA:H41	23:B:1012:CLA:H62	1.65	0.44
23:B:1014:CLA:CBD	23:B:1014:CLA:HAA1	2.47	0.44
2:B:272:ARG:O	2:B:276:ASP:OD2	2.35	0.44
2:B:302:TRP:CE3	2:B:305:ILE:HD12	2.52	0.44
2:B:440:ASP:OD2	2:B:442:ILE:N	2.51	0.44
23:A:1006:CLA:HED1	30:C:1057:DGD:HBH2	1.89	0.44
1:A:297:LEU:HD11	3:C:425:TRP:CZ3	2.51	0.44
25:D:1042:PQ9:H61	25:D:1042:PQ9:H91	1.68	0.44
4:D:267:LEU:HD23	4:D:268:HIS:HD2	1.82	0.44
4:D:304:ARG:HG2	4:D:311:PHE:CE2	2.51	0.44
4:D:61:HIS:O	4:D:62:GLY:C	2.53	0.44
23:B:1010:CLA:H13	30:H:1058:DGD:HA82	1.97	0.44
7:H:14:LEU:CD1	7:H:14:LEU:H	2.29	0.44
11:L:25:LEU:HD22	14:T:13:ILE:CD1	2.47	0.44
12:M:11:THR:O	12:M:13:LEU:N	2.50	0.44
13:O:184:ASP:O	13:O:185:PRO:C	2.54	0.44
13:O:70:CYS:N	13:O:266:TYR:O	2.45	0.44
16:V:102:MET:HE1	16:V:141:ILE:CB	2.47	0.44
16:V:48:THR:HB	16:V:51:GLN:H	1.82	0.44
23:A:1007:CLA:H11	8:I:9:TYR:CD2	2.52	0.44
24:A:1039:PHO:H91	4:D:153:PHE:CE2	2.51	0.44
1:A:257:ARG:O	4:D:132:ILE:HD13	2.18	0.44
1:A:327:GLY:O	1:A:330:VAL:HG22	2.17	0.44
1:A:44:ALA:O	1:A:45:THR:C	2.56	0.44
1:A:60:ILE:O	1:A:61:ASP:C	2.55	0.44
2:B:118:TRP:CG	2:B:119:ASP:N	2.85	0.44
2:B:130:GLU:HB2	2:B:131:PRO:HD2	1.98	0.44
2:B:442:ILE:O	2:B:443:PHE:C	2.55	0.44
2:B:87:ASP:O	2:B:88:PRO:C	2.55	0.44
23:C:1030:CLA:H142	23:C:1030:CLA:H112	1.84	0.44
3:C:123:ALA:HA	26:K:1052:BCR:C35	2.47	0.44
3:C:343:ARG:HA	3:C:348:GLU:O	2.17	0.44
3:C:42:LEU:HD13	3:C:151:TRP:CH2	2.52	0.44
3:C:451:ALA:CA	3:C:456:GLU:HG2	2.46	0.44
3:C:456:GLU:O	3:C:457:LYS:CG	2.65	0.44
4:D:195:PRO:CB	11:L:31:PHE:CE1	2.99	0.44
4:D:261:PHE:CE2	4:D:267:LEU:HA	2.52	0.44
1:A:315:ASN:O	4:D:63:LEU:CD2	2.65	0.44
5:E:15:THR:OG1	9:J:10:LEU:CD2	2.65	0.44
7:H:49:TYR:C	7:H:51:SER:H	2.20	0.44
8:I:13:THR:O	8:I:14:PHE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:5:PRO:C	11:L:7:ARG:H	2.19	0.44
12:M:6:LEU:HA	12:M:9:ILE:CD1	2.48	0.44
1:A:57:PRO:CG	13:O:141:ARG:NH1	2.75	0.44
15:U:80:VAL:C	15:U:82:ASN:H	2.21	0.44
16:V:81:ARG:O	16:V:85:LEU:HG	2.18	0.44
23:A:1007:CLA:CMC	26:A:1044:BCR:H352	2.47	0.44
1:A:308:ASP:CG	1:A:309:ALA:H	2.21	0.44
23:B:1012:CLA:CED	23:B:1012:CLA:CAA	2.40	0.44
23:B:1016:CLA:C14	23:D:1008:CLA:CMB	2.71	0.44
2:B:154:GLY:O	2:B:159:THR:OG1	2.26	0.44
2:B:381:ILE:HA	2:B:382:PRO:HD3	1.71	0.44
2:B:422:ARG:NH1	2:B:422:ARG:HB3	2.33	0.44
2:B:475:PHE:CD1	4:D:140:PRO:HD3	2.52	0.44
2:B:54:PRO:HD2	2:B:57:ARG:CG	2.47	0.44
3:C:439:VAL:HG22	23:C:1032:CLA:HBC1	1.98	0.44
23:D:1005:CLA:HBC2	23:D:1005:CLA:HMC1	1.98	0.44
23:D:1008:CLA:H91	17:X:30:LEU:HD23	1.98	0.44
4:D:153:PHE:CD1	4:D:153:PHE:C	2.91	0.44
4:D:29:PHE:HE2	4:D:132:ILE:HG12	1.82	0.44
4:D:320:LEU:O	4:D:321:LEU:C	2.55	0.44
5:E:21:VAL:C	5:E:23:HIS:N	2.70	0.44
5:E:5:THR:C	5:E:7:GLU:H	2.19	0.44
12:M:23:ILE:O	12:M:27:VAL:HG23	2.16	0.44
13:O:65:ARG:NE	13:O:110:GLU:N	2.66	0.44
13:O:80:GLU:O	13:O:82:PRO:HD3	2.18	0.44
15:U:45:GLU:O	15:U:45:GLU:HG2	2.17	0.44
16:V:105:PRO:CG	16:V:115:ALA:CA	2.93	0.44
16:V:105:PRO:HG2	16:V:115:ALA:CA	2.46	0.44
16:V:133:LEU:N	16:V:133:LEU:HD12	2.29	0.44
17:X:24:LEU:O	17:X:28:VAL:N	2.34	0.44
1:A:38:ILE:HG21	26:A:1044:BCR:H333	2.00	0.44
1:A:205:VAL:C	1:A:207:GLY:H	2.20	0.44
1:A:254:TYR:C	1:A:254:TYR:CD2	2.91	0.44
1:A:36:ILE:HD13	8:I:19:PHE:HB2	2.00	0.44
1:A:65:GLU:O	1:A:65:GLU:CG	2.62	0.44
23:B:1012:CLA:H92	23:B:1018:CLA:H61	2.00	0.44
23:B:1021:CLA:H112	23:B:1021:CLA:H91	1.79	0.44
2:B:112:CYS:O	2:B:113:TRP:C	2.56	0.44
2:B:87:ASP:O	2:B:87:ASP:CG	2.55	0.44
23:C:1025:CLA:CED	23:C:1025:CLA:OBD	2.66	0.44
23:C:1035:CLA:H91	26:K:1052:BCR:H383	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:GLU:HA	3:C:221:GLU:OE1	2.18	0.44
5:E:9:PRO:HD3	6:F:13:TYR:CD1	2.52	0.44
6:F:28:VAL:O	6:F:31:ILE:HG22	2.17	0.44
26:H:1049:BCR:H392	26:H:1049:BCR:C23	2.47	0.44
8:I:7:THR:OG1	8:I:8:VAL:N	2.50	0.44
11:L:31:PHE:O	11:L:35:PHE:CD1	2.70	0.44
13:O:179:THR:CG2	13:O:180:ALA:H	2.29	0.44
15:U:57:LEU:HD13	15:U:91:VAL:CG2	2.48	0.44
1:A:273:PHE:C	1:A:275:LEU:N	2.71	0.44
2:B:370:LEU:HD12	2:B:392:PHE:CZ	2.53	0.44
23:C:1030:CLA:HMB2	23:C:1031:CLA:C1B	2.47	0.44
3:C:128:GLY:CA	23:C:1037:CLA:HAC1	2.45	0.44
26:C:1054:BCR:H371	26:C:1054:BCR:H24C	1.57	0.44
3:C:217:PRO:O	30:C:1055:DGD:HG11	2.17	0.44
3:C:126:GLY:O	3:C:129:GLY:N	2.44	0.44
4:D:204:VAL:O	4:D:204:VAL:CG1	2.64	0.44
5:E:16:SER:HB3	5:E:19:TYR:CB	2.47	0.44
12:M:25:LEU:O	12:M:28:GLN:HG3	2.18	0.44
13:O:196:SER:O	13:O:197:ALA:C	2.55	0.44
13:O:215:ARG:HH11	13:O:215:ARG:CG	2.24	0.44
16:V:89:THR:HA	16:V:90:PRO:C	2.38	0.44
18:Y:38:LEU:HA	18:Y:41:VAL:HG12	1.99	0.44
1:A:76:ASN:HB3	1:A:79:THR:CG2	2.48	0.44
1:A:97:TRP:HA	8:I:1:MET:CG	2.48	0.44
2:B:464:PHE:CD1	23:B:1019:CLA:CBC	3.01	0.44
23:B:1021:CLA:H62	29:B:1060:MGE:CDB	2.22	0.44
2:B:215:PHE:CZ	2:B:219:VAL:HG21	2.53	0.44
2:B:224:ARG:O	2:B:228:ALA:HB2	2.17	0.44
2:B:373:LYS:CG	2:B:374:ASN:N	2.81	0.44
2:B:442:ILE:HG22	2:B:442:ILE:O	2.17	0.44
2:B:475:PHE:HD1	4:D:140:PRO:HD3	1.81	0.44
2:B:479:PHE:C	2:B:481:GLY:N	2.70	0.44
2:B:5:TRP:C	2:B:7:ARG:H	2.20	0.44
23:C:1026:CLA:HBB2	23:C:1034:CLA:H11	1.98	0.44
30:C:1055:DGD:HB32	30:C:1055:DGD:C7B	2.45	0.44
3:C:56:HIS:C	3:C:58:GLY:H	2.21	0.44
3:C:61:VAL:HG22	23:C:1027:CLA:HMD1	2.00	0.44
1:A:254:TYR:OH	4:D:129:GLN:HB3	2.17	0.44
2:B:482:ILE:HD13	4:D:138:VAL:HG12	1.98	0.44
4:D:287:VAL:CG2	4:D:288:GLY:N	2.80	0.44
2:B:257:TRP:CH2	4:D:291:LEU:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:LEU:HD13	4:D:92:LEU:O	2.18	0.44
7:H:49:TYR:CD1	30:H:1058:DGD:O1B	2.70	0.44
2:B:223:GLN:CG	7:H:24:GLY:CA	2.94	0.44
23:A:1003:CLA:C19	24:A:1038:PHO:CMA	2.95	0.44
1:A:235:TYR:C	1:A:237:TYR:N	2.69	0.44
1:A:322:ASN:O	1:A:325:ASN:HB2	2.17	0.44
1:A:43:ALA:HA	26:A:1044:BCR:C15	2.48	0.44
23:B:1012:CLA:O1A	23:B:1013:CLA:HBA1	2.17	0.44
23:B:1023:CLA:CBA	23:B:1023:CLA:O2D	2.66	0.44
2:B:297:THR:HG22	2:B:300:GLU:HB2	1.99	0.44
2:B:357:ARG:O	2:B:425:ILE:CD1	2.65	0.44
2:B:384:ARG:NH1	4:D:348:ARG:CD	2.81	0.44
3:C:333:GLY:O	13:O:179:THR:OG1	2.35	0.44
1:A:63:ILE:HG22	3:C:335:THR:HG21	2.00	0.44
3:C:48:LYS:HD3	3:C:132:HIS:O	2.17	0.44
4:D:155:SER:HA	4:D:159:ILE:HG13	2.00	0.44
4:D:18:LEU:O	4:D:19:ASP:C	2.56	0.44
1:A:328:MET:CB	4:D:325:ILE:CG1	2.92	0.44
13:O:133:THR:CG2	13:O:134:VAL:N	2.80	0.44
14:T:9:ILE:O	14:T:13:ILE:HG12	2.18	0.44
16:V:135:GLU:O	16:V:136:LYS:C	2.56	0.44
20:Z:22:GLY:O	20:Z:23:VAL:C	2.56	0.44
1:A:16:ARG:O	1:A:17:PHE:C	2.56	0.44
1:A:15:GLU:O	1:A:19:ASN:ND2	2.50	0.44
23:B:1011:CLA:H2A	23:B:1011:CLA:O1D	2.18	0.44
23:B:1018:CLA:H102	23:B:1018:CLA:H62	1.27	0.44
2:B:20:ILE:HG12	23:B:1023:CLA:CMD	2.48	0.44
2:B:143:LEU:O	2:B:146:ALA:HB3	2.18	0.44
2:B:15:ASP:C	2:B:17:GLY:N	2.71	0.44
2:B:241:SER:O	2:B:242:ILE:C	2.56	0.44
23:C:1029:CLA:HMD2	26:C:1054:BCR:HC7	2.00	0.44
3:C:229:ASN:CG	3:C:231:GLU:HG2	2.38	0.44
3:C:234:VAL:C	3:C:236:GLY:N	2.70	0.44
3:C:289:PHE:CE2	3:C:293:ASN:ND2	2.84	0.44
3:C:46:SER:H	3:C:140:LEU:HD22	1.83	0.44
3:C:71:GLU:O	3:C:74:HIS:N	2.49	0.44
4:D:52:THR:HG22	4:D:67:TYR:CZ	2.52	0.44
5:E:19:TYR:C	5:E:21:VAL:N	2.71	0.44
8:I:27:ASP:O	8:I:29:ALA:N	2.51	0.44
23:C:1035:CLA:H102	26:K:1052:BCR:H403	1.95	0.44
12:M:11:THR:O	12:M:12:ALA:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:127:ILE:CD1	13:O:127:ILE:N	2.50	0.44
13:O:65:ARG:NH1	13:O:66:ILE:N	2.66	0.44
16:V:79:ASP:OD1	16:V:84:THR:HG21	2.17	0.44
17:X:29:VAL:O	17:X:33:THR:HG22	2.17	0.44
18:Y:21:GLN:O	18:Y:24:MET:N	2.50	0.44
1:A:339:PHE:CD2	28:A:1065:BR:BR	3.25	0.44
1:A:188:ALA:HB2	1:A:328:MET:CG	2.36	0.44
1:A:323:ARG:CG	1:A:323:ARG:NH1	2.76	0.44
23:B:1020:CLA:C5	23:B:1020:CLA:O2A	2.45	0.44
29:B:1060:MGE:H7B2	29:B:1060:MGE:H4B1	1.71	0.44
2:B:153:PHE:CD2	2:B:202:HIS:ND1	2.84	0.44
2:B:278:SER:O	2:B:279:TYR:C	2.57	0.44
2:B:333:GLY:O	2:B:441:GLY:N	2.51	0.44
2:B:488:PRO:HD2	2:B:489:GLU:OE2	2.18	0.44
23:C:1033:CLA:C5	23:C:1033:CLA:O2A	2.66	0.44
23:C:1036:CLA:H161	23:C:1036:CLA:H202	1.69	0.44
3:C:160:ILE:HG22	3:C:164:HIS:CE1	2.52	0.44
3:C:259:TRP:CE3	3:C:260:ALA:HB2	2.52	0.44
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.50	0.44
4:D:89:LEU:HA	4:D:112:THR:HG21	1.99	0.44
4:D:322:ASN:OD1	4:D:322:ASN:N	2.49	0.44
4:D:43:LEU:N	4:D:43:LEU:HD22	2.18	0.44
7:H:21:VAL:HG12	7:H:22:ALA:N	2.33	0.44
7:H:35:MET:HG2	26:H:1049:BCR:C33	2.20	0.44
3:C:55:ALA:CB	26:K:1052:BCR:H371	2.44	0.44
15:U:100:ARG:O	15:U:104:ILE:HG13	2.18	0.44
15:U:82:ASN:CB	15:U:85:TYR:OH	2.60	0.44
16:V:134:THR:O	16:V:137:ASP:HB2	2.17	0.44
10:K:39:VAL:CB	18:Y:36:ILE:HD11	2.48	0.44
23:A:1007:CLA:HBA1	23:A:1007:CLA:H3A	1.60	0.43
1:A:113:GLN:CA	1:A:116:ILE:HG22	2.45	0.43
1:A:200:LEU:HD22	1:A:285:PHE:HD1	1.83	0.43
1:A:237:TYR:CD1	4:D:264:LYS:HG2	2.53	0.43
1:A:302:PHE:O	1:A:305:SER:HB3	2.18	0.43
23:B:1009:CLA:H62	23:B:1009:CLA:H2	1.70	0.43
23:B:1021:CLA:C19	29:B:1060:MGE:H132	2.46	0.43
2:B:165:GLY:HA3	2:B:180:PRO:N	2.32	0.43
2:B:191:ASN:O	2:B:193:TYR:N	2.50	0.43
2:B:233:ASN:C	2:B:235:GLU:N	2.71	0.43
2:B:237:VAL:HG22	23:B:1020:CLA:CMD	2.48	0.43
2:B:258:TYR:C	2:B:259:GLY:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:PHE:CD1	2:B:312:TYR:HB3	2.52	0.43
3:C:45:LEU:HD11	3:C:139:THR:HG23	2.00	0.43
3:C:368:PRO:C	3:C:370:ARG:H	2.20	0.43
3:C:436:PHE:HA	3:C:439:VAL:HG12	2.00	0.43
3:C:71:GLU:HB3	3:C:89:ILE:CD1	2.48	0.43
4:D:196:PHE:N	4:D:196:PHE:CD1	2.85	0.43
4:D:21:TRP:O	4:D:24:ARG:HB2	2.18	0.43
4:D:275:PRO:C	4:D:277:THR:N	2.72	0.43
4:D:88:SER:HA	7:H:50:ASN:HD21	1.81	0.43
6:F:41:GLN:NE2	9:J:27:LEU:O	2.51	0.43
23:H:1017:CLA:H41	23:H:1017:CLA:H62	1.79	0.43
9:J:20:GLY:O	9:J:24:ILE:HB	2.18	0.43
9:J:30:TYR:CD2	9:J:31:GLY:N	2.85	0.43
13:O:145:LEU:O	13:O:147:THR:HG22	2.18	0.43
13:O:56:TYR:OH	13:O:64:TYR:HE2	2.00	0.43
26:T:6046:BCR:H321	26:T:6046:BCR:C8	2.48	0.43
11:L:29:LEU:HD13	14:T:9:ILE:HG22	2.00	0.43
15:U:53:GLU:HG2	15:U:54:LYS:HG3	1.99	0.43
24:A:1039:PHO:HAA2	4:D:125:PHE:CZ	2.52	0.43
1:A:192:ILE:HG12	1:A:293:MET:HE1	1.99	0.43
23:B:1020:CLA:H141	23:B:1021:CLA:HBB2	2.00	0.43
2:B:233:ASN:O	2:B:235:GLU:N	2.51	0.43
2:B:368:VAL:HG13	2:B:381:ILE:H	1.84	0.43
2:B:448:ARG:HH11	2:B:448:ARG:CG	2.31	0.43
2:B:72:THR:HA	2:B:93:PHE:CZ	2.54	0.43
23:C:1036:CLA:H62	23:C:1036:CLA:H41	1.72	0.43
3:C:183:GLY:O	3:C:184:GLY:O	2.35	0.43
3:C:245:ILE:HG22	3:C:246:ALA:N	2.32	0.43
3:C:53:HIS:CE1	23:C:1033:CLA:H162	2.53	0.43
3:C:88:LEU:HG	23:C:1027:CLA:HBC3	1.99	0.43
4:D:210:LEU:C	4:D:212:ALA:N	2.69	0.43
4:D:292:ASN:OD1	4:D:294:ARG:NH1	2.47	0.43
4:D:33:SER:OG	4:D:128:ARG:HD3	2.18	0.43
4:D:34:GLY:O	4:D:38:PHE:HB2	2.18	0.43
4:D:44:ALA:C	4:D:46:GLY:N	2.69	0.43
5:E:83:LEU:CD2	5:E:84:LYS:N	2.81	0.43
9:J:19:MET:CA	9:J:22:ILE:HG22	2.46	0.43
10:K:28:ILE:O	10:K:31:LEU:HB2	2.18	0.43
11:L:29:LEU:HD13	14:T:9:ILE:CG2	2.48	0.43
13:O:144:LEU:N	13:O:144:LEU:HD23	2.33	0.43
13:O:46:PRO:HG2	13:O:266:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:53:VAL:C	20:Z:55:GLY:N	2.69	0.43
24:A:1039:PHO:H3A	24:A:1039:PHO:HBA2	1.53	0.43
1:A:131:TRP:CZ3	1:A:132:GLU:HA	2.53	0.43
1:A:151:LEU:HD11	1:A:155:PHE:HE2	1.83	0.43
1:A:277:ALA:O	1:A:281:VAL:HB	2.17	0.43
1:A:306:VAL:HG23	1:A:316:THR:HG23	1.99	0.43
23:B:1020:CLA:H161	23:B:1020:CLA:H141	1.69	0.43
2:B:371:THR:CG2	2:B:371:THR:O	2.65	0.43
23:C:1028:CLA:HED3	30:C:1056:DGD:HD5	2.01	0.43
3:C:182:PHE:CD2	3:C:182:PHE:N	2.85	0.43
3:C:322:GLN:NE2	3:C:381:LYS:CD	2.79	0.43
3:C:417:VAL:HG22	3:C:418:ASN:N	2.32	0.43
4:D:221:THR:CG2	4:D:244:TYR:CB	2.96	0.43
4:D:71:CYS:HB3	4:D:76:VAL:CG2	2.47	0.43
5:E:27:ILE:CB	5:E:28:PRO:CD	2.83	0.43
2:B:258:TYR:HD2	30:H:1058:DGD:HD1	1.83	0.43
13:O:124:GLU:HG2	13:O:125:ASP:N	2.34	0.43
16:V:143:GLY:O	16:V:147:VAL:CG2	2.65	0.43
3:C:135:ARG:NH1	20:Z:33:TRP:HB3	2.25	0.43
1:A:323:ARG:HE	1:A:326:LEU:HD12	1.83	0.43
23:B:1024:CLA:O2A	23:B:1024:CLA:HMA2	2.18	0.43
2:B:103:LEU:HD23	23:B:1014:CLA:H72	1.99	0.43
2:B:102:VAL:HG13	2:B:103:LEU:N	2.33	0.43
2:B:135:LEU:HB2	2:B:136:PRO:CD	2.49	0.43
2:B:215:PHE:CD2	2:B:215:PHE:C	2.91	0.43
2:B:256:MET:HE2	2:B:256:MET:HB3	1.45	0.43
2:B:318:ASN:HD21	2:B:320:ALA:HB2	1.82	0.43
2:B:318:ASN:OD1	2:B:320:ALA:HB3	2.19	0.43
2:B:373:LYS:HD3	2:B:374:ASN:N	2.33	0.43
2:B:372:ASP:OD1	2:B:376:VAL:HG12	2.19	0.43
2:B:340:TRP:HB2	2:B:430:PHE:CE2	2.53	0.43
2:B:453:PHE:O	2:B:453:PHE:CG	2.70	0.43
2:B:50:PRO:O	2:B:308:LYS:NZ	2.50	0.43
23:C:1033:CLA:H193	23:C:1036:CLA:CHD	2.49	0.43
3:C:135:ARG:NH2	3:C:135:ARG:HG3	2.32	0.43
3:C:250:TRP:HE1	23:C:1030:CLA:HED1	1.73	0.43
3:C:52:ALA:HB1	23:C:1033:CLA:HBB1	2.00	0.43
1:A:258:LEU:HD12	4:D:128:ARG:HH11	1.83	0.43
2:B:258:TYR:OH	4:D:162:LEU:O	2.34	0.43
4:D:180:ARG:HD3	4:D:184:PHE:HB2	2.00	0.43
5:E:8:ARG:CB	5:E:9:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1051:BCR:C10	26:K:1051:BCR:H331	2.49	0.43
14:T:3:THR:HG22	14:T:4:ILE:N	2.31	0.43
15:U:92:LEU:HD12	15:U:92:LEU:N	2.26	0.43
17:X:28:VAL:HG12	17:X:29:VAL:N	2.34	0.43
24:A:1038:PHO:H93	24:A:1038:PHO:H62	1.57	0.43
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.31	0.43
1:A:214:MET:HE2	25:A:1043:PQ9:H143	2.01	0.43
23:B:1012:CLA:C1	23:B:1013:CLA:H11	2.41	0.43
2:B:101:ILE:HG23	26:B:1047:BCR:H373	2.00	0.43
2:B:392:PHE:O	2:B:394:GLN:N	2.51	0.43
2:B:455:HIS:ND1	2:B:455:HIS:N	2.67	0.43
2:B:472:ARG:HG2	2:B:479:PHE:CE2	2.54	0.43
3:C:406:SER:HB3	30:C:1056:DGD:HE1	1.99	0.43
3:C:188:THR:HG23	3:C:189:TRP:CD1	2.53	0.43
3:C:382:ASN:C	3:C:384:ILE:N	2.72	0.43
4:D:101:PHE:O	4:D:101:PHE:CD1	2.70	0.43
4:D:148:ALA:N	4:D:149:PRO:HD2	2.33	0.43
4:D:14:TRP:HA	4:D:17:ILE:HD12	1.99	0.43
4:D:210:LEU:CD1	4:D:274:VAL:HG21	2.49	0.43
4:D:253:TRP:C	4:D:255:GLN:H	2.21	0.43
5:E:43:ALA:O	5:E:44:TYR:C	2.57	0.43
5:E:71:GLU:HG3	5:E:74:GLN:CB	2.48	0.43
8:I:9:TYR:O	8:I:10:ILE:C	2.56	0.43
8:I:34:ARG:HG3	8:I:34:ARG:HH11	1.83	0.43
4:D:195:PRO:HB2	11:L:31:PHE:CE1	2.53	0.43
2:B:325:PHE:HE1	11:L:34:TYR:HB3	1.74	0.43
13:O:145:LEU:CD2	13:O:145:LEU:H	2.25	0.43
13:O:70:CYS:C	13:O:71:LEU:HD12	2.38	0.43
13:O:78:VAL:HG23	13:O:94:THR:HG21	1.99	0.43
15:U:72:TYR:CD2	15:U:73:PRO:CD	3.01	0.43
18:Y:32:GLY:N	18:Y:33:PRO:CD	2.82	0.43
20:Z:14:ILE:O	20:Z:18:VAL:HG23	2.19	0.43
1:A:292:THR:HG22	1:A:293:MET:N	2.33	0.43
1:A:317:TRP:CE3	1:A:317:TRP:HA	2.53	0.43
23:B:1021:CLA:C19	29:B:1060:MGE:H133	2.25	0.43
2:B:122:LEU:N	2:B:122:LEU:CD1	2.82	0.43
2:B:135:LEU:CB	2:B:136:PRO:HD3	2.46	0.43
2:B:17:GLY:C	2:B:19:LEU:H	2.22	0.43
2:B:229:LEU:HD23	2:B:231:MET:H	1.82	0.43
2:B:272:ARG:HH12	4:D:164:GLN:HA	1.84	0.43
23:C:1033:CLA:H41	23:C:1033:CLA:H62	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:1057:DGD:HG12	9:J:33:TYR:OH	2.18	0.43
4:D:239:GLN:O	4:D:240:ALA:C	2.56	0.43
5:E:22:ILE:HD12	5:E:22:ILE:HA	1.89	0.43
5:E:63:ILE:O	5:E:65:LEU:N	2.49	0.43
9:J:19:MET:O	9:J:22:ILE:HG22	2.18	0.43
1:A:78:ILE:HG13	11:L:34:TYR:CZ	2.53	0.43
2:B:118:TRP:HH2	11:L:5:PRO:HD2	1.77	0.43
14:T:8:PHE:O	14:T:9:ILE:C	2.55	0.43
16:V:117:VAL:O	16:V:119:PRO:HD3	2.18	0.43
16:V:128:PRO:O	16:V:129:LYS:C	2.56	0.43
16:V:145:ILE:N	16:V:145:ILE:HD12	2.34	0.43
23:A:1006:CLA:H193	23:A:1006:CLA:H161	1.66	0.43
23:A:1006:CLA:H3A	23:A:1006:CLA:HBA2	1.64	0.43
1:A:148:SER:OG	1:A:284:TRP:NE1	2.50	0.43
1:A:224:ILE:O	2:B:482:ILE:N	2.52	0.43
1:A:62:GLY:O	1:A:63:ILE:C	2.56	0.43
23:B:1015:CLA:H141	23:B:1015:CLA:H161	1.73	0.43
23:B:1019:CLA:CBD	23:B:1019:CLA:CAA	2.97	0.43
2:B:18:ARG:H	2:B:18:ARG:HD3	1.83	0.43
2:B:201:HIS:CG	2:B:202:HIS:N	2.87	0.43
2:B:65:PHE:HA	2:B:68:ARG:HD2	1.99	0.43
2:B:68:ARG:CZ	23:B:1011:CLA:CED	2.96	0.43
23:C:1032:CLA:CMA	23:C:1032:CLA:HED3	2.48	0.43
3:C:344:SER:C	3:C:346:THR:N	2.72	0.43
4:D:235:PHE:O	4:D:236:ASN:HB2	2.19	0.43
3:C:473:ASP:CB	14:T:26:PRO:HG3	2.45	0.43
15:U:97:LEU:CB	15:U:102:LYS:HG2	2.41	0.43
16:V:118:HIS:HD1	16:V:118:HIS:C	2.22	0.43
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	2.00	0.43
1:A:159:LEU:HD11	1:A:163:ILE:HD11	2.00	0.43
1:A:79:THR:O	1:A:80:GLY:O	2.36	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.74	0.43
23:B:1011:CLA:OBD	23:B:1011:CLA:HED3	2.15	0.43
23:B:1019:CLA:C19	23:B:1021:CLA:C6	2.97	0.43
23:B:1023:CLA:C11	23:B:1023:CLA:H161	2.43	0.43
29:B:1060:MGE:H102	29:B:1060:MGE:H7A1	1.60	0.43
2:B:118:TRP:N	2:B:118:TRP:CD1	2.87	0.43
2:B:368:VAL:CG1	2:B:368:VAL:O	2.62	0.43
2:B:458:PHE:CD1	2:B:458:PHE:N	2.86	0.43
2:B:488:PRO:CG	2:B:489:GLU:H	2.30	0.43
3:C:52:ALA:O	3:C:55:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:LEU:HD13	4:D:109:GLY:N	2.33	0.43
4:D:103:ARG:HD3	5:E:73:LYS:CD	2.48	0.43
2:B:222:PRO:HD3	7:H:27:THR:CG2	2.49	0.43
7:H:5:THR:HG23	7:H:8:GLY:HA3	2.01	0.43
26:K:1051:BCR:C1	26:K:1052:BCR:H10C	2.48	0.43
10:K:18:PHE:C	10:K:20:PRO:CD	2.87	0.43
13:O:133:THR:CG2	13:O:134:VAL:H	2.32	0.43
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.33	0.43
20:Z:19:MET:O	20:Z:23:VAL:HG23	2.18	0.43
20:Z:40:ILE:HD13	20:Z:40:ILE:HA	1.91	0.43
1:A:137:LEU:O	1:A:139:MET:HG2	2.18	0.43
1:A:127:MET:HE1	1:A:148:SER:HA	2.00	0.43
1:A:317:TRP:C	1:A:319:ASP:H	2.22	0.43
1:A:81:ALA:HB1	1:A:175:GLY:CA	2.40	0.43
2:B:7:ARG:CD	23:B:1019:CLA:HED3	2.46	0.43
23:B:1021:CLA:H141	23:B:1021:CLA:H161	1.81	0.43
2:B:122:LEU:HA	7:H:12:ARG:CZ	2.49	0.43
2:B:275:TRP:CE2	2:B:315:ILE:HD12	2.53	0.43
27:A:1063:LHG:C27	23:C:1032:CLA:H62	2.49	0.43
3:C:436:PHE:HA	3:C:439:VAL:CG1	2.49	0.43
3:C:60:ILE:HG23	23:C:1027:CLA:CMD	2.49	0.43
23:D:1008:CLA:H112	23:D:1008:CLA:H143	1.58	0.43
23:D:1008:CLA:H91	17:X:30:LEU:HG	2.00	0.43
5:E:14:ILE:HG13	5:E:15:THR:N	2.32	0.43
6:F:11:VAL:CG1	6:F:12:SER:H	2.20	0.43
23:B:1011:CLA:H121	26:H:1049:BCR:H313	2.00	0.43
7:H:7:LEU:CD2	7:H:11:LEU:HD22	2.49	0.43
8:I:2:GLU:O	8:I:6:ILE:CD1	2.67	0.43
9:J:39:SER:C	9:J:40:LEU:HD22	2.38	0.43
15:U:50:ALA:HB1	15:U:113:THR:CG2	2.46	0.43
20:Z:1:MET:SD	20:Z:60:PHE:CD2	3.12	0.43
1:A:257:ARG:HB3	4:D:132:ILE:HG21	2.01	0.43
1:A:315:ASN:O	4:D:63:LEU:HG	2.19	0.43
1:A:330:VAL:HG23	1:A:331:MET:N	2.33	0.43
1:A:58:VAL:HB	1:A:83:VAL:CG1	2.47	0.43
23:B:1012:CLA:CGA	23:B:1013:CLA:HBA2	2.49	0.43
23:B:1018:CLA:H143	23:B:1018:CLA:H111	1.74	0.43
23:B:1020:CLA:HAA1	23:B:1020:CLA:CBD	2.49	0.43
2:B:189:GLY:O	2:B:197:GLY:HA3	2.18	0.43
23:C:1032:CLA:H2	23:C:1035:CLA:C2C	2.49	0.43
3:C:63:TRP:CB	23:C:1034:CLA:CED	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:PHE:CD1	23:C:1036:CLA:HBB1	2.53	0.43
3:C:173:LEU:HD23	3:C:176:VAL:HG21	2.00	0.43
3:C:403:SER:OG	3:C:407:VAL:HB	2.18	0.43
4:D:152:VAL:CG1	4:D:153:PHE:N	2.82	0.43
4:D:214:HIS:HA	4:D:217:THR:CG2	2.49	0.43
1:A:239:PHE:CZ	4:D:247:VAL:HA	2.54	0.43
4:D:251:ARG:HA	4:D:254:SER:HG	1.83	0.43
4:D:251:ARG:O	4:D:255:GLN:OE1	2.36	0.43
5:E:35:TRP:CD1	5:E:35:TRP:O	2.72	0.43
11:L:13:ASN:ND2	29:L:1061:MGE:O5D	2.52	0.43
12:M:8:PHE:HB3	12:M:9:ILE:H	1.68	0.43
13:O:265:PHE:CG	13:O:266:TYR:N	2.87	0.43
15:U:109:LEU:C	15:U:111:HIS:H	2.23	0.43
15:U:113:THR:CG2	15:U:114:VAL:H	2.32	0.43
15:U:55:ILE:HD11	15:U:64:ALA:O	2.19	0.43
3:C:78:GLU:HB3	16:V:128:PRO:CB	2.49	0.43
17:X:16:LEU:O	17:X:19:PHE:HB3	2.19	0.43
1:A:113:GLN:HA	1:A:116:ILE:CG2	2.46	0.42
1:A:135:TYR:C	1:A:137:LEU:N	2.72	0.42
1:A:279:ARG:CD	4:D:208:ALA:CB	2.80	0.42
1:A:77:ILE:HB	11:L:33:SER:OG	2.19	0.42
2:B:103:LEU:HD23	23:B:1014:CLA:C7	2.49	0.42
23:B:1011:CLA:CMD	23:B:1014:CLA:HMB1	2.49	0.42
23:B:1015:CLA:HAA1	23:B:1015:CLA:HBD	2.01	0.42
2:B:265:ILE:HG12	7:H:62:TRP:CZ3	2.54	0.42
2:B:422:ARG:C	2:B:424:ALA:H	2.22	0.42
2:B:78:TRP:HB2	2:B:79:SER:H	1.70	0.42
23:C:1033:CLA:H122	23:C:1033:CLA:C9	2.02	0.42
23:C:1033:CLA:C19	23:C:1033:CLA:H143	2.49	0.42
23:C:1037:CLA:O1A	23:C:1037:CLA:H3A	2.19	0.42
3:C:419:PHE:CE2	3:C:421:SER:HA	2.53	0.42
26:D:1050:BCR:C40	26:D:1050:BCR:H372	2.29	0.42
4:D:17:ILE:HG22	17:X:41:SER:CB	2.33	0.42
4:D:245:SER:HB2	4:D:248:THR:OG1	2.18	0.42
4:D:258:GLY:C	4:D:259:ILE:HD13	2.38	0.42
31:E:1040:HEM:HMA1	31:E:1040:HEM:O1A	2.16	0.42
5:E:71:GLU:O	5:E:72:ALA:C	2.57	0.42
8:I:15:PHE:O	8:I:18:LEU:HB2	2.19	0.42
23:C:1035:CLA:C9	26:K:1052:BCR:H402	2.42	0.42
13:O:198:ILE:O	13:O:198:ILE:HD12	2.19	0.42
15:U:113:THR:CG2	15:U:114:VAL:N	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:19:ILE:HG23	18:Y:20:ALA:H	1.84	0.42
1:A:99:ALA:C	1:A:101:SER:H	2.22	0.42
24:A:1039:PHO:H61	24:A:1039:PHO:H102	1.65	0.42
1:A:40:THR:HG21	1:A:121:LEU:CD2	2.49	0.42
1:A:70:SER:OG	1:A:71:LEU:N	2.52	0.42
23:B:1011:CLA:CGA	23:B:1011:CLA:C3A	2.92	0.42
23:B:1014:CLA:H8	23:B:1014:CLA:H51	1.55	0.42
23:B:1021:CLA:CBD	23:B:1021:CLA:HAA2	2.49	0.42
23:B:1022:CLA:H13	23:B:1022:CLA:H71	1.92	0.42
2:B:137:LYS:HD3	7:H:14:LEU:O	2.19	0.42
2:B:159:THR:HB	2:B:161:LEU:HD22	2.02	0.42
2:B:18:ARG:HD2	11:L:4:ASN:ND2	2.28	0.42
2:B:210:ILE:O	2:B:211:ILE:C	2.57	0.42
2:B:229:LEU:C	2:B:229:LEU:HD23	2.39	0.42
23:C:1030:CLA:CMB	23:C:1031:CLA:C1B	2.97	0.42
3:C:53:HIS:CB	23:C:1036:CLA:CMD	2.91	0.42
3:C:98:GLY:O	3:C:106:VAL:HG12	2.19	0.42
3:C:236:GLY:C	3:C:238:ILE:N	2.71	0.42
3:C:261:ARG:NH1	3:C:261:ARG:N	2.66	0.42
3:C:227:VAL:CG2	3:C:293:ASN:HD21	2.32	0.42
3:C:465:PRO:HB3	8:I:32:PRO:HB3	2.01	0.42
3:C:63:TRP:HB2	23:C:1034:CLA:HED1	1.98	0.42
4:D:22:LEU:CD1	4:D:32:TRP:CE3	3.02	0.42
2:B:461:LEU:HD23	4:D:280:TRP:CZ3	2.54	0.42
5:E:51:ARG:C	5:E:53:ASP:H	2.22	0.42
5:E:8:ARG:HA	5:E:8:ARG:NE	2.32	0.42
10:K:11:LEU:O	10:K:12:PRO:C	2.56	0.42
10:K:31:LEU:O	10:K:34:ALA:HB3	2.19	0.42
11:L:24:ILE:CD1	12:M:18:PRO:CG	2.96	0.42
11:L:25:LEU:O	11:L:25:LEU:HD23	2.20	0.42
11:L:28:ALA:O	11:L:29:LEU:C	2.58	0.42
13:O:114:ASN:OD1	13:O:118:SER:O	2.36	0.42
13:O:129:PHE:O	13:O:130:GLN:CG	2.63	0.42
13:O:166:THR:CG2	13:O:167:ASP:N	2.82	0.42
20:Z:49:ALA:O	20:Z:53:VAL:N	2.48	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.02	0.42
1:A:153:SER:O	1:A:156:ALA:HB3	2.18	0.42
1:A:260:PHE:HD1	1:A:261:GLN:O	2.02	0.42
1:A:38:ILE:HG22	1:A:39:PRO:N	2.33	0.42
23:B:1015:CLA:H111	23:B:1015:CLA:H142	1.59	0.42
2:B:23:HIS:CE1	23:B:1018:CLA:H193	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:1060:MGE:H261	29:B:1060:MGE:C3A	2.43	0.42
2:B:226:TYR:HA	2:B:231:MET:HG2	2.01	0.42
2:B:25:MET:C	2:B:27:THR:N	2.69	0.42
3:C:197:ARG:CG	3:C:198:VAL:N	2.81	0.42
3:C:340:TYR:N	3:C:340:TYR:CD2	2.88	0.42
3:C:47:GLY:O	3:C:50:LEU:HB3	2.20	0.42
25:D:1042:PQ9:H261	25:D:1042:PQ9:H241	1.71	0.42
4:D:77:ALA:HB1	4:D:173:PHE:O	2.19	0.42
4:D:87:HIS:HB2	30:H:1058:DGD:O2D	2.19	0.42
12:M:17:VAL:N	12:M:18:PRO:CD	2.82	0.42
13:O:135:GLN:HG3	13:O:140:GLU:O	2.19	0.42
15:U:83:ALA:HB1	15:U:84:PRO:HD2	2.01	0.42
23:C:1036:CLA:C19	26:Z:1053:BCR:H372	2.47	0.42
20:Z:52:LEU:C	20:Z:55:GLY:H	2.22	0.42
1:A:172:MET:HG3	1:A:172:MET:O	2.18	0.42
1:A:177:SER:HA	1:A:180:PHE:CE2	2.55	0.42
1:A:97:TRP:HZ3	8:I:8:VAL:HG11	1.84	0.42
23:B:1012:CLA:HBA1	23:B:1013:CLA:HBA2	2.00	0.42
2:B:354:LEU:CB	2:B:370:LEU:HD22	2.34	0.42
2:B:51:VAL:HG12	2:B:52:LEU:HG	2.01	0.42
23:C:1027:CLA:H152	26:Z:1053:BCR:H332	2.00	0.42
3:C:264:PHE:CZ	26:C:1054:BCR:H321	2.55	0.42
30:C:1057:DGD:CHB	30:C:1057:DGD:HAG2	2.49	0.42
30:C:1057:DGD:HG31	9:J:33:TYR:CE2	2.55	0.42
3:C:248:GLY:C	3:C:252:ILE:HD12	2.39	0.42
3:C:339:LYS:HD2	3:C:340:TYR:HE2	1.84	0.42
3:C:435:PHE:O	3:C:437:PHE:N	2.52	0.42
3:C:89:ILE:N	3:C:90:PRO:CD	2.82	0.42
4:D:36:LEU:C	4:D:39:PRO:HD2	2.40	0.42
4:D:77:ALA:CB	4:D:173:PHE:O	2.68	0.42
23:B:1016:CLA:H172	23:H:1017:CLA:H18	2.00	0.42
10:K:27:VAL:HG22	10:K:27:VAL:O	2.19	0.42
13:O:196:SER:O	13:O:197:ALA:O	2.37	0.42
13:O:34:ASP:O	13:O:37:VAL:HG12	2.19	0.42
11:L:18:TYR:CE2	14:T:19:PHE:O	2.70	0.42
15:U:103:GLN:O	15:U:105:LEU:N	2.52	0.42
15:U:89:GLU:O	15:U:92:LEU:HD13	2.20	0.42
16:V:134:THR:H	16:V:137:ASP:HB2	1.84	0.42
17:X:11:THR:O	17:X:12:ILE:CG2	2.67	0.42
17:X:32:LEU:HD12	17:X:32:LEU:HA	1.91	0.42
20:Z:61:VAL:CG2	20:Z:62:VAL:H	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1063:LHG:H102	27:A:1063:LHG:O9	2.19	0.42
1:A:157:VAL:HG13	1:A:172:MET:CB	2.48	0.42
1:A:268:SER:O	1:A:271:LEU:HB3	2.19	0.42
1:A:316:THR:HG22	4:D:75:THR:HB	2.02	0.42
1:A:58:VAL:HG12	1:A:59:ASP:N	2.34	0.42
23:B:1011:CLA:CMD	23:B:1014:CLA:HBB1	2.50	0.42
23:B:1024:CLA:H161	23:B:1024:CLA:H121	1.84	0.42
2:B:332:LYS:HA	2:B:437:LEU:HD13	2.01	0.42
2:B:335:GLY:O	2:B:432:PHE:HD2	2.02	0.42
2:B:53:ASN:HD21	2:B:58:GLN:NE2	2.17	0.42
23:C:1037:CLA:C10	23:C:1037:CLA:C14	2.85	0.42
3:C:210:PHE:O	3:C:213:LEU:HD21	2.18	0.42
3:C:230:LEU:HA	3:C:233:VAL:HG12	2.01	0.42
3:C:49:LEU:HA	3:C:52:ALA:HB3	2.00	0.42
3:C:59:LEU:O	23:C:1034:CLA:HED2	2.20	0.42
23:A:1006:CLA:C20	26:D:1050:BCR:H402	2.49	0.42
4:D:157:PHE:CE2	4:D:173:PHE:CE1	3.06	0.42
24:A:1038:PHO:NC	4:D:209:LEU:HD12	2.35	0.42
2:B:324:LEU:HA	4:D:293:LEU:CD1	2.49	0.42
5:E:69:ARG:N	5:E:69:ARG:NE	2.68	0.42
6:F:40:MET:HB3	29:J:1059:MGE:H1	1.81	0.42
9:J:30:TYR:C	9:J:32:ALA:N	2.73	0.42
19:N:17:UNK:C	19:N:19:UNK:N	2.82	0.42
13:O:188:ARG:HB2	13:O:188:ARG:HE	1.41	0.42
16:V:110:GLY:O	16:V:111:GLU:O	2.37	0.42
1:A:109:GLY:C	1:A:111:PRO:HD2	2.40	0.42
1:A:234:ASN:OD1	29:L:1061:MGE:O3D	2.30	0.42
1:A:91:LEU:HD23	30:C:1055:DGD:O2D	2.19	0.42
23:B:1023:CLA:C7	26:B:1048:BCR:C34	2.91	0.42
3:C:295:THR:C	3:C:297:TYR:N	2.72	0.42
3:C:436:PHE:O	3:C:439:VAL:HG12	2.18	0.42
26:D:1050:BCR:H363	6:F:33:PHE:HB3	2.02	0.42
4:D:111:TRP:C	4:D:113:PHE:N	2.71	0.42
4:D:128:ARG:CG	4:D:128:ARG:HH11	2.32	0.42
1:A:257:ARG:C	4:D:132:ILE:HD13	2.40	0.42
7:H:13:PRO:C	7:H:15:ASN:N	2.72	0.42
9:J:31:GLY:C	29:J:1059:MGE:H3	2.23	0.42
13:O:169:LYS:HA	13:O:224:SER:HA	2.00	0.42
1:A:143:ILE:CD1	4:D:216:ALA:O	2.68	0.42
1:A:181:ASN:O	1:A:182:PHE:C	2.58	0.42
1:A:197:PHE:C	1:A:199:GLN:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH2	1:A:261:GLN:OE1	2.52	0.42
1:A:31:GLY:HA3	1:A:132:GLU:CD	2.40	0.42
2:B:156:PHE:O	2:B:160:GLY:N	2.45	0.42
2:B:256:MET:CE	2:B:268:PHE:HD1	2.33	0.42
2:B:455:HIS:H	2:B:455:HIS:HD1	1.68	0.42
23:C:1033:CLA:H193	23:C:1036:CLA:HHD	2.02	0.42
1:A:152:ALA:HA	30:C:1055:DGD:HBS2	2.02	0.42
3:C:169:GLY:O	3:C:173:LEU:HG	2.19	0.42
3:C:254:THR:HG22	3:C:255:THR:N	2.33	0.42
4:D:156:VAL:CG2	23:D:1004:CLA:HED2	2.50	0.42
4:D:251:ARG:NE	4:D:255:GLN:NE2	2.55	0.42
4:D:322:ASN:O	4:D:326:ARG:HB2	2.19	0.42
4:D:45:LEU:O	4:D:49:LEU:HD12	2.20	0.42
4:D:63:LEU:HD23	4:D:64:ALA:N	2.34	0.42
4:D:56:THR:HA	4:D:69:GLU:OE2	2.20	0.42
5:E:35:TRP:CD1	5:E:35:TRP:C	2.92	0.42
6:F:41:GLN:HE22	9:J:27:LEU:CA	2.32	0.42
8:I:13:THR:O	8:I:15:PHE:N	2.52	0.42
8:I:16:VAL:HG23	8:I:17:LEU:H	1.83	0.42
26:D:1050:BCR:C39	29:J:1059:MGE:H6B1	2.49	0.42
12:M:7:GLY:O	12:M:8:PHE:O	2.37	0.42
13:O:113:VAL:HG22	13:O:119:LEU:CD2	2.50	0.42
13:O:147:THR:HG1	13:O:149:LYS:H	1.64	0.42
13:O:92:VAL:HG22	13:O:93:PRO:CD	2.49	0.42
14:T:4:ILE:HG23	14:T:5:THR:N	2.35	0.42
24:A:1039:PHO:H143	4:D:173:PHE:CD1	2.55	0.42
1:A:27:ARG:HH11	1:A:27:ARG:CB	2.31	0.42
1:A:74:GLY:O	1:A:75:ASN:C	2.58	0.42
1:A:98:GLU:O	1:A:99:ALA:C	2.58	0.42
23:B:1011:CLA:H101	23:B:1011:CLA:C14	2.45	0.42
2:B:149:LEU:HD22	23:B:1012:CLA:H162	2.01	0.42
23:B:1023:CLA:H52	23:B:1024:CLA:H193	2.01	0.42
26:B:1045:BCR:C30	26:B:1045:BCR:C37	2.61	0.42
26:B:1045:BCR:C10	26:B:1045:BCR:H331	2.50	0.42
2:B:101:ILE:HG23	26:B:1047:BCR:C37	2.50	0.42
23:B:1024:CLA:H161	26:B:1048:BCR:H332	2.01	0.42
26:B:1048:BCR:H24C	26:B:1048:BCR:H371	1.59	0.42
2:B:45:PHE:HA	2:B:58:GLN:OE1	2.19	0.42
2:B:56:TRP:O	2:B:56:TRP:HE3	2.02	0.42
2:B:99:ALA:HB1	23:B:1014:CLA:C2	2.36	0.42
3:C:113:VAL:HG23	3:C:114:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:O	3:C:183:GLY:O	2.38	0.42
3:C:258:GLY:O	3:C:262:ARG:NH2	2.53	0.42
3:C:390:ARG:O	3:C:393:ALA:HB3	2.20	0.42
3:C:89:ILE:CB	3:C:90:PRO:HD3	2.39	0.42
4:D:129:GLN:HE21	4:D:142:ASN:CG	2.21	0.42
4:D:150:ILE:O	4:D:154:VAL:CG2	2.66	0.42
4:D:245:SER:C	4:D:247:VAL:H	2.22	0.42
2:B:461:LEU:HD23	4:D:280:TRP:HZ3	1.85	0.42
5:E:32:ILE:HA	5:E:35:TRP:HB3	2.02	0.42
13:O:187:GLY:CA	13:O:194:TYR:HB2	2.50	0.42
31:V:1041:HEM:CMA	31:V:1041:HEM:CBA	2.97	0.42
1:A:310:LYS:CB	16:V:28:GLU:HG3	2.50	0.42
20:Z:5:PHE:CD1	20:Z:57:LEU:HD22	2.54	0.42
27:A:1063:LHG:H272	23:C:1032:CLA:H62	2.02	0.42
1:A:33:PHE:HE1	8:I:23:PHE:CE2	2.37	0.42
1:A:32:TRP:O	1:A:35:VAL:HG23	2.20	0.42
1:A:96:ILE:HG23	1:A:97:TRP:N	2.34	0.42
2:B:473:THR:HG21	23:B:1016:CLA:CED	2.50	0.42
2:B:154:GLY:HA2	2:B:158:LEU:HB2	2.02	0.42
2:B:236:THR:HG23	2:B:237:VAL:N	2.34	0.42
2:B:256:MET:SD	2:B:268:PHE:HD1	2.43	0.42
2:B:281:GLN:O	2:B:284:ILE:HG12	2.20	0.42
23:C:1032:CLA:H2A	23:C:1032:CLA:HED1	1.72	0.42
23:C:1032:CLA:H2	23:C:1035:CLA:HAC1	2.01	0.42
23:C:1028:CLA:H43	30:C:1057:DGD:HA42	1.99	0.42
3:C:354:GLU:C	3:C:356:MET:H	2.23	0.42
23:D:1005:CLA:H42	25:D:1042:PQ9:H191	2.01	0.42
4:D:175:VAL:HG12	4:D:179:PHE:CZ	2.55	0.42
4:D:274:VAL:CB	4:D:275:PRO:CD	2.86	0.42
7:H:38:PHE:CD1	26:H:1049:BCR:C10	3.01	0.42
14:T:15:ALA:C	14:T:17:PHE:N	2.74	0.42
15:U:39:LEU:N	15:U:39:LEU:CD1	2.71	0.42
16:V:132:ASN:O	16:V:133:LEU:O	2.38	0.42
25:A:1043:PQ9:H61	25:A:1043:PQ9:H91	1.69	0.42
1:A:214:MET:HB3	25:A:1043:PQ9:H12	2.01	0.42
1:A:258:LEU:HA	4:D:128:ARG:HH12	1.85	0.42
1:A:259:ILE:O	1:A:260:PHE:O	2.38	0.42
1:A:285:PHE:HZ	23:C:1034:CLA:H203	1.84	0.42
2:B:144:PHE:HA	2:B:213:GLY:HA3	2.02	0.42
2:B:222:PRO:CG	2:B:225:LEU:HD12	2.33	0.42
3:C:174:LEU:O	3:C:177:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:HD2	3:C:178:LYS:HA	1.88	0.42
3:C:270:ALA:O	3:C:274:TYR:CD1	2.72	0.42
4:D:251:ARG:HG2	4:D:255:GLN:OE1	2.20	0.42
5:E:16:SER:HB3	5:E:19:TYR:HB2	2.02	0.42
23:B:1023:CLA:H162	7:H:7:LEU:HD11	2.01	0.42
10:K:37:PHE:HB3	26:K:1051:BCR:H402	2.02	0.42
29:L:1061:MGE:H263	29:L:1061:MGE:H212	2.00	0.42
13:O:65:ARG:CD	13:O:110:GLU:HA	2.50	0.42
13:O:97:VAL:CG1	13:O:98:THR:H	2.33	0.42
20:Z:55:GLY:CA	26:Z:1053:BCR:C31	2.89	0.42
20:Z:17:PHE:CD2	20:Z:17:PHE:O	2.65	0.42
20:Z:3:ILE:O	20:Z:5:PHE:N	2.53	0.42
10:K:15:TYR:OH	20:Z:58:ASN:OD1	2.32	0.42
23:A:1007:CLA:HBD	23:A:1007:CLA:HAA1	2.01	0.41
1:A:126:TYR:O	1:A:130:GLN:CB	2.67	0.41
1:A:281:VAL:CG1	1:A:282:GLY:N	2.82	0.41
1:A:37:MET:O	1:A:41:LEU:CD2	2.68	0.41
23:B:1009:CLA:C2A	23:B:1009:CLA:CED	2.94	0.41
2:B:150:CYS:CA	23:B:1011:CLA:HBC3	2.50	0.41
2:B:223:GLN:HG2	7:H:24:GLY:HA2	2.01	0.41
2:B:30:VAL:HG12	23:B:1013:CLA:CMD	2.47	0.41
2:B:390:TYR:O	2:B:391:SER:O	2.38	0.41
2:B:400:SER:HB2	2:B:402:TYR:HE2	1.85	0.41
2:B:79:SER:C	2:B:81:THR:N	2.71	0.41
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.41
3:C:186:TYR:HE2	3:C:188:THR:HB	1.85	0.41
3:C:286:ALA:C	3:C:288:CYS:N	2.71	0.41
3:C:449:ARG:HG2	23:C:1029:CLA:HED1	2.01	0.41
3:C:86:LEU:HD12	3:C:86:LEU:N	2.34	0.41
23:D:1005:CLA:H91	23:D:1005:CLA:H121	2.02	0.41
4:D:20:ASP:HA	4:D:23:LYS:HZ2	1.84	0.41
4:D:218:VAL:O	4:D:221:THR:CG2	2.67	0.41
4:D:313:THR:O	4:D:314:PHE:C	2.57	0.41
5:E:37:PHE:CE2	5:E:46:VAL:HG21	2.55	0.41
5:E:53:ASP:O	16:V:28:GLU:OE1	2.38	0.41
5:E:72:ALA:O	5:E:75:GLN:HB2	2.20	0.41
6:F:11:VAL:CG1	6:F:12:SER:N	2.81	0.41
7:H:39:LEU:HD22	7:H:39:LEU:HA	1.72	0.41
26:K:1052:BCR:H331	26:K:1052:BCR:C34	2.50	0.41
23:B:1022:CLA:HAC2	29:L:1061:MGE:H122	2.02	0.41
11:L:1:MET:O	11:L:1:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:33:GLN:O	12:M:34:LYS:C	2.58	0.41
7:H:40:VAL:CG2	17:X:23:LEU:HD21	2.50	0.41
1:A:186:PHE:CE2	1:A:190:HIS:CD2	3.07	0.41
1:A:254:TYR:O	1:A:257:ARG:N	2.53	0.41
1:A:96:ILE:HG13	1:A:105:TRP:CE2	2.55	0.41
23:B:1012:CLA:H112	23:B:1023:CLA:O1A	2.20	0.41
2:B:9:HIS:ND1	23:B:1019:CLA:H11	2.34	0.41
2:B:464:PHE:CD2	29:B:1060:MGE:H5B1	2.53	0.41
2:B:118:TRP:CH2	11:L:5:PRO:CD	2.98	0.41
2:B:119:ASP:O	2:B:120:LEU:HD23	2.20	0.41
2:B:210:ILE:HD13	2:B:210:ILE:HA	1.91	0.41
2:B:226:TYR:CE2	2:B:231:MET:O	2.70	0.41
2:B:27:THR:OG1	23:B:1020:CLA:H11	2.20	0.41
23:A:1006:CLA:H18	26:D:1050:BCR:C29	2.49	0.41
4:D:108:GLY:O	4:D:109:GLY:C	2.57	0.41
4:D:202:ALA:HB3	25:D:1042:PQ9:H311	2.02	0.41
4:D:205:LEU:HB2	23:D:1005:CLA:H12	2.02	0.41
1:A:272:HIS:CD2	4:D:214:HIS:NE2	2.88	0.41
4:D:67:TYR:CZ	29:J:1059:MGE:H1G1	2.53	0.41
17:X:20:PHE:O	17:X:23:LEU:N	2.52	0.41
20:Z:5:PHE:HD1	20:Z:57:LEU:HD13	1.85	0.41
23:A:1006:CLA:H122	23:A:1006:CLA:H161	1.58	0.41
2:B:250:PHE:HE2	23:B:1010:CLA:C20	2.31	0.41
2:B:191:ASN:ND2	2:B:191:ASN:C	2.74	0.41
2:B:250:PHE:HZ	30:H:1058:DGD:CIA	2.25	0.41
2:B:317:ASN:HA	2:B:330:MET:HE1	2.02	0.41
2:B:478:VAL:O	2:B:479:PHE:C	2.59	0.41
2:B:59:GLY:O	23:B:1015:CLA:HED2	2.21	0.41
23:C:1025:CLA:H61	23:C:1025:CLA:H41	1.86	0.41
30:C:1056:DGD:HA72	30:C:1056:DGD:HAT1	1.20	0.41
3:C:214:LEU:HD23	3:C:214:LEU:O	2.20	0.41
3:C:428:THR:CG2	3:C:429:SER:H	2.21	0.41
23:D:1004:CLA:H93	23:D:1004:CLA:H62	1.88	0.41
25:D:1042:PQ9:H212	25:D:1042:PQ9:H191	1.97	0.41
4:D:308:ASP:C	4:D:310:GLU:H	2.23	0.41
4:D:39:PRO:HG2	4:D:40:CYS:H	1.85	0.41
7:H:15:ASN:ND2	7:H:15:ASN:O	2.53	0.41
7:H:61:SER:CB	30:H:1058:DGD:O3E	2.68	0.41
10:K:25:LEU:HB3	10:K:26:PRO:CD	2.49	0.41
11:L:12:LEU:HD13	11:L:12:LEU:C	2.40	0.41
13:O:161:SER:O	13:O:163:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:92:VAL:CG2	13:O:93:PRO:CD	2.96	0.41
15:U:132:LEU:O	15:U:132:LEU:HD23	2.20	0.41
16:V:141:ILE:O	16:V:144:HIS:N	2.54	0.41
16:V:151:ILE:HG22	16:V:152:LEU:N	2.35	0.41
1:A:149:ALA:HA	1:A:284:TRP:HD1	1.81	0.41
2:B:393:GLU:C	2:B:396:GLY:H	2.24	0.41
2:B:5:TRP:CD1	2:B:5:TRP:N	2.88	0.41
23:C:1025:CLA:H203	23:C:1031:CLA:H152	2.01	0.41
3:C:185:LEU:O	3:C:196:VAL:HG23	2.21	0.41
3:C:289:PHE:HE2	3:C:293:ASN:HD22	1.66	0.41
3:C:431:PHE:HD2	3:C:431:PHE:C	2.23	0.41
4:D:29:PHE:CD1	4:D:30:VAL:N	2.88	0.41
5:E:75:GLN:O	5:E:79:PHE:HD1	2.03	0.41
8:I:4:LEU:CD1	8:I:8:VAL:HG23	2.50	0.41
12:M:11:THR:HG22	12:M:12:ALA:H	1.82	0.41
14:T:1:MET:HB2	14:T:2:GLU:H	1.40	0.41
15:U:109:LEU:C	15:U:111:HIS:N	2.74	0.41
31:V:1041:HEM:CMA	31:V:1041:HEM:HBA2	2.50	0.41
16:V:121:LEU:HD13	16:V:121:LEU:HA	1.81	0.41
20:Z:12:LEU:HD12	20:Z:51:VAL:CA	2.50	0.41
1:A:214:MET:SD	24:A:1039:PHO:HMD3	2.60	0.41
1:A:127:MET:CE	1:A:148:SER:HA	2.51	0.41
1:A:197:PHE:CZ	30:C:1056:DGD:HAS1	2.55	0.41
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.41
23:B:1011:CLA:HED2	23:B:1011:CLA:CAD	2.48	0.41
23:B:1013:CLA:H72	23:B:1020:CLA:C17	2.50	0.41
23:C:1025:CLA:C1B	23:C:1025:CLA:H42	2.46	0.41
30:C:1055:DGD:O1B	30:C:1055:DGD:HB41	2.17	0.41
3:C:48:LYS:NZ	3:C:138:GLU:OE1	2.53	0.41
3:C:262:ARG:C	3:C:263:ALA:O	2.56	0.41
3:C:224:ILE:CD1	3:C:285:ILE:HD11	2.40	0.41
3:C:442:LEU:O	3:C:443:TRP:C	2.59	0.41
2:B:362:PHE:CE1	4:D:184:PHE:CE1	3.08	0.41
4:D:190:ASN:HD21	4:D:193:LEU:HD22	1.85	0.41
4:D:199:MET:O	4:D:202:ALA:HB3	2.20	0.41
4:D:21:TRP:O	4:D:22:LEU:C	2.58	0.41
4:D:250:ASN:OD1	4:D:251:ARG:N	2.54	0.41
4:D:59:TYR:CD1	4:D:59:TYR:N	2.89	0.41
5:E:60:GLN:O	5:E:60:GLN:NE2	2.53	0.41
5:E:75:GLN:C	5:E:79:PHE:HD1	2.23	0.41
8:I:2:GLU:O	8:I:6:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:13:LEU:HA	12:M:13:LEU:HD23	1.83	0.41
13:O:109:GLY:HA3	13:O:123:GLU:CA	2.50	0.41
16:V:159:GLY:HA2	16:V:163:TYR:CE1	2.52	0.41
16:V:78:LEU:HA	16:V:78:LEU:HD23	1.74	0.41
20:Z:39:LEU:HD12	20:Z:42:LEU:CB	2.50	0.41
1:A:116:ILE:O	1:A:117:PHE:C	2.58	0.41
1:A:13:LEU:H	1:A:13:LEU:CD2	2.27	0.41
1:A:245:THR:HG22	4:D:264:LYS:CD	2.48	0.41
1:A:42:LEU:O	1:A:43:ALA:C	2.59	0.41
2:B:125:ASP:OD1	2:B:126:PRO:HD2	2.21	0.41
2:B:133:LEU:CB	2:B:138:MET:HE1	2.49	0.41
2:B:216:HIS:HE1	23:H:1017:CLA:HMA3	1.85	0.41
2:B:220:ARG:HG3	7:H:22:ALA:HB2	2.03	0.41
2:B:284:ILE:O	2:B:287:ARG:HB2	2.20	0.41
3:C:225:VAL:HG12	3:C:225:VAL:O	2.21	0.41
3:C:283:GLY:HA3	3:C:434:ALA:CB	2.35	0.41
4:D:156:VAL:HG21	23:D:1004:CLA:OBD	2.20	0.41
4:D:218:VAL:O	4:D:220:ASN:N	2.53	0.41
4:D:221:THR:HG23	4:D:222:LEU:H	1.86	0.41
4:D:324:GLY:C	4:D:326:ARG:N	2.71	0.41
4:D:42:TYR:CD2	4:D:43:LEU:HD13	2.55	0.41
30:C:1057:DGD:HD4	9:J:39:SER:HB3	2.03	0.41
12:M:22:LEU:C	12:M:24:ILE:N	2.74	0.41
13:O:259:VAL:HG12	13:O:261:ILE:HG13	2.03	0.41
16:V:141:ILE:O	16:V:144:HIS:HB3	2.21	0.41
16:V:158:GLY:HA3	16:V:162:TYR:HE2	1.85	0.41
1:A:161:TYR:HD1	1:A:294:ALA:HA	1.86	0.41
1:A:78:ILE:HD11	11:L:34:TYR:CE2	2.56	0.41
23:B:1009:CLA:C4B	26:H:1049:BCR:C38	2.98	0.41
23:B:1023:CLA:NC	23:B:1024:CLA:HBC1	2.34	0.41
26:B:1045:BCR:C39	26:B:1045:BCR:H373	2.29	0.41
2:B:230:ARG:NH1	2:B:230:ARG:CA	2.81	0.41
2:B:257:TRP:NE1	2:B:273:TYR:OH	2.51	0.41
2:B:476:ARG:CG	2:B:477:ASP:N	2.83	0.41
23:C:1025:CLA:C2D	23:C:1026:CLA:H71	2.51	0.41
3:C:222:GLY:O	3:C:223:TRP:O	2.38	0.41
3:C:350:ILE:CD1	3:C:356:MET:HA	2.51	0.41
3:C:60:ILE:HG23	3:C:61:VAL:N	2.36	0.41
4:D:91:LEU:HD12	23:D:1008:CLA:HED2	2.01	0.41
23:D:1005:CLA:H43	25:D:1042:PQ9:H191	2.01	0.41
4:D:299:ILE:C	4:D:301:GLN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:1051:BCR:C37	26:K:1051:BCR:C30	2.60	0.41
10:K:18:PHE:O	10:K:19:ASP:C	2.58	0.41
29:D:1062:MGE:H1G2	11:L:15:THR:CG2	2.50	0.41
13:O:98:THR:HG22	13:O:99:ARG:O	2.20	0.41
1:A:304:HIS:O	1:A:306:VAL:N	2.54	0.41
1:A:317:TRP:HA	4:D:63:LEU:HD11	2.02	0.41
2:B:257:TRP:CH2	4:D:291:LEU:CA	3.04	0.41
2:B:260:SER:O	2:B:262:THR:N	2.54	0.41
2:B:284:ILE:CG2	2:B:309:LEU:HD22	2.39	0.41
2:B:307:GLU:O	2:B:310:ALA:N	2.54	0.41
2:B:354:LEU:HA	2:B:372:ASP:HA	2.03	0.41
2:B:35:GLY:O	2:B:39:LEU:HG	2.20	0.41
2:B:246:PHE:CD2	2:B:463:PHE:HA	2.55	0.41
3:C:131:TYR:O	3:C:133:ALA:N	2.53	0.41
3:C:185:LEU:HD12	3:C:199:ILE:CD1	2.50	0.41
3:C:340:TYR:C	3:C:341:LEU:HG	2.40	0.41
3:C:366:LEU:HD23	3:C:370:ARG:NH2	2.35	0.41
3:C:374:GLY:O	3:C:375:LEU:C	2.58	0.41
3:C:56:HIS:C	3:C:58:GLY:N	2.74	0.41
3:C:74:HIS:O	3:C:75:PHE:C	2.57	0.41
4:D:55:VAL:HG11	4:D:105:CYS:SG	2.61	0.41
4:D:122:LEU:HD12	4:D:122:LEU:HA	1.83	0.41
4:D:16:ASP:HA	4:D:19:ASP:HB3	2.03	0.41
4:D:195:PRO:HB3	11:L:31:PHE:CE1	2.56	0.41
1:A:212:CYS:HB2	4:D:207:GLY:O	2.21	0.41
4:D:189:HIS:CE1	4:D:294:ARG:NH1	2.89	0.41
5:E:19:TYR:O	5:E:23:HIS:HB2	2.21	0.41
5:E:49:THR:HA	5:E:50:PRO:HD3	1.79	0.41
8:I:6:ILE:O	8:I:7:THR:C	2.57	0.41
9:J:30:TYR:CD2	9:J:30:TYR:C	2.93	0.41
13:O:55:ALA:HB1	13:O:162:ILE:O	2.20	0.41
14:T:15:ALA:O	14:T:18:PHE:N	2.53	0.41
15:U:98:THR:O	15:U:99:GLU:C	2.59	0.41
31:V:1041:HEM:HHC	31:V:1041:HEM:CBB	2.50	0.41
16:V:149:PRO:HD3	16:V:156:TRP:CD1	2.55	0.41
16:V:29:LEU:HG	16:V:29:LEU:O	2.21	0.41
18:Y:19:ILE:CG2	18:Y:20:ALA:H	2.32	0.41
1:A:207:GLY:HA2	23:A:1006:CLA:H43	2.02	0.41
1:A:142:TRP:CH2	27:A:1063:LHG:HC11	2.55	0.41
1:A:128:GLY:HA2	23:C:1029:CLA:HMB2	2.03	0.41
1:A:207:GLY:O	1:A:211:PHE:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:HIS:C	1:A:252:HIS:ND1	2.74	0.41
1:A:271:LEU:HD21	25:A:1043:PQ9:C10	2.51	0.41
23:B:1011:CLA:O2A	23:B:1011:CLA:H3A	2.21	0.41
2:B:103:LEU:C	2:B:106:LEU:HB3	2.41	0.41
2:B:136:PRO:HG3	23:B:1018:CLA:HBC1	2.03	0.41
2:B:181:VAL:HB	2:B:199:VAL:HG21	2.03	0.41
2:B:373:LYS:O	2:B:374:ASN:HB2	2.21	0.41
2:B:478:VAL:HG12	4:D:139:ARG:CD	2.50	0.41
23:C:1026:CLA:H3A	23:C:1026:CLA:HBA2	1.60	0.41
23:C:1025:CLA:C17	23:C:1031:CLA:HMB3	2.45	0.41
23:C:1032:CLA:HAB	23:C:1034:CLA:CMC	2.51	0.41
3:C:355:THR:HG22	3:C:355:THR:O	2.21	0.41
3:C:394:GLU:HB2	16:V:127:PHE:HZ	1.86	0.41
1:A:160:ILE:HG13	3:C:431:PHE:CE1	2.55	0.41
3:C:439:VAL:HG22	23:C:1032:CLA:CBC	2.50	0.41
4:D:148:ALA:HB2	4:D:276:VAL:CA	2.50	0.41
4:D:168:PHE:C	4:D:170:ALA:H	2.25	0.41
4:D:293:LEU:O	4:D:293:LEU:CD1	2.69	0.41
5:E:69:ARG:NE	5:E:69:ARG:H	2.19	0.41
5:E:68:ASP:CB	5:E:69:ARG:HH21	2.30	0.41
7:H:7:LEU:HA	7:H:10:ILE:HD12	2.02	0.41
10:K:19:ASP:HA	10:K:22:VAL:CG1	2.48	0.41
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.02	0.41
2:B:434:THR:HG23	13:O:204:LYS:HE2	2.02	0.41
14:T:18:PHE:O	14:T:22:PHE:CD2	2.68	0.41
17:X:30:LEU:HD22	17:X:30:LEU:HA	1.88	0.41
1:A:210:LEU:HD13	24:A:1039:PHO:ND	2.35	0.41
1:A:297:LEU:HD13	30:C:1056:DGD:HAW2	2.02	0.41
1:A:60:ILE:CG1	1:A:61:ASP:N	2.53	0.41
1:A:99:ALA:CB	1:A:105:TRP:N	2.83	0.41
2:B:239:SER:HB2	23:B:1016:CLA:HED2	2.02	0.41
23:B:1018:CLA:CBD	23:B:1018:CLA:HAA2	2.51	0.41
23:B:1019:CLA:C5	23:B:1021:CLA:CED	2.94	0.41
2:B:165:GLY:HA3	2:B:179:GLN:C	2.41	0.41
2:B:359:MET:HB3	2:B:425:ILE:HG22	2.03	0.41
2:B:449:GLY:O	2:B:450:TRP:C	2.60	0.41
23:C:1025:CLA:H142	23:C:1025:CLA:H111	1.90	0.41
3:C:61:VAL:CA	23:C:1027:CLA:HMD2	2.49	0.41
3:C:53:HIS:HB3	23:C:1036:CLA:HMD1	2.00	0.41
3:C:251:HIS:CE1	23:C:1030:CLA:NA	2.88	0.41
3:C:293:ASN:ND2	3:C:296:VAL:HG22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:O	3:C:305:THR:HG23	2.20	0.41
25:D:1042:PQ9:H111	25:D:1042:PQ9:H152	1.80	0.41
1:A:220:THR:HG22	4:D:141:TYR:CE2	2.56	0.41
1:A:83:VAL:HG23	4:D:314:PHE:HE1	1.85	0.41
4:D:43:LEU:O	4:D:47:GLY:N	2.50	0.41
5:E:15:THR:O	5:E:16:SER:C	2.60	0.41
13:O:121:PHE:CB	13:O:153:ALA:HB3	2.44	0.41
13:O:213:VAL:O	13:O:213:VAL:HG22	2.21	0.41
13:O:216:PHE:HD1	13:O:216:PHE:O	2.04	0.41
17:X:23:LEU:HA	17:X:23:LEU:HD12	1.78	0.41
18:Y:39:LEU:HD21	20:Z:25:VAL:CG1	2.49	0.41
20:Z:62:VAL:O	20:Z:62:VAL:HG13	2.21	0.41
1:A:320:ILE:O	1:A:321:ILE:C	2.58	0.41
1:A:32:TRP:HE3	1:A:35:VAL:HG21	1.86	0.41
23:B:1019:CLA:H112	23:B:1019:CLA:H143	1.54	0.41
2:B:137:LYS:O	2:B:138:MET:C	2.59	0.41
2:B:143:LEU:HD13	2:B:143:LEU:C	2.42	0.41
2:B:342:GLY:HA3	2:B:403:GLY:O	2.21	0.41
2:B:466:HIS:NE2	23:B:1016:CLA:ND	2.69	0.41
23:C:1027:CLA:CBA	23:C:1027:CLA:HBD	2.51	0.41
23:C:1032:CLA:C17	23:C:1034:CLA:H192	2.51	0.41
3:C:126:GLY:O	3:C:127:PHE:C	2.59	0.41
3:C:318:LEU:C	3:C:318:LEU:HD23	2.41	0.41
3:C:414:ILE:CG1	3:C:415:ASN:N	2.84	0.41
3:C:75:PHE:HB2	3:C:86:LEU:HD21	2.02	0.41
4:D:253:TRP:C	4:D:255:GLN:N	2.73	0.41
5:E:51:ARG:C	5:E:53:ASP:N	2.74	0.41
4:D:154:VAL:HG21	30:H:1058:DGD:HAF1	2.01	0.41
7:H:38:PHE:HD1	26:H:1049:BCR:C10	2.32	0.41
26:D:1050:BCR:C37	29:J:1059:MGE:H3A1	2.51	0.41
13:O:65:ARG:HD2	13:O:110:GLU:HA	2.02	0.41
16:V:125:ASP:HB3	16:V:131:ARG:NE	2.36	0.41
16:V:160:LYS:CB	16:V:160:LYS:HZ3	2.11	0.41
18:Y:35:ILE:HG13	18:Y:36:ILE:N	2.36	0.41
1:A:199:GLN:HG3	1:A:200:LEU:N	2.35	0.40
1:A:231:GLU:CG	1:A:235:TYR:HE1	2.33	0.40
1:A:261:GLN:O	1:A:262:TYR:HB2	2.20	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.02	0.40
23:B:1012:CLA:H112	23:B:1023:CLA:O2A	2.13	0.40
2:B:145:LEU:HD13	23:B:1023:CLA:HMB2	2.02	0.40
2:B:25:MET:HE2	26:B:1045:BCR:H291	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ALA:HB3	2:B:156:PHE:CD2	2.55	0.40
2:B:160:GLY:C	2:B:162:PHE:H	2.25	0.40
2:B:188:ASP:C	2:B:190:PHE:N	2.75	0.40
2:B:223:GLN:C	2:B:227:LYS:HG2	2.42	0.40
2:B:68:ARG:HH22	2:B:262:THR:HB	1.85	0.40
23:C:1026:CLA:H92	23:C:1026:CLA:H61	1.57	0.40
23:C:1025:CLA:HBA2	23:C:1026:CLA:H93	2.03	0.40
3:C:60:ILE:HG23	23:C:1027:CLA:HMD1	2.03	0.40
23:C:1029:CLA:H71	23:C:1029:CLA:C4	2.51	0.40
3:C:356:MET:HG2	3:C:357:ARG:N	2.37	0.40
3:C:425:TRP:CZ2	23:C:1028:CLA:O1A	2.73	0.40
1:A:288:LEU:HD21	3:C:432:VAL:HG13	2.02	0.40
2:B:257:TRP:CH2	4:D:291:LEU:HG	2.25	0.40
4:D:292:ASN:O	4:D:294:ARG:N	2.54	0.40
4:D:83:ASN:CG	4:D:336:HIS:CE1	2.95	0.40
5:E:19:TYR:CE1	5:E:20:TRP:CD1	3.07	0.40
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.40
23:B:1018:CLA:C2B	23:H:1017:CLA:HMB2	2.50	0.40
1:A:97:TRP:CZ3	8:I:8:VAL:HG11	2.55	0.40
11:L:15:THR:CA	11:L:18:TYR:HB2	2.50	0.40
13:O:64:TYR:CD1	13:O:64:TYR:N	2.89	0.40
11:L:18:TYR:CD2	14:T:20:ALA:HB2	2.56	0.40
14:T:1:MET:HA	14:T:4:ILE:HG22	2.03	0.40
13:O:175:PRO:HB3	15:U:123:GLU:HG2	2.02	0.40
10:K:39:VAL:CA	18:Y:36:ILE:CD1	2.97	0.40
20:Z:61:VAL:CG2	20:Z:62:VAL:N	2.81	0.40
1:A:101:SER:C	1:A:103:ASP:N	2.72	0.40
1:A:140:ARG:HH21	27:A:1063:LHG:C1	2.34	0.40
1:A:27:ARG:HD2	14:T:24:ARG:NH2	2.37	0.40
2:B:26:HIS:ND1	23:B:1020:CLA:HMA1	2.36	0.40
23:B:1022:CLA:C9	23:B:1022:CLA:C3	2.96	0.40
2:B:330:MET:HG2	2:B:444:ARG:O	2.21	0.40
2:B:360:PRO:O	2:B:361:ALA:C	2.59	0.40
2:B:440:ASP:C	2:B:440:ASP:OD2	2.59	0.40
3:C:88:LEU:CG	23:C:1027:CLA:HBC3	2.50	0.40
3:C:59:LEU:HB3	23:C:1034:CLA:O1D	2.20	0.40
3:C:270:ALA:O	3:C:273:SER:N	2.54	0.40
3:C:84:GLN:O	3:C:86:LEU:N	2.52	0.40
3:C:89:ILE:O	3:C:92:ILE:HG13	2.21	0.40
26:D:1050:BCR:H24C	26:D:1050:BCR:H382	1.95	0.40
23:D:1005:CLA:C7	29:D:1062:MGE:H202	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:CB	4:D:149:PRO:CD	2.94	0.40
4:D:291:LEU:CD1	4:D:291:LEU:N	2.84	0.40
4:D:45:LEU:C	4:D:45:LEU:CD1	2.82	0.40
4:D:53:THR:C	4:D:66:SER:OG	2.60	0.40
7:H:10:ILE:H	7:H:10:ILE:HG13	1.55	0.40
29:D:1062:MGE:H222	29:L:1061:MGE:CGB	2.51	0.40
12:M:14:PHE:O	12:M:14:PHE:CG	2.73	0.40
29:D:1062:MGE:H4A2	14:T:17:PHE:CD2	2.57	0.40
15:U:72:TYR:HD2	15:U:73:PRO:CD	2.34	0.40
1:A:135:TYR:O	1:A:137:LEU:N	2.54	0.40
1:A:14:TRP:CD1	1:A:18:CYS:SG	3.10	0.40
1:A:202:VAL:HG11	23:A:1006:CLA:C3D	2.52	0.40
1:A:244:GLU:O	1:A:246:TYR:N	2.55	0.40
1:A:247:ASN:ND2	1:A:250:ALA:CB	2.85	0.40
23:B:1019:CLA:CMB	23:B:1020:CLA:C4B	3.00	0.40
2:B:123:PHE:HD1	2:B:123:PHE:HA	1.76	0.40
2:B:223:GLN:HG2	7:H:24:GLY:N	2.36	0.40
2:B:306:PRO:O	2:B:307:GLU:C	2.59	0.40
2:B:318:ASN:HD21	2:B:320:ALA:CB	2.33	0.40
2:B:329:PRO:O	2:B:331:ASN:N	2.55	0.40
2:B:457:VAL:HG23	2:B:457:VAL:H	1.55	0.40
2:B:463:PHE:CE1	23:B:1016:CLA:CBB	2.93	0.40
3:C:223:TRP:HB3	3:C:224:ILE:H	1.75	0.40
1:A:87:ASN:ND2	3:C:357:ARG:CG	2.84	0.40
1:A:212:CYS:SG	4:D:271:MET:O	2.67	0.40
7:H:14:LEU:HD12	7:H:14:LEU:N	2.34	0.40
13:O:104:LEU:HD22	13:O:128:ASP:HA	2.03	0.40
13:O:167:ASP:O	13:O:168:PHE:CG	2.74	0.40
13:O:208:LEU:CD1	13:O:208:LEU:H	2.35	0.40
13:O:250:ASP:OD1	13:O:253:ALA:HB2	2.21	0.40
15:U:112:PHE:N	15:U:112:PHE:HD2	2.18	0.40
16:V:128:PRO:HB3	16:V:131:ARG:NE	2.36	0.40
18:Y:39:LEU:CD1	20:Z:28:ALA:HB3	2.50	0.40
1:A:202:VAL:HG12	1:A:206:PHE:CD1	2.57	0.40
26:B:1047:BCR:H371	26:B:1047:BCR:H24C	1.63	0.40
2:B:193:TYR:C	2:B:261:ALA:HB2	2.42	0.40
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.56	0.40
2:B:321:LYS:HB3	2:B:321:LYS:HZ2	1.86	0.40
2:B:476:ARG:C	2:B:476:ARG:HD2	2.41	0.40
2:B:69:LEU:HD11	23:B:1011:CLA:HMD1	2.04	0.40
23:C:1035:CLA:HAA1	23:C:1035:CLA:CBD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:293:ASN:OD1	3:C:295:THR:N	2.54	0.40
3:C:394:GLU:CD	16:V:127:PHE:CE2	2.95	0.40
3:C:418:ASN:HD22	3:C:419:PHE:N	2.20	0.40
3:C:45:LEU:HD12	3:C:45:LEU:H	1.86	0.40
29:D:1062:MGE:H2G	29:D:1062:MGE:H1D	1.29	0.40
4:D:155:SER:HA	4:D:159:ILE:CG1	2.51	0.40
4:D:237:PRO:O	4:D:238:THR:CB	2.70	0.40
4:D:280:TRP:O	4:D:283:ALA:HB3	2.20	0.40
4:D:46:GLY:O	4:D:49:LEU:N	2.55	0.40
4:D:83:ASN:CB	4:D:336:HIS:CE1	3.04	0.40
5:E:30:LEU:HA	5:E:30:LEU:HD22	1.65	0.40
23:H:1017:CLA:HAA1	23:H:1017:CLA:CBD	2.52	0.40
23:C:1034:CLA:HMB3	10:K:33:PHE:HB2	2.03	0.40
11:L:28:ALA:HB2	12:M:15:VAL:HG22	2.04	0.40
12:M:17:VAL:HB	12:M:18:PRO:CD	2.51	0.40
13:O:250:ASP:O	13:O:251:MET:C	2.58	0.40
13:O:73:PRO:HG3	13:O:102:THR:HG1	1.85	0.40
15:U:130:ASN:O	15:U:131:GLY:O	2.38	0.40
15:U:58:ASN:OD1	15:U:85:TYR:N	2.54	0.40
18:Y:44:GLY:CA	20:Z:30:PRO:HD3	2.50	0.40
20:Z:2:THR:O	20:Z:5:PHE:HB3	2.21	0.40
20:Z:7:LEU:HA	20:Z:10:ALA:HB3	2.04	0.40
23:A:1006:CLA:HMC3	4:D:157:PHE:CE1	2.57	0.40
1:A:134:SER:CB	1:A:141:PRO:HA	2.44	0.40
1:A:310:LYS:HA	16:V:29:LEU:CB	2.35	0.40
23:B:1010:CLA:HMB1	23:B:1010:CLA:CBB	2.33	0.40
2:B:149:LEU:CB	23:B:1011:CLA:HBC1	2.51	0.40
23:B:1012:CLA:CED	23:B:1013:CLA:H11	2.49	0.40
23:B:1019:CLA:H122	23:B:1021:CLA:H102	2.04	0.40
2:B:19:LEU:HD13	2:B:19:LEU:C	2.42	0.40
2:B:392:PHE:O	2:B:393:GLU:CB	2.69	0.40
2:B:67:ALA:O	2:B:68:ARG:C	2.60	0.40
23:C:1036:CLA:H151	26:Z:1053:BCR:H362	2.03	0.40
30:C:1055:DGD:HBG2	30:C:1055:DGD:HBN1	1.71	0.40
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.22	0.40
3:C:397:THR:OG1	3:C:398:HIS:N	2.55	0.40
23:D:1005:CLA:CBB	23:D:1005:CLA:HMB1	2.51	0.40
4:D:218:VAL:CA	4:D:221:THR:HG22	2.52	0.40
4:D:58:TRP:CZ2	5:E:55:TYR:HB3	2.56	0.40
6:F:44:GLN:O	6:F:45:ARG:CB	2.69	0.40
2:B:6:TYR:CZ	11:L:11:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:21:LEU:CD2	12:M:22:LEU:HD12	2.50	0.40
12:M:31:SER:C	12:M:33:GLN:H	2.25	0.40
13:O:162:ILE:HG22	13:O:162:ILE:O	2.22	0.40
13:O:190:LEU:HD11	15:U:42:VAL:HG22	2.03	0.40
15:U:90:ASP:O	15:U:93:ASN:HB2	2.21	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%)	210 (63%)	84 (25%)	39 (12%)	0	7
1	a	333/344 (97%)	214 (64%)	75 (22%)	44 (13%)	0	5
2	B	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	6
2	b	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	6
3	C	445/447 (100%)	306 (69%)	89 (20%)	50 (11%)	0	7
3	c	445/447 (100%)	316 (71%)	82 (18%)	47 (11%)	0	9
4	D	338/340 (99%)	199 (59%)	87 (26%)	52 (15%)	0	4
4	d	338/340 (99%)	214 (63%)	79 (23%)	45 (13%)	0	5
5	E	80/83 (96%)	44 (55%)	22 (28%)	14 (18%)	0	3
5	e	80/83 (96%)	51 (64%)	18 (22%)	11 (14%)	0	5
6	F	33/44 (75%)	26 (79%)	6 (18%)	1 (3%)	5	38
6	f	33/44 (75%)	26 (79%)	5 (15%)	2 (6%)	1	21
7	H	62/64 (97%)	39 (63%)	15 (24%)	8 (13%)	0	6
7	h	62/64 (97%)	38 (61%)	19 (31%)	5 (8%)	1	14
8	I	33/35 (94%)	19 (58%)	8 (24%)	6 (18%)	0	2
8	i	33/35 (94%)	24 (73%)	6 (18%)	3 (9%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	32/40 (80%)	26 (81%)	2 (6%)	4 (12%)	0	6
9	j	32/40 (80%)	26 (81%)	3 (9%)	3 (9%)	1	11
10	K	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	0	7
10	k	34/36 (94%)	23 (68%)	7 (21%)	4 (12%)	0	7
11	L	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	1	13
11	l	35/37 (95%)	22 (63%)	9 (26%)	4 (11%)	0	7
12	M	34/36 (94%)	19 (56%)	8 (24%)	7 (21%)	0	2
12	m	34/36 (94%)	24 (71%)	7 (21%)	3 (9%)	1	12
13	O	240/242 (99%)	155 (65%)	47 (20%)	38 (16%)	0	4
13	o	240/242 (99%)	163 (68%)	45 (19%)	32 (13%)	0	5
14	T	28/30 (93%)	18 (64%)	5 (18%)	5 (18%)	0	2
14	t	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	4	34
15	U	96/98 (98%)	56 (58%)	24 (25%)	16 (17%)	0	3
15	u	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	4
16	V	135/137 (98%)	91 (67%)	25 (18%)	19 (14%)	0	4
16	v	135/137 (98%)	90 (67%)	28 (21%)	17 (13%)	0	6
17	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	4	38
17	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	4	38
18	Y	26/28 (93%)	19 (73%)	5 (19%)	2 (8%)	1	15
18	y	26/28 (93%)	19 (73%)	3 (12%)	4 (15%)	0	4
20	Z	60/62 (97%)	39 (65%)	10 (17%)	11 (18%)	0	2
20	z	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	10
All	All	5118/5250 (98%)	3365 (66%)	1106 (22%)	647 (13%)	0	6

All (647) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	75	ASN
1	A	79	THR
1	A	80	GLY
1	A	84	PRO
1	A	91	LEU
1	A	96	ILE

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	129	ARG
1	A	151	LEU
1	A	169	SER
1	A	224	ILE
1	A	261	GLN
1	A	279	ARG
1	A	305	SER
1	A	335	ASN
2	B	34	ALA
2	B	48	SER
2	B	87	ASP
2	B	93	PHE
2	B	121	GLU
2	B	151	PHE
2	B	157	HIS
2	B	171	PRO
2	B	224	ARG
2	B	230	ARG
2	B	279	TYR
2	B	327	THR
2	B	361	ALA
2	B	407	ASN
2	B	443	PHE
2	B	478	VAL
2	B	479	PHE
2	B	487	SER
3	C	33	PHE
3	C	42	LEU
3	C	99	VAL
3	C	127	PHE
3	C	138	GLU
3	C	411	ALA
3	C	457	LYS
3	C	461	ARG
4	D	22	LEU
4	D	25	ASP
4	D	113	PHE
4	D	222	LEU
4	D	233	ARG
4	D	236	ASN
4	D	239	GLN

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Mol	Chain	Res	Type
4	D	262	SER
4	D	299	ILE
4	D	325	ILE
4	D	330	ALA
4	D	338	ASN
5	E	9	PRO
5	E	11	SER
5	E	13	ILE
5	E	20	TRP
5	E	60	GLN
5	E	82	GLN
5	E	83	LEU
7	H	17	GLU
7	H	18	TYR
7	H	26	GLY
10	K	13	GLU
10	K	27	VAL
12	M	8	PHE
12	M	11	THR
12	M	12	ALA
12	M	34	LYS
13	O	52	ALA
13	O	88	GLU
13	O	110	GLU
13	O	151	LEU
13	O	175	PRO
13	O	188	ARG
13	O	197	ALA
13	O	247	SER
14	T	2	GLU
15	U	53	GLU
15	U	60	THR
15	U	72	TYR
15	U	73	PRO
15	U	132	LEU
16	V	109	ASP
16	V	111	GLU
16	V	124	ALA
16	V	133	LEU
17	X	43	ILE
20	Z	31	GLN
20	Z	32	ASP

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Mol	Chain	Res	Type
1	a	5031	GLY
1	a	5060	ILE
1	a	5075	ASN
1	a	5080	GLY
1	a	5084	PRO
1	a	5129	ARG
1	a	5224	ILE
1	a	5229	GLU
1	a	5261	GLN
1	a	5277	ALA
1	a	5305	SER
2	b	5045	SER
2	b	5096	ALA
2	b	5118	GLU
2	b	5119	LEU
2	b	5154	HIS
2	b	5168	PRO
2	b	5221	ARG
2	b	5227	ARG
2	b	5276	TYR
2	b	5324	THR
2	b	5358	ALA
2	b	5359	PHE
2	b	5383	ALA
2	b	5388	SER
2	b	5440	PHE
2	b	5475	VAL
2	b	5476	PHE
2	b	5484	SER
3	c	5099	VAL
3	c	5138	GLU
3	c	5264	PHE
3	c	5295	THR
3	c	5407	VAL
3	c	5411	ALA
3	c	5457	LYS
3	c	5461	ARG
4	d	5021	TRP
4	d	5022	LEU
4	d	5025	ASP
4	d	5026	ARG
4	d	5090	LEU

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Mol	Chain	Res	Type
4	d	5169	PHE
4	d	5222	LEU
4	d	5233	ARG
4	d	5235	PHE
4	d	5236	ASN
4	d	5239	GLN
4	d	5242	GLU
4	d	5262	SER
4	d	5330	ALA
4	d	5338	ASN
5	e	5009	PRO
5	e	5011	SER
5	e	5060	GLN
7	h	5026	GLY
10	k	5013	GLU
12	m	5005	GLN
13	o	5088	GLU
13	o	5106	GLN
13	o	5110	GLU
13	o	5151	LEU
13	o	5175	PRO
13	o	5188	ARG
13	o	5247	SER
15	u	5053	GLU
15	u	5060	THR
15	u	5072	TYR
15	u	5073	PRO
15	u	5116	GLU
16	v	5088	ALA
16	v	5109	ASP
16	v	5122	ARG
16	v	5124	ALA
16	v	5133	LEU
1	A	44	ALA
1	A	72	LEU
1	A	88	ALA
1	A	114	LEU
1	A	150	PRO
1	A	229	GLU
1	A	260	PHE
1	A	318	ALA
2	B	6	TYR

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Mol	Chain	Res	Type
2	B	59	GLY
2	B	89	GLY
2	B	122	LEU
2	B	150	CYS
2	B	165	GLY
2	B	174	LEU
2	B	219	VAL
2	B	259	GLY
2	B	261	ALA
2	B	280	PHE
2	B	322	GLY
2	B	330	MET
2	B	386	ALA
2	B	391	SER
2	B	396	GLY
2	B	488	PRO
3	C	40	ALA
3	C	80	PRO
3	C	184	GLY
3	C	196	VAL
3	C	217	PRO
3	C	223	TRP
3	C	256	PRO
3	C	384	ILE
3	C	400	PRO
3	C	406	SER
3	C	472	LEU
4	D	23	LYS
4	D	26	ARG
4	D	109	GLY
4	D	169	PHE
4	D	211	CYS
4	D	228	GLY
4	D	235	PHE
4	D	242	GLU
4	D	274	VAL
4	D	300	SER
4	D	345	VAL
4	D	349	GLY
5	E	44	TYR
5	E	45	ASP
7	H	6	TRP

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Mol	Chain	Res	Type
9	J	31	GLY
9	J	35	GLY
12	M	3	VAL
12	M	5	GLN
13	O	60	SER
13	O	106	GLN
13	O	115	SER
13	O	162	ILE
13	O	169	LYS
13	O	185	PRO
13	O	201	PRO
13	O	206	GLU
13	O	224	SER
13	O	256	PRO
14	T	11	ALA
15	U	90	ASP
15	U	110	GLU
15	U	124	GLY
15	U	130	ASN
15	U	131	GLY
16	V	41	GLU
16	V	67	HIS
16	V	110	GLY
16	V	123	SER
16	V	153	GLY
18	Y	45	ASN
20	Z	6	GLN
20	Z	55	GLY
20	Z	61	VAL
1	a	5061	ASP
1	a	5088	ALA
1	a	5096	ILE
1	a	5100	ALA
1	a	5150	PRO
1	a	5245	THR
1	a	5260	PHE
1	a	5275	LEU
1	a	5318	ALA
1	a	5335	ASN
2	b	5003	TYR
2	b	5008	VAL
2	b	5031	ALA

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Mol	Chain	Res	Type
2	b	5040	ALA
2	b	5056	GLY
2	b	5148	PHE
2	b	5162	GLY
2	b	5183	GLY
2	b	5231	ILE
2	b	5237	SER
2	b	5247	PHE
2	b	5261	PRO
2	b	5277	PHE
2	b	5319	GLY
2	b	5393	GLY
3	c	5040	ALA
3	c	5085	GLY
3	c	5172	ALA
3	c	5184	GLY
3	c	5217	PRO
3	c	5257	PHE
3	c	5266	TRP
3	c	5277	GLY
3	c	5333	GLY
3	c	5355	THR
3	c	5383	ASP
3	c	5432	VAL
4	d	5100	ASP
4	d	5168	PHE
4	d	5228	GLY
4	d	5238	THR
4	d	5240	ALA
4	d	5274	VAL
4	d	5325	ILE
4	d	5329	MET
4	d	5345	VAL
4	d	5349	GLY
5	e	5013	ILE
5	e	5020	TRP
5	e	5044	TYR
6	f	5041	GLN
6	f	5043	ILE
7	h	5006	TRP
7	h	5014	LEU
9	j	5031	GLY

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Mol	Chain	Res	Type
9	j	5035	GLY
11	l	5006	ASN
11	l	5030	LEU
12	m	5014	PHE
12	m	5034	LYS
13	o	5049	ASP
13	o	5052	ALA
13	o	5169	LYS
13	o	5177	TYR
13	o	5179	THR
13	o	5185	PRO
13	o	5197	ALA
13	o	5209	ALA
15	u	5063	ALA
15	u	5090	ASP
15	u	5099	GLU
15	u	5132	LEU
16	v	5041	GLU
16	v	5064	ALA
16	v	5153	GLY
16	v	5154	ASP
17	x	5043	ILE
18	y	5025	ARG
20	z	5006	GLN
20	z	5050	LEU
1	A	45	THR
1	A	61	ASP
1	A	112	TYR
1	A	217	SER
1	A	245	THR
1	A	274	PHE
1	A	321	ILE
2	B	28	ALA
2	B	80	ILE
2	B	161	LEU
2	B	204	ALA
2	B	223	GLN
2	B	266	GLU
2	B	307	GLU
2	B	372	ASP
3	C	29	GLU
3	C	46	SER

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Mol	Chain	Res	Type
3	C	75	PHE
3	C	139	THR
3	C	161	LEU
3	C	172	ALA
3	C	228	ASN
3	C	277	GLY
3	C	287	THR
3	C	355	THR
3	C	429	SER
3	C	436	PHE
3	C	452	ALA
3	C	456	GLU
3	C	471	SER
4	D	21	TRP
4	D	58	TRP
4	D	66	SER
4	D	114	ILE
4	D	165	SER
4	D	168	PHE
4	D	173	PHE
4	D	219	GLU
4	D	238	THR
4	D	273	PHE
4	D	292	ASN
4	D	329	MET
5	E	31	PHE
6	F	19	ARG
7	H	19	GLY
8	I	24	LEU
9	J	18	GLY
10	K	12	PRO
10	K	36	ALA
11	L	31	PHE
13	O	49	ASP
13	O	100	GLU
13	O	116	ASP
13	O	117	GLY
13	O	146	PHE
13	O	150	ASN
13	O	209	ALA
13	O	229	LYS
13	O	232	GLY

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Mol	Chain	Res	Type
14	T	16	LEU
14	T	26	PRO
15	U	94	ILE
15	U	99	GLU
15	U	123	GLU
16	V	64	ALA
16	V	65	SER
16	V	81	ARG
16	V	112	GLN
16	V	154	ASP
18	Y	43	ARG
20	Z	4	LEU
1	a	5045	THR
1	a	5081	ALA
1	a	5091	LEU
1	a	5168	PHE
1	a	5217	SER
1	a	5279	ARG
1	a	5280	VAL
1	a	5321	ILE
1	a	5334	ARG
2	b	5171	LEU
2	b	5193	GLY
2	b	5220	GLN
2	b	5404	ASN
2	b	5433	THR
2	b	5485	PRO
3	c	5033	PHE
3	c	5042	LEU
3	c	5287	THR
3	c	5316	THR
3	c	5400	PRO
3	c	5429	SER
4	d	5041	ALA
4	d	5062	GLY
4	d	5071	CYS
4	d	5095	PRO
4	d	5096	GLU
4	d	5192	THR
4	d	5292	ASN
4	d	5300	SER
5	e	5012	ASP

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Mol	Chain	Res	Type
5	e	5045	ASP
5	e	5082	GLN
8	i	5024	LEU
8	i	5027	ASP
10	k	5012	PRO
11	l	5031	PHE
13	o	5086	ARG
13	o	5157	PRO
13	o	5229	LYS
14	t	5026	PRO
15	u	5130	ASN
16	v	5051	GLN
16	v	5065	SER
16	v	5112	GLN
16	v	5129	LYS
20	z	5032	ASP
20	z	5055	GLY
1	A	152	ALA
1	A	153	SER
2	B	11	VAL
2	B	43	ALA
2	B	249	ALA
2	B	250	PHE
2	B	392	PHE
2	B	414	PRO
3	C	57	ALA
3	C	101	PRO
3	C	212	TYR
3	C	298	PRO
3	C	435	PHE
3	C	443	TRP
3	C	465	PRO
4	D	30	VAL
4	D	188	PHE
4	D	240	ALA
4	D	275	PRO
4	D	281	MET
4	D	344	GLU
4	D	348	ARG
5	E	10	PHE
7	H	14	LEU
8	I	27	ASP

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Mol	Chain	Res	Type
9	J	34	ALA
11	L	3	PRO
11	L	30	LEU
12	M	9	ILE
13	O	96	LEU
13	O	138	GLY
13	O	157	PRO
13	O	179	THR
13	O	251	MET
14	T	9	ILE
15	U	92	LEU
16	V	69	GLY
20	Z	23	VAL
1	a	5142	TRP
1	a	5165	GLN
1	a	5236	GLY
2	b	5052	MET
2	b	5143	ALA
2	b	5155	LEU
3	c	5057	ALA
3	c	5075	PHE
3	c	5256	PRO
3	c	5260	ALA
3	c	5324	LEU
3	c	5384	ILE
4	d	5030	VAL
4	d	5101	PHE
4	d	5181	PHE
4	d	5273	PHE
4	d	5275	PRO
4	d	5277	THR
7	h	5020	LYS
7	h	5063	LYS
8	i	5010	ILE
10	k	5027	VAL
11	l	5003	PRO
13	o	5096	LEU
13	o	5100	GLU
15	u	5092	LEU
16	v	5162	TYR
18	y	5012	ILE
1	A	63	ILE

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Mol	Chain	Res	Type
1	A	179	THR
1	A	280	VAL
2	B	50	PRO
2	B	71	VAL
2	B	234	ILE
2	B	360	PRO
2	B	439	SER
2	B	484	PRO
3	C	257	PHE
3	C	296	VAL
3	C	333	GLY
4	D	111	TRP
5	E	43	ALA
8	I	2	GLU
8	I	5	LYS
13	O	122	VAL
16	V	83	GLU
16	V	121	LEU
16	V	162	TYR
20	Z	42	LEU
1	a	5070	SER
1	a	5072	LEU
1	a	5079	THR
1	a	5164	GLY
2	b	5084	ASP
2	b	5256	GLY
2	b	5257	SER
2	b	5270	TYR
2	b	5313	GLY
2	b	5327	MET
2	b	5346	LYS
2	b	5371	ASN
2	b	5439	ILE
2	b	5481	PRO
3	c	5109	PHE
3	c	5132	HIS
3	c	5471	SER
4	d	5080	THR
4	d	5306	ALA
9	j	5034	ALA
13	o	5060	SER
13	o	5187	GLY

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Mol	Chain	Res	Type
13	o	5224	SER
13	o	5228	ALA
13	o	5243	SER
15	u	5094	ILE
18	y	5027	ASN
20	z	5010	ALA
1	A	31	GLY
1	A	176	ILE
2	B	99	ALA
3	C	216	SER
4	D	37	LEU
7	H	58	VAL
8	I	30	ARG
13	O	41	LEU
13	O	269	ILE
15	U	104	ILE
16	V	128	PRO
20	Z	3	ILE
1	a	5172	MET
1	a	5185	VAL
1	a	5293	MET
1	a	5333	GLU
2	b	5192	PRO
2	b	5334	ALA
2	b	5411	PRO
2	b	5452	HIS
3	c	5046	SER
3	c	5077	PRO
4	d	5152	VAL
5	e	5072	ALA
10	k	5022	VAL
13	o	5117	GLY
13	o	5143	PRO
13	o	5201	PRO
16	v	5110	GLY
3	C	85	GLY
4	D	47	GLY
4	D	187	GLY
13	O	109	GLY
15	U	43	VAL
20	Z	24	PRO
1	a	5138	GLY

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Mol	Chain	Res	Type
2	b	5013	PRO
2	b	5123	PRO
2	b	5133	PRO
3	c	5216	SER
3	c	5414	ILE
3	c	5465	PRO
4	d	5299	ILE
5	e	5052	PRO
13	o	5122	VAL
13	o	5162	ILE
15	u	5122	VAL
18	y	5026	GLY
1	A	236	GLY
2	B	211	ILE
2	B	367	PRO
3	C	77	PRO
4	D	62	GLY
4	D	132	ILE
4	D	152	VAL
5	E	52	PRO
3	c	5196	VAL
3	c	5199	ILE
13	o	5256	PRO
15	u	5131	GLY
2	B	126	PRO
2	B	192	PRO
3	C	249	ILE
3	C	306	GLY
4	D	237	PRO
5	E	27	ILE
1	a	5327	GLY
3	c	5367	GLU
3	c	5408	GLY
3	c	5470	PRO
13	o	5109	GLY
15	u	5084	PRO
16	v	5148	GLU
20	z	5061	VAL
3	C	414	ILE
4	D	39	PRO
7	H	60	VAL
8	I	10	ILE

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Mol	Chain	Res	Type
13	O	143	PRO
13	O	187	GLY
1	a	5066	PRO
2	b	5219	PRO
4	d	5309	PRO
16	v	5128	PRO
20	Z	22	GLY
3	c	5298	PRO
3	c	5304	PRO
4	d	5237	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	223 (83%)	47 (17%)	2	14
1	a	270/279 (97%)	216 (80%)	54 (20%)	1	9
2	B	386/388 (100%)	330 (86%)	56 (14%)	3	23
2	b	386/388 (100%)	332 (86%)	54 (14%)	4	25
3	C	349/349 (100%)	285 (82%)	64 (18%)	2	12
3	c	349/349 (100%)	292 (84%)	57 (16%)	2	17
4	D	275/275 (100%)	224 (82%)	51 (18%)	2	11
4	d	275/275 (100%)	231 (84%)	44 (16%)	2	18
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	10
5	e	72/73 (99%)	62 (86%)	10 (14%)	4	25
6	F	29/38 (76%)	21 (72%)	8 (28%)	0	3
6	f	29/38 (76%)	22 (76%)	7 (24%)	1	5
7	H	54/54 (100%)	40 (74%)	14 (26%)	0	4
7	h	54/54 (100%)	41 (76%)	13 (24%)	1	5
8	I	32/32 (100%)	26 (81%)	6 (19%)	1	11
8	i	32/32 (100%)	26 (81%)	6 (19%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	15 (62%)	9 (38%)	0	1
9	j	24/28 (86%)	14 (58%)	10 (42%)	0	0
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	3
10	k	29/29 (100%)	21 (72%)	8 (28%)	0	3
11	L	35/35 (100%)	28 (80%)	7 (20%)	1	9
11	l	35/35 (100%)	28 (80%)	7 (20%)	1	9
12	M	33/33 (100%)	30 (91%)	3 (9%)	10	42
12	m	33/33 (100%)	30 (91%)	3 (9%)	10	42
13	O	200/206 (97%)	172 (86%)	28 (14%)	4	25
13	o	200/206 (97%)	168 (84%)	32 (16%)	2	18
14	T	27/27 (100%)	19 (70%)	8 (30%)	0	3
14	t	27/27 (100%)	21 (78%)	6 (22%)	1	7
15	U	85/85 (100%)	72 (85%)	13 (15%)	3	21
15	u	85/85 (100%)	73 (86%)	12 (14%)	4	24
16	V	117/117 (100%)	97 (83%)	20 (17%)	2	15
16	v	117/117 (100%)	100 (86%)	17 (14%)	3	23
17	X	27/27 (100%)	18 (67%)	9 (33%)	0	2
17	x	27/27 (100%)	16 (59%)	11 (41%)	0	0
18	Y	21/21 (100%)	13 (62%)	8 (38%)	0	1
18	y	21/21 (100%)	14 (67%)	7 (33%)	0	2
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	8
20	z	52/52 (100%)	39 (75%)	13 (25%)	0	5
All	All	4234/4296 (99%)	3479 (82%)	755 (18%)	2	13

All (755) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	27	ARG
1	A	46	ILE
1	A	52	PHE
1	A	56	PRO
1	A	60	ILE
1	A	73	TYR

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Mol	Chain	Res	Type
1	A	83	VAL
1	A	89	ILE
1	A	92	HIS
1	A	93	PHE
1	A	102	LEU
1	A	121	LEU
1	A	129	ARG
1	A	131	TRP
1	A	139	MET
1	A	144	CYS
1	A	155	PHE
1	A	157	VAL
1	A	165	GLN
1	A	174	LEU
1	A	180	PHE
1	A	186	PHE
1	A	191	ASN
1	A	192	ILE
1	A	193	LEU
1	A	197	PHE
1	A	199	GLN
1	A	206	PHE
1	A	227	THR
1	A	247	ASN
1	A	254	TYR
1	A	257	ARG
1	A	266	ASN
1	A	273	PHE
1	A	278	TRP
1	A	279	ARG
1	A	283	VAL
1	A	292	THR
1	A	298	ASN
1	A	316	THR
1	A	317	TRP
1	A	319	ASP
1	A	322	ASN
1	A	328	MET
1	A	334	ARG
1	A	337	HIS
2	B	6	TYR
2	B	8	VAL

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Mol	Chain	Res	Type
2	B	18	ARG
2	B	24	LEU
2	B	51	VAL
2	B	81	THR
2	B	83	GLU
2	B	106	LEU
2	B	109	LEU
2	B	116	VAL
2	B	122	LEU
2	B	123	PHE
2	B	124	ARG
2	B	135	LEU
2	B	148	LEU
2	B	156	PHE
2	B	161	LEU
2	B	171	PRO
2	B	174	LEU
2	B	184	GLU
2	B	185	TRP
2	B	191	ASN
2	B	226	TYR
2	B	230	ARG
2	B	246	PHE
2	B	251	VAL
2	B	256	MET
2	B	265	ILE
2	B	271	THR
2	B	272	ARG
2	B	277	SER
2	B	286	ARG
2	B	288	VAL
2	B	289	GLN
2	B	318	ASN
2	B	336	ILE
2	B	345	VAL
2	B	346	PHE
2	B	356	VAL
2	B	359	MET
2	B	367	PRO
2	B	377	VAL
2	B	390	TYR
2	B	405	GLU

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Mol	Chain	Res	Type
2	B	415	PRO
2	B	417	VAL
2	B	435	GLU
2	B	439	SER
2	B	443	PHE
2	B	444	ARG
2	B	446	SER
2	B	448	ARG
2	B	463	PHE
2	B	464	PHE
2	B	469	HIS
2	B	477	ASP
3	C	33	PHE
3	C	42	LEU
3	C	45	LEU
3	C	48	LYS
3	C	56	HIS
3	C	59	LEU
3	C	67	MET
3	C	72	LEU
3	C	76	ILE
3	C	78	GLU
3	C	80	PRO
3	C	88	LEU
3	C	92	ILE
3	C	95	LEU
3	C	107	ASP
3	C	113	VAL
3	C	119	LEU
3	C	135	ARG
3	C	140	LEU
3	C	157	MET
3	C	160	ILE
3	C	210	PHE
3	C	214	LEU
3	C	224	ILE
3	C	227	VAL
3	C	231	GLU
3	C	237	HIS
3	C	244	CYS
3	C	245	ILE
3	C	257	PHE

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Mol	Chain	Res	Type
3	C	259	TRP
3	C	262	ARG
3	C	265	ILE
3	C	289	PHE
3	C	313	GLN
3	C	320	ARG
3	C	328	VAL
3	C	334	PRO
3	C	337	LEU
3	C	343	ARG
3	C	350	ILE
3	C	356	MET
3	C	357	ARG
3	C	368	PRO
3	C	369	LEU
3	C	382	ASN
3	C	383	ASP
3	C	391	ARG
3	C	413	GLU
3	C	416	SER
3	C	418	ASN
3	C	419	PHE
3	C	428	THR
3	C	430	HIS
3	C	431	PHE
3	C	441	HIS
3	C	442	LEU
3	C	447	ARG
3	C	449	ARG
3	C	456	GLU
3	C	460	ASP
3	C	461	ARG
3	C	467	LEU
3	C	472	LEU
4	D	21	TRP
4	D	23	LYS
4	D	24	ARG
4	D	35	ILE
4	D	43	LEU
4	D	45	LEU
4	D	53	THR
4	D	55	VAL

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Mol	Chain	Res	Type
4	D	83	ASN
4	D	85	MET
4	D	89	LEU
4	D	90	LEU
4	D	91	LEU
4	D	96	GLU
4	D	102	THR
4	D	103	ARG
4	D	122	LEU
4	D	134	ARG
4	D	138	VAL
4	D	159	ILE
4	D	168	PHE
4	D	175	VAL
4	D	180	ARG
4	D	183	LEU
4	D	188	PHE
4	D	211	CYS
4	D	213	ILE
4	D	217	THR
4	D	221	THR
4	D	222	LEU
4	D	232	PHE
4	D	233	ARG
4	D	235	PHE
4	D	248	THR
4	D	266	TRP
4	D	267	LEU
4	D	277	THR
4	D	279	LEU
4	D	280	TRP
4	D	281	MET
4	D	289	LEU
4	D	291	LEU
4	D	294	ARG
4	D	300	SER
4	D	307	GLU
4	D	311	PHE
4	D	313	THR
4	D	316	THR
4	D	319	LEU
4	D	337	GLU

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Mol	Chain	Res	Type
4	D	340	VAL
5	E	8	ARG
5	E	12	ASP
5	E	13	ILE
5	E	24	SER
5	E	30	LEU
5	E	35	TRP
5	E	45	ASP
5	E	51	ARG
5	E	58	GLN
5	E	60	GLN
5	E	69	ARG
5	E	80	LEU
5	E	81	GLU
5	E	83	LEU
6	F	18	VAL
6	F	19	ARG
6	F	25	THR
6	F	26	LEU
6	F	32	PHE
6	F	37	ILE
6	F	40	MET
6	F	43	ILE
7	H	4	ARG
7	H	5	THR
7	H	10	ILE
7	H	11	LEU
7	H	12	ARG
7	H	17	GLU
7	H	18	TYR
7	H	25	TRP
7	H	33	VAL
7	H	39	LEU
7	H	45	ILE
7	H	49	TYR
7	H	50	ASN
7	H	52	THR
8	I	6	ILE
8	I	13	THR
8	I	14	PHE
8	I	23	PHE
8	I	24	LEU

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Mol	Chain	Res	Type
8	I	35	LYS
9	J	8	ILE
9	J	11	TRP
9	J	12	ILE
9	J	13	VAL
9	J	22	ILE
9	J	23	VAL
9	J	30	TYR
9	J	39	SER
9	J	40	LEU
10	K	11	LEU
10	K	19	ASP
10	K	28	ILE
10	K	31	LEU
10	K	32	PHE
10	K	33	PHE
10	K	37	PHE
10	K	38	VAL
11	L	7	ARG
11	L	8	GLN
11	L	14	ARG
11	L	21	LEU
11	L	24	ILE
11	L	31	PHE
11	L	32	SER
12	M	1	MET
12	M	8	PHE
12	M	32	GLN
13	O	31	LEU
13	O	34	ASP
13	O	63	THR
13	O	88	GLU
13	O	91	PHE
13	O	100	GLU
13	O	108	GLN
13	O	120	THR
13	O	121	PHE
13	O	122	VAL
13	O	127	ILE
13	O	136	MET
13	O	144	LEU
13	O	157	PRO

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Mol	Chain	Res	Type
13	O	158	ASN
13	O	167	ASP
13	O	169	LYS
13	O	178	ARG
13	O	183	LEU
13	O	186	LYS
13	O	194	TYR
13	O	200	LEU
13	O	206	GLU
13	O	210	ARG
13	O	213	VAL
13	O	215	ARG
13	O	251	MET
13	O	254	HIS
14	T	1	MET
14	T	3	THR
14	T	4	ILE
14	T	7	VAL
14	T	14	ILE
14	T	16	LEU
14	T	28	ARG
14	T	29	ILE
15	U	39	LEU
15	U	58	ASN
15	U	61	ASN
15	U	73	PRO
15	U	90	ASP
15	U	98	THR
15	U	99	GLU
15	U	101	GLN
15	U	109	LEU
15	U	118	GLU
15	U	121	LEU
15	U	127	ARG
15	U	132	LEU
16	V	28	GLU
16	V	30	THR
16	V	33	VAL
16	V	34	LEU
16	V	35	THR
16	V	38	LEU
16	V	44	THR

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Mol	Chain	Res	Type
16	V	48	THR
16	V	58	LEU
16	V	59	PHE
16	V	61	TYR
16	V	92	ARG
16	V	101	TYR
16	V	102	MET
16	V	109	ASP
16	V	119	PRO
16	V	121	LEU
16	V	122	ARG
16	V	135	GLU
16	V	160	LYS
17	X	13	THR
17	X	24	LEU
17	X	28	VAL
17	X	30	LEU
17	X	32	LEU
17	X	34	PHE
17	X	37	LEU
17	X	38	ILE
17	X	44	ASP
18	Y	19	ILE
18	Y	21	GLN
18	Y	24	MET
18	Y	36	ILE
18	Y	37	PHE
18	Y	38	LEU
18	Y	39	LEU
18	Y	46	LEU
20	Z	3	ILE
20	Z	9	LEU
20	Z	12	LEU
20	Z	17	PHE
20	Z	27	TYR
20	Z	31	GLN
20	Z	34	ASP
20	Z	35	ARG
20	Z	38	GLN
20	Z	47	TRP
20	Z	57	LEU
1	a	5017	PHE

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Mol	Chain	Res	Type
1	a	5027	ARG
1	a	5032	TRP
1	a	5038	ILE
1	a	5046	ILE
1	a	5048	PHE
1	a	5060	ILE
1	a	5065	GLU
1	a	5075	ASN
1	a	5089	ILE
1	a	5092	HIS
1	a	5093	PHE
1	a	5102	LEU
1	a	5121	LEU
1	a	5129	ARG
1	a	5130	GLN
1	a	5131	TRP
1	a	5133	LEU
1	a	5145	VAL
1	a	5157	VAL
1	a	5165	GLN
1	a	5172	MET
1	a	5174	LEU
1	a	5186	PHE
1	a	5192	ILE
1	a	5193	LEU
1	a	5197	PHE
1	a	5199	GLN
1	a	5205	VAL
1	a	5206	PHE
1	a	5210	LEU
1	a	5215	HIS
1	a	5226	GLU
1	a	5227	THR
1	a	5232	SER
1	a	5254	TYR
1	a	5257	ARG
1	a	5260	PHE
1	a	5266	ASN
1	a	5268	SER
1	a	5269	ARG
1	a	5271	LEU
1	a	5278	TRP

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Mol	Chain	Res	Type
1	a	5279	ARG
1	a	5283	VAL
1	a	5292	THR
1	a	5298	ASN
1	a	5316	THR
1	a	5317	TRP
1	a	5319	ASP
1	a	5322	ASN
1	a	5334	ARG
1	a	5337	HIS
1	a	5341	LEU
2	b	5003	TYR
2	b	5005	VAL
2	b	5015	ARG
2	b	5033	SER
2	b	5048	VAL
2	b	5060	LEU
2	b	5113	VAL
2	b	5119	LEU
2	b	5120	PHE
2	b	5121	ARG
2	b	5132	LEU
2	b	5135	MET
2	b	5145	LEU
2	b	5153	PHE
2	b	5168	PRO
2	b	5181	GLU
2	b	5182	TRP
2	b	5188	ASN
2	b	5223	TYR
2	b	5227	ARG
2	b	5230	ASN
2	b	5243	PHE
2	b	5248	VAL
2	b	5262	ILE
2	b	5265	PHE
2	b	5268	THR
2	b	5269	ARG
2	b	5271	GLN
2	b	5274	SER
2	b	5283	ARG
2	b	5289	LEU

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Mol	Chain	Res	Type
2	b	5306	LEU
2	b	5343	PHE
2	b	5356	MET
2	b	5359	PHE
2	b	5387	TYR
2	b	5394	VAL
2	b	5398	PHE
2	b	5402	GLU
2	b	5411	PRO
2	b	5414	VAL
2	b	5426	ILE
2	b	5429	PHE
2	b	5430	ASP
2	b	5432	GLU
2	b	5436	SER
2	b	5440	PHE
2	b	5441	ARG
2	b	5445	ARG
2	b	5460	PHE
2	b	5461	PHE
2	b	5466	HIS
2	b	5469	ARG
2	b	5474	ASP
3	c	5033	PHE
3	c	5042	LEU
3	c	5045	LEU
3	c	5048	LYS
3	c	5056	HIS
3	c	5059	LEU
3	c	5067	MET
3	c	5072	LEU
3	c	5078	GLU
3	c	5084	GLN
3	c	5088	LEU
3	c	5113	VAL
3	c	5119	LEU
3	c	5124	VAL
3	c	5135	ARG
3	c	5140	LEU
3	c	5149	TYR
3	c	5160	ILE
3	c	5174	LEU

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Mol	Chain	Res	Type
3	c	5207	ARG
3	c	5210	PHE
3	c	5212	TYR
3	c	5214	LEU
3	c	5224	ILE
3	c	5231	GLU
3	c	5237	HIS
3	c	5245	ILE
3	c	5256	PRO
3	c	5257	PHE
3	c	5262	ARG
3	c	5274	TYR
3	c	5296	VAL
3	c	5315	MET
3	c	5321	ASP
3	c	5328	VAL
3	c	5332	GLN
3	c	5334	PRO
3	c	5337	LEU
3	c	5343	ARG
3	c	5350	ILE
3	c	5355	THR
3	c	5357	ARG
3	c	5369	LEU
3	c	5382	ASN
3	c	5383	ASP
3	c	5405	ASN
3	c	5406	SER
3	c	5413	GLU
3	c	5416	SER
3	c	5418	ASN
3	c	5419	PHE
3	c	5428	THR
3	c	5431	PHE
3	c	5447	ARG
3	c	5456	GLU
3	c	5467	LEU
3	c	5472	LEU
4	d	5021	TRP
4	d	5023	LYS
4	d	5024	ARG
4	d	5043	LEU

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Mol	Chain	Res	Type
4	d	5045	LEU
4	d	5053	THR
4	d	5068	LEU
4	d	5071	CYS
4	d	5085	MET
4	d	5089	LEU
4	d	5090	LEU
4	d	5092	LEU
4	d	5096	GLU
4	d	5101	PHE
4	d	5102	THR
4	d	5103	ARG
4	d	5110	LEU
4	d	5113	PHE
4	d	5130	PHE
4	d	5134	ARG
4	d	5138	VAL
4	d	5159	ILE
4	d	5168	PHE
4	d	5175	VAL
4	d	5180	ARG
4	d	5188	PHE
4	d	5191	TRP
4	d	5213	ILE
4	d	5217	THR
4	d	5222	LEU
4	d	5232	PHE
4	d	5233	ARG
4	d	5235	PHE
4	d	5236	ASN
4	d	5248	THR
4	d	5266	TRP
4	d	5269	PHE
4	d	5279	LEU
4	d	5280	TRP
4	d	5281	MET
4	d	5291	LEU
4	d	5319	LEU
4	d	5340	VAL
4	d	5345	VAL
5	e	5008	ARG
5	e	5012	ASP

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Mol	Chain	Res	Type
5	e	5017	VAL
5	e	5030	LEU
5	e	5058	GLN
5	e	5060	GLN
5	e	5068	ASP
5	e	5069	ARG
5	e	5081	GLU
5	e	5083	LEU
6	f	5018	VAL
6	f	5019	ARG
6	f	5025	THR
6	f	5026	LEU
6	f	5032	PHE
6	f	5033	PHE
6	f	5043	ILE
7	h	5004	ARG
7	h	5005	THR
7	h	5009	ASP
7	h	5010	ILE
7	h	5011	LEU
7	h	5017	GLU
7	h	5025	TRP
7	h	5033	VAL
7	h	5039	LEU
7	h	5045	ILE
7	h	5049	TYR
7	h	5050	ASN
7	h	5056	ASP
8	i	5006	ILE
8	i	5013	THR
8	i	5014	PHE
8	i	5023	PHE
8	i	5024	LEU
8	i	5035	LYS
9	j	5007	ARG
9	j	5008	ILE
9	j	5011	TRP
9	j	5012	ILE
9	j	5013	VAL
9	j	5022	ILE
9	j	5023	VAL
9	j	5024	ILE

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Mol	Chain	Res	Type
9	j	5036	LEU
9	j	5040	LEU
10	k	5011	LEU
10	k	5012	PRO
10	k	5019	ASP
10	k	5028	ILE
10	k	5031	LEU
10	k	5032	PHE
10	k	5037	PHE
10	k	5038	VAL
11	l	5007	ARG
11	l	5008	GLN
11	l	5014	ARG
11	l	5017	LEU
11	l	5021	LEU
11	l	5026	VAL
11	l	5031	PHE
12	m	5001	MET
12	m	5008	PHE
12	m	5011	THR
13	o	5031	LEU
13	o	5034	ASP
13	o	5081	GLU
13	o	5088	GLU
13	o	5091	PHE
13	o	5114	ASN
13	o	5127	ILE
13	o	5128	ASP
13	o	5133	THR
13	o	5136	MET
13	o	5144	LEU
13	o	5145	LEU
13	o	5148	VAL
13	o	5156	GLN
13	o	5157	PRO
13	o	5158	ASN
13	o	5167	ASP
13	o	5169	LYS
13	o	5172	PHE
13	o	5178	ARG
13	o	5183	LEU
13	o	5186	LYS

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Mol	Chain	Res	Type
13	o	5194	TYR
13	o	5198	ILE
13	o	5206	GLU
13	o	5210	ARG
13	o	5213	VAL
13	o	5215	ARG
13	o	5222	GLN
13	o	5254	HIS
13	o	5258	GLU
13	o	5269	ILE
14	t	5001	MET
14	t	5004	ILE
14	t	5014	ILE
14	t	5016	LEU
14	t	5028	ARG
14	t	5029	ILE
15	u	5039	LEU
15	u	5058	ASN
15	u	5061	ASN
15	u	5062	ILE
15	u	5073	PRO
15	u	5090	ASP
15	u	5095	PRO
15	u	5099	GLU
15	u	5109	LEU
15	u	5118	GLU
15	u	5127	ARG
15	u	5132	LEU
16	v	5030	THR
16	v	5036	VAL
16	v	5038	LEU
16	v	5052	TYR
16	v	5058	LEU
16	v	5059	PHE
16	v	5061	TYR
16	v	5063	CYS
16	v	5066	CYS
16	v	5067	HIS
16	v	5083	GLU
16	v	5092	ARG
16	v	5118	HIS
16	v	5121	LEU

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Mol	Chain	Res	Type
16	v	5122	ARG
16	v	5135	GLU
16	v	5160	LYS
17	x	5011	THR
17	x	5013	THR
17	x	5023	LEU
17	x	5024	LEU
17	x	5028	VAL
17	x	5030	LEU
17	x	5032	LEU
17	x	5034	PHE
17	x	5037	LEU
17	x	5038	ILE
17	x	5042	GLN
18	y	5001	ILE
18	y	5003	GLN
18	y	5010	ILE
18	y	5018	ILE
18	y	5019	PHE
18	y	5024	ARG
18	y	5028	LEU
20	z	5003	ILE
20	z	5009	LEU
20	z	5012	LEU
20	z	5016	SER
20	z	5017	PHE
20	z	5027	TYR
20	z	5031	GLN
20	z	5034	ASP
20	z	5035	ARG
20	z	5038	GLN
20	z	5047	TRP
20	z	5048	ILE
20	z	5057	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	76	ASN
1	A	92	HIS
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	303	ASN
1	A	315	ASN
1	A	322	ASN
2	B	58	GLN
2	B	114	HIS
2	B	191	ASN
2	B	201	HIS
2	B	289	GLN
2	B	318	ASN
2	B	343	HIS
2	B	348	ASN
2	B	394	GLN
2	B	395	GLN
2	B	409	GLN
3	C	44	ASN
3	C	201	ASN
3	C	322	GLN
3	C	441	HIS
4	D	72	ASN
4	D	87	HIS
4	D	98	GLN
4	D	129	GLN
4	D	142	ASN
4	D	197	HIS
4	D	220	ASN
4	D	224	GLN
4	D	236	ASN
4	D	255	GLN
4	D	332	GLN
4	D	334	GLN
5	E	60	GLN
5	E	82	GLN
6	F	41	GLN
7	H	15	ASN
11	L	4	ASN
12	M	5	GLN
12	M	32	GLN
13	O	43	ASN
13	O	72	GLN
13	O	158	ASN
13	O	212	ASN

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Mol	Chain	Res	Type
13	O	245	GLN
15	U	58	ASN
15	U	67	GLN
15	U	82	ASN
15	U	108	ASN
16	V	51	GLN
16	V	60	GLN
16	V	104	ASN
16	V	144	HIS
17	X	42	GLN
1	a	5019	ASN
1	a	5075	ASN
1	a	5076	ASN
1	a	5087	ASN
1	a	5092	HIS
1	a	5130	GLN
1	a	5165	GLN
1	a	5247	ASN
1	a	5296	ASN
1	a	5315	ASN
1	a	5322	ASN
2	b	5055	GLN
2	b	5111	HIS
2	b	5176	GLN
2	b	5188	ASN
2	b	5230	ASN
2	b	5286	GLN
2	b	5340	HIS
2	b	5391	GLN
2	b	5392	GLN
3	c	5044	ASN
3	c	5118	HIS
3	c	5313	GLN
3	c	5322	GLN
3	c	5332	GLN
3	c	5398	HIS
3	c	5441	HIS
4	d	5087	HIS
4	d	5098	GLN
4	d	5164	GLN
4	d	5197	HIS
4	d	5220	ASN

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Mol	Chain	Res	Type
4	d	5224	GLN
4	d	5236	ASN
4	d	5239	GLN
4	d	5255	GLN
4	d	5268	HIS
4	d	5322	ASN
4	d	5332	GLN
4	d	5334	GLN
4	d	5336	HIS
5	e	5060	GLN
6	f	5041	GLN
7	h	5015	ASN
11	l	5037	ASN
12	m	5005	GLN
12	m	5028	GLN
12	m	5032	GLN
12	m	5033	GLN
13	o	5108	GLN
13	o	5150	ASN
13	o	5158	ASN
13	o	5173	ASN
13	o	5212	ASN
13	o	5257	HIS
15	u	5058	ASN
15	u	5067	GLN
15	u	5108	ASN
15	u	5111	HIS
15	u	5130	ASN
16	v	5051	GLN
16	v	5060	GLN
16	v	5104	ASN
17	x	5042	GLN
20	z	5006	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 130 ligands modelled in this entry, 6 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	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	A	1006	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	A	1007	-	58,73,73	1.71	12 (20%)	66,113,113	2.34	21 (31%)
24	PHO	A	1038	-	67,69,69	2.88	24 (35%)	85,99,99	2.88	20 (23%)
24	PHO	A	1039	-	67,69,69	2.89	23 (34%)	85,99,99	2.98	22 (25%)
25	PQ9	A	1043	-	45,45,45	4.00	16 (35%)	57,57,57	5.07	23 (40%)
26	BCR	A	1044	-	41,41,41	4.05	16 (39%)	56,56,56	6.11	30 (53%)
27	LHG	A	1063	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	B	1009	-	58,73,73	1.85	14 (24%)	66,113,113	2.22	19 (28%)
23	CLA	B	1010	-	58,73,73	1.70	12 (20%)	66,113,113	2.42	22 (33%)
23	CLA	B	1011	2	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1012	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1013	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1014	-	58,73,73	1.75	14 (24%)	66,113,113	2.33	19 (28%)
23	CLA	B	1015	-	58,73,73	1.78	13 (22%)	66,113,113	2.50	24 (36%)
23	CLA	B	1016	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	B	1018	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	B	1019	-	58,73,73	1.80	11 (18%)	66,113,113	2.62	26 (39%)
23	CLA	B	1020	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1021	-	58,73,73	1.87	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	B	1022	-	58,73,73	1.69	12 (20%)	66,113,113	2.36	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	1023	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	B	1024	-	58,73,73	1.72	13 (22%)	66,113,113	2.50	24 (36%)
26	BCR	B	1045	-	41,41,41	4.25	15 (36%)	56,56,56	6.39	28 (50%)
26	BCR	B	1047	-	41,41,41	4.21	16 (39%)	56,56,56	7.04	25 (44%)
26	BCR	B	1048	-	41,41,41	4.26	17 (41%)	56,56,56	6.25	25 (44%)
29	MGE	B	1060	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
23	CLA	C	1025	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1026	-	58,73,73	1.67	12 (20%)	66,113,113	2.44	21 (31%)
23	CLA	C	1027	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1028	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1029	-	58,73,73	1.74	12 (20%)	66,113,113	2.39	20 (30%)
23	CLA	C	1030	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	C	1031	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1032	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1033	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	C	1034	-	58,73,73	1.91	15 (25%)	66,113,113	2.50	21 (31%)
23	CLA	C	1035	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1036	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1037	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
26	BCR	C	1054	-	41,41,41	4.22	17 (41%)	56,56,56	6.76	26 (46%)
30	DGD	C	1055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	C	1056	-	67,67,67	0.85	2 (2%)	81,81,81	0.92	3 (3%)
30	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	D	1004	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	D	1005	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	D	1008	-	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
25	PQ9	D	1042	-	45,45,45	3.85	17 (37%)	57,57,57	5.13	28 (49%)
26	BCR	D	1050	-	41,41,41	4.17	16 (39%)	56,56,56	6.16	28 (50%)
29	MGE	D	1062	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
31	HEM	E	1040	6	27,50,50	2.17	5 (18%)	17,82,82	1.40	1 (5%)
23	CLA	H	1017	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
26	BCR	H	1049	-	41,41,41	4.26	16 (39%)	56,56,56	6.11	24 (42%)
30	DGD	H	1058	-	67,67,67	0.84	2 (2%)	81,81,81	0.91	3 (3%)
29	MGE	J	1059	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
26	BCR	K	1051	-	41,41,41	4.22	16 (39%)	56,56,56	6.33	29 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	K	1052	-	41,41,41	4.26	16 (39%)	56,56,56	5.46	24 (42%)
29	MGE	L	1061	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)
26	BCR	T	6046	-	41,41,41	4.28	17 (41%)	56,56,56	7.47	30 (53%)
31	HEM	V	1041	16	27,50,50	2.18	5 (18%)	17,82,82	1.40	1 (5%)
26	BCR	Z	1053	-	41,41,41	4.26	15 (36%)	56,56,56	6.42	30 (53%)
21	OEC	a	6001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	a	6003	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	a	6006	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	a	6007	-	58,73,73	1.71	11 (18%)	66,113,113	2.34	21 (31%)
24	PHO	a	6039	-	67,69,69	2.89	23 (34%)	85,99,99	2.98	22 (25%)
25	PQ9	a	6043	-	45,45,45	4.13	21 (46%)	57,57,57	5.01	22 (38%)
26	BCR	a	6044	-	41,41,41	4.05	16 (39%)	56,56,56	6.11	30 (53%)
27	LHG	a	6063	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	b	6009	-	58,73,73	1.85	14 (24%)	66,113,113	2.22	19 (28%)
23	CLA	b	6010	-	58,73,73	1.71	12 (20%)	66,113,113	2.42	22 (33%)
23	CLA	b	6011	2	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	b	6012	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	b	6013	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6014	-	58,73,73	1.75	14 (24%)	66,113,113	2.33	19 (28%)
23	CLA	b	6015	-	58,73,73	1.77	13 (22%)	66,113,113	2.51	24 (36%)
23	CLA	b	6016	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6017	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6018	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	b	6019	-	58,73,73	1.80	11 (18%)	66,113,113	2.62	25 (37%)
23	CLA	b	6020	2	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6021	-	58,73,73	1.87	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	b	6022	-	58,73,73	1.69	12 (20%)	66,113,113	2.36	23 (34%)
23	CLA	b	6023	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6024	-	58,73,73	1.72	13 (22%)	66,113,113	2.50	24 (36%)
26	BCR	b	6045	-	41,41,41	4.25	16 (39%)	56,56,56	6.39	28 (50%)
26	BCR	b	6047	-	41,41,41	4.21	16 (39%)	56,56,56	7.04	25 (44%)
26	BCR	b	6048	-	41,41,41	4.26	17 (41%)	56,56,56	6.25	25 (44%)
29	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
23	CLA	c	6025	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6026	-	58,73,73	1.67	12 (20%)	66,113,113	2.43	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	6027	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6028	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6029	-	58,73,73	1.74	12 (20%)	66,113,113	2.40	20 (30%)
23	CLA	c	6030	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6031	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6032	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6033	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6034	-	58,73,73	1.84	12 (20%)	66,113,113	2.28	17 (25%)
23	CLA	c	6035	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6036	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6037	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
26	BCR	c	6054	-	41,41,41	4.22	17 (41%)	56,56,56	6.75	26 (46%)
30	DGD	c	6055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	c	6056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	c	6057	-	67,67,67	0.85	2 (2%)	81,81,81	0.92	3 (3%)
23	CLA	d	6004	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	d	6005	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	d	6008	-	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
24	PHO	d	6038	-	67,69,69	2.89	24 (35%)	85,99,99	2.88	20 (23%)
25	PQ9	d	6042	-	45,45,45	3.87	15 (33%)	57,57,57	5.13	27 (47%)
26	BCR	d	6050	-	41,41,41	4.17	16 (39%)	56,56,56	6.16	28 (50%)
29	MGE	d	6059	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
29	MGE	d	6061	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)
29	MGE	d	6062	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
31	HEM	e	6040	6	27,50,50	2.17	5 (18%)	17,82,82	1.41	1 (5%)
26	BCR	h	6049	-	41,41,41	4.26	16 (39%)	56,56,56	6.11	24 (42%)
30	DGD	h	6058	-	67,67,67	0.84	2 (2%)	81,81,81	0.92	3 (3%)
26	BCR	k	6051	-	41,41,41	4.22	16 (39%)	56,56,56	6.33	29 (51%)
26	BCR	k	6052	-	41,41,41	4.27	16 (39%)	56,56,56	5.11	24 (42%)
26	BCR	t	1046	-	41,41,41	4.27	16 (39%)	56,56,56	6.42	27 (48%)
31	HEM	v	6041	-	27,50,50	2.18	5 (18%)	17,82,82	1.39	1 (5%)
26	BCR	z	6053	-	41,41,41	4.25	15 (36%)	56,56,56	6.42	30 (53%)

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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1006	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1007	-	4/4/20/25	1/37/135/135	0/0/9/9
24	PHO	A	1038	-	2/2/17/22	1/53/103/103	0/5/6/6
24	PHO	A	1039	-	1/1/17/22	0/53/103/103	0/5/6/6
25	PQ9	A	1043	-	-	0/41/61/61	0/1/1/1
26	BCR	A	1044	-	-	2/29/63/63	0/2/2/2
27	LHG	A	1063	-	-	0/53/53/53	0/0/0/0
23	CLA	B	1009	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1010	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1011	2	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1012	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1013	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1018	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1019	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1020	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1021	-	5/5/20/25	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	1/37/135/135	0/0/9/9
23	CLA	B	1024	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	B	1045	-	-	0/29/63/63	0/2/2/2
26	BCR	B	1047	-	-	2/29/63/63	0/2/2/2
26	BCR	B	1048	-	-	1/29/63/63	0/2/2/2
29	MGE	B	1060	-	-	1/43/63/63	0/1/1/1
23	CLA	C	1025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1026	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1027	-	6/6/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1028	-	6/6/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	1031	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	C	1032	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1033	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1034	-	7/7/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1035	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1036	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1037	-	5/5/20/25	0/37/135/135	0/0/9/9
26	BCR	C	1054	-	-	0/29/63/63	0/2/2/2
30	DGD	C	1055	-	-	0/55/95/95	0/2/2/2
30	DGD	C	1056	-	-	0/55/95/95	0/2/2/2
30	DGD	C	1057	-	-	0/55/95/95	0/2/2/2
23	CLA	D	1004	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PQ9	D	1042	-	-	0/41/61/61	0/1/1/1
26	BCR	D	1050	-	-	0/29/63/63	0/2/2/2
29	MGE	D	1062	-	-	0/43/63/63	0/1/1/1
31	HEM	E	1040	6	-	0/6/54/54	0/0/8/8
23	CLA	H	1017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	H	1049	-	-	0/29/63/63	0/2/2/2
30	DGD	H	1058	-	-	0/55/95/95	0/2/2/2
29	MGE	J	1059	-	-	0/43/63/63	0/1/1/1
26	BCR	K	1051	-	-	0/29/63/63	0/2/2/2
26	BCR	K	1052	-	-	0/29/63/63	0/2/2/2
29	MGE	L	1061	-	-	0/43/63/63	0/1/1/1
26	BCR	T	6046	-	-	0/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	0/6/54/54	0/0/8/8
26	BCR	Z	1053	-	-	1/29/63/63	0/2/2/2
21	OEC	a	6001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	a	6003	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6006	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6007	-	4/4/20/25	1/37/135/135	0/0/9/9
24	PHO	a	6039	-	1/1/17/22	0/53/103/103	0/5/6/6
25	PQ9	a	6043	-	-	0/41/61/61	0/1/1/1
26	BCR	a	6044	-	-	2/29/63/63	0/2/2/2
27	LHG	a	6063	-	-	0/53/53/53	0/0/0/0
23	CLA	b	6009	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6010	-	3/3/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6011	2	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6012	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6013	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6017	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6018	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6019	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6020	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6021	-	5/5/20/25	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	1/37/135/135	0/0/9/9
23	CLA	b	6024	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	b	6045	-	-	0/29/63/63	0/2/2/2
26	BCR	b	6047	-	-	2/29/63/63	0/2/2/2
26	BCR	b	6048	-	-	1/29/63/63	0/2/2/2
29	MGE	b	6060	-	-	1/43/63/63	0/1/1/1
23	CLA	c	6025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6026	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6027	-	6/6/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6028	-	6/6/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6031	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	c	6032	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6033	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6034	-	7/7/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6035	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6036	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6037	-	5/5/20/25	0/37/135/135	0/0/9/9
26	BCR	c	6054	-	-	0/29/63/63	0/2/2/2
30	DGD	c	6055	-	-	0/55/95/95	0/2/2/2
30	DGD	c	6056	-	-	0/55/95/95	0/2/2/2
30	DGD	c	6057	-	-	0/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	6004	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	d	6038	-	2/2/17/22	1/53/103/103	0/5/6/6
25	PQ9	d	6042	-	-	0/41/61/61	0/1/1/1
26	BCR	d	6050	-	-	0/29/63/63	0/2/2/2
29	MGE	d	6059	-	-	0/43/63/63	0/1/1/1
29	MGE	d	6061	-	-	0/43/63/63	0/1/1/1
29	MGE	d	6062	-	-	0/43/63/63	0/1/1/1
31	HEM	e	6040	6	-	0/6/54/54	0/0/8/8
26	BCR	h	6049	-	-	0/29/63/63	0/2/2/2
30	DGD	h	6058	-	-	0/55/95/95	0/2/2/2
26	BCR	k	6051	-	-	0/29/63/63	0/2/2/2
26	BCR	k	6052	-	-	0/29/63/63	0/2/2/2
26	BCR	t	1046	-	-	0/29/63/63	0/2/2/2
31	HEM	v	6041	-	-	0/6/54/54	0/0/8/8
26	BCR	z	6053	-	-	1/29/63/63	0/2/2/2

All (1521) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6047	BCR	C8-C9	-9.33	1.25	1.45
26	B	1047	BCR	C8-C9	-9.32	1.25	1.45
26	B	1048	BCR	C8-C9	-9.29	1.25	1.45
26	b	6048	BCR	C8-C9	-9.29	1.25	1.45
26	k	6051	BCR	C12-C13	-9.26	1.25	1.45
26	b	6048	BCR	C12-C13	-9.26	1.25	1.45
26	B	1048	BCR	C19-C18	-9.24	1.25	1.45
26	b	6048	BCR	C19-C18	-9.24	1.25	1.45
26	B	1048	BCR	C12-C13	-9.24	1.25	1.45
26	K	1051	BCR	C12-C13	-9.23	1.25	1.45
26	k	6052	BCR	C8-C9	-9.22	1.25	1.45
26	c	6054	BCR	C12-C13	-9.21	1.25	1.45
26	b	6045	BCR	C19-C18	-9.21	1.25	1.45
26	C	1054	BCR	C12-C13	-9.21	1.25	1.45
26	k	6052	BCR	C19-C18	-9.21	1.25	1.45
26	T	6046	BCR	C12-C13	-9.20	1.25	1.45
26	t	1046	BCR	C8-C9	-9.20	1.25	1.45
26	b	6045	BCR	C8-C9	-9.20	1.25	1.45
26	z	6053	BCR	C8-C9	-9.20	1.25	1.45
26	T	6046	BCR	C19-C18	-9.20	1.25	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	6049	BCR	C12-C13	-9.20	1.25	1.45
26	k	6052	BCR	C12-C13	-9.20	1.25	1.45
26	Z	1053	BCR	C8-C9	-9.20	1.25	1.45
26	K	1052	BCR	C19-C18	-9.20	1.25	1.45
26	H	1049	BCR	C19-C18	-9.20	1.25	1.45
26	B	1045	BCR	C19-C18	-9.20	1.25	1.45
26	b	6045	BCR	C12-C13	-9.20	1.25	1.45
26	H	1049	BCR	C12-C13	-9.20	1.25	1.45
26	K	1052	BCR	C8-C9	-9.19	1.25	1.45
26	h	6049	BCR	C19-C18	-9.19	1.25	1.45
26	t	1046	BCR	C19-C18	-9.19	1.25	1.45
26	t	1046	BCR	C12-C13	-9.19	1.26	1.45
26	B	1045	BCR	C12-C13	-9.18	1.26	1.45
26	B	1045	BCR	C8-C9	-9.18	1.26	1.45
26	T	6046	BCR	C8-C9	-9.17	1.26	1.45
26	K	1052	BCR	C12-C13	-9.17	1.26	1.45
26	Z	1053	BCR	C19-C18	-9.17	1.26	1.45
26	h	6049	BCR	C8-C9	-9.17	1.26	1.45
26	H	1049	BCR	C8-C9	-9.17	1.26	1.45
26	z	6053	BCR	C19-C18	-9.17	1.26	1.45
26	b	6047	BCR	C12-C13	-9.16	1.26	1.45
26	B	1047	BCR	C12-C13	-9.16	1.26	1.45
26	Z	1053	BCR	C12-C13	-9.15	1.26	1.45
26	z	6053	BCR	C12-C13	-9.15	1.26	1.45
26	C	1054	BCR	C8-C9	-9.14	1.26	1.45
26	c	6054	BCR	C8-C9	-9.13	1.26	1.45
26	k	6051	BCR	C19-C18	-9.12	1.26	1.45
26	K	1051	BCR	C19-C18	-9.12	1.26	1.45
26	D	1050	BCR	C12-C13	-9.09	1.26	1.45
26	d	6050	BCR	C12-C13	-9.05	1.26	1.45
26	c	6054	BCR	C19-C18	-9.03	1.26	1.45
26	K	1051	BCR	C8-C9	-9.03	1.26	1.45
26	C	1054	BCR	C19-C18	-9.02	1.26	1.45
26	k	6051	BCR	C8-C9	-9.02	1.26	1.45
26	B	1047	BCR	C19-C18	-9.00	1.26	1.45
26	b	6047	BCR	C19-C18	-9.00	1.26	1.45
26	d	6050	BCR	C19-C18	-8.99	1.26	1.45
26	D	1050	BCR	C19-C18	-8.98	1.26	1.45
26	D	1050	BCR	C8-C9	-8.90	1.26	1.45
26	d	6050	BCR	C8-C9	-8.89	1.26	1.45
26	a	6044	BCR	C12-C13	-8.87	1.26	1.45
26	A	1044	BCR	C19-C18	-8.87	1.26	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	6044	BCR	C19-C18	-8.87	1.26	1.45
26	a	6044	BCR	C8-C9	-8.86	1.26	1.45
26	A	1044	BCR	C8-C9	-8.86	1.26	1.45
26	A	1044	BCR	C12-C13	-8.86	1.26	1.45
26	k	6052	BCR	C20-C21	-8.27	1.18	1.43
26	H	1049	BCR	C20-C21	-8.26	1.18	1.43
26	H	1049	BCR	C16-C17	-8.26	1.18	1.43
26	B	1045	BCR	C16-C17	-8.25	1.18	1.43
26	h	6049	BCR	C20-C21	-8.25	1.18	1.43
26	T	6046	BCR	C20-C21	-8.25	1.18	1.43
26	h	6049	BCR	C16-C17	-8.25	1.18	1.43
26	Z	1053	BCR	C16-C17	-8.25	1.18	1.43
26	b	6045	BCR	C16-C17	-8.25	1.18	1.43
26	t	1046	BCR	C16-C17	-8.24	1.18	1.43
26	K	1052	BCR	C20-C21	-8.24	1.18	1.43
26	B	1045	BCR	C20-C21	-8.24	1.18	1.43
26	T	6046	BCR	C16-C17	-8.24	1.18	1.43
26	b	6045	BCR	C20-C21	-8.23	1.18	1.43
26	z	6053	BCR	C20-C21	-8.23	1.18	1.43
26	Z	1053	BCR	C20-C21	-8.23	1.18	1.43
26	k	6052	BCR	C16-C17	-8.23	1.18	1.43
26	z	6053	BCR	C16-C17	-8.23	1.18	1.43
26	k	6051	BCR	C20-C21	-8.22	1.18	1.43
26	K	1052	BCR	C16-C17	-8.21	1.18	1.43
26	t	1046	BCR	C20-C21	-8.21	1.18	1.43
26	K	1051	BCR	C20-C21	-8.20	1.18	1.43
26	b	6048	BCR	C16-C17	-8.19	1.18	1.43
26	B	1048	BCR	C16-C17	-8.18	1.18	1.43
26	d	6050	BCR	C16-C17	-8.18	1.18	1.43
26	D	1050	BCR	C16-C17	-8.15	1.18	1.43
26	K	1051	BCR	C16-C17	-8.12	1.18	1.43
26	k	6051	BCR	C16-C17	-8.12	1.18	1.43
26	C	1054	BCR	C16-C17	-8.12	1.18	1.43
26	c	6054	BCR	C16-C17	-8.12	1.18	1.43
26	b	6047	BCR	C16-C17	-8.12	1.18	1.43
26	B	1047	BCR	C16-C17	-8.08	1.18	1.43
26	B	1048	BCR	C20-C21	-8.08	1.18	1.43
26	b	6048	BCR	C20-C21	-8.08	1.18	1.43
26	b	6047	BCR	C20-C21	-8.06	1.19	1.43
26	B	1047	BCR	C20-C21	-8.03	1.19	1.43
26	D	1050	BCR	C20-C21	-8.01	1.19	1.43
26	d	6050	BCR	C20-C21	-8.00	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	6054	BCR	C20-C21	-7.98	1.19	1.43
26	C	1054	BCR	C20-C21	-7.98	1.19	1.43
26	a	6044	BCR	C20-C21	-7.93	1.19	1.43
26	a	6044	BCR	C16-C17	-7.92	1.19	1.43
26	A	1044	BCR	C20-C21	-7.92	1.19	1.43
26	A	1044	BCR	C16-C17	-7.92	1.19	1.43
26	B	1048	BCR	C17-C18	-7.49	1.25	1.35
26	t	1046	BCR	C21-C22	-7.48	1.25	1.35
26	b	6048	BCR	C17-C18	-7.46	1.25	1.35
26	Z	1053	BCR	C17-C18	-7.45	1.25	1.35
26	K	1052	BCR	C17-C18	-7.45	1.25	1.35
26	b	6045	BCR	C21-C22	-7.44	1.25	1.35
26	z	6053	BCR	C17-C18	-7.43	1.25	1.35
26	B	1045	BCR	C21-C22	-7.42	1.25	1.35
26	T	6046	BCR	C17-C18	-7.41	1.26	1.35
26	h	6049	BCR	C21-C22	-7.41	1.26	1.35
26	k	6052	BCR	C17-C18	-7.40	1.26	1.35
26	Z	1053	BCR	C21-C22	-7.40	1.26	1.35
26	T	6046	BCR	C21-C22	-7.40	1.26	1.35
26	t	1046	BCR	C17-C18	-7.39	1.26	1.35
26	K	1052	BCR	C21-C22	-7.39	1.26	1.35
26	B	1045	BCR	C17-C18	-7.39	1.26	1.35
26	h	6049	BCR	C17-C18	-7.38	1.26	1.35
26	H	1049	BCR	C21-C22	-7.38	1.26	1.35
26	b	6045	BCR	C17-C18	-7.38	1.26	1.35
26	z	6053	BCR	C21-C22	-7.37	1.26	1.35
26	k	6052	BCR	C21-C22	-7.36	1.26	1.35
26	H	1049	BCR	C17-C18	-7.36	1.26	1.35
26	K	1051	BCR	C21-C22	-7.35	1.26	1.35
26	k	6051	BCR	C21-C22	-7.35	1.26	1.35
26	B	1048	BCR	C21-C22	-7.28	1.26	1.35
26	D	1050	BCR	C17-C18	-7.27	1.26	1.35
26	b	6048	BCR	C21-C22	-7.27	1.26	1.35
26	C	1054	BCR	C17-C18	-7.25	1.26	1.35
26	B	1047	BCR	C21-C22	-7.24	1.26	1.35
26	d	6050	BCR	C17-C18	-7.23	1.26	1.35
26	c	6054	BCR	C17-C18	-7.21	1.26	1.35
26	K	1051	BCR	C17-C18	-7.20	1.26	1.35
26	k	6051	BCR	C17-C18	-7.19	1.26	1.35
26	B	1047	BCR	C17-C18	-7.18	1.26	1.35
26	b	6047	BCR	C21-C22	-7.18	1.26	1.35
26	b	6047	BCR	C17-C18	-7.13	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	6050	BCR	C21-C22	-7.07	1.26	1.35
26	D	1050	BCR	C21-C22	-7.06	1.26	1.35
26	C	1054	BCR	C21-C22	-7.03	1.26	1.35
26	c	6054	BCR	C21-C22	-7.02	1.26	1.35
26	A	1044	BCR	C21-C22	-6.83	1.26	1.35
26	a	6044	BCR	C21-C22	-6.81	1.26	1.35
26	A	1044	BCR	C17-C18	-6.81	1.26	1.35
26	a	6044	BCR	C17-C18	-6.76	1.26	1.35
26	k	6052	BCR	C16-C15	-6.73	1.18	1.35
26	t	1046	BCR	C16-C15	-6.72	1.18	1.35
26	c	6054	BCR	C16-C15	-6.71	1.18	1.35
26	z	6053	BCR	C16-C15	-6.70	1.18	1.35
26	K	1052	BCR	C16-C15	-6.70	1.18	1.35
26	C	1054	BCR	C16-C15	-6.70	1.18	1.35
26	Z	1053	BCR	C16-C15	-6.69	1.18	1.35
26	T	6046	BCR	C16-C15	-6.69	1.18	1.35
26	b	6045	BCR	C16-C15	-6.68	1.18	1.35
26	B	1045	BCR	C16-C15	-6.68	1.18	1.35
26	H	1049	BCR	C16-C15	-6.68	1.18	1.35
26	h	6049	BCR	C16-C15	-6.67	1.18	1.35
26	k	6051	BCR	C16-C15	-6.61	1.18	1.35
26	K	1051	BCR	C16-C15	-6.59	1.18	1.35
26	D	1050	BCR	C16-C15	-6.58	1.18	1.35
26	d	6050	BCR	C16-C15	-6.56	1.18	1.35
26	B	1048	BCR	C16-C15	-6.53	1.18	1.35
26	b	6048	BCR	C16-C15	-6.52	1.18	1.35
26	B	1047	BCR	C16-C15	-6.50	1.19	1.35
26	b	6047	BCR	C16-C15	-6.47	1.19	1.35
25	A	1043	PQ9	C24-C23	-6.39	1.34	1.50
26	h	6049	BCR	C20-C19	-6.34	1.18	1.34
26	T	6046	BCR	C20-C19	-6.33	1.18	1.34
26	H	1049	BCR	C20-C19	-6.33	1.18	1.34
26	H	1049	BCR	C11-C12	-6.33	1.18	1.34
26	z	6053	BCR	C11-C12	-6.33	1.18	1.34
26	T	6046	BCR	C11-C12	-6.33	1.18	1.34
26	k	6052	BCR	C11-C12	-6.33	1.18	1.34
26	t	1046	BCR	C20-C19	-6.32	1.18	1.34
26	a	6044	BCR	C16-C15	-6.32	1.19	1.35
26	Z	1053	BCR	C11-C12	-6.32	1.18	1.34
26	t	1046	BCR	C11-C12	-6.32	1.18	1.34
26	A	1044	BCR	C16-C15	-6.32	1.19	1.35
26	h	6049	BCR	C11-C12	-6.31	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6045	BCR	C11-C12	-6.31	1.18	1.34
26	B	1045	BCR	C20-C19	-6.31	1.18	1.34
26	z	6053	BCR	C20-C19	-6.30	1.18	1.34
26	K	1052	BCR	C11-C12	-6.30	1.18	1.34
26	b	6045	BCR	C20-C19	-6.30	1.18	1.34
26	B	1045	BCR	C11-C12	-6.30	1.18	1.34
26	Z	1053	BCR	C20-C19	-6.30	1.18	1.34
26	K	1052	BCR	C20-C19	-6.29	1.18	1.34
26	k	6052	BCR	C20-C19	-6.28	1.18	1.34
26	k	6051	BCR	C11-C12	-6.28	1.18	1.34
26	K	1051	BCR	C11-C12	-6.27	1.18	1.34
26	b	6048	BCR	C20-C19	-6.27	1.18	1.34
26	B	1048	BCR	C11-C12	-6.24	1.18	1.34
26	B	1048	BCR	C20-C19	-6.23	1.18	1.34
26	d	6050	BCR	C11-C12	-6.22	1.18	1.34
26	b	6048	BCR	C11-C12	-6.22	1.18	1.34
26	D	1050	BCR	C11-C12	-6.20	1.18	1.34
26	b	6047	BCR	C11-C12	-6.20	1.18	1.34
26	B	1047	BCR	C11-C12	-6.19	1.18	1.34
26	C	1054	BCR	C11-C12	-6.13	1.18	1.34
26	K	1051	BCR	C20-C19	-6.12	1.18	1.34
26	c	6054	BCR	C11-C12	-6.10	1.19	1.34
26	k	6051	BCR	C20-C19	-6.08	1.19	1.34
25	D	1042	PQ9	C9-C10	-6.08	1.37	1.50
26	c	6054	BCR	C20-C19	-6.08	1.19	1.34
26	B	1047	BCR	C20-C19	-6.06	1.19	1.34
26	C	1054	BCR	C20-C19	-6.06	1.19	1.34
26	b	6047	BCR	C20-C19	-6.05	1.19	1.34
26	D	1050	BCR	C20-C19	-6.03	1.19	1.34
26	d	6050	BCR	C20-C19	-6.02	1.19	1.34
25	a	6043	PQ9	C24-C23	-5.99	1.35	1.50
26	A	1044	BCR	C20-C19	-5.97	1.19	1.34
26	a	6044	BCR	C20-C19	-5.96	1.19	1.34
25	d	6042	PQ9	C9-C10	-5.95	1.38	1.50
26	a	6044	BCR	C11-C12	-5.90	1.19	1.34
25	D	1042	PQ9	C24-C23	-5.90	1.35	1.50
26	A	1044	BCR	C11-C12	-5.90	1.19	1.34
26	c	6054	BCR	C15-C14	-5.84	1.25	1.43
26	C	1054	BCR	C15-C14	-5.84	1.25	1.43
26	K	1051	BCR	C15-C14	-5.80	1.25	1.43
26	K	1052	BCR	C15-C14	-5.79	1.25	1.43
26	z	6053	BCR	C15-C14	-5.79	1.25	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	1053	BCR	C15-C14	-5.79	1.25	1.43
26	Z	1053	BCR	C11-C10	-5.79	1.25	1.43
26	k	6051	BCR	C15-C14	-5.79	1.25	1.43
26	k	6052	BCR	C15-C14	-5.79	1.25	1.43
26	b	6045	BCR	C15-C14	-5.79	1.25	1.43
26	K	1052	BCR	C11-C10	-5.78	1.25	1.43
26	h	6049	BCR	C15-C14	-5.78	1.26	1.43
26	B	1045	BCR	C15-C14	-5.78	1.26	1.43
26	t	1046	BCR	C15-C14	-5.78	1.26	1.43
26	H	1049	BCR	C15-C14	-5.77	1.26	1.43
26	b	6048	BCR	C11-C10	-5.77	1.26	1.43
26	z	6053	BCR	C11-C10	-5.77	1.26	1.43
26	H	1049	BCR	C11-C10	-5.77	1.26	1.43
26	t	1046	BCR	C11-C10	-5.77	1.26	1.43
26	T	6046	BCR	C15-C14	-5.76	1.26	1.43
26	B	1045	BCR	C11-C10	-5.76	1.26	1.43
26	k	6052	BCR	C11-C10	-5.76	1.26	1.43
26	B	1048	BCR	C11-C10	-5.76	1.26	1.43
26	h	6049	BCR	C11-C10	-5.76	1.26	1.43
26	T	6046	BCR	C11-C10	-5.75	1.26	1.43
26	k	6051	BCR	C11-C10	-5.74	1.26	1.43
26	K	1051	BCR	C11-C10	-5.74	1.26	1.43
26	b	6045	BCR	C11-C10	-5.74	1.26	1.43
26	b	6047	BCR	C11-C10	-5.73	1.26	1.43
25	a	6043	PQ9	C9-C10	-5.72	1.38	1.50
26	B	1047	BCR	C11-C10	-5.72	1.26	1.43
26	d	6050	BCR	C15-C14	-5.72	1.26	1.43
26	c	6054	BCR	C11-C10	-5.72	1.26	1.43
26	D	1050	BCR	C15-C14	-5.71	1.26	1.43
25	d	6042	PQ9	C24-C23	-5.71	1.36	1.50
26	C	1054	BCR	C11-C10	-5.69	1.26	1.43
26	D	1050	BCR	C11-C10	-5.67	1.26	1.43
26	b	6048	BCR	C15-C14	-5.67	1.26	1.43
26	d	6050	BCR	C11-C10	-5.66	1.26	1.43
25	A	1043	PQ9	C9-C10	-5.66	1.38	1.50
26	b	6047	BCR	C15-C14	-5.65	1.26	1.43
26	B	1047	BCR	C15-C14	-5.65	1.26	1.43
26	B	1048	BCR	C15-C14	-5.65	1.26	1.43
26	A	1044	BCR	C15-C14	-5.52	1.26	1.43
26	a	6044	BCR	C15-C14	-5.51	1.26	1.43
26	a	6044	BCR	C11-C10	-5.44	1.27	1.43
26	A	1044	BCR	C11-C10	-5.43	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1043	PQ9	C29-C28	-5.36	1.37	1.50
26	k	6052	BCR	C23-C22	-5.32	1.34	1.45
26	c	6054	BCR	C23-C22	-5.32	1.34	1.45
26	B	1048	BCR	C23-C22	-5.31	1.34	1.45
26	C	1054	BCR	C23-C22	-5.31	1.34	1.45
26	b	6048	BCR	C23-C22	-5.29	1.34	1.45
26	Z	1053	BCR	C23-C22	-5.28	1.34	1.45
26	z	6053	BCR	C23-C22	-5.25	1.34	1.45
26	K	1052	BCR	C23-C22	-5.24	1.34	1.45
26	H	1049	BCR	C23-C22	-5.24	1.34	1.45
26	b	6047	BCR	C23-C22	-5.21	1.34	1.45
26	B	1047	BCR	C23-C22	-5.20	1.34	1.45
26	h	6049	BCR	C23-C22	-5.20	1.34	1.45
26	k	6051	BCR	C23-C22	-5.18	1.34	1.45
26	K	1051	BCR	C23-C22	-5.18	1.34	1.45
26	d	6050	BCR	C23-C22	-5.13	1.34	1.45
26	t	1046	BCR	C23-C22	-5.09	1.34	1.45
26	D	1050	BCR	C23-C22	-5.09	1.34	1.45
26	T	6046	BCR	C23-C22	-5.06	1.34	1.45
25	d	6042	PQ9	C34-C33	-4.98	1.38	1.50
26	B	1045	BCR	C23-C22	-4.98	1.35	1.45
26	b	6045	BCR	C23-C22	-4.98	1.35	1.45
26	a	6044	BCR	C23-C22	-4.96	1.35	1.45
26	A	1044	BCR	C23-C22	-4.94	1.35	1.45
25	D	1042	PQ9	C34-C33	-4.87	1.38	1.50
25	d	6042	PQ9	C21-C22	-4.73	1.34	1.50
31	v	6041	HEM	C3B-C2B	-4.70	1.33	1.40
31	e	6040	HEM	C3B-C2B	-4.68	1.33	1.40
31	V	1041	HEM	C3C-C2C	-4.67	1.33	1.40
31	V	1041	HEM	C3B-C2B	-4.66	1.33	1.40
31	E	1040	HEM	C3B-C2B	-4.66	1.33	1.40
31	v	6041	HEM	C3C-C2C	-4.63	1.34	1.40
31	E	1040	HEM	C3C-C2C	-4.61	1.34	1.40
25	D	1042	PQ9	C21-C22	-4.58	1.35	1.50
31	e	6040	HEM	C3C-C2C	-4.57	1.34	1.40
25	A	1043	PQ9	C35-C36	-4.48	1.38	1.53
25	a	6043	PQ9	C35-C36	-4.32	1.39	1.53
25	d	6042	PQ9	C35-C36	-4.13	1.39	1.53
25	a	6043	PQ9	C21-C22	-3.98	1.37	1.50
25	A	1043	PQ9	C34-C33	-3.90	1.40	1.50
25	a	6043	PQ9	C34-C33	-3.90	1.40	1.50
25	D	1042	PQ9	C35-C36	-3.84	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1043	PQ9	C21-C22	-3.67	1.38	1.50
23	b	6015	CLA	C4A-NA	-3.61	1.32	1.38
23	B	1015	CLA	C4A-NA	-3.60	1.32	1.38
23	a	6007	CLA	C4A-NA	-3.38	1.33	1.38
23	A	1007	CLA	C4A-NA	-3.37	1.33	1.38
23	B	1014	CLA	C4A-NA	-3.36	1.33	1.38
23	b	6014	CLA	C4A-NA	-3.34	1.33	1.38
24	d	6038	PHO	O2D-CGD	-3.33	1.24	1.33
23	C	1029	CLA	C4A-NA	-3.33	1.33	1.38
24	A	1038	PHO	O2D-CGD	-3.32	1.24	1.33
23	b	6024	CLA	C4A-NA	-3.32	1.33	1.38
23	B	1024	CLA	C4A-NA	-3.32	1.33	1.38
23	c	6029	CLA	C4A-NA	-3.30	1.33	1.38
23	b	6010	CLA	C4A-NA	-3.16	1.33	1.38
23	B	1010	CLA	C4A-NA	-3.16	1.33	1.38
24	d	6038	PHO	C1B-C2B	-3.12	1.39	1.45
24	A	1038	PHO	C1B-C2B	-3.11	1.39	1.45
24	a	6039	PHO	O2D-CGD	-3.08	1.25	1.33
24	A	1039	PHO	O2D-CGD	-3.07	1.25	1.33
26	b	6048	BCR	C24-C25	-3.04	1.34	1.45
26	B	1048	BCR	C24-C25	-3.02	1.34	1.45
26	h	6049	BCR	C24-C25	-3.01	1.34	1.45
26	K	1052	BCR	C24-C25	-3.01	1.34	1.45
26	Z	1053	BCR	C24-C25	-3.01	1.34	1.45
26	c	6054	BCR	C24-C25	-3.01	1.34	1.45
26	H	1049	BCR	C24-C25	-3.00	1.34	1.45
26	z	6053	BCR	C24-C25	-3.00	1.34	1.45
26	k	6052	BCR	C24-C25	-2.99	1.34	1.45
26	C	1054	BCR	C24-C25	-2.99	1.34	1.45
26	B	1047	BCR	C24-C25	-2.97	1.34	1.45
26	b	6047	BCR	C24-C25	-2.97	1.34	1.45
23	C	1034	CLA	O2D-CED	-2.93	1.38	1.45
24	d	6038	PHO	C3D-C4D	-2.92	1.34	1.43
24	A	1038	PHO	C3D-C4D	-2.92	1.34	1.43
23	b	6022	CLA	C4A-NA	-2.87	1.33	1.38
23	B	1022	CLA	C4A-NA	-2.87	1.33	1.38
26	b	6047	BCR	C1-C6	-2.84	1.49	1.53
26	B	1047	BCR	C1-C6	-2.84	1.49	1.53
24	a	6039	PHO	C1B-C2B	-2.84	1.39	1.45
24	A	1039	PHO	C1B-C2B	-2.84	1.39	1.45
26	T	6046	BCR	C24-C25	-2.82	1.35	1.45
26	t	1046	BCR	C24-C25	-2.81	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1039	PHO	C3D-C4D	-2.80	1.34	1.43
24	a	6039	PHO	C3D-C4D	-2.80	1.34	1.43
24	d	6038	PHO	O2A-CGA	-2.78	1.25	1.33
26	K	1051	BCR	C24-C25	-2.76	1.35	1.45
24	A	1038	PHO	O2A-CGA	-2.76	1.25	1.33
26	k	6051	BCR	C24-C25	-2.75	1.35	1.45
26	B	1045	BCR	C24-C25	-2.71	1.35	1.45
26	d	6050	BCR	C24-C25	-2.71	1.35	1.45
26	D	1050	BCR	C24-C25	-2.71	1.35	1.45
26	b	6045	BCR	C24-C25	-2.70	1.35	1.45
23	C	1026	CLA	C4A-NA	-2.69	1.34	1.38
23	c	6026	CLA	C4A-NA	-2.68	1.34	1.38
24	A	1039	PHO	O2A-CGA	-2.68	1.25	1.33
24	a	6039	PHO	O2A-CGA	-2.68	1.25	1.33
23	b	6019	CLA	C4A-NA	-2.67	1.34	1.38
26	C	1054	BCR	C30-C25	-2.66	1.50	1.53
23	B	1019	CLA	C4A-NA	-2.66	1.34	1.38
26	c	6054	BCR	C30-C25	-2.64	1.50	1.53
26	T	6046	BCR	C30-C25	-2.60	1.50	1.53
26	d	6050	BCR	C30-C25	-2.51	1.50	1.53
26	A	1044	BCR	C24-C25	-2.48	1.36	1.45
26	a	6044	BCR	C24-C25	-2.48	1.36	1.45
23	c	6034	CLA	C4A-NA	-2.47	1.34	1.38
26	D	1050	BCR	C30-C25	-2.45	1.50	1.53
23	B	1014	CLA	CHB-C4A	-2.43	1.30	1.33
26	b	6048	BCR	C1-C6	-2.43	1.50	1.53
26	t	1046	BCR	C30-C25	-2.41	1.50	1.53
26	T	6046	BCR	C1-C6	-2.40	1.50	1.53
23	b	6014	CLA	CHB-C4A	-2.40	1.30	1.33
26	B	1048	BCR	C1-C6	-2.39	1.50	1.53
25	a	6043	PQ9	C29-C28	-2.37	1.44	1.50
26	k	6051	BCR	C30-C25	-2.36	1.50	1.53
26	K	1051	BCR	C30-C25	-2.34	1.50	1.53
26	b	6048	BCR	C8-C7	-2.33	1.25	1.33
26	B	1048	BCR	C8-C7	-2.33	1.25	1.33
23	b	6009	CLA	C4A-NA	-2.33	1.34	1.38
26	b	6045	BCR	C8-C7	-2.32	1.25	1.33
26	Z	1053	BCR	C8-C7	-2.32	1.25	1.33
26	b	6047	BCR	C8-C7	-2.32	1.25	1.33
26	B	1047	BCR	C8-C7	-2.32	1.25	1.33
23	B	1009	CLA	C4A-NA	-2.32	1.34	1.38
26	B	1045	BCR	C8-C7	-2.32	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	1049	BCR	C8-C7	-2.32	1.25	1.33
26	z	6053	BCR	C8-C7	-2.31	1.25	1.33
26	K	1052	BCR	C8-C7	-2.31	1.25	1.33
24	A	1038	PHO	C3B-C4B	-2.31	1.38	1.43
26	t	1046	BCR	C8-C7	-2.30	1.26	1.33
26	h	6049	BCR	C8-C7	-2.30	1.26	1.33
24	d	6038	PHO	C3B-C4B	-2.30	1.38	1.43
26	a	6044	BCR	C30-C25	-2.29	1.50	1.53
26	k	6052	BCR	C8-C7	-2.29	1.26	1.33
24	A	1038	PHO	C4D-CHA	-2.29	1.37	1.43
26	T	6046	BCR	C8-C7	-2.28	1.26	1.33
25	A	1043	PQ9	C36-C37	-2.27	1.42	1.50
24	d	6038	PHO	C4D-CHA	-2.26	1.37	1.43
26	C	1054	BCR	C8-C7	-2.25	1.26	1.33
23	b	6015	CLA	C2A-C1A	-2.24	1.47	1.52
24	A	1039	PHO	C1C-NC	-2.24	1.33	1.38
24	a	6039	PHO	C1C-NC	-2.24	1.33	1.38
26	A	1044	BCR	C30-C25	-2.23	1.50	1.53
23	B	1015	CLA	C2A-C1A	-2.23	1.47	1.52
26	c	6054	BCR	C8-C7	-2.23	1.26	1.33
24	a	6039	PHO	C3B-C4B	-2.22	1.38	1.43
25	d	6042	PQ9	C29-C28	-2.21	1.45	1.50
24	d	6038	PHO	C1D-C2D	-2.21	1.41	1.45
26	B	1048	BCR	C30-C25	-2.21	1.50	1.53
26	C	1054	BCR	C1-C6	-2.20	1.50	1.53
26	k	6051	BCR	C8-C7	-2.20	1.26	1.33
24	A	1038	PHO	C1D-C2D	-2.19	1.41	1.45
24	A	1039	PHO	C3B-C4B	-2.18	1.38	1.43
26	K	1051	BCR	C8-C7	-2.18	1.26	1.33
23	a	6003	CLA	C4A-NA	-2.17	1.34	1.38
23	d	6004	CLA	C4A-NA	-2.17	1.34	1.38
26	b	6048	BCR	C30-C25	-2.16	1.50	1.53
23	c	6031	CLA	C4A-NA	-2.15	1.34	1.38
26	c	6054	BCR	C1-C6	-2.15	1.50	1.53
23	c	6027	CLA	C4A-NA	-2.14	1.34	1.38
24	A	1039	PHO	C1D-C2D	-2.14	1.41	1.45
23	d	6005	CLA	C4A-NA	-2.14	1.34	1.38
23	D	1005	CLA	C4A-NA	-2.14	1.34	1.38
23	C	1027	CLA	C4A-NA	-2.13	1.34	1.38
23	b	6021	CLA	C4A-NA	-2.13	1.34	1.38
23	B	1021	CLA	C4A-NA	-2.13	1.34	1.38
23	c	6033	CLA	C4A-NA	-2.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6025	CLA	C4A-NA	-2.13	1.34	1.38
23	C	1031	CLA	C4A-NA	-2.12	1.34	1.38
23	A	1003	CLA	C4A-NA	-2.12	1.34	1.38
23	C	1033	CLA	C4A-NA	-2.12	1.34	1.38
23	B	1023	CLA	C4A-NA	-2.12	1.34	1.38
23	D	1004	CLA	C4A-NA	-2.12	1.34	1.38
23	C	1025	CLA	C4A-NA	-2.12	1.34	1.38
23	B	1018	CLA	C4A-NA	-2.12	1.34	1.38
23	b	6011	CLA	C4A-NA	-2.12	1.34	1.38
24	a	6039	PHO	C1D-C2D	-2.11	1.41	1.45
23	A	1006	CLA	C4A-NA	-2.11	1.35	1.38
23	B	1012	CLA	C4A-NA	-2.11	1.35	1.38
23	b	6017	CLA	C4A-NA	-2.11	1.35	1.38
23	B	1016	CLA	C4A-NA	-2.11	1.35	1.38
23	B	1011	CLA	C4A-NA	-2.11	1.35	1.38
23	b	6020	CLA	C4A-NA	-2.10	1.35	1.38
23	C	1032	CLA	C4A-NA	-2.10	1.35	1.38
23	C	1028	CLA	C4A-NA	-2.10	1.35	1.38
23	C	1036	CLA	C4A-NA	-2.10	1.35	1.38
23	B	1013	CLA	C4A-NA	-2.10	1.35	1.38
23	b	6012	CLA	C4A-NA	-2.10	1.35	1.38
23	B	1020	CLA	C4A-NA	-2.09	1.35	1.38
23	b	6014	CLA	CBD-CGD	-2.09	1.45	1.52
23	C	1037	CLA	C4A-NA	-2.09	1.35	1.38
24	d	6038	PHO	C1C-NC	-2.09	1.34	1.38
23	b	6023	CLA	C4A-NA	-2.09	1.35	1.38
23	H	1017	CLA	C4A-NA	-2.09	1.35	1.38
23	b	6016	CLA	C4A-NA	-2.09	1.35	1.38
23	B	1014	CLA	CBD-CGD	-2.08	1.46	1.52
23	C	1030	CLA	C4A-NA	-2.08	1.35	1.38
23	c	6032	CLA	C4A-NA	-2.08	1.35	1.38
23	b	6018	CLA	C4A-NA	-2.08	1.35	1.38
23	c	6037	CLA	C4A-NA	-2.08	1.35	1.38
25	a	6043	PQ9	C36-C37	-2.08	1.43	1.50
26	A	1044	BCR	C8-C7	-2.08	1.26	1.33
23	c	6028	CLA	C4A-NA	-2.07	1.35	1.38
23	D	1008	CLA	C4A-NA	-2.07	1.35	1.38
23	b	6013	CLA	C4A-NA	-2.07	1.35	1.38
26	d	6050	BCR	C8-C7	-2.07	1.26	1.33
23	c	6030	CLA	C4A-NA	-2.07	1.35	1.38
26	D	1050	BCR	C8-C7	-2.06	1.26	1.33
23	C	1034	CLA	C4A-NA	-2.06	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6036	CLA	C4A-NA	-2.06	1.35	1.38
24	A	1038	PHO	C1C-NC	-2.06	1.34	1.38
26	a	6044	BCR	C8-C7	-2.06	1.26	1.33
24	A	1039	PHO	C4D-CHA	-2.06	1.38	1.43
23	a	6006	CLA	C4A-NA	-2.05	1.35	1.38
23	C	1035	CLA	C4A-NA	-2.05	1.35	1.38
24	a	6039	PHO	C4D-CHA	-2.05	1.38	1.43
25	D	1042	PQ9	C15-C13	-2.04	1.46	1.51
23	d	6008	CLA	C4A-NA	-2.04	1.35	1.38
26	K	1052	BCR	C30-C25	-2.03	1.51	1.53
23	c	6035	CLA	C4A-NA	-2.02	1.35	1.38
24	A	1038	PHO	C1A-NA	-2.02	1.33	1.37
26	H	1049	BCR	C30-C25	-2.02	1.51	1.53
26	k	6052	BCR	C30-C25	-2.02	1.51	1.53
24	d	6038	PHO	C1A-NA	-2.02	1.33	1.37
26	b	6045	BCR	C1-C6	-2.01	1.51	1.53
26	h	6049	BCR	C1-C6	-2.00	1.51	1.53
23	A	1007	CLA	CHD-C4C	2.02	1.46	1.41
23	b	6024	CLA	C4C-C3C	2.04	1.48	1.45
25	a	6043	PQ9	C5-C4	2.05	1.52	1.48
23	b	6010	CLA	C4B-CHC	2.07	1.45	1.40
23	B	1024	CLA	C4C-C3C	2.07	1.48	1.45
23	B	1010	CLA	C4B-CHC	2.07	1.45	1.40
23	B	1022	CLA	CHD-C4C	2.08	1.47	1.41
23	c	6026	CLA	C4B-CHC	2.08	1.45	1.40
23	a	6007	CLA	C4B-CHC	2.08	1.45	1.40
23	C	1026	CLA	C4B-CHC	2.10	1.45	1.40
23	b	6015	CLA	C1B-CHB	2.10	1.45	1.40
23	A	1007	CLA	C4B-CHC	2.10	1.45	1.40
23	b	6022	CLA	CHD-C4C	2.11	1.47	1.41
23	B	1015	CLA	C1B-CHB	2.11	1.45	1.40
23	c	6026	CLA	CHD-C4C	2.13	1.47	1.41
23	C	1026	CLA	CHD-C4C	2.13	1.47	1.41
23	b	6009	CLA	C1C-C2C	2.14	1.48	1.44
23	B	1009	CLA	C1C-C2C	2.15	1.48	1.44
23	B	1019	CLA	C4B-CHC	2.15	1.45	1.40
24	A	1039	PHO	C1C-C2C	2.16	1.50	1.45
24	A	1038	PHO	C1C-C2C	2.16	1.50	1.45
23	b	6019	CLA	C4B-CHC	2.16	1.45	1.40
24	d	6038	PHO	C1C-C2C	2.16	1.50	1.45
24	a	6039	PHO	C1C-C2C	2.17	1.50	1.45
25	D	1042	PQ9	C11-C12	2.18	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6011	CLA	C1C-C2C	2.20	1.48	1.44
23	C	1029	CLA	CHD-C4C	2.20	1.47	1.41
25	a	6043	PQ9	C35-C33	2.20	1.56	1.51
23	B	1011	CLA	C1C-C2C	2.21	1.48	1.44
23	H	1017	CLA	C1C-C2C	2.21	1.48	1.44
23	c	6029	CLA	CHD-C4C	2.21	1.47	1.41
23	C	1030	CLA	C1C-C2C	2.21	1.48	1.44
23	B	1024	CLA	C1B-CHB	2.22	1.46	1.40
23	c	6031	CLA	C1C-C2C	2.22	1.48	1.44
23	A	1006	CLA	C1C-C2C	2.22	1.48	1.44
23	b	6017	CLA	C1C-C2C	2.22	1.48	1.44
23	D	1004	CLA	C1C-C2C	2.22	1.48	1.44
23	B	1018	CLA	C1C-C2C	2.22	1.48	1.44
23	C	1034	CLA	C1C-C2C	2.22	1.48	1.44
23	b	6018	CLA	C1C-C2C	2.22	1.48	1.44
23	c	6032	CLA	C1C-C2C	2.22	1.48	1.44
23	d	6004	CLA	C1C-C2C	2.23	1.48	1.44
23	C	1037	CLA	C1C-C2C	2.23	1.48	1.44
23	b	6010	CLA	C1B-CHB	2.23	1.46	1.40
25	a	6043	PQ9	C40-C38	2.23	1.56	1.51
23	c	6031	CLA	C4C-C3C	2.23	1.48	1.45
23	B	1010	CLA	C1B-CHB	2.23	1.46	1.40
23	C	1035	CLA	C1C-C2C	2.23	1.48	1.44
23	b	6016	CLA	C1C-C2C	2.23	1.48	1.44
23	B	1016	CLA	C1C-C2C	2.23	1.48	1.44
23	B	1023	CLA	C1C-C2C	2.23	1.48	1.44
23	c	6037	CLA	C1C-C2C	2.23	1.48	1.44
23	c	6030	CLA	C1C-C2C	2.23	1.48	1.44
23	b	6012	CLA	C1C-C2C	2.23	1.48	1.44
23	b	6024	CLA	C1B-CHB	2.23	1.46	1.40
23	d	6008	CLA	C4C-C3C	2.24	1.48	1.45
23	c	6028	CLA	C1C-C2C	2.24	1.48	1.44
23	c	6033	CLA	C4C-C3C	2.24	1.48	1.45
23	C	1031	CLA	C1C-C2C	2.24	1.48	1.44
23	C	1033	CLA	C4C-C3C	2.24	1.48	1.45
23	B	1021	CLA	C1C-C2C	2.24	1.48	1.44
23	B	1020	CLA	C1C-C2C	2.24	1.48	1.44
23	D	1005	CLA	C1C-C2C	2.25	1.48	1.44
23	c	6027	CLA	C1C-C2C	2.25	1.48	1.44
23	c	6036	CLA	C4C-C3C	2.25	1.48	1.45
23	C	1027	CLA	C1C-C2C	2.25	1.48	1.44
23	B	1014	CLA	CHD-C4C	2.25	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6021	CLA	C1C-C2C	2.25	1.48	1.44
23	b	6014	CLA	CHD-C4C	2.25	1.47	1.41
23	c	6035	CLA	C1C-C2C	2.25	1.48	1.44
23	C	1028	CLA	C1C-C2C	2.25	1.48	1.44
23	D	1008	CLA	C1C-C2C	2.25	1.48	1.44
23	b	6023	CLA	C1C-C2C	2.25	1.48	1.44
23	d	6005	CLA	C1C-C2C	2.26	1.48	1.44
23	a	6006	CLA	C1C-C2C	2.26	1.48	1.44
23	C	1036	CLA	C1C-C2C	2.26	1.48	1.44
23	b	6020	CLA	C1C-C2C	2.26	1.48	1.44
23	c	6036	CLA	C1C-C2C	2.26	1.48	1.44
23	C	1031	CLA	C4C-C3C	2.26	1.48	1.45
23	B	1023	CLA	C4C-C3C	2.26	1.48	1.45
23	B	1012	CLA	C1C-C2C	2.26	1.48	1.44
23	D	1008	CLA	C4C-C3C	2.26	1.48	1.45
23	d	6008	CLA	C1C-C2C	2.26	1.48	1.44
23	B	1013	CLA	C1C-C2C	2.26	1.48	1.44
23	b	6018	CLA	C4C-C3C	2.26	1.48	1.45
23	b	6023	CLA	C4C-C3C	2.26	1.49	1.45
23	D	1004	CLA	C4C-C3C	2.26	1.49	1.45
23	A	1003	CLA	C1C-C2C	2.27	1.48	1.44
23	d	6004	CLA	C4C-C3C	2.27	1.49	1.45
23	B	1015	CLA	CHD-C4C	2.27	1.47	1.41
23	b	6015	CLA	CHD-C4C	2.27	1.47	1.41
23	a	6003	CLA	C1C-C2C	2.27	1.48	1.44
23	C	1032	CLA	C4C-C3C	2.27	1.49	1.45
23	C	1032	CLA	C1C-C2C	2.27	1.48	1.44
23	c	6028	CLA	C4C-C3C	2.27	1.49	1.45
23	b	6013	CLA	C1C-C2C	2.27	1.48	1.44
23	b	6020	CLA	C4C-C3C	2.27	1.49	1.45
23	B	1018	CLA	C4C-C3C	2.27	1.49	1.45
23	C	1033	CLA	C1C-C2C	2.27	1.48	1.44
23	c	6035	CLA	C4C-C3C	2.27	1.49	1.45
23	c	6033	CLA	C1C-C2C	2.27	1.48	1.44
23	a	6007	CLA	C1B-CHB	2.27	1.46	1.40
23	B	1020	CLA	C4C-C3C	2.27	1.49	1.45
23	b	6021	CLA	C4C-C3C	2.27	1.49	1.45
23	C	1025	CLA	C1C-C2C	2.28	1.48	1.44
23	b	6012	CLA	C4C-C3C	2.28	1.49	1.45
23	b	6011	CLA	C4C-C3C	2.28	1.49	1.45
23	B	1013	CLA	C4C-C3C	2.28	1.49	1.45
23	c	6026	CLA	C1B-CHB	2.29	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1035	CLA	C4C-C3C	2.29	1.49	1.45
23	c	6025	CLA	C1C-C2C	2.29	1.49	1.44
23	C	1036	CLA	C4C-C3C	2.29	1.49	1.45
23	C	1034	CLA	C4C-C3C	2.29	1.49	1.45
23	b	6013	CLA	C4C-C3C	2.29	1.49	1.45
23	C	1028	CLA	C4C-C3C	2.29	1.49	1.45
23	C	1026	CLA	C1B-CHB	2.29	1.46	1.40
23	B	1024	CLA	C4B-CHC	2.29	1.46	1.40
23	c	6032	CLA	C4C-C3C	2.29	1.49	1.45
23	b	6024	CLA	C4B-CHC	2.30	1.46	1.40
23	A	1006	CLA	C4C-C3C	2.30	1.49	1.45
23	C	1025	CLA	C4C-C3C	2.30	1.49	1.45
23	C	1030	CLA	C4C-C3C	2.30	1.49	1.45
23	c	6037	CLA	C4C-C3C	2.30	1.49	1.45
23	B	1011	CLA	C4C-C3C	2.30	1.49	1.45
23	D	1005	CLA	C4C-C3C	2.30	1.49	1.45
23	A	1007	CLA	C1B-CHB	2.30	1.46	1.40
23	B	1016	CLA	C4C-C3C	2.30	1.49	1.45
23	c	6030	CLA	C4C-C3C	2.30	1.49	1.45
23	A	1003	CLA	C4C-C3C	2.30	1.49	1.45
23	c	6025	CLA	C4C-C3C	2.30	1.49	1.45
23	H	1017	CLA	C4C-C3C	2.30	1.49	1.45
23	B	1012	CLA	C4C-C3C	2.31	1.49	1.45
23	a	6006	CLA	C4C-C3C	2.31	1.49	1.45
23	B	1021	CLA	C4C-C3C	2.31	1.49	1.45
23	C	1037	CLA	C4C-C3C	2.31	1.49	1.45
23	d	6005	CLA	C4C-C3C	2.31	1.49	1.45
23	b	6016	CLA	C4C-C3C	2.31	1.49	1.45
23	C	1027	CLA	C4C-C3C	2.33	1.49	1.45
23	C	1029	CLA	C4B-CHC	2.33	1.46	1.40
23	c	6029	CLA	C4B-CHC	2.34	1.46	1.40
23	c	6027	CLA	C4C-C3C	2.34	1.49	1.45
23	b	6017	CLA	C4C-C3C	2.34	1.49	1.45
25	a	6043	PQ9	C20-C18	2.35	1.56	1.51
23	a	6003	CLA	C4C-C3C	2.36	1.49	1.45
23	b	6022	CLA	C1B-CHB	2.36	1.46	1.40
23	c	6034	CLA	C1B-CHB	2.37	1.46	1.40
23	c	6034	CLA	CHD-C4C	2.37	1.48	1.41
23	B	1022	CLA	C1B-CHB	2.39	1.46	1.40
23	b	6022	CLA	C4B-CHC	2.41	1.46	1.40
23	B	1022	CLA	C4B-CHC	2.42	1.46	1.40
23	C	1029	CLA	C1B-CHB	2.42	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6029	CLA	C1B-CHB	2.42	1.46	1.40
23	b	6009	CLA	CHD-C4C	2.42	1.48	1.41
23	B	1009	CLA	CHD-C4C	2.43	1.48	1.41
23	b	6010	CLA	CHD-C4C	2.44	1.48	1.41
23	B	1010	CLA	CHD-C4C	2.44	1.48	1.41
25	a	6043	PQ9	C11-C2	2.45	1.53	1.51
23	b	6009	CLA	C4B-CHC	2.45	1.46	1.40
23	b	6009	CLA	C4C-C3C	2.46	1.49	1.45
23	B	1009	CLA	C4C-C3C	2.46	1.49	1.45
23	B	1009	CLA	C4B-CHC	2.47	1.46	1.40
23	a	6003	CLA	C1B-CHB	2.47	1.46	1.40
23	c	6032	CLA	C1B-CHB	2.48	1.46	1.40
23	b	6024	CLA	CHD-C4C	2.49	1.48	1.41
23	B	1024	CLA	CHD-C4C	2.49	1.48	1.41
23	A	1003	CLA	C1B-CHB	2.49	1.46	1.40
23	b	6015	CLA	C4B-CHC	2.49	1.46	1.40
23	b	6023	CLA	C1B-CHB	2.49	1.46	1.40
23	C	1027	CLA	C1B-CHB	2.49	1.46	1.40
23	c	6037	CLA	C1B-CHB	2.49	1.46	1.40
23	d	6005	CLA	C1B-CHB	2.50	1.46	1.40
23	C	1037	CLA	C1B-CHB	2.50	1.46	1.40
23	c	6033	CLA	C1B-CHB	2.50	1.46	1.40
23	c	6025	CLA	C1B-CHB	2.50	1.46	1.40
23	B	1013	CLA	C1B-CHB	2.50	1.46	1.40
23	c	6031	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6021	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6020	CLA	CHD-C4C	2.50	1.48	1.41
23	a	6006	CLA	C1B-CHB	2.50	1.46	1.40
23	C	1033	CLA	C1B-CHB	2.50	1.46	1.40
23	D	1005	CLA	C1B-CHB	2.50	1.46	1.40
23	b	6013	CLA	C1B-CHB	2.50	1.46	1.40
23	B	1020	CLA	C1B-CHB	2.50	1.46	1.40
23	C	1025	CLA	C1B-CHB	2.50	1.46	1.40
23	B	1011	CLA	C1B-CHB	2.51	1.46	1.40
23	b	6020	CLA	C1B-CHB	2.51	1.46	1.40
23	C	1031	CLA	C1B-CHB	2.51	1.46	1.40
23	b	6023	CLA	CHD-C4C	2.51	1.48	1.41
23	c	6032	CLA	CHD-C4C	2.51	1.48	1.41
23	D	1004	CLA	C1B-CHB	2.51	1.46	1.40
23	B	1015	CLA	C4B-CHC	2.51	1.46	1.40
23	B	1021	CLA	CHD-C4C	2.52	1.48	1.41
23	b	6012	CLA	CHD-C4C	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1021	CLA	C1B-CHB	2.52	1.46	1.40
23	C	1032	CLA	C1B-CHB	2.52	1.46	1.40
23	b	6014	CLA	C1C-C2C	2.52	1.49	1.44
23	c	6033	CLA	CHD-C4C	2.52	1.48	1.41
23	B	1023	CLA	C1B-CHB	2.52	1.46	1.40
23	D	1008	CLA	CHD-C4C	2.52	1.48	1.41
23	A	1006	CLA	CHD-C4C	2.52	1.48	1.41
23	b	6021	CLA	CHD-C4C	2.52	1.48	1.41
23	C	1027	CLA	CHD-C4C	2.52	1.48	1.41
23	b	6011	CLA	C1B-CHB	2.52	1.46	1.40
23	B	1016	CLA	C1B-CHB	2.52	1.46	1.40
23	C	1034	CLA	C1B-CHB	2.52	1.46	1.40
23	A	1006	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1012	CLA	C1B-CHB	2.53	1.46	1.40
23	a	6003	CLA	CHD-C4C	2.53	1.48	1.41
23	d	6004	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1012	CLA	CHD-C4C	2.53	1.48	1.41
23	C	1036	CLA	C1B-CHB	2.53	1.46	1.40
23	b	6009	CLA	C1B-CHB	2.53	1.46	1.40
23	B	1020	CLA	CHD-C4C	2.53	1.48	1.41
23	C	1025	CLA	CHD-C4C	2.53	1.48	1.41
23	B	1014	CLA	C1C-C2C	2.53	1.49	1.44
23	b	6017	CLA	CHD-C4C	2.53	1.48	1.41
23	B	1016	CLA	CHD-C4C	2.53	1.48	1.41
23	C	1028	CLA	C1B-CHB	2.53	1.46	1.40
23	b	6017	CLA	C1B-CHB	2.53	1.46	1.40
23	b	6016	CLA	CHD-C4C	2.53	1.48	1.41
23	B	1023	CLA	CHD-C4C	2.53	1.48	1.41
23	b	6012	CLA	C1B-CHB	2.53	1.46	1.40
23	c	6025	CLA	CHD-C4C	2.53	1.48	1.41
23	d	6005	CLA	CHD-C4C	2.53	1.48	1.41
23	B	1009	CLA	C1B-CHB	2.54	1.46	1.40
23	B	1011	CLA	CHD-C4C	2.54	1.48	1.41
23	C	1032	CLA	CHD-C4C	2.54	1.48	1.41
23	a	6006	CLA	CHD-C4C	2.54	1.48	1.41
23	c	6027	CLA	C1B-CHB	2.54	1.46	1.40
23	d	6008	CLA	CHD-C4C	2.54	1.48	1.41
23	B	1018	CLA	C1B-CHB	2.54	1.46	1.40
23	A	1003	CLA	CHD-C4C	2.54	1.48	1.41
23	B	1013	CLA	CHD-C4C	2.54	1.48	1.41
23	D	1005	CLA	CHD-C4C	2.54	1.48	1.41
23	b	6013	CLA	CHD-C4C	2.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1030	CLA	C1B-CHB	2.54	1.46	1.40
23	b	6016	CLA	C1B-CHB	2.54	1.46	1.40
23	H	1017	CLA	C1B-CHB	2.54	1.46	1.40
23	b	6011	CLA	CHD-C4C	2.54	1.48	1.41
23	D	1004	CLA	CHD-C4C	2.54	1.48	1.41
23	c	6027	CLA	CHD-C4C	2.54	1.48	1.41
23	c	6037	CLA	CHD-C4C	2.54	1.48	1.41
23	C	1035	CLA	CHD-C4C	2.54	1.48	1.41
23	c	6035	CLA	CHD-C4C	2.55	1.48	1.41
23	C	1033	CLA	CHD-C4C	2.55	1.48	1.41
23	c	6030	CLA	CHD-C4C	2.55	1.48	1.41
23	D	1008	CLA	C1B-CHB	2.55	1.46	1.40
23	H	1017	CLA	CHD-C4C	2.55	1.48	1.41
23	c	6030	CLA	C1B-CHB	2.55	1.46	1.40
23	c	6035	CLA	C1B-CHB	2.55	1.46	1.40
23	C	1037	CLA	CHD-C4C	2.55	1.48	1.41
23	C	1030	CLA	CHD-C4C	2.55	1.48	1.41
23	C	1031	CLA	CHD-C4C	2.55	1.48	1.41
23	C	1036	CLA	CHD-C4C	2.55	1.48	1.41
23	c	6034	CLA	C4B-CHC	2.55	1.46	1.40
23	C	1035	CLA	C1B-CHB	2.55	1.46	1.40
23	c	6036	CLA	C1B-CHB	2.55	1.46	1.40
23	c	6028	CLA	C1B-CHB	2.55	1.46	1.40
23	B	1018	CLA	CHD-C4C	2.56	1.48	1.41
23	C	1034	CLA	CHD-C4C	2.56	1.48	1.41
23	C	1028	CLA	CHD-C4C	2.56	1.48	1.41
23	c	6031	CLA	CHD-C4C	2.56	1.48	1.41
23	c	6028	CLA	CHD-C4C	2.56	1.48	1.41
23	c	6036	CLA	CHD-C4C	2.56	1.48	1.41
23	b	6018	CLA	CHD-C4C	2.57	1.48	1.41
23	d	6004	CLA	CHD-C4C	2.57	1.48	1.41
23	b	6014	CLA	C4B-CHC	2.57	1.47	1.40
23	b	6018	CLA	C1B-CHB	2.57	1.47	1.40
23	d	6008	CLA	C1B-CHB	2.58	1.47	1.40
23	B	1014	CLA	C4B-CHC	2.58	1.47	1.40
25	d	6042	PQ9	C3-C4	2.62	1.52	1.44
23	B	1019	CLA	C1B-CHB	2.63	1.47	1.40
23	c	6035	CLA	C4B-CHC	2.64	1.47	1.40
23	b	6011	CLA	C4B-CHC	2.64	1.47	1.40
23	c	6028	CLA	C4B-CHC	2.65	1.47	1.40
24	A	1038	PHO	C4C-C3C	2.65	1.49	1.45
23	b	6019	CLA	C1B-CHB	2.65	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	1042	PQ9	C3-C4	2.65	1.52	1.44
23	b	6016	CLA	C4B-CHC	2.65	1.47	1.40
23	a	6003	CLA	C4B-CHC	2.65	1.47	1.40
23	C	1028	CLA	C4B-CHC	2.65	1.47	1.40
23	C	1035	CLA	C4B-CHC	2.65	1.47	1.40
24	d	6038	PHO	C4C-C3C	2.66	1.49	1.45
23	B	1011	CLA	C4B-CHC	2.66	1.47	1.40
23	d	6004	CLA	C4B-CHC	2.66	1.47	1.40
23	B	1021	CLA	C4B-CHC	2.66	1.47	1.40
23	c	6031	CLA	C4B-CHC	2.66	1.47	1.40
23	B	1018	CLA	C4B-CHC	2.67	1.47	1.40
23	b	6021	CLA	C4B-CHC	2.67	1.47	1.40
23	B	1016	CLA	C4B-CHC	2.67	1.47	1.40
23	C	1034	CLA	C4B-CHC	2.67	1.47	1.40
23	b	6023	CLA	C4B-CHC	2.67	1.47	1.40
23	d	6005	CLA	C4B-CHC	2.67	1.47	1.40
23	D	1004	CLA	C4B-CHC	2.67	1.47	1.40
23	A	1003	CLA	C4B-CHC	2.68	1.47	1.40
25	D	1042	PQ9	C35-C33	2.68	1.57	1.51
23	D	1005	CLA	C4B-CHC	2.68	1.47	1.40
23	c	6027	CLA	C4B-CHC	2.68	1.47	1.40
23	c	6037	CLA	C4B-CHC	2.68	1.47	1.40
23	B	1023	CLA	C4B-CHC	2.68	1.47	1.40
23	c	6036	CLA	C4B-CHC	2.68	1.47	1.40
23	b	6018	CLA	C4B-CHC	2.68	1.47	1.40
23	B	1020	CLA	C4B-CHC	2.68	1.47	1.40
23	C	1036	CLA	C4B-CHC	2.68	1.47	1.40
23	B	1012	CLA	C4B-CHC	2.68	1.47	1.40
23	b	6020	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1037	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1027	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1032	CLA	C4B-CHC	2.69	1.47	1.40
23	b	6017	CLA	C4B-CHC	2.69	1.47	1.40
23	A	1006	CLA	C4B-CHC	2.69	1.47	1.40
23	C	1031	CLA	C4B-CHC	2.69	1.47	1.40
23	H	1017	CLA	C4B-CHC	2.69	1.47	1.40
23	b	6012	CLA	C4B-CHC	2.70	1.47	1.40
23	D	1008	CLA	C4B-CHC	2.70	1.47	1.40
23	c	6033	CLA	C4B-CHC	2.70	1.47	1.40
23	a	6006	CLA	C4B-CHC	2.71	1.47	1.40
23	C	1030	CLA	C4B-CHC	2.71	1.47	1.40
23	C	1033	CLA	C4B-CHC	2.71	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1025	CLA	C4B-CHC	2.71	1.47	1.40
23	B	1013	CLA	C4B-CHC	2.71	1.47	1.40
23	c	6032	CLA	C4B-CHC	2.71	1.47	1.40
23	c	6025	CLA	C4B-CHC	2.72	1.47	1.40
23	b	6013	CLA	C4B-CHC	2.73	1.47	1.40
23	d	6008	CLA	C4B-CHC	2.74	1.47	1.40
23	c	6030	CLA	C4B-CHC	2.74	1.47	1.40
25	d	6042	PQ9	C40-C38	2.79	1.57	1.51
25	a	6043	PQ9	C3-C4	2.80	1.52	1.44
23	B	1010	CLA	C3D-C2D	2.80	1.45	1.39
23	B	1014	CLA	C3B-C2B	2.81	1.44	1.40
25	A	1043	PQ9	C11-C12	2.81	1.55	1.50
23	b	6010	CLA	C3D-C2D	2.82	1.45	1.39
23	b	6014	CLA	C3B-C2B	2.83	1.44	1.40
24	A	1038	PHO	CHB-C4A	2.87	1.47	1.40
24	d	6038	PHO	CHB-C4A	2.87	1.47	1.40
25	A	1043	PQ9	C3-C4	2.89	1.53	1.44
25	D	1042	PQ9	C40-C38	2.89	1.57	1.51
24	a	6039	PHO	CHB-C4A	2.90	1.47	1.40
24	A	1039	PHO	CHB-C4A	2.91	1.47	1.40
24	A	1039	PHO	C4C-C3C	2.93	1.50	1.45
24	a	6039	PHO	C4C-C3C	2.94	1.50	1.45
24	d	6038	PHO	CHD-C4C	2.96	1.47	1.40
24	A	1038	PHO	CHD-C4C	2.98	1.47	1.40
23	a	6007	CLA	OBD-CAD	2.99	1.26	1.22
24	a	6039	PHO	CHD-C4C	3.02	1.47	1.40
24	A	1039	PHO	CHD-C4C	3.03	1.47	1.40
23	A	1007	CLA	OBD-CAD	3.03	1.26	1.22
23	a	6007	CLA	C3D-C2D	3.03	1.45	1.39
23	A	1007	CLA	C3D-C2D	3.05	1.45	1.39
23	b	6015	CLA	C3D-C2D	3.05	1.45	1.39
23	b	6019	CLA	C1D-C2D	3.05	1.49	1.42
23	B	1019	CLA	C1D-C2D	3.06	1.49	1.42
25	a	6043	PQ9	C11-C12	3.07	1.55	1.50
23	B	1015	CLA	C3D-C2D	3.07	1.45	1.39
23	b	6022	CLA	C3D-C2D	3.08	1.45	1.39
23	B	1022	CLA	C3D-C2D	3.11	1.45	1.39
24	A	1039	PHO	C3D-C2D	3.13	1.47	1.38
24	a	6039	PHO	C3D-C2D	3.14	1.47	1.38
23	B	1022	CLA	C3B-C2B	3.17	1.44	1.40
23	c	6026	CLA	C3B-C2B	3.19	1.44	1.40
23	C	1026	CLA	C3B-C2B	3.19	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6026	CLA	C1D-C2D	3.19	1.50	1.42
23	b	6022	CLA	C3B-C2B	3.20	1.44	1.40
23	C	1026	CLA	C1D-C2D	3.22	1.50	1.42
24	d	6038	PHO	C3D-C2D	3.23	1.48	1.38
23	B	1024	CLA	C1D-C2D	3.24	1.50	1.42
24	A	1038	PHO	C3D-C2D	3.24	1.48	1.38
23	A	1007	CLA	C1D-C2D	3.24	1.50	1.42
23	b	6024	CLA	C1D-C2D	3.25	1.50	1.42
23	C	1029	CLA	C3B-C2B	3.26	1.44	1.40
23	a	6007	CLA	C1D-C2D	3.26	1.50	1.42
23	B	1024	CLA	C3D-C2D	3.27	1.46	1.39
23	b	6024	CLA	C3D-C2D	3.27	1.46	1.39
23	C	1029	CLA	C1D-C2D	3.27	1.50	1.42
23	c	6029	CLA	C1D-C2D	3.28	1.50	1.42
23	c	6029	CLA	C3B-C2B	3.29	1.44	1.40
23	b	6014	CLA	C3D-C2D	3.31	1.46	1.39
23	B	1014	CLA	C3D-C2D	3.32	1.46	1.39
23	b	6015	CLA	C1D-C2D	3.40	1.50	1.42
23	B	1015	CLA	C1D-C2D	3.41	1.50	1.42
23	B	1014	CLA	C1D-C2D	3.43	1.50	1.42
23	b	6014	CLA	C1D-C2D	3.43	1.50	1.42
23	B	1024	CLA	C3B-C2B	3.43	1.45	1.40
23	b	6024	CLA	C3B-C2B	3.46	1.45	1.40
23	B	1022	CLA	C1D-C2D	3.47	1.50	1.42
31	v	6041	HEM	C3B-CAB	3.48	1.54	1.47
23	c	6034	CLA	C3D-C2D	3.49	1.46	1.39
23	b	6022	CLA	C1D-C2D	3.49	1.50	1.42
31	V	1041	HEM	C3B-CAB	3.51	1.54	1.47
31	E	1040	HEM	C3B-CAB	3.53	1.54	1.47
23	b	6014	CLA	OBD-CAD	3.54	1.27	1.22
25	D	1042	PQ9	C6-C5	3.54	1.58	1.50
31	e	6040	HEM	C3B-CAB	3.54	1.54	1.47
31	e	6040	HEM	C3C-CAC	3.55	1.54	1.47
23	c	6034	CLA	C1D-C2D	3.55	1.50	1.42
31	v	6041	HEM	C3C-CAC	3.56	1.54	1.47
31	E	1040	HEM	C3C-CAC	3.56	1.54	1.47
23	B	1014	CLA	OBD-CAD	3.57	1.27	1.22
31	V	1041	HEM	C3C-CAC	3.57	1.54	1.47
23	A	1007	CLA	C3B-C2B	3.58	1.45	1.40
23	B	1015	CLA	C3B-C2B	3.60	1.45	1.40
23	c	6026	CLA	O2A-CGA	3.60	1.43	1.33
23	b	6015	CLA	C3B-C2B	3.60	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1026	CLA	O2A-CGA	3.61	1.43	1.33
23	a	6007	CLA	C3B-C2B	3.61	1.45	1.40
23	B	1009	CLA	C1D-C2D	3.63	1.51	1.42
25	d	6042	PQ9	C6-C5	3.63	1.58	1.50
23	B	1010	CLA	CHC-C1C	3.66	1.45	1.35
25	a	6043	PQ9	C6-C5	3.66	1.58	1.50
23	C	1026	CLA	C3D-C2D	3.66	1.47	1.39
23	b	6009	CLA	C1D-C2D	3.66	1.51	1.42
23	C	1029	CLA	OBD-CAD	3.66	1.27	1.22
23	b	6010	CLA	O2A-CGA	3.67	1.44	1.33
23	B	1010	CLA	O2A-CGA	3.68	1.44	1.33
23	c	6026	CLA	C3D-C2D	3.68	1.47	1.39
23	b	6010	CLA	CHC-C1C	3.68	1.45	1.35
23	B	1010	CLA	C1D-C2D	3.69	1.51	1.42
23	c	6029	CLA	OBD-CAD	3.70	1.27	1.22
23	b	6010	CLA	C1D-C2D	3.71	1.51	1.42
23	b	6013	CLA	C3D-C2D	3.72	1.47	1.39
25	A	1043	PQ9	C6-C5	3.72	1.58	1.50
23	C	1029	CLA	O2A-CGA	3.73	1.44	1.33
23	B	1019	CLA	CHC-C1C	3.74	1.46	1.35
23	b	6019	CLA	CHC-C1C	3.74	1.46	1.35
23	b	6009	CLA	C3D-C2D	3.74	1.47	1.39
23	c	6029	CLA	O2A-CGA	3.75	1.44	1.33
23	B	1010	CLA	OBD-CAD	3.75	1.27	1.22
23	b	6019	CLA	C3D-C2D	3.75	1.47	1.39
23	B	1013	CLA	C3D-C2D	3.75	1.47	1.39
23	C	1027	CLA	C3D-C2D	3.75	1.47	1.39
23	c	6027	CLA	C3D-C2D	3.75	1.47	1.39
23	B	1009	CLA	C3D-C2D	3.76	1.47	1.39
23	b	6011	CLA	C3D-C2D	3.76	1.47	1.39
23	c	6035	CLA	C3D-C2D	3.76	1.47	1.39
23	c	6032	CLA	C1D-C2D	3.76	1.51	1.42
23	c	6025	CLA	C3D-C2D	3.76	1.47	1.39
23	C	1025	CLA	C3D-C2D	3.77	1.47	1.39
23	c	6036	CLA	C3D-C2D	3.77	1.47	1.39
23	c	6028	CLA	C3D-C2D	3.77	1.47	1.39
23	C	1035	CLA	C3D-C2D	3.77	1.47	1.39
23	b	6010	CLA	OBD-CAD	3.77	1.27	1.22
23	d	6005	CLA	C3D-C2D	3.77	1.47	1.39
23	D	1004	CLA	C3D-C2D	3.77	1.47	1.39
23	C	1032	CLA	C3D-C2D	3.78	1.47	1.39
23	D	1008	CLA	C3D-C2D	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1012	CLA	C3D-C2D	3.78	1.47	1.39
23	b	6011	CLA	C1D-C2D	3.78	1.51	1.42
23	b	6021	CLA	C3D-C2D	3.78	1.47	1.39
23	b	6024	CLA	C3C-C2C	3.78	1.44	1.36
23	b	6021	CLA	C1D-C2D	3.78	1.51	1.42
23	C	1036	CLA	C3D-C2D	3.78	1.47	1.39
23	B	1021	CLA	C3D-C2D	3.79	1.47	1.39
23	D	1005	CLA	C3D-C2D	3.79	1.47	1.39
23	B	1023	CLA	C3D-C2D	3.79	1.47	1.39
23	B	1024	CLA	C3C-C2C	3.79	1.44	1.36
23	B	1018	CLA	C3D-C2D	3.79	1.47	1.39
23	C	1030	CLA	C3D-C2D	3.79	1.47	1.39
23	a	6003	CLA	C3D-C2D	3.79	1.47	1.39
23	b	6020	CLA	C3D-C2D	3.80	1.47	1.39
23	C	1032	CLA	C1D-C2D	3.80	1.51	1.42
23	C	1034	CLA	C1D-C2D	3.80	1.51	1.42
23	C	1028	CLA	C3D-C2D	3.80	1.47	1.39
23	c	6030	CLA	C3D-C2D	3.80	1.47	1.39
23	c	6032	CLA	C3D-C2D	3.80	1.47	1.39
23	B	1011	CLA	C3D-C2D	3.80	1.47	1.39
23	A	1006	CLA	C3D-C2D	3.80	1.47	1.39
23	C	1033	CLA	C3D-C2D	3.80	1.47	1.39
23	B	1019	CLA	C3D-C2D	3.80	1.47	1.39
23	b	6018	CLA	C3D-C2D	3.80	1.47	1.39
23	H	1017	CLA	C3D-C2D	3.80	1.47	1.39
23	a	6006	CLA	C3D-C2D	3.81	1.47	1.39
23	B	1011	CLA	C1D-C2D	3.81	1.51	1.42
23	B	1010	CLA	C3B-C2B	3.81	1.45	1.40
23	d	6004	CLA	C3D-C2D	3.81	1.47	1.39
23	B	1020	CLA	C3D-C2D	3.81	1.47	1.39
23	C	1034	CLA	C3D-C2D	3.81	1.47	1.39
23	C	1037	CLA	C3D-C2D	3.81	1.47	1.39
23	d	6008	CLA	C3D-C2D	3.81	1.47	1.39
23	b	6016	CLA	C3D-C2D	3.81	1.47	1.39
23	B	1016	CLA	C3D-C2D	3.81	1.47	1.39
23	B	1021	CLA	C1D-C2D	3.81	1.51	1.42
23	b	6023	CLA	C3D-C2D	3.81	1.47	1.39
23	C	1030	CLA	C1D-C2D	3.81	1.51	1.42
23	c	6029	CLA	C3D-C2D	3.82	1.47	1.39
23	c	6030	CLA	C1D-C2D	3.82	1.51	1.42
23	c	6037	CLA	C1D-C2D	3.82	1.51	1.42
23	d	6008	CLA	C1D-C2D	3.82	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6012	CLA	C3D-C2D	3.82	1.47	1.39
23	b	6013	CLA	C1D-C2D	3.82	1.51	1.42
23	D	1008	CLA	C1D-C2D	3.82	1.51	1.42
23	C	1031	CLA	C3D-C2D	3.82	1.47	1.39
23	b	6020	CLA	C1D-C2D	3.83	1.51	1.42
23	A	1003	CLA	C3D-C2D	3.83	1.47	1.39
23	d	6004	CLA	C1D-C2D	3.83	1.51	1.42
23	b	6010	CLA	C3B-C2B	3.83	1.45	1.40
23	C	1037	CLA	C1D-C2D	3.83	1.51	1.42
23	B	1013	CLA	C1D-C2D	3.83	1.51	1.42
23	a	6006	CLA	C1D-C2D	3.83	1.51	1.42
23	c	6033	CLA	C3D-C2D	3.83	1.47	1.39
23	c	6035	CLA	C1D-C2D	3.83	1.51	1.42
23	c	6031	CLA	C3D-C2D	3.83	1.47	1.39
23	c	6037	CLA	C3D-C2D	3.83	1.47	1.39
23	B	1016	CLA	C1D-C2D	3.84	1.51	1.42
23	C	1027	CLA	C1D-C2D	3.84	1.51	1.42
23	b	6022	CLA	O2A-CGA	3.84	1.44	1.33
23	A	1006	CLA	C1D-C2D	3.84	1.51	1.42
23	b	6014	CLA	O2A-CGA	3.84	1.44	1.33
23	D	1004	CLA	C1D-C2D	3.84	1.51	1.42
23	B	1022	CLA	O2A-CGA	3.84	1.44	1.33
23	b	6012	CLA	C1D-C2D	3.84	1.51	1.42
23	B	1018	CLA	C1D-C2D	3.84	1.51	1.42
23	c	6033	CLA	C1D-C2D	3.84	1.51	1.42
23	B	1014	CLA	O2A-CGA	3.84	1.44	1.33
23	B	1020	CLA	C1D-C2D	3.84	1.51	1.42
23	c	6025	CLA	C1D-C2D	3.85	1.51	1.42
23	C	1025	CLA	C1D-C2D	3.85	1.51	1.42
23	C	1033	CLA	C1D-C2D	3.85	1.51	1.42
23	C	1028	CLA	C1D-C2D	3.85	1.51	1.42
23	b	6016	CLA	C1D-C2D	3.85	1.51	1.42
23	B	1024	CLA	CHC-C1C	3.86	1.46	1.35
23	C	1031	CLA	C1D-C2D	3.86	1.51	1.42
23	b	6017	CLA	C3D-C2D	3.86	1.47	1.39
23	A	1003	CLA	C1D-C2D	3.86	1.51	1.42
23	c	6027	CLA	C1D-C2D	3.86	1.51	1.42
23	b	6018	CLA	C1D-C2D	3.86	1.51	1.42
23	C	1035	CLA	C1D-C2D	3.86	1.51	1.42
23	B	1012	CLA	C1D-C2D	3.86	1.51	1.42
23	D	1005	CLA	C1D-C2D	3.86	1.51	1.42
23	C	1029	CLA	C3D-C2D	3.86	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6022	CLA	CHC-C1C	3.86	1.46	1.35
23	b	6023	CLA	C1D-C2D	3.86	1.51	1.42
23	B	1022	CLA	CHC-C1C	3.86	1.46	1.35
23	H	1017	CLA	C1D-C2D	3.87	1.51	1.42
23	d	6005	CLA	C1D-C2D	3.87	1.51	1.42
23	a	6003	CLA	C1D-C2D	3.87	1.51	1.42
23	C	1036	CLA	C1D-C2D	3.87	1.51	1.42
23	c	6036	CLA	C1D-C2D	3.87	1.51	1.42
23	B	1023	CLA	C1D-C2D	3.87	1.51	1.42
23	c	6031	CLA	C1D-C2D	3.88	1.51	1.42
23	c	6028	CLA	C1D-C2D	3.88	1.51	1.42
23	b	6017	CLA	C1D-C2D	3.88	1.51	1.42
23	b	6024	CLA	CHC-C1C	3.89	1.46	1.35
23	c	6026	CLA	CHC-C1C	3.90	1.46	1.35
23	C	1026	CLA	CHC-C1C	3.90	1.46	1.35
23	B	1022	CLA	OBD-CAD	3.94	1.27	1.22
23	b	6022	CLA	OBD-CAD	3.94	1.27	1.22
23	c	6026	CLA	O2D-CGD	3.95	1.43	1.33
23	C	1026	CLA	O2D-CGD	3.96	1.43	1.33
29	d	6061	MGE	O2G-C1B	3.97	1.45	1.34
23	B	1024	CLA	O2A-CGA	3.97	1.44	1.33
23	B	1015	CLA	CHC-C1C	3.97	1.46	1.35
23	b	6024	CLA	O2A-CGA	3.98	1.44	1.33
23	b	6015	CLA	CHC-C1C	3.98	1.46	1.35
23	A	1007	CLA	CHC-C1C	3.98	1.46	1.35
23	B	1009	CLA	CHC-C1C	3.98	1.46	1.35
30	C	1057	DGD	O2G-C1B	3.98	1.45	1.34
29	L	1061	MGE	O2G-C1B	3.99	1.45	1.34
23	a	6007	CLA	CHC-C1C	3.99	1.46	1.35
30	h	6058	DGD	O2G-C1B	3.99	1.45	1.34
23	b	6009	CLA	CHC-C1C	3.99	1.46	1.35
29	B	1060	MGE	O2G-C1B	3.99	1.45	1.34
29	D	1062	MGE	O2G-C1B	3.99	1.45	1.34
30	c	6055	DGD	O2G-C1B	3.99	1.45	1.34
30	c	6057	DGD	O2G-C1B	3.99	1.45	1.34
30	C	1056	DGD	O2G-C1B	4.00	1.45	1.34
30	c	6056	DGD	O2G-C1B	4.00	1.45	1.34
27	a	6063	LHG	O7-C7	4.00	1.45	1.34
30	H	1058	DGD	O2G-C1B	4.00	1.45	1.34
29	d	6062	MGE	O2G-C1B	4.01	1.45	1.34
27	A	1063	LHG	O7-C7	4.01	1.45	1.34
29	J	1059	MGE	O2G-C1B	4.01	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	6060	MGE	O2G-C1B	4.02	1.45	1.34
29	d	6059	MGE	O2G-C1B	4.02	1.45	1.34
30	C	1055	DGD	O2G-C1B	4.02	1.45	1.34
24	d	6038	PHO	CBB-CAB	4.03	1.50	1.30
24	A	1038	PHO	CBB-CAB	4.03	1.50	1.30
23	C	1029	CLA	CHC-C1C	4.05	1.46	1.35
24	A	1039	PHO	CBB-CAB	4.06	1.50	1.30
23	b	6015	CLA	OBD-CAD	4.07	1.28	1.22
23	c	6029	CLA	CHC-C1C	4.07	1.46	1.35
24	a	6039	PHO	CBB-CAB	4.07	1.50	1.30
23	c	6026	CLA	OBD-CAD	4.07	1.28	1.22
23	B	1019	CLA	O2A-CGA	4.08	1.45	1.33
23	b	6019	CLA	O2A-CGA	4.08	1.45	1.33
23	b	6015	CLA	O2A-CGA	4.08	1.45	1.33
23	C	1026	CLA	OBD-CAD	4.09	1.28	1.22
23	B	1015	CLA	O2A-CGA	4.09	1.45	1.33
23	B	1015	CLA	OBD-CAD	4.10	1.28	1.22
23	b	6024	CLA	OBD-CAD	4.10	1.28	1.22
23	B	1024	CLA	OBD-CAD	4.12	1.28	1.22
23	c	6034	CLA	CHC-C1C	4.14	1.47	1.35
25	D	1042	PQ9	C22-C23	4.17	1.43	1.33
23	A	1007	CLA	O2A-CGA	4.18	1.45	1.33
23	a	6007	CLA	O2A-CGA	4.18	1.45	1.33
23	b	6009	CLA	O2A-CGA	4.18	1.45	1.33
23	B	1009	CLA	O2A-CGA	4.19	1.45	1.33
25	d	6042	PQ9	C22-C23	4.20	1.43	1.33
23	c	6037	CLA	CHC-C1C	4.24	1.47	1.35
23	A	1006	CLA	CHC-C1C	4.24	1.47	1.35
23	b	6011	CLA	CHC-C1C	4.24	1.47	1.35
23	C	1037	CLA	CHC-C1C	4.24	1.47	1.35
23	C	1036	CLA	CHC-C1C	4.24	1.47	1.35
23	b	6018	CLA	CHC-C1C	4.24	1.47	1.35
23	b	6021	CLA	CHC-C1C	4.24	1.47	1.35
23	d	6008	CLA	CHC-C1C	4.25	1.47	1.35
23	B	1011	CLA	CHC-C1C	4.25	1.47	1.35
23	b	6020	CLA	CHC-C1C	4.25	1.47	1.35
23	C	1031	CLA	CHC-C1C	4.25	1.47	1.35
23	C	1027	CLA	CHC-C1C	4.25	1.47	1.35
23	B	1021	CLA	CHC-C1C	4.25	1.47	1.35
23	c	6032	CLA	CHC-C1C	4.25	1.47	1.35
23	c	6034	CLA	OBD-CAD	4.25	1.28	1.22
23	b	6012	CLA	CHC-C1C	4.25	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	6006	CLA	CHC-C1C	4.25	1.47	1.35
23	C	1032	CLA	CHC-C1C	4.25	1.47	1.35
23	D	1005	CLA	CHC-C1C	4.26	1.47	1.35
23	B	1012	CLA	CHC-C1C	4.26	1.47	1.35
23	A	1003	CLA	CHC-C1C	4.26	1.47	1.35
23	b	6013	CLA	CHC-C1C	4.26	1.47	1.35
23	b	6023	CLA	CHC-C1C	4.26	1.47	1.35
23	c	6033	CLA	CHC-C1C	4.26	1.47	1.35
23	B	1016	CLA	CHC-C1C	4.26	1.47	1.35
23	b	6019	CLA	O2D-CGD	4.26	1.43	1.33
23	B	1020	CLA	CHC-C1C	4.26	1.47	1.35
23	B	1013	CLA	CHC-C1C	4.26	1.47	1.35
23	D	1008	CLA	CHC-C1C	4.26	1.47	1.35
23	a	6003	CLA	CHC-C1C	4.26	1.47	1.35
23	d	6004	CLA	CHC-C1C	4.26	1.47	1.35
23	B	1018	CLA	CHC-C1C	4.26	1.47	1.35
23	c	6031	CLA	CHC-C1C	4.27	1.47	1.35
23	B	1019	CLA	O2D-CGD	4.27	1.43	1.33
23	c	6030	CLA	CHC-C1C	4.27	1.47	1.35
23	c	6036	CLA	CHC-C1C	4.27	1.47	1.35
23	C	1025	CLA	CHC-C1C	4.27	1.47	1.35
23	C	1033	CLA	CHC-C1C	4.27	1.47	1.35
24	d	6038	PHO	CHC-C4B	4.27	1.50	1.40
23	c	6028	CLA	CHC-C1C	4.27	1.47	1.35
23	b	6015	CLA	O2D-CGD	4.27	1.43	1.33
23	C	1030	CLA	CHC-C1C	4.27	1.47	1.35
23	D	1004	CLA	CHC-C1C	4.27	1.47	1.35
23	c	6033	CLA	O2A-CGA	4.27	1.45	1.33
23	b	6014	CLA	CHC-C1C	4.27	1.47	1.35
23	B	1022	CLA	C3C-C2C	4.27	1.45	1.36
23	B	1023	CLA	CHC-C1C	4.28	1.47	1.35
23	c	6025	CLA	CHC-C1C	4.28	1.47	1.35
23	C	1034	CLA	CHC-C1C	4.28	1.47	1.35
23	d	6005	CLA	CHC-C1C	4.28	1.47	1.35
23	B	1014	CLA	O2D-CGD	4.28	1.43	1.33
23	B	1014	CLA	CHC-C1C	4.28	1.47	1.35
23	C	1028	CLA	CHC-C1C	4.28	1.47	1.35
23	c	6034	CLA	O2A-CGA	4.28	1.45	1.33
23	B	1015	CLA	O2D-CGD	4.28	1.43	1.33
23	c	6026	CLA	C3C-C2C	4.28	1.45	1.36
23	b	6022	CLA	C3C-C2C	4.28	1.45	1.36
23	b	6016	CLA	CHC-C1C	4.28	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1038	PHO	CHC-C4B	4.28	1.50	1.40
23	c	6027	CLA	CHC-C1C	4.28	1.47	1.35
23	d	6004	CLA	O2A-CGA	4.28	1.45	1.33
23	C	1035	CLA	CHC-C1C	4.29	1.47	1.35
23	b	6014	CLA	O2D-CGD	4.29	1.43	1.33
23	H	1017	CLA	CHC-C1C	4.29	1.47	1.35
23	c	6035	CLA	CHC-C1C	4.29	1.47	1.35
23	C	1033	CLA	O2A-CGA	4.29	1.45	1.33
27	A	1063	LHG	O8-C23	4.30	1.45	1.33
23	B	1010	CLA	O2D-CGD	4.30	1.44	1.33
23	B	1011	CLA	O2A-CGA	4.30	1.45	1.33
23	a	6003	CLA	O2A-CGA	4.30	1.45	1.33
23	C	1034	CLA	O2A-CGA	4.30	1.45	1.33
23	C	1036	CLA	O2A-CGA	4.30	1.45	1.33
23	D	1004	CLA	O2A-CGA	4.30	1.45	1.33
23	c	6035	CLA	O2A-CGA	4.30	1.45	1.33
23	d	6008	CLA	O2A-CGA	4.30	1.45	1.33
23	b	6017	CLA	CHC-C1C	4.31	1.47	1.35
23	b	6017	CLA	O2A-CGA	4.31	1.45	1.33
23	b	6013	CLA	O2A-CGA	4.31	1.45	1.33
23	a	6006	CLA	O2A-CGA	4.31	1.45	1.33
23	c	6027	CLA	O2A-CGA	4.31	1.45	1.33
23	B	1020	CLA	O2A-CGA	4.31	1.45	1.33
30	C	1055	DGD	O1G-C1A	4.31	1.45	1.33
23	B	1013	CLA	O2A-CGA	4.31	1.45	1.33
23	c	6030	CLA	O2A-CGA	4.31	1.45	1.33
23	C	1031	CLA	O2A-CGA	4.31	1.45	1.33
23	D	1008	CLA	O2A-CGA	4.32	1.45	1.33
23	C	1028	CLA	O2A-CGA	4.32	1.45	1.33
23	c	6036	CLA	O2A-CGA	4.32	1.45	1.33
30	c	6055	DGD	O1G-C1A	4.32	1.45	1.33
23	b	6020	CLA	O2A-CGA	4.32	1.45	1.33
23	b	6010	CLA	O2D-CGD	4.32	1.44	1.33
29	b	6060	MGE	O1G-C1A	4.32	1.45	1.33
23	C	1030	CLA	O2A-CGA	4.32	1.45	1.33
29	J	1059	MGE	O1G-C1A	4.32	1.45	1.33
23	A	1006	CLA	O2A-CGA	4.32	1.45	1.33
23	B	1021	CLA	O2A-CGA	4.32	1.45	1.33
30	C	1057	DGD	O1G-C1A	4.32	1.45	1.33
23	b	6012	CLA	O2A-CGA	4.32	1.45	1.33
27	a	6063	LHG	O8-C23	4.32	1.45	1.33
23	B	1012	CLA	O2A-CGA	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1023	CLA	O2A-CGA	4.32	1.45	1.33
23	b	6021	CLA	O2A-CGA	4.32	1.45	1.33
23	H	1017	CLA	O2A-CGA	4.32	1.45	1.33
23	B	1018	CLA	O2A-CGA	4.32	1.45	1.33
23	c	6028	CLA	O2A-CGA	4.32	1.45	1.33
23	b	6011	CLA	O2A-CGA	4.32	1.45	1.33
23	C	1026	CLA	C3C-C2C	4.33	1.46	1.36
29	D	1062	MGE	O1G-C1A	4.33	1.45	1.33
23	C	1025	CLA	O2A-CGA	4.33	1.45	1.33
29	L	1061	MGE	O1G-C1A	4.33	1.45	1.33
23	C	1035	CLA	O2A-CGA	4.33	1.45	1.33
23	b	6023	CLA	O2A-CGA	4.33	1.45	1.33
23	c	6025	CLA	O2A-CGA	4.33	1.45	1.33
23	b	6018	CLA	O2A-CGA	4.33	1.45	1.33
29	d	6061	MGE	O1G-C1A	4.33	1.45	1.33
30	h	6058	DGD	O1G-C1A	4.33	1.45	1.33
30	H	1058	DGD	O1G-C1A	4.33	1.45	1.33
29	d	6059	MGE	O1G-C1A	4.33	1.45	1.33
30	c	6057	DGD	O1G-C1A	4.33	1.45	1.33
23	C	1037	CLA	O2A-CGA	4.33	1.45	1.33
23	b	6016	CLA	O2A-CGA	4.33	1.45	1.33
23	B	1016	CLA	O2A-CGA	4.33	1.45	1.33
23	c	6031	CLA	O2A-CGA	4.33	1.45	1.33
23	A	1003	CLA	O2A-CGA	4.33	1.45	1.33
23	c	6032	CLA	O2A-CGA	4.33	1.45	1.33
30	C	1056	DGD	O1G-C1A	4.33	1.45	1.33
30	c	6056	DGD	O1G-C1A	4.33	1.45	1.33
23	d	6005	CLA	O2A-CGA	4.33	1.45	1.33
23	D	1005	CLA	O2A-CGA	4.34	1.45	1.33
23	C	1032	CLA	O2A-CGA	4.34	1.45	1.33
23	C	1027	CLA	O2A-CGA	4.34	1.45	1.33
29	B	1060	MGE	O1G-C1A	4.34	1.45	1.33
23	B	1010	CLA	C3C-C2C	4.34	1.46	1.36
23	c	6037	CLA	O2A-CGA	4.34	1.45	1.33
29	d	6062	MGE	O1G-C1A	4.34	1.45	1.33
23	b	6010	CLA	C3C-C2C	4.37	1.46	1.36
23	B	1015	CLA	C3C-C2C	4.40	1.46	1.36
23	b	6015	CLA	C3C-C2C	4.40	1.46	1.36
23	a	6007	CLA	C3C-C2C	4.40	1.46	1.36
24	A	1039	PHO	CHC-C4B	4.41	1.50	1.40
24	a	6039	PHO	CHC-C4B	4.42	1.50	1.40
23	A	1007	CLA	C3C-C2C	4.42	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1022	CLA	O2D-CGD	4.43	1.44	1.33
23	b	6022	CLA	O2D-CGD	4.43	1.44	1.33
23	B	1009	CLA	OBD-CAD	4.46	1.28	1.22
23	b	6009	CLA	OBD-CAD	4.52	1.28	1.22
23	B	1019	CLA	C3C-C2C	4.54	1.46	1.36
24	A	1038	PHO	CHC-C1C	4.54	1.47	1.38
24	d	6038	PHO	CHC-C1C	4.54	1.47	1.38
23	b	6019	CLA	C3C-C2C	4.55	1.46	1.36
23	c	6029	CLA	O2D-CGD	4.55	1.44	1.33
23	C	1029	CLA	O2D-CGD	4.56	1.44	1.33
23	c	6029	CLA	C3C-C2C	4.57	1.46	1.36
23	C	1029	CLA	C3C-C2C	4.58	1.46	1.36
23	D	1005	CLA	OBD-CAD	4.59	1.28	1.22
23	b	6013	CLA	OBD-CAD	4.59	1.28	1.22
23	b	6017	CLA	OBD-CAD	4.60	1.28	1.22
23	c	6025	CLA	OBD-CAD	4.60	1.28	1.22
23	a	6003	CLA	OBD-CAD	4.61	1.28	1.22
23	c	6030	CLA	OBD-CAD	4.61	1.28	1.22
23	c	6032	CLA	OBD-CAD	4.61	1.28	1.22
23	A	1003	CLA	OBD-CAD	4.61	1.28	1.22
23	C	1025	CLA	OBD-CAD	4.61	1.28	1.22
23	B	1021	CLA	OBD-CAD	4.61	1.28	1.22
23	a	6006	CLA	OBD-CAD	4.62	1.28	1.22
23	c	6036	CLA	OBD-CAD	4.62	1.28	1.22
23	C	1036	CLA	OBD-CAD	4.62	1.28	1.22
23	D	1008	CLA	OBD-CAD	4.62	1.28	1.22
23	B	1011	CLA	OBD-CAD	4.63	1.28	1.22
23	c	6028	CLA	OBD-CAD	4.63	1.28	1.22
23	d	6005	CLA	OBD-CAD	4.63	1.28	1.22
23	b	6021	CLA	OBD-CAD	4.63	1.28	1.22
23	B	1013	CLA	OBD-CAD	4.64	1.28	1.22
23	d	6008	CLA	OBD-CAD	4.64	1.28	1.22
24	A	1039	PHO	CHC-C1C	4.64	1.47	1.38
23	H	1017	CLA	OBD-CAD	4.64	1.28	1.22
23	b	6011	CLA	OBD-CAD	4.64	1.28	1.22
23	C	1032	CLA	OBD-CAD	4.64	1.28	1.22
23	C	1034	CLA	OBD-CAD	4.65	1.29	1.22
23	C	1030	CLA	OBD-CAD	4.65	1.29	1.22
23	c	6033	CLA	OBD-CAD	4.65	1.29	1.22
23	C	1033	CLA	OBD-CAD	4.65	1.29	1.22
23	b	6020	CLA	OBD-CAD	4.65	1.29	1.22
23	B	1020	CLA	OBD-CAD	4.65	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	6039	PHO	CHC-C1C	4.65	1.47	1.38
23	C	1028	CLA	OBD-CAD	4.65	1.29	1.22
23	C	1037	CLA	OBD-CAD	4.66	1.29	1.22
23	B	1018	CLA	OBD-CAD	4.66	1.29	1.22
23	b	6021	CLA	C3B-C2B	4.66	1.46	1.40
23	b	6018	CLA	OBD-CAD	4.66	1.29	1.22
23	C	1027	CLA	OBD-CAD	4.66	1.29	1.22
23	d	6008	CLA	C3B-C2B	4.67	1.46	1.40
23	c	6037	CLA	OBD-CAD	4.67	1.29	1.22
23	B	1023	CLA	OBD-CAD	4.67	1.29	1.22
23	B	1014	CLA	C3C-C2C	4.67	1.46	1.36
23	b	6014	CLA	C3C-C2C	4.67	1.46	1.36
23	c	6032	CLA	C3B-C2B	4.67	1.46	1.40
23	c	6027	CLA	OBD-CAD	4.67	1.29	1.22
23	A	1007	CLA	O2D-CGD	4.67	1.44	1.33
23	C	1025	CLA	C3B-C2B	4.67	1.46	1.40
23	B	1012	CLA	OBD-CAD	4.68	1.29	1.22
23	a	6007	CLA	O2D-CGD	4.68	1.44	1.33
23	C	1031	CLA	OBD-CAD	4.68	1.29	1.22
23	C	1035	CLA	OBD-CAD	4.69	1.29	1.22
23	B	1016	CLA	C3B-C2B	4.69	1.46	1.40
23	C	1027	CLA	C3B-C2B	4.69	1.46	1.40
23	D	1004	CLA	OBD-CAD	4.69	1.29	1.22
23	b	6012	CLA	C3B-C2B	4.69	1.46	1.40
23	B	1021	CLA	C3B-C2B	4.69	1.46	1.40
23	b	6023	CLA	OBD-CAD	4.69	1.29	1.22
23	b	6012	CLA	OBD-CAD	4.70	1.29	1.22
23	C	1033	CLA	C3B-C2B	4.70	1.46	1.40
23	c	6025	CLA	C3B-C2B	4.70	1.46	1.40
23	B	1016	CLA	OBD-CAD	4.70	1.29	1.22
23	C	1028	CLA	C3B-C2B	4.70	1.46	1.40
23	b	6016	CLA	C3B-C2B	4.70	1.46	1.40
23	b	6019	CLA	OBD-CAD	4.70	1.29	1.22
23	b	6017	CLA	C3B-C2B	4.71	1.46	1.40
23	B	1013	CLA	C3B-C2B	4.71	1.46	1.40
23	D	1004	CLA	C3B-C2B	4.71	1.46	1.40
23	B	1019	CLA	OBD-CAD	4.71	1.29	1.22
23	b	6018	CLA	C3B-C2B	4.71	1.46	1.40
23	B	1024	CLA	O2D-CGD	4.71	1.45	1.33
23	B	1012	CLA	C3B-C2B	4.71	1.46	1.40
23	c	6033	CLA	C3B-C2B	4.71	1.46	1.40
23	b	6024	CLA	O2D-CGD	4.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	1030	CLA	C3B-C2B	4.72	1.46	1.40
23	A	1006	CLA	OBD-CAD	4.72	1.29	1.22
23	B	1011	CLA	C3B-C2B	4.72	1.46	1.40
23	c	6031	CLA	OBD-CAD	4.72	1.29	1.22
23	b	6011	CLA	C3B-C2B	4.72	1.46	1.40
23	c	6036	CLA	C3B-C2B	4.72	1.46	1.40
23	c	6028	CLA	C3B-C2B	4.72	1.46	1.40
23	A	1006	CLA	C3B-C2B	4.73	1.46	1.40
23	B	1018	CLA	C3B-C2B	4.73	1.46	1.40
23	c	6035	CLA	OBD-CAD	4.73	1.29	1.22
23	b	6016	CLA	OBD-CAD	4.73	1.29	1.22
23	A	1003	CLA	C3B-C2B	4.73	1.46	1.40
23	D	1008	CLA	C3B-C2B	4.73	1.46	1.40
23	H	1017	CLA	C3B-C2B	4.73	1.46	1.40
23	b	6013	CLA	C3B-C2B	4.73	1.46	1.40
23	b	6023	CLA	C3B-C2B	4.73	1.46	1.40
23	C	1034	CLA	C3B-C2B	4.73	1.46	1.40
23	C	1032	CLA	C3B-C2B	4.73	1.46	1.40
23	c	6027	CLA	C3B-C2B	4.74	1.46	1.40
23	C	1036	CLA	C3B-C2B	4.74	1.46	1.40
23	c	6030	CLA	C3B-C2B	4.74	1.46	1.40
23	B	1020	CLA	C3B-C2B	4.74	1.46	1.40
23	d	6004	CLA	OBD-CAD	4.74	1.29	1.22
23	d	6005	CLA	C3B-C2B	4.74	1.46	1.40
23	C	1035	CLA	C3B-C2B	4.75	1.46	1.40
23	d	6004	CLA	C3B-C2B	4.75	1.46	1.40
23	B	1023	CLA	C3B-C2B	4.75	1.46	1.40
23	c	6031	CLA	C3B-C2B	4.75	1.46	1.40
23	a	6006	CLA	C3B-C2B	4.76	1.47	1.40
23	C	1037	CLA	C3B-C2B	4.76	1.47	1.40
23	D	1005	CLA	C3B-C2B	4.76	1.47	1.40
23	b	6009	CLA	C3C-C2C	4.76	1.46	1.36
23	a	6003	CLA	C3B-C2B	4.77	1.47	1.40
23	b	6020	CLA	C3B-C2B	4.77	1.47	1.40
23	c	6035	CLA	C3B-C2B	4.77	1.47	1.40
23	B	1009	CLA	C3C-C2C	4.77	1.46	1.36
23	c	6037	CLA	C3B-C2B	4.78	1.47	1.40
23	C	1031	CLA	C3B-C2B	4.78	1.47	1.40
23	b	6017	CLA	C3C-C2C	4.85	1.47	1.36
23	A	1006	CLA	C3C-C2C	4.85	1.47	1.36
23	d	6005	CLA	C3C-C2C	4.85	1.47	1.36
23	c	6027	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	6011	CLA	C3C-C2C	4.86	1.47	1.36
23	D	1005	CLA	C3C-C2C	4.86	1.47	1.36
23	b	6016	CLA	C3C-C2C	4.86	1.47	1.36
23	B	1011	CLA	C3C-C2C	4.86	1.47	1.36
23	B	1009	CLA	C3B-C2B	4.86	1.47	1.40
23	a	6003	CLA	C3C-C2C	4.87	1.47	1.36
23	c	6025	CLA	C3C-C2C	4.87	1.47	1.36
23	c	6028	CLA	C3C-C2C	4.87	1.47	1.36
23	b	6012	CLA	C3C-C2C	4.87	1.47	1.36
23	C	1028	CLA	C3C-C2C	4.87	1.47	1.36
23	b	6018	CLA	C3C-C2C	4.87	1.47	1.36
23	b	6009	CLA	C3B-C2B	4.87	1.47	1.40
23	c	6033	CLA	C3C-C2C	4.87	1.47	1.36
23	B	1021	CLA	C3C-C2C	4.88	1.47	1.36
23	B	1013	CLA	C3C-C2C	4.88	1.47	1.36
23	C	1036	CLA	C3C-C2C	4.88	1.47	1.36
23	c	6031	CLA	C3C-C2C	4.88	1.47	1.36
23	C	1032	CLA	C3C-C2C	4.88	1.47	1.36
23	b	6021	CLA	C3C-C2C	4.88	1.47	1.36
23	B	1018	CLA	C3C-C2C	4.88	1.47	1.36
23	H	1017	CLA	C3C-C2C	4.88	1.47	1.36
23	B	1016	CLA	C3C-C2C	4.88	1.47	1.36
23	C	1030	CLA	C3C-C2C	4.88	1.47	1.36
23	a	6006	CLA	C3C-C2C	4.89	1.47	1.36
23	B	1023	CLA	C3C-C2C	4.89	1.47	1.36
23	A	1003	CLA	C3C-C2C	4.89	1.47	1.36
23	d	6004	CLA	C3C-C2C	4.89	1.47	1.36
23	C	1033	CLA	C3C-C2C	4.89	1.47	1.36
23	B	1012	CLA	C3C-C2C	4.89	1.47	1.36
23	c	6037	CLA	C3C-C2C	4.89	1.47	1.36
23	c	6032	CLA	C3C-C2C	4.89	1.47	1.36
23	d	6008	CLA	C3C-C2C	4.90	1.47	1.36
23	C	1027	CLA	C3C-C2C	4.90	1.47	1.36
23	b	6023	CLA	C3C-C2C	4.90	1.47	1.36
23	C	1034	CLA	C3C-C2C	4.90	1.47	1.36
23	c	6030	CLA	C3C-C2C	4.90	1.47	1.36
23	B	1020	CLA	C3C-C2C	4.90	1.47	1.36
23	b	6013	CLA	C3C-C2C	4.90	1.47	1.36
23	b	6020	CLA	C3C-C2C	4.91	1.47	1.36
23	C	1035	CLA	C3C-C2C	4.91	1.47	1.36
23	D	1008	CLA	C3C-C2C	4.91	1.47	1.36
23	C	1025	CLA	C3C-C2C	4.91	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6036	CLA	C3C-C2C	4.91	1.47	1.36
23	C	1037	CLA	C3C-C2C	4.91	1.47	1.36
23	C	1031	CLA	C3C-C2C	4.91	1.47	1.36
23	B	1009	CLA	O2D-CGD	4.91	1.45	1.33
23	c	6035	CLA	C3C-C2C	4.92	1.47	1.36
23	D	1004	CLA	C3C-C2C	4.92	1.47	1.36
23	b	6009	CLA	O2D-CGD	4.93	1.45	1.33
23	c	6034	CLA	C3B-C2B	4.93	1.47	1.40
23	B	1019	CLA	C3B-C2B	4.96	1.47	1.40
23	c	6034	CLA	C3C-C2C	4.97	1.47	1.36
23	b	6019	CLA	C3B-C2B	4.99	1.47	1.40
23	D	1008	CLA	O2D-CGD	5.01	1.45	1.33
23	b	6023	CLA	O2D-CGD	5.01	1.45	1.33
23	a	6006	CLA	O2D-CGD	5.02	1.45	1.33
23	B	1023	CLA	O2D-CGD	5.02	1.45	1.33
23	b	6017	CLA	O2D-CGD	5.02	1.45	1.33
23	H	1017	CLA	O2D-CGD	5.02	1.45	1.33
23	B	1016	CLA	O2D-CGD	5.02	1.45	1.33
23	d	6008	CLA	O2D-CGD	5.03	1.45	1.33
25	A	1043	PQ9	C22-C23	5.03	1.45	1.33
23	C	1032	CLA	O2D-CGD	5.03	1.45	1.33
23	c	6034	CLA	O2D-CGD	5.03	1.45	1.33
23	c	6032	CLA	O2D-CGD	5.03	1.45	1.33
23	d	6005	CLA	O2D-CGD	5.03	1.45	1.33
23	b	6016	CLA	O2D-CGD	5.03	1.45	1.33
23	c	6025	CLA	O2D-CGD	5.03	1.45	1.33
23	a	6003	CLA	O2D-CGD	5.04	1.45	1.33
23	c	6028	CLA	O2D-CGD	5.04	1.45	1.33
23	c	6030	CLA	O2D-CGD	5.04	1.45	1.33
23	b	6013	CLA	O2D-CGD	5.04	1.45	1.33
23	B	1012	CLA	O2D-CGD	5.04	1.45	1.33
23	A	1003	CLA	O2D-CGD	5.04	1.45	1.33
23	c	6027	CLA	O2D-CGD	5.04	1.45	1.33
23	C	1028	CLA	O2D-CGD	5.04	1.45	1.33
23	D	1005	CLA	O2D-CGD	5.04	1.45	1.33
23	C	1027	CLA	O2D-CGD	5.04	1.45	1.33
23	C	1037	CLA	O2D-CGD	5.04	1.45	1.33
23	B	1013	CLA	O2D-CGD	5.04	1.45	1.33
23	c	6037	CLA	O2D-CGD	5.05	1.45	1.33
23	D	1004	CLA	O2D-CGD	5.05	1.45	1.33
23	C	1031	CLA	O2D-CGD	5.05	1.45	1.33
23	c	6031	CLA	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	6035	CLA	O2D-CGD	5.05	1.45	1.33
23	b	6012	CLA	O2D-CGD	5.05	1.45	1.33
23	A	1006	CLA	O2D-CGD	5.05	1.45	1.33
23	B	1020	CLA	O2D-CGD	5.06	1.45	1.33
23	C	1034	CLA	O2D-CGD	5.06	1.45	1.33
23	B	1018	CLA	O2D-CGD	5.06	1.45	1.33
23	C	1030	CLA	O2D-CGD	5.06	1.45	1.33
23	C	1025	CLA	O2D-CGD	5.06	1.45	1.33
23	c	6033	CLA	O2D-CGD	5.06	1.45	1.33
23	C	1035	CLA	O2D-CGD	5.06	1.45	1.33
23	b	6011	CLA	O2D-CGD	5.06	1.45	1.33
23	B	1011	CLA	O2D-CGD	5.06	1.45	1.33
23	B	1021	CLA	O2D-CGD	5.07	1.45	1.33
23	b	6018	CLA	O2D-CGD	5.07	1.45	1.33
23	C	1036	CLA	O2D-CGD	5.07	1.45	1.33
23	C	1033	CLA	O2D-CGD	5.07	1.45	1.33
23	c	6036	CLA	O2D-CGD	5.07	1.45	1.33
23	d	6004	CLA	O2D-CGD	5.07	1.45	1.33
23	b	6020	CLA	O2D-CGD	5.08	1.45	1.33
23	b	6021	CLA	O2D-CGD	5.08	1.45	1.33
25	a	6043	PQ9	C22-C23	5.34	1.46	1.33
31	E	1040	HEM	C3D-C2D	5.44	1.53	1.37
31	V	1041	HEM	C3D-C2D	5.45	1.53	1.37
31	e	6040	HEM	C3D-C2D	5.45	1.53	1.37
31	v	6041	HEM	C3D-C2D	5.45	1.53	1.37
24	A	1038	PHO	CHD-C1D	5.79	1.49	1.38
24	d	6038	PHO	CHD-C1D	5.82	1.50	1.38
24	A	1038	PHO	C2-C3	5.82	1.47	1.33
24	d	6038	PHO	C2-C3	5.83	1.47	1.33
24	A	1039	PHO	C2-C3	5.88	1.47	1.33
24	a	6039	PHO	C2-C3	5.90	1.47	1.33
24	a	6039	PHO	CHD-C1D	5.95	1.50	1.38
24	A	1039	PHO	CHD-C1D	5.96	1.50	1.38
24	d	6038	PHO	CHB-C1B	6.00	1.50	1.38
24	A	1038	PHO	CHB-C1B	6.02	1.50	1.38
24	a	6039	PHO	CHB-C1B	6.20	1.50	1.38
24	A	1039	PHO	CHB-C1B	6.21	1.50	1.38
24	A	1039	PHO	O1A-CGA	6.38	1.41	1.22
24	a	6039	PHO	O1A-CGA	6.39	1.41	1.22
24	A	1038	PHO	O1A-CGA	6.39	1.41	1.22
24	d	6038	PHO	O1A-CGA	6.41	1.41	1.22
24	d	6038	PHO	C3C-C2C	7.38	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1038	PHO	C3C-C2C	7.40	1.52	1.36
24	a	6039	PHO	C3C-C2C	7.41	1.52	1.36
24	A	1039	PHO	C3C-C2C	7.43	1.52	1.36
25	D	1042	PQ9	C3-C2	7.45	1.54	1.34
25	A	1043	PQ9	C3-C2	7.61	1.54	1.34
25	a	6043	PQ9	C3-C2	7.72	1.55	1.34
25	d	6042	PQ9	C3-C2	7.80	1.55	1.34
25	D	1042	PQ9	C12-C13	8.02	1.52	1.33
25	D	1042	PQ9	C17-C18	8.07	1.52	1.33
24	A	1038	PHO	O1D-CGD	8.09	1.41	1.21
24	A	1039	PHO	O1D-CGD	8.09	1.41	1.21
24	d	6038	PHO	O1D-CGD	8.11	1.41	1.21
24	a	6039	PHO	O1D-CGD	8.12	1.41	1.21
25	d	6042	PQ9	C17-C18	8.35	1.53	1.33
25	d	6042	PQ9	C12-C13	8.36	1.53	1.33
25	A	1043	PQ9	C37-C38	8.40	1.53	1.33
25	A	1043	PQ9	C17-C18	9.09	1.55	1.33
25	A	1043	PQ9	C12-C13	9.13	1.55	1.33
25	a	6043	PQ9	C37-C38	9.15	1.55	1.33
25	d	6042	PQ9	C37-C38	9.29	1.55	1.33
25	a	6043	PQ9	C12-C13	9.63	1.56	1.33
25	D	1042	PQ9	C37-C38	9.66	1.56	1.33
25	a	6043	PQ9	C17-C18	9.73	1.57	1.33
24	d	6038	PHO	OBD-CAD	10.91	1.41	1.22
24	a	6039	PHO	OBD-CAD	10.92	1.41	1.22
24	A	1038	PHO	OBD-CAD	10.93	1.41	1.22
24	A	1039	PHO	OBD-CAD	10.94	1.41	1.22
25	d	6042	PQ9	C27-C28	13.25	1.65	1.33
25	D	1042	PQ9	C27-C28	13.29	1.65	1.33
25	A	1043	PQ9	C27-C28	13.50	1.66	1.33
25	a	6043	PQ9	C27-C28	14.16	1.67	1.33

All (2272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	6042	PQ9	C29-C28-C30	-23.79	74.25	115.29
25	D	1042	PQ9	C29-C28-C30	-23.27	75.15	115.29
25	a	6043	PQ9	C29-C28-C30	-21.18	78.75	115.29
25	A	1043	PQ9	C29-C28-C30	-20.21	80.43	115.29
26	z	6053	BCR	C40-C30-C25	-15.89	84.54	110.31
26	Z	1053	BCR	C40-C30-C25	-15.89	84.55	110.31
25	d	6042	PQ9	C29-C28-C27	-15.14	83.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1038	PHO	CAC-C3C-C4C	-15.09	108.98	125.19
24	d	6038	PHO	CAC-C3C-C4C	-15.09	108.99	125.19
25	D	1042	PQ9	C29-C28-C27	-15.06	84.13	123.70
25	a	6043	PQ9	C29-C28-C27	-14.99	84.33	123.70
24	A	1039	PHO	CAC-C3C-C4C	-14.62	109.48	125.19
24	a	6039	PHO	CAC-C3C-C4C	-14.62	109.49	125.19
25	A	1043	PQ9	C29-C28-C27	-14.04	86.83	123.70
24	a	6039	PHO	CMC-C2C-C1C	-10.11	109.41	125.05
24	A	1039	PHO	CMC-C2C-C1C	-10.09	109.45	125.05
23	B	1019	CLA	C1C-NC-C4C	-9.77	101.55	107.05
23	b	6019	CLA	C1C-NC-C4C	-9.72	101.58	107.05
24	A	1039	PHO	CAC-C3C-C2C	-9.69	111.01	127.51
24	a	6039	PHO	CAC-C3C-C2C	-9.68	111.02	127.51
24	A	1038	PHO	CMC-C2C-C1C	-9.48	110.39	125.05
24	d	6038	PHO	CMC-C2C-C1C	-9.47	110.40	125.05
23	b	6024	CLA	C1C-NC-C4C	-9.23	101.85	107.05
23	B	1024	CLA	C1C-NC-C4C	-9.22	101.86	107.05
23	C	1026	CLA	C1C-NC-C4C	-9.03	101.97	107.05
25	A	1043	PQ9	C11-C12-C13	-9.02	111.51	126.79
23	c	6026	CLA	C1C-NC-C4C	-9.01	101.97	107.05
23	B	1009	CLA	C1C-NC-C4C	-8.82	102.08	107.05
23	b	6009	CLA	C1C-NC-C4C	-8.77	102.11	107.05
24	A	1039	PHO	CMD-C2D-C3D	-8.71	108.04	127.89
24	a	6039	PHO	CMD-C2D-C3D	-8.71	108.04	127.89
24	d	6038	PHO	CMD-C2D-C3D	-8.70	108.06	127.89
24	A	1038	PHO	CMD-C2D-C3D	-8.70	108.07	127.89
25	a	6043	PQ9	C11-C12-C13	-8.46	112.45	126.79
23	b	6022	CLA	C1C-NC-C4C	-8.32	102.36	107.05
23	B	1022	CLA	C1C-NC-C4C	-8.31	102.37	107.05
23	b	6011	CLA	C1C-NC-C4C	-8.26	102.40	107.05
23	b	6018	CLA	C1C-NC-C4C	-8.24	102.41	107.05
23	d	6008	CLA	C1C-NC-C4C	-8.23	102.41	107.05
23	C	1030	CLA	C1C-NC-C4C	-8.23	102.42	107.05
23	b	6014	CLA	C1C-NC-C4C	-8.22	102.42	107.05
23	H	1017	CLA	C1C-NC-C4C	-8.22	102.42	107.05
23	B	1018	CLA	C1C-NC-C4C	-8.22	102.42	107.05
23	B	1014	CLA	C1C-NC-C4C	-8.22	102.42	107.05
23	C	1034	CLA	C1C-NC-C4C	-8.21	102.43	107.05
25	d	6042	PQ9	C11-C12-C13	-8.21	112.89	126.79
23	C	1033	CLA	C1C-NC-C4C	-8.20	102.43	107.05
23	D	1008	CLA	C1C-NC-C4C	-8.19	102.44	107.05
23	c	6033	CLA	C1C-NC-C4C	-8.18	102.44	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1023	CLA	C1C-NC-C4C	-8.18	102.44	107.05
23	c	6036	CLA	C1C-NC-C4C	-8.18	102.44	107.05
23	c	6027	CLA	C1C-NC-C4C	-8.17	102.45	107.05
23	b	6017	CLA	C1C-NC-C4C	-8.17	102.45	107.05
23	C	1035	CLA	C1C-NC-C4C	-8.17	102.45	107.05
23	c	6030	CLA	C1C-NC-C4C	-8.17	102.45	107.05
23	b	6023	CLA	C1C-NC-C4C	-8.16	102.45	107.05
23	C	1028	CLA	C1C-NC-C4C	-8.16	102.45	107.05
23	B	1011	CLA	C1C-NC-C4C	-8.16	102.46	107.05
23	A	1003	CLA	C1C-NC-C4C	-8.15	102.46	107.05
23	c	6032	CLA	C1C-NC-C4C	-8.15	102.46	107.05
24	d	6038	PHO	CAC-C3C-C2C	-8.15	113.64	127.51
23	B	1020	CLA	C1C-NC-C4C	-8.15	102.46	107.05
23	a	6003	CLA	C1C-NC-C4C	-8.14	102.46	107.05
23	C	1032	CLA	C1C-NC-C4C	-8.14	102.46	107.05
23	d	6004	CLA	C1C-NC-C4C	-8.14	102.46	107.05
23	B	1013	CLA	C1C-NC-C4C	-8.14	102.46	107.05
23	c	6028	CLA	C1C-NC-C4C	-8.14	102.47	107.05
24	A	1038	PHO	CAC-C3C-C2C	-8.14	113.66	127.51
23	b	6016	CLA	C1C-NC-C4C	-8.13	102.47	107.05
23	A	1006	CLA	C1C-NC-C4C	-8.13	102.47	107.05
23	C	1025	CLA	C1C-NC-C4C	-8.12	102.47	107.05
23	c	6031	CLA	C1C-NC-C4C	-8.12	102.48	107.05
23	a	6006	CLA	C1C-NC-C4C	-8.12	102.48	107.05
23	b	6020	CLA	C1C-NC-C4C	-8.12	102.48	107.05
23	D	1004	CLA	C1C-NC-C4C	-8.12	102.48	107.05
23	C	1037	CLA	C1C-NC-C4C	-8.11	102.48	107.05
23	b	6012	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	C	1031	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	D	1005	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	d	6005	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	B	1012	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	C	1036	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	c	6035	CLA	C1C-NC-C4C	-8.10	102.49	107.05
23	c	6025	CLA	C1C-NC-C4C	-8.09	102.49	107.05
23	C	1027	CLA	C1C-NC-C4C	-8.09	102.49	107.05
23	B	1021	CLA	C1C-NC-C4C	-8.08	102.50	107.05
23	b	6013	CLA	C1C-NC-C4C	-8.08	102.50	107.05
23	b	6021	CLA	C1C-NC-C4C	-8.07	102.51	107.05
23	B	1016	CLA	C1C-NC-C4C	-8.06	102.51	107.05
23	c	6034	CLA	C1C-NC-C4C	-8.04	102.52	107.05
23	c	6037	CLA	C1C-NC-C4C	-8.04	102.52	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1007	CLA	C1C-NC-C4C	-7.98	102.56	107.05
23	a	6007	CLA	C1C-NC-C4C	-7.92	102.59	107.05
23	C	1029	CLA	C1C-NC-C4C	-7.82	102.65	107.05
23	c	6029	CLA	C1C-NC-C4C	-7.81	102.65	107.05
23	b	6015	CLA	C1C-NC-C4C	-7.76	102.68	107.05
23	b	6010	CLA	C1C-NC-C4C	-7.72	102.70	107.05
23	B	1015	CLA	C1C-NC-C4C	-7.71	102.71	107.05
23	B	1010	CLA	C1C-NC-C4C	-7.71	102.71	107.05
25	D	1042	PQ9	C11-C12-C13	-7.70	113.75	126.79
26	Z	1053	BCR	C40-C30-C39	-7.53	85.80	108.52
26	z	6053	BCR	C40-C30-C39	-7.52	85.82	108.52
26	T	6046	BCR	C30-C25-C26	-6.41	113.58	122.59
25	D	1042	PQ9	C16-C17-C18	-6.36	111.92	127.66
23	c	6029	CLA	O1D-CGD-CBD	-6.33	112.84	124.58
26	A	1044	BCR	C30-C25-C26	-6.32	113.71	122.59
25	d	6042	PQ9	C16-C17-C18	-6.30	112.08	127.66
23	C	1029	CLA	O1D-CGD-CBD	-6.30	112.90	124.58
26	a	6044	BCR	C30-C25-C26	-6.29	113.75	122.59
23	b	6019	CLA	O2D-CGD-O1D	-6.16	111.60	123.82
23	B	1019	CLA	O2D-CGD-O1D	-6.15	111.61	123.82
26	t	1046	BCR	C30-C25-C26	-6.00	114.17	122.59
26	d	6050	BCR	C33-C5-C6	-5.94	117.86	124.51
26	D	1050	BCR	C33-C5-C6	-5.92	117.88	124.51
26	z	6053	BCR	C40-C30-C29	-5.90	85.77	108.78
26	Z	1053	BCR	C40-C30-C29	-5.90	85.78	108.78
26	T	6046	BCR	C1-C6-C5	-5.72	114.55	122.59
23	B	1010	CLA	O1D-CGD-CBD	-5.64	114.12	124.58
23	b	6010	CLA	O1D-CGD-CBD	-5.61	114.17	124.58
23	b	6015	CLA	O1D-CGD-CBD	-5.56	114.27	124.58
23	B	1015	CLA	O1D-CGD-CBD	-5.54	114.30	124.58
24	A	1039	PHO	CMC-C2C-C3C	-5.50	111.00	126.11
24	a	6039	PHO	CMC-C2C-C3C	-5.48	111.03	126.11
23	b	6015	CLA	CAA-C2A-C1A	-5.44	94.14	111.97
23	B	1015	CLA	CAA-C2A-C1A	-5.44	94.14	111.97
23	B	1014	CLA	O1D-CGD-CBD	-5.44	114.50	124.58
23	b	6014	CLA	O1D-CGD-CBD	-5.43	114.52	124.58
26	T	6046	BCR	C4-C5-C6	-5.40	114.81	122.74
26	T	6046	BCR	C28-C27-C26	-5.38	104.55	113.99
26	d	6050	BCR	C11-C10-C9	-5.28	119.78	127.31
26	D	1050	BCR	C11-C10-C9	-5.26	119.80	127.31
26	K	1051	BCR	C33-C5-C6	-5.24	118.64	124.51
26	k	6051	BCR	C33-C5-C6	-5.21	118.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	1051	BCR	C15-C14-C13	-5.21	119.88	127.31
23	A	1007	CLA	O1D-CGD-CBD	-5.20	114.94	124.58
23	a	6007	CLA	O1D-CGD-CBD	-5.19	114.96	124.58
26	T	6046	BCR	C15-C14-C13	-5.18	119.91	127.31
26	k	6051	BCR	C15-C14-C13	-5.18	119.92	127.31
26	h	6049	BCR	C15-C14-C13	-5.17	119.92	127.31
26	z	6053	BCR	C11-C10-C9	-5.15	119.96	127.31
26	B	1045	BCR	C11-C10-C9	-5.15	119.97	127.31
26	H	1049	BCR	C11-C10-C9	-5.14	119.97	127.31
26	b	6045	BCR	C11-C10-C9	-5.14	119.97	127.31
26	H	1049	BCR	C15-C14-C13	-5.14	119.97	127.31
26	h	6049	BCR	C11-C10-C9	-5.14	119.98	127.31
26	C	1054	BCR	C15-C14-C13	-5.13	119.98	127.31
26	c	6054	BCR	C15-C14-C13	-5.13	119.98	127.31
26	k	6052	BCR	C11-C10-C9	-5.13	119.99	127.31
26	t	1046	BCR	C11-C10-C9	-5.13	119.99	127.31
26	K	1052	BCR	C15-C14-C13	-5.12	120.00	127.31
23	b	6022	CLA	C1C-C2C-C3C	-5.12	101.45	106.93
26	B	1045	BCR	C15-C14-C13	-5.11	120.02	127.31
26	K	1052	BCR	C11-C10-C9	-5.11	120.02	127.31
26	Z	1053	BCR	C11-C10-C9	-5.11	120.02	127.31
26	Z	1053	BCR	C15-C14-C13	-5.11	120.02	127.31
26	k	6052	BCR	C15-C14-C13	-5.11	120.02	127.31
26	t	1046	BCR	C15-C14-C13	-5.11	120.02	127.31
26	b	6045	BCR	C15-C14-C13	-5.10	120.03	127.31
26	z	6053	BCR	C15-C14-C13	-5.10	120.03	127.31
23	B	1022	CLA	C1C-C2C-C3C	-5.09	101.48	106.93
26	c	6054	BCR	C33-C5-C6	-5.02	118.89	124.51
26	C	1054	BCR	C33-C5-C6	-4.99	118.92	124.51
26	d	6050	BCR	C15-C14-C13	-4.98	120.20	127.31
26	D	1050	BCR	C15-C14-C13	-4.97	120.22	127.31
24	A	1038	PHO	CMC-C2C-C3C	-4.96	112.47	126.11
24	d	6038	PHO	CMC-C2C-C3C	-4.95	112.49	126.11
26	b	6048	BCR	C38-C26-C25	-4.94	118.97	124.51
26	B	1048	BCR	C38-C26-C25	-4.93	118.99	124.51
23	C	1026	CLA	O1D-CGD-CBD	-4.91	115.47	124.58
23	c	6026	CLA	O1D-CGD-CBD	-4.90	115.48	124.58
23	B	1019	CLA	CHD-C4C-C3C	-4.89	117.66	124.88
23	b	6019	CLA	CHD-C4C-C3C	-4.87	117.69	124.88
23	c	6029	CLA	C1C-C2C-C3C	-4.85	101.74	106.93
23	C	1029	CLA	C1C-C2C-C3C	-4.85	101.74	106.93
26	k	6051	BCR	C11-C10-C9	-4.79	120.48	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	1051	BCR	C11-C10-C9	-4.79	120.48	127.31
26	T	6046	BCR	C11-C10-C9	-4.76	120.51	127.31
26	B	1048	BCR	C33-C5-C6	-4.71	119.23	124.51
26	b	6048	BCR	C33-C5-C6	-4.68	119.27	124.51
26	t	1046	BCR	C28-C27-C26	-4.67	105.80	113.99
25	d	6042	PQ9	C39-C38-C37	-4.66	111.44	123.70
26	b	6048	BCR	C11-C10-C9	-4.66	120.66	127.31
26	B	1048	BCR	C11-C10-C9	-4.64	120.68	127.31
26	B	1048	BCR	C24-C23-C22	-4.64	119.24	126.21
26	b	6048	BCR	C24-C23-C22	-4.64	119.24	126.21
23	B	1022	CLA	O2A-CGA-O1A	-4.63	112.28	123.58
23	b	6022	CLA	O2A-CGA-O1A	-4.63	112.29	123.58
26	B	1047	BCR	C33-C5-C6	-4.61	119.35	124.51
25	D	1042	PQ9	C31-C32-C33	-4.60	116.28	127.66
26	b	6047	BCR	C33-C5-C6	-4.57	119.39	124.51
26	C	1054	BCR	C24-C23-C22	-4.55	119.38	126.21
26	c	6054	BCR	C24-C23-C22	-4.53	119.41	126.21
26	K	1051	BCR	C30-C25-C26	-4.50	116.27	122.59
26	B	1047	BCR	C11-C10-C9	-4.49	120.90	127.31
23	B	1014	CLA	C1C-C2C-C3C	-4.49	102.13	106.93
23	c	6029	CLA	O2D-CGD-O1D	-4.48	114.92	123.82
23	C	1029	CLA	O2D-CGD-O1D	-4.48	114.92	123.82
23	b	6010	CLA	C2A-C1A-CHA	-4.48	116.04	123.92
23	B	1010	CLA	C2A-C1A-CHA	-4.48	116.04	123.92
26	b	6047	BCR	C11-C10-C9	-4.47	120.92	127.31
23	b	6010	CLA	C1C-C2C-C3C	-4.47	102.14	106.93
23	c	6034	CLA	CHD-C4C-C3C	-4.47	118.28	124.88
26	T	6046	BCR	C27-C26-C25	-4.47	116.18	122.74
26	c	6054	BCR	C30-C25-C26	-4.46	116.33	122.59
26	k	6051	BCR	C30-C25-C26	-4.46	116.33	122.59
25	D	1042	PQ9	C39-C38-C37	-4.45	112.00	123.70
23	B	1010	CLA	C1C-C2C-C3C	-4.45	102.16	106.93
23	b	6014	CLA	C1C-C2C-C3C	-4.45	102.17	106.93
23	A	1007	CLA	CHD-C4C-C3C	-4.43	118.34	124.88
23	a	6007	CLA	CHD-C4C-C3C	-4.42	118.35	124.88
26	C	1054	BCR	C30-C25-C26	-4.42	116.38	122.59
23	C	1026	CLA	CHD-C4C-C3C	-4.39	118.40	124.88
23	c	6026	CLA	CHD-C4C-C3C	-4.37	118.42	124.88
23	b	6024	CLA	C1C-C2C-C3C	-4.37	102.26	106.93
25	a	6043	PQ9	C20-C21-C22	-4.35	97.31	111.87
23	B	1024	CLA	C1C-C2C-C3C	-4.35	102.28	106.93
23	A	1007	CLA	C1C-C2C-C3C	-4.34	102.29	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6007	CLA	C1C-C2C-C3C	-4.33	102.30	106.93
23	B	1015	CLA	O2D-CGD-O1D	-4.31	115.26	123.82
23	b	6015	CLA	O2D-CGD-O1D	-4.30	115.29	123.82
26	C	1054	BCR	C11-C10-C9	-4.29	121.18	127.31
23	B	1014	CLA	CHD-C4C-C3C	-4.27	118.58	124.88
26	c	6054	BCR	C11-C10-C9	-4.27	121.22	127.31
23	B	1022	CLA	CHD-C4C-C3C	-4.26	118.59	124.88
25	d	6042	PQ9	C31-C32-C33	-4.26	117.11	127.66
23	b	6014	CLA	CHD-C4C-C3C	-4.26	118.59	124.88
23	b	6022	CLA	CHD-C4C-C3C	-4.26	118.60	124.88
26	b	6047	BCR	C15-C14-C13	-4.25	121.25	127.31
26	D	1050	BCR	C38-C26-C25	-4.25	119.75	124.51
26	B	1047	BCR	C15-C14-C13	-4.24	121.26	127.31
23	c	6029	CLA	C2A-C1A-CHA	-4.23	116.48	123.92
23	c	6034	CLA	C1C-C2C-C3C	-4.22	102.41	106.93
23	C	1029	CLA	C2A-C1A-CHA	-4.22	116.50	123.92
23	B	1010	CLA	O2A-CGA-O1A	-4.21	113.30	123.58
23	B	1022	CLA	C2A-C1A-CHA	-4.21	116.51	123.92
23	b	6010	CLA	O2A-CGA-O1A	-4.21	113.31	123.58
23	C	1026	CLA	C1C-C2C-C3C	-4.21	102.43	106.93
26	d	6050	BCR	C38-C26-C25	-4.21	119.80	124.51
26	t	1046	BCR	C27-C26-C25	-4.21	116.57	122.74
23	c	6026	CLA	C1C-C2C-C3C	-4.20	102.43	106.93
23	b	6022	CLA	C2A-C1A-CHA	-4.20	116.53	123.92
23	b	6015	CLA	CAA-C2A-C3A	-4.19	101.32	112.81
23	B	1015	CLA	CAA-C2A-C3A	-4.19	101.33	112.81
26	B	1048	BCR	C15-C14-C13	-4.18	121.34	127.31
25	A	1043	PQ9	C20-C21-C22	-4.17	97.90	111.87
26	h	6049	BCR	C24-C23-C22	-4.17	119.95	126.21
26	z	6053	BCR	C24-C23-C22	-4.16	119.96	126.21
26	b	6048	BCR	C15-C14-C13	-4.16	121.38	127.31
26	H	1049	BCR	C24-C23-C22	-4.15	119.97	126.21
26	Z	1053	BCR	C24-C23-C22	-4.15	119.97	126.21
23	C	1026	CLA	CAA-CBA-CGA	-4.15	100.96	113.35
23	c	6026	CLA	CAA-CBA-CGA	-4.15	100.97	113.35
23	B	1024	CLA	O1D-CGD-CBD	-4.14	116.90	124.58
26	B	1045	BCR	C30-C25-C26	-4.14	116.78	122.59
23	b	6024	CLA	O1D-CGD-CBD	-4.14	116.91	124.58
24	a	6039	PHO	C3D-C2D-C1D	-4.13	99.66	105.85
26	b	6045	BCR	C30-C25-C26	-4.13	116.79	122.59
26	k	6052	BCR	C24-C23-C22	-4.12	120.02	126.21
26	K	1052	BCR	C24-C23-C22	-4.11	120.03	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1039	PHO	C3D-C2D-C1D	-4.11	99.69	105.85
23	c	6026	CLA	O2D-CGD-O1D	-4.11	115.66	123.82
23	C	1026	CLA	O2D-CGD-O1D	-4.10	115.67	123.82
25	d	6042	PQ9	C2-C3-C4	-4.09	114.17	122.47
23	b	6009	CLA	C1C-C2C-C3C	-4.09	102.56	106.93
23	B	1009	CLA	C1C-C2C-C3C	-4.07	102.57	106.93
26	A	1044	BCR	C28-C27-C26	-4.07	106.85	113.99
23	c	6026	CLA	O2A-CGA-O1A	-4.07	113.66	123.58
26	z	6053	BCR	C33-C5-C6	-4.07	119.95	124.51
26	h	6049	BCR	C33-C5-C6	-4.07	119.96	124.51
24	A	1039	PHO	C4C-C3C-C2C	-4.07	102.28	106.80
23	b	6013	CLA	C1C-C2C-C3C	-4.06	102.58	106.93
23	C	1026	CLA	O2A-CGA-O1A	-4.06	113.68	123.58
26	a	6044	BCR	C28-C27-C26	-4.06	106.88	113.99
26	Z	1053	BCR	C33-C5-C6	-4.05	119.97	124.51
26	b	6047	BCR	C24-C23-C22	-4.05	120.12	126.21
25	D	1042	PQ9	C2-C3-C4	-4.05	114.25	122.47
26	k	6052	BCR	C33-C5-C6	-4.05	119.97	124.51
26	z	6053	BCR	C38-C26-C25	-4.04	119.98	124.51
26	Z	1053	BCR	C38-C26-C25	-4.04	119.99	124.51
26	h	6049	BCR	C38-C26-C25	-4.04	119.99	124.51
24	a	6039	PHO	C4C-C3C-C2C	-4.04	102.31	106.80
26	H	1049	BCR	C33-C5-C6	-4.04	119.99	124.51
23	c	6035	CLA	C1C-C2C-C3C	-4.04	102.61	106.93
26	t	1046	BCR	C33-C5-C6	-4.03	119.99	124.51
23	c	6025	CLA	C1C-C2C-C3C	-4.03	102.61	106.93
26	H	1049	BCR	C38-C26-C25	-4.03	120.00	124.51
26	b	6045	BCR	C33-C5-C6	-4.03	120.00	124.51
23	B	1019	CLA	O1D-CGD-CBD	-4.03	117.11	124.58
23	B	1013	CLA	C1C-C2C-C3C	-4.03	102.62	106.93
23	C	1025	CLA	C1C-C2C-C3C	-4.03	102.62	106.93
25	a	6043	PQ9	C2-C3-C4	-4.02	114.32	122.47
23	D	1004	CLA	C1C-C2C-C3C	-4.02	102.63	106.93
23	C	1032	CLA	C1C-C2C-C3C	-4.02	102.63	106.93
26	B	1045	BCR	C33-C5-C6	-4.02	120.01	124.51
23	b	6019	CLA	O1D-CGD-CBD	-4.02	117.13	124.58
26	B	1045	BCR	C38-C26-C25	-4.02	120.01	124.51
23	D	1008	CLA	C1C-C2C-C3C	-4.02	102.63	106.93
23	c	6036	CLA	C1C-C2C-C3C	-4.02	102.63	106.93
26	b	6045	BCR	C38-C26-C25	-4.02	120.01	124.51
26	K	1052	BCR	C38-C26-C25	-4.01	120.01	124.51
23	d	6008	CLA	C1C-C2C-C3C	-4.01	102.64	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1035	CLA	C1C-C2C-C3C	-4.01	102.64	106.93
26	K	1052	BCR	C33-C5-C6	-4.01	120.02	124.51
23	B	1020	CLA	C1C-C2C-C3C	-4.01	102.64	106.93
23	c	6032	CLA	C1C-C2C-C3C	-4.00	102.64	106.93
26	B	1047	BCR	C24-C23-C22	-4.00	120.20	126.21
23	C	1033	CLA	C1C-C2C-C3C	-4.00	102.65	106.93
23	c	6030	CLA	C1C-C2C-C3C	-4.00	102.65	106.93
23	B	1023	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	a	6006	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	C	1028	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	c	6033	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	c	6037	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
26	k	6052	BCR	C38-C26-C25	-3.99	120.04	124.51
23	b	6020	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	C	1031	CLA	C1C-C2C-C3C	-3.99	102.66	106.93
23	d	6005	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	b	6023	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	B	1018	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	B	1019	CLA	C2A-C1A-CHA	-3.98	116.92	123.92
23	d	6004	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	b	6009	CLA	CHD-C4C-C3C	-3.98	119.01	124.88
23	C	1037	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	C	1027	CLA	C1C-C2C-C3C	-3.98	102.67	106.93
23	c	6028	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	B	1011	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	B	1009	CLA	CHD-C4C-C3C	-3.97	119.01	124.88
23	C	1036	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	b	6019	CLA	C2A-C1A-CHA	-3.97	116.93	123.92
23	H	1017	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	B	1015	CLA	CHD-C4C-C3C	-3.97	119.02	124.88
23	c	6027	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	B	1012	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	c	6031	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	B	1019	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	b	6017	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	C	1034	CLA	C1C-C2C-C3C	-3.97	102.68	106.93
23	b	6016	CLA	C1C-C2C-C3C	-3.96	102.69	106.93
23	C	1030	CLA	C1C-C2C-C3C	-3.96	102.69	106.93
23	b	6011	CLA	C1C-C2C-C3C	-3.96	102.69	106.93
23	B	1016	CLA	C1C-C2C-C3C	-3.96	102.69	106.93
23	b	6015	CLA	CHD-C4C-C3C	-3.96	119.04	124.88
23	b	6021	CLA	C1C-C2C-C3C	-3.96	102.69	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	1005	CLA	C1C-C2C-C3C	-3.96	102.69	106.93
23	A	1003	CLA	C1C-C2C-C3C	-3.96	102.70	106.93
23	b	6012	CLA	C1C-C2C-C3C	-3.95	102.70	106.93
23	B	1021	CLA	C1C-C2C-C3C	-3.95	102.70	106.93
23	C	1029	CLA	CHD-C4C-C3C	-3.95	119.06	124.88
23	B	1024	CLA	C1-C2-C3	-3.94	118.70	125.96
23	c	6029	CLA	CHD-C4C-C3C	-3.94	119.06	124.88
23	A	1006	CLA	C1C-C2C-C3C	-3.94	102.71	106.93
23	b	6018	CLA	C1C-C2C-C3C	-3.94	102.71	106.93
23	a	6003	CLA	C1C-C2C-C3C	-3.94	102.71	106.93
24	d	6038	PHO	C3D-C2D-C1D	-3.93	99.96	105.85
24	A	1038	PHO	C3D-C2D-C1D	-3.93	99.96	105.85
23	b	6019	CLA	C1C-C2C-C3C	-3.93	102.72	106.93
25	A	1043	PQ9	C2-C3-C4	-3.93	114.51	122.47
23	b	6024	CLA	C1-C2-C3	-3.93	118.72	125.96
23	b	6010	CLA	O2D-CGD-O1D	-3.89	116.09	123.82
23	B	1010	CLA	O2D-CGD-O1D	-3.89	116.09	123.82
23	b	6024	CLA	O2D-CGD-O1D	-3.89	116.10	123.82
23	b	6013	CLA	CHD-C4C-C3C	-3.88	119.15	124.88
23	C	1034	CLA	CHD-C4C-C3C	-3.88	119.15	124.88
23	B	1024	CLA	O2D-CGD-O1D	-3.88	116.12	123.82
23	C	1025	CLA	CHD-C4C-C3C	-3.88	119.15	124.88
23	c	6030	CLA	CHD-C4C-C3C	-3.88	119.16	124.88
23	a	6003	CLA	CHD-C4C-C3C	-3.88	119.16	124.88
23	c	6034	CLA	C1-C2-C3	-3.87	118.82	125.96
23	B	1012	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	A	1003	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	C	1033	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	C	1030	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	c	6025	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	C	1037	CLA	CHD-C4C-C3C	-3.87	119.17	124.88
23	c	6031	CLA	CHD-C4C-C3C	-3.86	119.18	124.88
23	b	6017	CLA	CHD-C4C-C3C	-3.86	119.18	124.88
26	A	1044	BCR	C3-C4-C5	-3.86	107.22	113.99
23	C	1029	CLA	C1-C2-C3	-3.86	118.85	125.96
23	B	1023	CLA	CHD-C4C-C3C	-3.86	119.19	124.88
23	B	1013	CLA	CHD-C4C-C3C	-3.85	119.19	124.88
23	B	1016	CLA	CHD-C4C-C3C	-3.85	119.19	124.88
23	C	1031	CLA	CHD-C4C-C3C	-3.85	119.19	124.88
23	B	1015	CLA	C1C-C2C-C3C	-3.85	102.81	106.93
23	H	1017	CLA	CHD-C4C-C3C	-3.85	119.19	124.88
23	a	6006	CLA	CHD-C4C-C3C	-3.85	119.19	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6011	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
26	a	6044	BCR	C3-C4-C5	-3.85	107.24	113.99
23	D	1004	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
23	b	6015	CLA	C1C-C2C-C3C	-3.85	102.81	106.93
23	c	6037	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
23	b	6018	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
23	C	1028	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
23	c	6027	CLA	CHD-C4C-C3C	-3.85	119.20	124.88
23	B	1019	CLA	CMA-C3A-C4A	-3.84	101.44	111.77
23	B	1011	CLA	CHD-C4C-C3C	-3.84	119.21	124.88
23	c	6029	CLA	C1-C2-C3	-3.84	118.88	125.96
23	b	6019	CLA	CMA-C3A-C4A	-3.84	101.45	111.77
23	c	6036	CLA	CHD-C4C-C3C	-3.84	119.21	124.88
23	d	6004	CLA	CHD-C4C-C3C	-3.84	119.21	124.88
23	C	1036	CLA	CHD-C4C-C3C	-3.84	119.21	124.88
23	B	1018	CLA	CHD-C4C-C3C	-3.84	119.21	124.88
23	c	6033	CLA	CHD-C4C-C3C	-3.84	119.22	124.88
23	B	1021	CLA	CHD-C4C-C3C	-3.84	119.22	124.88
23	b	6023	CLA	CHD-C4C-C3C	-3.83	119.22	124.88
23	B	1020	CLA	CHD-C4C-C3C	-3.83	119.22	124.88
23	C	1027	CLA	CHD-C4C-C3C	-3.83	119.22	124.88
23	D	1008	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	b	6012	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	A	1006	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	c	6035	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	c	6028	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	D	1005	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	b	6016	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	C	1035	CLA	CHD-C4C-C3C	-3.83	119.23	124.88
23	c	6032	CLA	CHD-C4C-C3C	-3.82	119.23	124.88
23	C	1032	CLA	CHD-C4C-C3C	-3.82	119.24	124.88
23	b	6021	CLA	CHD-C4C-C3C	-3.82	119.25	124.88
23	d	6008	CLA	CHD-C4C-C3C	-3.81	119.25	124.88
23	b	6020	CLA	CHD-C4C-C3C	-3.81	119.26	124.88
26	a	6044	BCR	C15-C14-C13	-3.81	121.88	127.31
23	d	6005	CLA	CHD-C4C-C3C	-3.79	119.28	124.88
26	D	1050	BCR	C30-C25-C26	-3.79	117.27	122.59
26	c	6054	BCR	C38-C26-C25	-3.78	120.27	124.51
26	d	6050	BCR	C30-C25-C26	-3.78	117.28	122.59
26	A	1044	BCR	C15-C14-C13	-3.77	121.93	127.31
25	a	6043	PQ9	C14-C13-C12	-3.77	113.80	123.70
26	B	1047	BCR	C38-C26-C25	-3.76	120.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	1054	BCR	C38-C26-C25	-3.76	120.30	124.51
25	d	6042	PQ9	C35-C36-C37	-3.76	99.29	111.87
26	b	6047	BCR	C38-C26-C25	-3.75	120.31	124.51
23	B	1010	CLA	C1-C2-C3	-3.74	119.06	125.96
23	b	6010	CLA	C1-C2-C3	-3.74	119.06	125.96
26	T	6046	BCR	C3-C4-C5	-3.73	107.46	113.99
26	K	1051	BCR	C38-C26-C25	-3.72	120.35	124.51
23	b	6015	CLA	C2A-C1A-CHA	-3.71	117.38	123.92
25	D	1042	PQ9	C35-C36-C37	-3.71	99.44	111.87
23	B	1015	CLA	C2A-C1A-CHA	-3.70	117.40	123.92
23	B	1014	CLA	C1-C2-C3	-3.70	119.13	125.96
26	k	6051	BCR	C38-C26-C25	-3.70	120.36	124.51
23	b	6014	CLA	C1-C2-C3	-3.68	119.17	125.96
23	a	6007	CLA	O2D-CGD-O1D	-3.68	116.51	123.82
23	A	1007	CLA	O2D-CGD-O1D	-3.67	116.53	123.82
26	b	6045	BCR	C37-C22-C21	-3.67	117.78	122.92
25	a	6043	PQ9	C19-C18-C17	-3.66	114.08	123.70
26	B	1045	BCR	C37-C22-C21	-3.66	117.80	122.92
25	A	1043	PQ9	C11-C2-C3	-3.66	118.43	123.27
25	d	6042	PQ9	C26-C27-C28	-3.63	118.68	127.66
23	B	1022	CLA	CAA-C2A-C1A	-3.62	100.10	111.97
23	b	6022	CLA	CAA-C2A-C1A	-3.62	100.12	111.97
24	d	6038	PHO	OBD-CAD-C3D	-3.61	119.63	128.47
23	B	1014	CLA	O2A-CGA-O1A	-3.61	114.78	123.58
24	A	1038	PHO	OBD-CAD-C3D	-3.61	119.63	128.47
23	b	6014	CLA	O2A-CGA-O1A	-3.61	114.78	123.58
25	A	1043	PQ9	C19-C18-C17	-3.61	114.23	123.70
25	a	6043	PQ9	C11-C2-C3	-3.60	118.51	123.27
25	A	1043	PQ9	C14-C13-C12	-3.59	114.26	123.70
23	B	1024	CLA	CHD-C4C-C3C	-3.59	119.59	124.88
26	A	1044	BCR	C1-C6-C5	-3.58	117.56	122.59
23	b	6024	CLA	CHD-C4C-C3C	-3.56	119.62	124.88
26	a	6044	BCR	C1-C6-C5	-3.55	117.61	122.59
23	b	6010	CLA	CHD-C4C-C3C	-3.54	119.65	124.88
23	B	1010	CLA	CHD-C4C-C3C	-3.54	119.65	124.88
23	b	6014	CLA	O2D-CGD-O1D	-3.54	116.79	123.82
24	d	6038	PHO	C1C-C2C-C3C	-3.54	102.39	106.50
24	A	1038	PHO	C1C-C2C-C3C	-3.53	102.40	106.50
23	B	1014	CLA	O2D-CGD-O1D	-3.53	116.81	123.82
23	c	6033	CLA	C2A-C1A-CHA	-3.53	117.71	123.92
25	D	1042	PQ9	C34-C33-C32	-3.53	114.43	123.70
23	c	6035	CLA	C2A-C1A-CHA	-3.52	117.72	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1021	CLA	C2A-C1A-CHA	-3.52	117.73	123.92
23	b	6021	CLA	C2A-C1A-CHA	-3.51	117.73	123.92
23	C	1027	CLA	C2A-C1A-CHA	-3.51	117.74	123.92
23	c	6027	CLA	C2A-C1A-CHA	-3.51	117.74	123.92
23	D	1008	CLA	C2A-C1A-CHA	-3.51	117.75	123.92
23	c	6034	CLA	C2A-C1A-CHA	-3.51	117.75	123.92
23	A	1007	CLA	C2A-C1A-CHA	-3.51	117.75	123.92
23	C	1035	CLA	C2A-C1A-CHA	-3.51	117.75	123.92
23	C	1033	CLA	C2A-C1A-CHA	-3.51	117.75	123.92
23	d	6008	CLA	C2A-C1A-CHA	-3.50	117.76	123.92
23	a	6007	CLA	C2A-C1A-CHA	-3.50	117.76	123.92
23	c	6028	CLA	C2A-C1A-CHA	-3.50	117.76	123.92
25	D	1042	PQ9	C26-C27-C28	-3.50	119.00	127.66
26	k	6051	BCR	C37-C22-C21	-3.50	118.02	122.92
23	B	1012	CLA	C2A-C1A-CHA	-3.50	117.77	123.92
23	B	1020	CLA	C2A-C1A-CHA	-3.49	117.77	123.92
23	C	1028	CLA	C2A-C1A-CHA	-3.49	117.77	123.92
26	K	1051	BCR	C37-C22-C21	-3.49	118.04	122.92
23	c	6037	CLA	C2A-C1A-CHA	-3.49	117.78	123.92
23	d	6005	CLA	C2A-C1A-CHA	-3.49	117.78	123.92
23	C	1032	CLA	C2A-C1A-CHA	-3.49	117.78	123.92
23	C	1030	CLA	C2A-C1A-CHA	-3.49	117.78	123.92
23	b	6017	CLA	C2A-C1A-CHA	-3.48	117.79	123.92
23	B	1013	CLA	C2A-C1A-CHA	-3.48	117.79	123.92
23	C	1025	CLA	C2A-C1A-CHA	-3.48	117.79	123.92
24	d	6038	PHO	C4C-C3C-C2C	-3.48	102.93	106.80
23	C	1037	CLA	C2A-C1A-CHA	-3.48	117.79	123.92
23	C	1031	CLA	C2A-C1A-CHA	-3.48	117.79	123.92
24	A	1038	PHO	C4C-C3C-C2C	-3.48	102.93	106.80
23	D	1004	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	A	1003	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	b	6012	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	C	1036	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	d	6004	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	A	1006	CLA	C2A-C1A-CHA	-3.48	117.80	123.92
23	a	6003	CLA	C2A-C1A-CHA	-3.47	117.80	123.92
23	H	1017	CLA	C2A-C1A-CHA	-3.47	117.80	123.92
23	D	1005	CLA	C2A-C1A-CHA	-3.47	117.80	123.92
23	c	6030	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	B	1011	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	B	1023	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	b	6019	CLA	C4C-C3C-C2C	-3.47	101.75	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6006	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	b	6020	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	B	1018	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	c	6032	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	c	6036	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	C	1034	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	c	6025	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	b	6011	CLA	C2A-C1A-CHA	-3.47	117.81	123.92
23	B	1016	CLA	C2A-C1A-CHA	-3.46	117.82	123.92
23	b	6016	CLA	C2A-C1A-CHA	-3.46	117.83	123.92
23	b	6013	CLA	C2A-C1A-CHA	-3.46	117.83	123.92
23	B	1019	CLA	C4C-C3C-C2C	-3.46	101.77	106.90
23	c	6031	CLA	C2A-C1A-CHA	-3.46	117.83	123.92
23	b	6010	CLA	CAA-CBA-CGA	-3.46	103.03	113.35
23	b	6023	CLA	C2A-C1A-CHA	-3.45	117.84	123.92
23	b	6018	CLA	C2A-C1A-CHA	-3.45	117.85	123.92
23	B	1010	CLA	CAA-CBA-CGA	-3.45	103.06	113.35
23	B	1022	CLA	C1-C2-C3	-3.44	119.61	125.96
23	b	6022	CLA	C1-C2-C3	-3.44	119.62	125.96
25	A	1043	PQ9	C39-C38-C37	-3.42	114.70	123.70
26	B	1047	BCR	C28-C27-C26	-3.42	107.99	113.99
23	B	1014	CLA	CMA-C3A-C4A	-3.42	102.58	111.77
26	b	6047	BCR	C28-C27-C26	-3.42	107.99	113.99
23	B	1024	CLA	CAA-C2A-C3A	-3.42	103.44	112.81
23	b	6014	CLA	CMA-C3A-C4A	-3.41	102.60	111.77
23	b	6024	CLA	CAA-C2A-C3A	-3.41	103.46	112.81
23	B	1019	CLA	CAA-CBA-CGA	-3.40	103.20	113.35
23	b	6019	CLA	CAA-CBA-CGA	-3.40	103.21	113.35
26	b	6047	BCR	C30-C25-C26	-3.39	117.83	122.59
26	b	6047	BCR	C27-C26-C25	-3.38	117.77	122.74
26	B	1047	BCR	C30-C25-C26	-3.37	117.85	122.59
25	d	6042	PQ9	C14-C13-C12	-3.37	114.86	123.70
26	B	1047	BCR	C27-C26-C25	-3.35	117.82	122.74
26	A	1044	BCR	C11-C10-C9	-3.35	122.53	127.31
26	a	6044	BCR	C11-C10-C9	-3.34	122.54	127.31
23	B	1009	CLA	C2A-C1A-CHA	-3.34	118.04	123.92
26	a	6044	BCR	C37-C22-C21	-3.34	118.25	122.92
23	b	6009	CLA	C2A-C1A-CHA	-3.33	118.06	123.92
26	T	6046	BCR	C37-C22-C21	-3.32	118.27	122.92
26	A	1044	BCR	C37-C22-C21	-3.32	118.28	122.92
23	c	6029	CLA	O2A-CGA-O1A	-3.28	115.58	123.58
23	C	1029	CLA	O2A-CGA-O1A	-3.28	115.58	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	6039	PHO	C1C-C2C-C3C	-3.25	102.73	106.50
26	K	1051	BCR	C28-C27-C26	-3.25	108.29	113.99
24	A	1039	PHO	OBD-CAD-C3D	-3.25	120.52	128.47
26	k	6051	BCR	C28-C27-C26	-3.25	108.30	113.99
24	A	1039	PHO	C1C-C2C-C3C	-3.24	102.74	106.50
24	a	6039	PHO	OBD-CAD-C3D	-3.22	120.59	128.47
26	d	6050	BCR	C37-C22-C21	-3.20	118.44	122.92
26	t	1046	BCR	C37-C22-C21	-3.20	118.45	122.92
25	d	6042	PQ9	C19-C18-C17	-3.18	115.34	123.70
26	D	1050	BCR	C37-C22-C21	-3.18	118.47	122.92
25	D	1042	PQ9	C11-C2-C3	-3.17	119.07	123.27
26	a	6044	BCR	C4-C5-C6	-3.16	118.10	122.74
25	D	1042	PQ9	C14-C13-C12	-3.16	115.40	123.70
26	D	1050	BCR	C34-C9-C10	-3.16	118.50	122.92
26	d	6050	BCR	C34-C9-C10	-3.16	118.50	122.92
25	A	1043	PQ9	C31-C32-C33	-3.14	119.89	127.66
26	A	1044	BCR	C4-C5-C6	-3.12	118.16	122.74
26	a	6044	BCR	C38-C26-C25	-3.06	121.08	124.51
23	c	6034	CLA	O2D-CGD-O1D	-3.06	117.74	123.82
26	A	1044	BCR	C38-C26-C25	-3.06	121.08	124.51
23	B	1024	CLA	C2A-C1A-CHA	-3.04	118.57	123.92
23	b	6024	CLA	C2A-C1A-CHA	-3.04	118.58	123.92
26	C	1054	BCR	C27-C26-C25	-3.03	118.29	122.74
26	c	6054	BCR	C27-C26-C25	-3.03	118.29	122.74
25	d	6042	PQ9	C34-C33-C32	-3.02	115.77	123.70
26	b	6048	BCR	C3-C4-C5	-3.00	108.72	113.99
26	B	1048	BCR	C3-C4-C5	-3.00	108.73	113.99
25	a	6043	PQ9	C39-C38-C37	-3.00	115.83	123.70
24	a	6039	PHO	C1-C2-C3	-2.99	120.45	125.96
23	c	6030	CLA	C1-C2-C3	-2.98	120.47	125.96
23	c	6027	CLA	C1-C2-C3	-2.98	120.47	125.96
23	a	6006	CLA	C1-C2-C3	-2.98	120.47	125.96
23	B	1010	CLA	CMD-C2D-C3D	-2.97	119.47	124.88
23	C	1031	CLA	C1-C2-C3	-2.97	120.48	125.96
23	b	6018	CLA	C1-C2-C3	-2.97	120.48	125.96
23	c	6037	CLA	C1-C2-C3	-2.97	120.49	125.96
23	C	1030	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	6032	CLA	C1-C2-C3	-2.96	120.50	125.96
23	d	6008	CLA	C1-C2-C3	-2.96	120.50	125.96
23	D	1004	CLA	C1-C2-C3	-2.96	120.50	125.96
23	d	6004	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	6035	CLA	C1-C2-C3	-2.96	120.50	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1032	CLA	C1-C2-C3	-2.96	120.50	125.96
23	C	1027	CLA	C1-C2-C3	-2.96	120.50	125.96
23	B	1015	CLA	CBA-CAA-C2A	-2.96	105.03	113.82
23	B	1018	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	6031	CLA	C1-C2-C3	-2.96	120.50	125.96
23	b	6016	CLA	C1-C2-C3	-2.96	120.50	125.96
23	C	1025	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	6028	CLA	C1-C2-C3	-2.96	120.50	125.96
25	D	1042	PQ9	C19-C18-C17	-2.96	115.92	123.70
23	A	1006	CLA	C1-C2-C3	-2.96	120.50	125.96
24	A	1039	PHO	C1-C2-C3	-2.96	120.50	125.96
23	b	6011	CLA	C1-C2-C3	-2.96	120.50	125.96
23	C	1028	CLA	C1-C2-C3	-2.96	120.51	125.96
23	D	1008	CLA	C1-C2-C3	-2.96	120.51	125.96
23	b	6012	CLA	C1-C2-C3	-2.96	120.51	125.96
23	B	1016	CLA	C1-C2-C3	-2.96	120.51	125.96
23	B	1020	CLA	C1-C2-C3	-2.96	120.51	125.96
23	a	6003	CLA	C1-C2-C3	-2.96	120.51	125.96
23	C	1035	CLA	C1-C2-C3	-2.96	120.51	125.96
23	c	6036	CLA	C1-C2-C3	-2.95	120.51	125.96
23	b	6010	CLA	CMD-C2D-C3D	-2.95	119.50	124.88
23	D	1005	CLA	C1-C2-C3	-2.95	120.52	125.96
23	b	6015	CLA	CBA-CAA-C2A	-2.95	105.06	113.82
23	C	1034	CLA	C1-C2-C3	-2.95	120.52	125.96
23	B	1013	CLA	C1-C2-C3	-2.95	120.52	125.96
25	A	1043	PQ9	C15-C16-C17	-2.95	101.99	111.87
23	C	1033	CLA	C1-C2-C3	-2.95	120.52	125.96
23	C	1037	CLA	C1-C2-C3	-2.95	120.52	125.96
23	c	6025	CLA	C1-C2-C3	-2.95	120.53	125.96
23	b	6020	CLA	C1-C2-C3	-2.95	120.53	125.96
23	b	6017	CLA	C1-C2-C3	-2.95	120.53	125.96
23	B	1021	CLA	C1-C2-C3	-2.95	120.53	125.96
23	A	1003	CLA	C1-C2-C3	-2.95	120.53	125.96
23	B	1012	CLA	C1-C2-C3	-2.94	120.53	125.96
23	c	6033	CLA	C1-C2-C3	-2.94	120.53	125.96
23	b	6013	CLA	C1-C2-C3	-2.94	120.54	125.96
23	b	6023	CLA	C1-C2-C3	-2.94	120.54	125.96
23	C	1036	CLA	C1-C2-C3	-2.94	120.54	125.96
23	B	1011	CLA	C1-C2-C3	-2.94	120.54	125.96
25	a	6043	PQ9	C15-C16-C17	-2.94	102.05	111.87
23	B	1023	CLA	C1-C2-C3	-2.94	120.55	125.96
23	d	6005	CLA	C1-C2-C3	-2.93	120.55	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	H	1017	CLA	C1-C2-C3	-2.93	120.57	125.96
23	b	6021	CLA	C1-C2-C3	-2.92	120.57	125.96
24	d	6038	PHO	CHD-C1D-ND	-2.91	118.50	124.63
24	A	1038	PHO	CHD-C1D-ND	-2.90	118.52	124.63
23	b	6022	CLA	CBC-CAC-C3C	-2.89	104.37	112.42
23	B	1022	CLA	CBC-CAC-C3C	-2.89	104.39	112.42
23	B	1009	CLA	C4C-C3C-C2C	-2.88	102.62	106.90
26	B	1048	BCR	C8-C7-C6	-2.88	119.20	127.25
25	d	6042	PQ9	C20-C21-C22	-2.88	102.24	111.87
26	b	6048	BCR	C8-C7-C6	-2.87	119.21	127.25
23	b	6009	CLA	C4C-C3C-C2C	-2.87	102.65	106.90
25	a	6043	PQ9	C31-C32-C33	-2.86	120.59	127.66
26	T	6046	BCR	C29-C30-C25	-2.85	106.02	110.48
23	b	6009	CLA	O2D-CGD-O1D	-2.84	118.18	123.82
23	B	1009	CLA	O2D-CGD-O1D	-2.84	118.18	123.82
26	T	6046	BCR	C2-C1-C6	-2.84	106.04	110.48
23	b	6015	CLA	C4C-C3C-C2C	-2.82	102.72	106.90
23	B	1015	CLA	C4C-C3C-C2C	-2.82	102.72	106.90
26	D	1050	BCR	C35-C13-C14	-2.82	118.98	122.92
26	b	6047	BCR	C8-C7-C6	-2.81	119.38	127.25
26	B	1047	BCR	C8-C7-C6	-2.81	119.39	127.25
26	d	6050	BCR	C35-C13-C14	-2.81	118.99	122.92
26	a	6044	BCR	C36-C18-C17	-2.80	119.00	122.92
26	A	1044	BCR	C36-C18-C17	-2.80	119.00	122.92
26	B	1045	BCR	C28-C27-C26	-2.80	109.09	113.99
23	C	1026	CLA	C4C-C3C-C2C	-2.79	102.76	106.90
26	t	1046	BCR	C38-C26-C25	-2.78	121.40	124.51
26	b	6045	BCR	C28-C27-C26	-2.78	109.12	113.99
23	c	6026	CLA	C4C-C3C-C2C	-2.76	102.80	106.90
24	A	1039	PHO	CHD-C1D-ND	-2.74	118.85	124.63
23	a	6003	CLA	C4C-C3C-C2C	-2.73	102.85	106.90
23	H	1017	CLA	C4C-C3C-C2C	-2.73	102.85	106.90
23	C	1030	CLA	C4C-C3C-C2C	-2.73	102.85	106.90
23	C	1034	CLA	C4C-C3C-C2C	-2.73	102.85	106.90
23	b	6017	CLA	C4C-C3C-C2C	-2.73	102.86	106.90
23	A	1003	CLA	C4C-C3C-C2C	-2.73	102.86	106.90
23	c	6034	CLA	C4C-C3C-C2C	-2.73	102.86	106.90
23	b	6018	CLA	C4C-C3C-C2C	-2.73	102.86	106.90
24	a	6039	PHO	CHD-C1D-ND	-2.72	118.88	124.63
23	c	6030	CLA	C4C-C3C-C2C	-2.72	102.86	106.90
23	C	1037	CLA	C4C-C3C-C2C	-2.72	102.87	106.90
23	b	6009	CLA	C1-C2-C3	-2.71	120.96	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6004	CLA	C4C-C3C-C2C	-2.71	102.88	106.90
23	C	1027	CLA	C4C-C3C-C2C	-2.71	102.89	106.90
23	c	6031	CLA	C4C-C3C-C2C	-2.71	102.89	106.90
23	C	1031	CLA	C4C-C3C-C2C	-2.71	102.89	106.90
23	B	1016	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
26	c	6054	BCR	C36-C18-C17	-2.70	119.14	122.92
23	C	1028	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	c	6027	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	B	1012	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	c	6028	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	B	1018	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	a	6006	CLA	C4C-C3C-C2C	-2.70	102.89	106.90
23	B	1009	CLA	C1-C2-C3	-2.70	120.98	125.96
23	b	6012	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	B	1021	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	C	1025	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	C	1033	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	C	1036	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	C	1035	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	c	6037	CLA	C4C-C3C-C2C	-2.70	102.90	106.90
23	c	6036	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
26	b	6047	BCR	C23-C24-C25	-2.69	119.71	127.25
23	b	6020	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	b	6016	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	B	1020	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	b	6011	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	B	1023	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	D	1004	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
23	D	1005	CLA	C4C-C3C-C2C	-2.69	102.91	106.90
26	C	1054	BCR	C36-C18-C17	-2.68	119.17	122.92
26	D	1050	BCR	C36-C18-C17	-2.68	119.17	122.92
23	b	6021	CLA	C4C-C3C-C2C	-2.68	102.92	106.90
23	c	6033	CLA	C4C-C3C-C2C	-2.68	102.92	106.90
23	A	1006	CLA	C4C-C3C-C2C	-2.68	102.92	106.90
23	b	6023	CLA	C4C-C3C-C2C	-2.68	102.92	106.90
23	D	1008	CLA	C4C-C3C-C2C	-2.68	102.93	106.90
23	B	1011	CLA	C4C-C3C-C2C	-2.68	102.93	106.90
23	c	6032	CLA	C4C-C3C-C2C	-2.68	102.93	106.90
26	B	1047	BCR	C23-C24-C25	-2.68	119.76	127.25
23	c	6035	CLA	C4C-C3C-C2C	-2.67	102.94	106.90
23	B	1013	CLA	C4C-C3C-C2C	-2.67	102.94	106.90
26	d	6050	BCR	C36-C18-C17	-2.67	119.18	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6008	CLA	C4C-C3C-C2C	-2.67	102.94	106.90
23	c	6026	CLA	CGD-CBD-CAD	-2.67	102.09	110.73
23	C	1032	CLA	C4C-C3C-C2C	-2.67	102.95	106.90
23	C	1026	CLA	CGD-CBD-CAD	-2.67	102.10	110.73
23	c	6025	CLA	C4C-C3C-C2C	-2.66	102.95	106.90
23	d	6005	CLA	C4C-C3C-C2C	-2.66	102.95	106.90
26	K	1051	BCR	C34-C9-C10	-2.66	119.20	122.92
26	k	6051	BCR	C34-C9-C10	-2.66	119.20	122.92
23	b	6009	CLA	O1D-CGD-CBD	-2.65	119.66	124.58
23	b	6013	CLA	C4C-C3C-C2C	-2.65	102.96	106.90
23	B	1009	CLA	O1D-CGD-CBD	-2.65	119.66	124.58
23	b	6022	CLA	C6-C5-C3	-2.65	106.40	112.82
23	A	1007	CLA	CAA-C2A-C3A	-2.65	105.56	112.81
23	a	6007	CLA	CAA-C2A-C3A	-2.64	105.56	112.81
23	B	1022	CLA	C6-C5-C3	-2.64	106.43	112.82
26	a	6044	BCR	C29-C30-C25	-2.64	106.35	110.48
26	b	6047	BCR	C37-C22-C21	-2.63	119.23	122.92
23	b	6019	CLA	C16-C15-C13	-2.63	107.10	115.73
23	B	1019	CLA	C16-C15-C13	-2.63	107.11	115.73
23	b	6019	CLA	OBD-CAD-C3D	-2.63	123.31	128.09
23	b	6024	CLA	CBC-CAC-C3C	-2.62	105.12	112.42
26	z	6053	BCR	C28-C27-C26	-2.62	109.39	113.99
23	B	1024	CLA	CBC-CAC-C3C	-2.62	105.13	112.42
23	B	1019	CLA	OBD-CAD-C3D	-2.62	123.33	128.09
26	A	1044	BCR	C29-C30-C25	-2.62	106.38	110.48
23	A	1007	CLA	C4C-C3C-C2C	-2.62	103.02	106.90
26	H	1049	BCR	C23-C24-C25	-2.61	119.93	127.25
26	B	1047	BCR	C37-C22-C21	-2.61	119.26	122.92
26	h	6049	BCR	C23-C24-C25	-2.61	119.94	127.25
23	b	6010	CLA	CHC-C1C-C2C	-2.61	119.49	126.75
26	A	1044	BCR	C33-C5-C6	-2.61	121.59	124.51
23	b	6014	CLA	C4C-C3C-C2C	-2.60	103.04	106.90
26	K	1052	BCR	C28-C27-C26	-2.60	109.42	113.99
26	h	6049	BCR	C8-C7-C6	-2.60	119.96	127.25
23	a	6007	CLA	C4C-C3C-C2C	-2.60	103.04	106.90
26	H	1049	BCR	C8-C7-C6	-2.60	119.97	127.25
26	b	6045	BCR	C3-C4-C5	-2.60	109.43	113.99
23	B	1010	CLA	CHC-C1C-C2C	-2.60	119.52	126.75
26	B	1045	BCR	C8-C7-C6	-2.60	119.98	127.25
26	t	1046	BCR	C8-C7-C6	-2.59	119.99	127.25
26	b	6045	BCR	C8-C7-C6	-2.59	119.99	127.25
26	k	6052	BCR	C8-C7-C6	-2.59	120.00	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	1052	BCR	C23-C24-C25	-2.59	120.00	127.25
26	Z	1053	BCR	C8-C7-C6	-2.59	120.00	127.25
26	d	6050	BCR	C3-C4-C5	-2.59	109.45	113.99
23	b	6010	CLA	C4C-C3C-C2C	-2.59	103.06	106.90
26	z	6053	BCR	C23-C24-C25	-2.59	120.00	127.25
26	z	6053	BCR	C8-C7-C6	-2.59	120.01	127.25
23	B	1010	CLA	C4C-C3C-C2C	-2.59	103.07	106.90
26	Z	1053	BCR	C23-C24-C25	-2.59	120.01	127.25
26	B	1045	BCR	C3-C4-C5	-2.58	109.46	113.99
24	d	6038	PHO	C1-C2-C3	-2.58	121.19	125.96
23	B	1014	CLA	C4C-C3C-C2C	-2.58	103.07	106.90
24	A	1038	PHO	C1-C2-C3	-2.58	121.20	125.96
26	k	6052	BCR	C28-C27-C26	-2.58	109.46	113.99
29	J	1059	MGE	C2G-O2G-C1B	-2.58	111.78	117.88
23	B	1015	CLA	C1-C2-C3	-2.58	121.20	125.96
26	h	6049	BCR	C3-C4-C5	-2.58	109.47	113.99
26	k	6052	BCR	C23-C24-C25	-2.58	120.03	127.25
26	K	1052	BCR	C8-C7-C6	-2.58	120.03	127.25
27	A	1063	LHG	C5-O7-C7	-2.58	111.78	117.88
30	h	6058	DGD	C2G-O2G-C1B	-2.58	111.78	117.88
26	Z	1053	BCR	C28-C27-C26	-2.58	109.47	113.99
30	C	1055	DGD	C2G-O2G-C1B	-2.58	111.78	117.88
30	c	6057	DGD	C2G-O2G-C1B	-2.58	111.79	117.88
29	b	6060	MGE	C2G-O2G-C1B	-2.58	111.79	117.88
26	B	1047	BCR	C36-C18-C17	-2.58	119.31	122.92
30	C	1056	DGD	C2G-O2G-C1B	-2.58	111.79	117.88
26	H	1049	BCR	C3-C4-C5	-2.57	109.47	113.99
29	B	1060	MGE	C2G-O2G-C1B	-2.57	111.79	117.88
29	d	6059	MGE	C2G-O2G-C1B	-2.57	111.80	117.88
30	C	1057	DGD	C2G-O2G-C1B	-2.57	111.80	117.88
29	D	1062	MGE	C2G-O2G-C1B	-2.57	111.80	117.88
26	b	6047	BCR	C36-C18-C17	-2.57	119.32	122.92
26	a	6044	BCR	C33-C5-C6	-2.57	121.63	124.51
26	D	1050	BCR	C3-C4-C5	-2.57	109.48	113.99
26	K	1052	BCR	C3-C4-C5	-2.57	109.48	113.99
26	k	6052	BCR	C3-C4-C5	-2.57	109.49	113.99
30	H	1058	DGD	C2G-O2G-C1B	-2.57	111.81	117.88
29	d	6062	MGE	C2G-O2G-C1B	-2.57	111.81	117.88
29	d	6061	MGE	C2G-O2G-C1B	-2.57	111.81	117.88
23	A	1007	CLA	C1-C2-C3	-2.56	121.23	125.96
29	L	1061	MGE	C2G-O2G-C1B	-2.56	111.82	117.88
23	a	6007	CLA	C1-C2-C3	-2.56	121.23	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	6063	LHG	C5-O7-C7	-2.56	111.82	117.88
26	C	1054	BCR	C23-C24-C25	-2.56	120.08	127.25
23	b	6015	CLA	C1-C2-C3	-2.56	121.24	125.96
26	A	1044	BCR	C27-C26-C25	-2.56	118.98	122.74
30	c	6055	DGD	C2G-O2G-C1B	-2.56	111.83	117.88
30	c	6056	DGD	C2G-O2G-C1B	-2.56	111.83	117.88
26	C	1054	BCR	C35-C13-C14	-2.56	119.34	122.92
26	a	6044	BCR	C27-C26-C25	-2.56	118.99	122.74
25	d	6042	PQ9	C11-C2-C3	-2.55	119.90	123.27
26	t	1046	BCR	C3-C4-C5	-2.55	109.52	113.99
23	B	1009	CLA	O2A-CGA-O1A	-2.55	117.36	123.58
26	c	6054	BCR	C23-C24-C25	-2.55	120.12	127.25
23	B	1022	CLA	CMD-C2D-C3D	-2.54	120.25	124.88
26	Z	1053	BCR	C3-C4-C5	-2.54	109.54	113.99
23	b	6009	CLA	O2A-CGA-O1A	-2.53	117.40	123.58
26	z	6053	BCR	C3-C4-C5	-2.53	109.55	113.99
26	c	6054	BCR	C35-C13-C14	-2.53	119.38	122.92
26	H	1049	BCR	C28-C27-C26	-2.53	109.56	113.99
26	h	6049	BCR	C28-C27-C26	-2.52	109.57	113.99
23	b	6022	CLA	CMD-C2D-C3D	-2.51	120.31	124.88
24	A	1039	PHO	C4D-ND-C1D	-2.50	102.47	106.98
26	D	1050	BCR	C28-C27-C26	-2.50	109.61	113.99
26	d	6050	BCR	C28-C27-C26	-2.50	109.61	113.99
23	c	6026	CLA	C2A-C1A-CHA	-2.49	119.53	123.92
24	a	6039	PHO	C4D-ND-C1D	-2.49	102.49	106.98
23	a	6007	CLA	O2A-CGA-O1A	-2.48	117.52	123.58
23	A	1007	CLA	O2A-CGA-O1A	-2.48	117.53	123.58
24	d	6038	PHO	C4D-ND-C1D	-2.48	102.51	106.98
23	C	1026	CLA	C2A-C1A-CHA	-2.48	119.56	123.92
24	A	1038	PHO	C4D-ND-C1D	-2.47	102.52	106.98
23	b	6020	CLA	O2D-CGD-O1D	-2.47	118.93	123.82
24	d	6038	PHO	CBB-CAB-C3B	-2.46	115.38	127.43
26	k	6051	BCR	C35-C13-C14	-2.46	119.47	122.92
24	A	1038	PHO	CBB-CAB-C3B	-2.46	115.38	127.43
26	A	1044	BCR	C35-C13-C14	-2.46	119.48	122.92
23	b	6018	CLA	O2D-CGD-O1D	-2.45	118.95	123.82
23	B	1023	CLA	O2D-CGD-O1D	-2.45	118.95	123.82
23	C	1026	CLA	CHC-C1C-C2C	-2.45	119.92	126.75
26	a	6044	BCR	C35-C13-C14	-2.45	119.50	122.92
23	C	1031	CLA	O2D-CGD-O1D	-2.45	118.97	123.82
23	B	1020	CLA	O2D-CGD-O1D	-2.45	118.97	123.82
23	c	6025	CLA	O2D-CGD-O1D	-2.44	118.97	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6011	CLA	O2D-CGD-O1D	-2.44	118.97	123.82
23	D	1008	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	b	6016	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	C	1025	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	C	1028	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
26	K	1051	BCR	C35-C13-C14	-2.44	119.51	122.92
23	B	1011	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	B	1018	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	b	6012	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	b	6023	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	d	6004	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	c	6026	CLA	CHC-C1C-C2C	-2.44	119.96	126.75
23	c	6036	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	C	1036	CLA	O2D-CGD-O1D	-2.44	118.98	123.82
23	c	6027	CLA	O2D-CGD-O1D	-2.44	118.99	123.82
23	b	6021	CLA	O2D-CGD-O1D	-2.44	118.99	123.82
23	B	1021	CLA	O2D-CGD-O1D	-2.44	118.99	123.82
23	d	6008	CLA	O2D-CGD-O1D	-2.43	118.99	123.82
23	c	6033	CLA	O2D-CGD-O1D	-2.43	118.99	123.82
23	C	1035	CLA	O2D-CGD-O1D	-2.43	118.99	123.82
23	c	6030	CLA	O2D-CGD-O1D	-2.43	118.99	123.82
23	c	6035	CLA	O2D-CGD-O1D	-2.43	118.99	123.82
23	A	1006	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	C	1030	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	b	6022	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	c	6031	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	C	1033	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	D	1004	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	c	6028	CLA	O2D-CGD-O1D	-2.43	119.00	123.82
23	b	6019	CLA	C1-C2-C3	-2.43	121.49	125.96
23	C	1034	CLA	O2D-CGD-O1D	-2.43	119.01	123.82
26	T	6046	BCR	C38-C26-C25	-2.43	121.79	124.51
23	a	6006	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	C	1037	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	B	1013	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	D	1005	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	B	1012	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	C	1027	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
23	B	1022	CLA	O2D-CGD-O1D	-2.42	119.03	123.82
23	b	6024	CLA	CHC-C1C-C2C	-2.42	120.03	126.75
23	B	1016	CLA	O2D-CGD-O1D	-2.41	119.03	123.82
23	B	1019	CLA	C1-C2-C3	-2.41	121.51	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	H	1017	CLA	O2D-CGD-O1D	-2.41	119.04	123.82
23	d	6005	CLA	O2D-CGD-O1D	-2.41	119.05	123.82
23	B	1024	CLA	CHC-C1C-C2C	-2.40	120.05	126.75
23	b	6013	CLA	O2D-CGD-O1D	-2.40	119.05	123.82
23	c	6037	CLA	O2D-CGD-O1D	-2.40	119.06	123.82
23	B	1009	CLA	CHC-C1C-C2C	-2.40	120.07	126.75
23	b	6015	CLA	O2A-CGA-O1A	-2.40	117.73	123.58
23	B	1015	CLA	O2A-CGA-O1A	-2.40	117.74	123.58
23	b	6009	CLA	CHC-C1C-C2C	-2.39	120.08	126.75
23	C	1032	CLA	O2D-CGD-O1D	-2.39	119.07	123.82
23	A	1003	CLA	O2D-CGD-O1D	-2.39	119.08	123.82
23	a	6003	CLA	O2D-CGD-O1D	-2.39	119.08	123.82
23	c	6034	CLA	O2A-CGA-O1A	-2.39	117.75	123.58
23	b	6017	CLA	O2D-CGD-O1D	-2.39	119.08	123.82
23	b	6022	CLA	CHC-C1C-C2C	-2.38	120.12	126.75
23	B	1022	CLA	CHC-C1C-C2C	-2.38	120.12	126.75
23	A	1007	CLA	CHC-C1C-C2C	-2.38	120.14	126.75
24	a	6039	PHO	O2D-CGD-O1D	-2.38	119.11	123.82
23	c	6032	CLA	O2D-CGD-O1D	-2.37	119.12	123.82
23	B	1014	CLA	C2A-C1A-CHA	-2.37	119.76	123.92
23	a	6007	CLA	CHC-C1C-C2C	-2.36	120.17	126.75
23	B	1024	CLA	C4C-C3C-C2C	-2.36	103.40	106.90
23	b	6014	CLA	C2A-C1A-CHA	-2.36	119.76	123.92
26	D	1050	BCR	C8-C7-C6	-2.36	120.65	127.25
26	c	6054	BCR	C8-C7-C6	-2.36	120.66	127.25
24	A	1039	PHO	O2D-CGD-O1D	-2.35	119.15	123.82
26	d	6050	BCR	C8-C7-C6	-2.35	120.67	127.25
23	b	6024	CLA	C4C-C3C-C2C	-2.35	103.42	106.90
26	t	1046	BCR	C29-C30-C25	-2.35	106.81	110.48
23	B	1022	CLA	C16-C15-C13	-2.34	108.05	115.73
23	b	6022	CLA	C16-C15-C13	-2.34	108.05	115.73
23	c	6034	CLA	CHC-C1C-C2C	-2.34	120.24	126.75
26	C	1054	BCR	C8-C7-C6	-2.34	120.71	127.25
23	B	1019	CLA	CHC-C1C-C2C	-2.33	120.28	126.75
23	b	6019	CLA	CHC-C1C-C2C	-2.32	120.28	126.75
23	c	6029	CLA	CHC-C1C-C2C	-2.31	120.32	126.75
23	C	1029	CLA	CHC-C1C-C2C	-2.30	120.34	126.75
25	D	1042	PQ9	C12-C11-C2	-2.30	105.17	111.88
23	c	6030	CLA	CHC-C1C-C2C	-2.30	120.36	126.75
26	B	1047	BCR	C3-C4-C5	-2.30	109.97	113.99
23	b	6017	CLA	CHC-C1C-C2C	-2.29	120.36	126.75
23	C	1025	CLA	CHC-C1C-C2C	-2.29	120.36	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1007	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
23	C	1035	CLA	CHC-C1C-C2C	-2.29	120.37	126.75
23	c	6029	CLA	C6-C5-C3	-2.29	107.27	112.82
23	a	6007	CLA	CAA-C2A-C1A	-2.29	104.47	111.97
26	C	1054	BCR	C29-C30-C25	-2.29	106.89	110.48
25	D	1042	PQ9	C15-C16-C17	-2.29	104.21	111.87
23	C	1027	CLA	CHC-C1C-C2C	-2.29	120.38	126.75
23	H	1017	CLA	CHC-C1C-C2C	-2.29	120.38	126.75
23	b	6013	CLA	CHC-C1C-C2C	-2.29	120.38	126.75
23	c	6035	CLA	CHC-C1C-C2C	-2.29	120.38	126.75
23	B	1013	CLA	CHC-C1C-C2C	-2.29	120.38	126.75
23	D	1004	CLA	CHC-C1C-C2C	-2.29	120.39	126.75
23	C	1033	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	c	6036	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	C	1030	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
26	c	6054	BCR	C29-C30-C25	-2.28	106.91	110.48
23	c	6032	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	c	6027	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	A	1003	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	c	6025	CLA	CHC-C1C-C2C	-2.28	120.39	126.75
23	c	6033	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	C	1032	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	C	1037	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	b	6020	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	a	6006	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	B	1020	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	B	1018	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	D	1008	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	C	1034	CLA	CHC-C1C-C2C	-2.28	120.40	126.75
23	C	1029	CLA	C6-C5-C3	-2.28	107.30	112.82
23	b	6012	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	C	1036	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	a	6003	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	d	6004	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	C	1028	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	C	1031	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
23	d	6005	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	D	1005	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	d	6008	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	B	1023	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	b	6016	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	B	1012	CLA	CHC-C1C-C2C	-2.27	120.43	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6037	CLA	CHC-C1C-C2C	-2.27	120.43	126.75
23	b	6018	CLA	CHC-C1C-C2C	-2.27	120.43	126.75
23	b	6023	CLA	CHC-C1C-C2C	-2.27	120.43	126.75
26	b	6047	BCR	C3-C4-C5	-2.27	110.01	113.99
23	B	1016	CLA	CHC-C1C-C2C	-2.27	120.43	126.75
23	b	6021	CLA	CHC-C1C-C2C	-2.27	120.44	126.75
23	c	6028	CLA	CHC-C1C-C2C	-2.27	120.44	126.75
23	B	1021	CLA	CHC-C1C-C2C	-2.26	120.45	126.75
23	B	1011	CLA	CHC-C1C-C2C	-2.26	120.45	126.75
23	c	6031	CLA	CHC-C1C-C2C	-2.26	120.45	126.75
23	c	6029	CLA	C4C-C3C-C2C	-2.26	103.55	106.90
26	C	1054	BCR	C37-C22-C21	-2.26	119.76	122.92
23	C	1029	CLA	C4C-C3C-C2C	-2.26	103.56	106.90
23	A	1006	CLA	CHC-C1C-C2C	-2.26	120.47	126.75
23	c	6025	CLA	O1D-CGD-CBD	-2.25	120.40	124.58
26	c	6054	BCR	C37-C22-C21	-2.25	119.77	122.92
23	b	6017	CLA	O1D-CGD-CBD	-2.25	120.42	124.58
23	d	6008	CLA	O1D-CGD-CBD	-2.25	120.42	124.58
23	b	6011	CLA	CHC-C1C-C2C	-2.24	120.50	126.75
23	c	6028	CLA	O1D-CGD-CBD	-2.24	120.42	124.58
23	C	1028	CLA	O1D-CGD-CBD	-2.24	120.43	124.58
23	C	1025	CLA	O1D-CGD-CBD	-2.24	120.43	124.58
26	a	6044	BCR	C34-C9-C10	-2.24	119.79	122.92
31	e	6040	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
23	c	6031	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
24	a	6039	PHO	CBB-CAB-C3B	-2.23	116.50	127.43
23	D	1008	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
23	b	6023	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
26	A	1044	BCR	C34-C9-C10	-2.23	119.80	122.92
23	c	6032	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
23	H	1017	CLA	O1D-CGD-CBD	-2.23	120.44	124.58
23	C	1030	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
23	c	6030	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
23	C	1031	CLA	O1D-CGD-CBD	-2.23	120.45	124.58
23	B	1024	CLA	O2A-CGA-O1A	-2.23	118.15	123.58
24	A	1039	PHO	CBB-CAB-C3B	-2.23	116.54	127.43
23	c	6035	CLA	O1D-CGD-CBD	-2.22	120.45	124.58
23	c	6027	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
23	C	1035	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
23	B	1023	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
23	c	6037	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
23	b	6024	CLA	O2A-CGA-O1A	-2.22	118.17	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	6048	BCR	C34-C9-C10	-2.22	119.82	122.92
23	d	6005	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
23	C	1032	CLA	O1D-CGD-CBD	-2.22	120.47	124.58
23	C	1034	CLA	O1D-CGD-CBD	-2.21	120.47	124.58
23	B	1021	CLA	O1D-CGD-CBD	-2.21	120.47	124.58
23	a	6006	CLA	O1D-CGD-CBD	-2.21	120.48	124.58
23	b	6018	CLA	O1D-CGD-CBD	-2.21	120.48	124.58
23	B	1012	CLA	O1D-CGD-CBD	-2.21	120.48	124.58
26	T	6046	BCR	C8-C7-C6	-2.21	121.07	127.25
26	b	6048	BCR	C23-C24-C25	-2.21	121.07	127.25
23	C	1033	CLA	O1D-CGD-CBD	-2.21	120.48	124.58
25	A	1043	PQ9	C26-C27-C28	-2.21	122.20	127.66
23	B	1018	CLA	O1D-CGD-CBD	-2.21	120.49	124.58
23	b	6021	CLA	O1D-CGD-CBD	-2.20	120.49	124.58
26	B	1048	BCR	C34-C9-C10	-2.20	119.84	122.92
23	D	1004	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
23	A	1006	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
23	D	1005	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
23	C	1027	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
23	b	6019	CLA	C6-C5-C3	-2.20	107.49	112.82
23	B	1011	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
23	B	1019	CLA	C6-C5-C3	-2.20	107.50	112.82
26	B	1048	BCR	C23-C24-C25	-2.20	121.10	127.25
23	b	6011	CLA	O1D-CGD-CBD	-2.20	120.51	124.58
23	b	6013	CLA	O1D-CGD-CBD	-2.20	120.51	124.58
31	E	1040	HEM	C1D-C2D-C3D	-2.19	105.47	107.00
23	C	1037	CLA	O1D-CGD-CBD	-2.19	120.51	124.58
23	C	1036	CLA	O1D-CGD-CBD	-2.19	120.51	124.58
23	B	1013	CLA	O1D-CGD-CBD	-2.19	120.52	124.58
23	c	6033	CLA	O1D-CGD-CBD	-2.19	120.52	124.58
23	b	6012	CLA	O1D-CGD-CBD	-2.19	120.52	124.58
23	A	1003	CLA	O1D-CGD-CBD	-2.19	120.53	124.58
26	K	1051	BCR	C8-C7-C6	-2.18	121.14	127.25
23	c	6036	CLA	O1D-CGD-CBD	-2.18	120.53	124.58
26	k	6051	BCR	C8-C7-C6	-2.18	121.15	127.25
23	a	6003	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
23	d	6004	CLA	O1D-CGD-CBD	-2.18	120.55	124.58
23	B	1016	CLA	O1D-CGD-CBD	-2.17	120.55	124.58
23	B	1015	CLA	C16-C15-C13	-2.17	108.60	115.73
23	B	1020	CLA	O1D-CGD-CBD	-2.17	120.56	124.58
23	b	6015	CLA	C16-C15-C13	-2.16	108.63	115.73
26	B	1048	BCR	C1-C6-C5	-2.16	119.55	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6020	CLA	O1D-CGD-CBD	-2.16	120.57	124.58
23	B	1022	CLA	O1D-CGD-CBD	-2.16	120.58	124.58
23	B	1015	CLA	CHC-C1C-C2C	-2.15	120.75	126.75
23	b	6022	CLA	O1D-CGD-CBD	-2.15	120.59	124.58
23	b	6015	CLA	CHC-C1C-C2C	-2.15	120.77	126.75
25	A	1043	PQ9	C41-C40-C38	-2.15	105.75	112.85
26	K	1051	BCR	C3-C4-C5	-2.15	110.23	113.99
26	b	6048	BCR	C1-C6-C5	-2.14	119.58	122.59
26	k	6051	BCR	C3-C4-C5	-2.14	110.24	113.99
23	b	6016	CLA	O1D-CGD-CBD	-2.14	120.61	124.58
24	d	6038	PHO	C1B-NB-C4B	-2.14	102.37	106.51
26	B	1048	BCR	C28-C27-C26	-2.13	110.25	113.99
25	A	1043	PQ9	C34-C33-C32	-2.13	118.09	123.70
26	B	1048	BCR	C37-C22-C21	-2.13	119.94	122.92
24	A	1038	PHO	C1B-NB-C4B	-2.13	102.38	106.51
26	b	6045	BCR	C24-C25-C26	-2.13	116.47	121.54
23	b	6019	CLA	O1A-CGA-CBA	-2.12	115.41	123.70
31	V	1041	HEM	C1D-C2D-C3D	-2.12	105.52	107.00
26	k	6052	BCR	C37-C22-C21	-2.12	119.95	122.92
24	A	1039	PHO	O1D-CGD-CBD	-2.12	120.65	124.58
31	v	6041	HEM	C1D-C2D-C3D	-2.12	105.52	107.00
23	B	1019	CLA	O1A-CGA-CBA	-2.11	115.45	123.70
26	b	6048	BCR	C37-C22-C21	-2.11	119.96	122.92
26	Z	1053	BCR	C34-C9-C10	-2.11	119.97	122.92
26	b	6045	BCR	C36-C18-C17	-2.11	119.97	122.92
24	a	6039	PHO	O1D-CGD-CBD	-2.11	120.67	124.58
26	B	1045	BCR	C24-C25-C26	-2.11	116.51	121.54
26	b	6045	BCR	C35-C13-C14	-2.11	119.97	122.92
26	b	6048	BCR	C28-C27-C26	-2.11	110.30	113.99
26	Z	1053	BCR	C37-C22-C21	-2.11	119.97	122.92
26	h	6049	BCR	C36-C18-C17	-2.10	119.98	122.92
26	k	6052	BCR	C34-C9-C10	-2.10	119.98	122.92
26	K	1052	BCR	C34-C9-C10	-2.10	119.98	122.92
26	k	6051	BCR	C29-C30-C25	-2.10	107.19	110.48
25	a	6043	PQ9	C41-C40-C38	-2.10	105.92	112.85
26	B	1045	BCR	C35-C13-C14	-2.10	119.98	122.92
25	a	6043	PQ9	C16-C17-C18	-2.09	122.48	127.66
26	B	1045	BCR	C36-C18-C17	-2.09	119.99	122.92
26	H	1049	BCR	C36-C18-C17	-2.09	119.99	122.92
26	b	6045	BCR	C34-C9-C10	-2.09	120.00	122.92
26	k	6052	BCR	C35-C13-C14	-2.09	120.00	122.92
26	K	1051	BCR	C29-C30-C25	-2.09	107.21	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1024	CLA	CAA-C2A-C1A	-2.08	105.14	111.97
26	z	6053	BCR	C34-C9-C10	-2.08	120.00	122.92
26	H	1049	BCR	C37-C22-C21	-2.08	120.00	122.92
26	c	6054	BCR	C34-C9-C10	-2.08	120.00	122.92
23	b	6021	CLA	CMD-C2D-C3D	-2.08	121.08	124.88
26	b	6048	BCR	C35-C13-C14	-2.08	120.01	122.92
26	t	1046	BCR	C34-C9-C10	-2.08	120.01	122.92
25	D	1042	PQ9	C20-C21-C22	-2.08	104.90	111.87
23	B	1015	CLA	CBC-CAC-C3C	-2.08	106.63	112.42
23	b	6024	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
23	b	6015	CLA	CBC-CAC-C3C	-2.08	106.64	112.42
23	c	6032	CLA	CMD-C2D-C3D	-2.08	121.10	124.88
26	d	6050	BCR	C24-C25-C26	-2.08	116.59	121.54
26	z	6053	BCR	C35-C13-C14	-2.08	120.02	122.92
26	C	1054	BCR	C34-C9-C10	-2.08	120.02	122.92
26	z	6053	BCR	C37-C22-C21	-2.07	120.02	122.92
26	k	6052	BCR	C36-C18-C17	-2.07	120.02	122.92
26	t	1046	BCR	C35-C13-C14	-2.07	120.02	122.92
26	K	1052	BCR	C36-C18-C17	-2.07	120.02	122.92
26	T	6046	BCR	C35-C13-C14	-2.07	120.02	122.92
26	Z	1053	BCR	C35-C13-C14	-2.07	120.02	122.92
26	h	6049	BCR	C37-C22-C21	-2.07	120.02	122.92
26	h	6049	BCR	C34-C9-C10	-2.07	120.02	122.92
26	K	1052	BCR	C35-C13-C14	-2.07	120.02	122.92
26	z	6053	BCR	C36-C18-C17	-2.07	120.02	122.92
26	B	1045	BCR	C34-C9-C10	-2.07	120.02	122.92
23	c	6026	CLA	C1-O2A-CGA	-2.07	112.00	116.77
23	C	1026	CLA	C1-O2A-CGA	-2.07	112.00	116.77
24	a	6039	PHO	C1B-NB-C4B	-2.07	102.50	106.51
26	H	1049	BCR	C34-C9-C10	-2.07	120.03	122.92
26	Z	1053	BCR	C36-C18-C17	-2.07	120.03	122.92
26	H	1049	BCR	C35-C13-C14	-2.06	120.03	122.92
25	A	1043	PQ9	C16-C17-C18	-2.06	122.55	127.66
23	a	6006	CLA	CMD-C2D-C3D	-2.06	121.12	124.88
23	C	1034	CLA	CMD-C2D-C3D	-2.06	121.12	124.88
23	b	6019	CLA	C11-C10-C8	-2.06	108.96	115.73
23	B	1019	CLA	C11-C10-C8	-2.06	108.96	115.73
24	A	1039	PHO	C1B-NB-C4B	-2.06	102.51	106.51
26	D	1050	BCR	C24-C25-C26	-2.06	116.62	121.54
23	d	6008	CLA	CMD-C2D-C3D	-2.06	121.12	124.88
26	h	6049	BCR	C35-C13-C14	-2.06	120.04	122.92
26	t	1046	BCR	C36-C18-C17	-2.06	120.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6015	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	d	6005	CLA	CMD-C2D-C3D	-2.06	121.13	124.88
26	B	1048	BCR	C35-C13-C14	-2.06	120.04	122.92
23	B	1015	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	b	6011	CLA	CMD-C2D-C3D	-2.06	121.13	124.88
26	K	1052	BCR	C37-C22-C21	-2.06	120.04	122.92
23	c	6025	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	B	1021	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	c	6030	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	B	1011	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	b	6022	CLA	C6-C7-C8	-2.05	108.99	115.73
23	D	1008	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	c	6035	CLA	CMD-C2D-C3D	-2.05	121.14	124.88
23	C	1028	CLA	CMD-C2D-C3D	-2.05	121.15	124.88
23	C	1030	CLA	CMD-C2D-C3D	-2.05	121.15	124.88
23	B	1022	CLA	C6-C7-C8	-2.05	109.01	115.73
23	b	6018	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	C	1025	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	a	6003	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	c	6037	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	b	6016	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	B	1018	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	d	6004	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
25	a	6043	PQ9	C35-C36-C37	-2.04	105.04	111.87
23	b	6012	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	C	1032	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	D	1005	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
26	T	6046	BCR	C36-C18-C17	-2.04	120.06	122.92
23	c	6036	CLA	CMD-C2D-C3D	-2.04	121.16	124.88
23	A	1006	CLA	CMD-C2D-C3D	-2.04	121.17	124.88
23	B	1016	CLA	CMD-C2D-C3D	-2.04	121.17	124.88
23	B	1022	CLA	C4C-C3C-C2C	-2.04	103.88	106.90
23	C	1027	CLA	CMD-C2D-C3D	-2.03	121.17	124.88
23	D	1004	CLA	CMD-C2D-C3D	-2.03	121.17	124.88
23	A	1003	CLA	CMD-C2D-C3D	-2.03	121.17	124.88
23	C	1035	CLA	CMD-C2D-C3D	-2.03	121.17	124.88
23	b	6010	CLA	O1A-CGA-CBA	-2.03	115.76	123.70
23	c	6027	CLA	CMD-C2D-C3D	-2.03	121.18	124.88
23	C	1031	CLA	CMD-C2D-C3D	-2.03	121.18	124.88
23	B	1013	CLA	CMD-C2D-C3D	-2.03	121.18	124.88
26	k	6051	BCR	C24-C25-C26	-2.03	116.70	121.54
23	b	6013	CLA	CMD-C2D-C3D	-2.03	121.18	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6024	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
23	B	1010	CLA	O1A-CGA-CBA	-2.03	115.78	123.70
23	b	6023	CLA	CMD-C2D-C3D	-2.03	121.18	124.88
23	c	6033	CLA	CMD-C2D-C3D	-2.03	121.19	124.88
26	k	6051	BCR	C27-C26-C25	-2.03	119.77	122.74
23	C	1037	CLA	CMD-C2D-C3D	-2.02	121.19	124.88
23	C	1036	CLA	CMD-C2D-C3D	-2.02	121.19	124.88
23	C	1029	CLA	C6-C7-C8	-2.02	109.09	115.73
23	B	1023	CLA	CMD-C2D-C3D	-2.02	121.20	124.88
23	C	1033	CLA	CMD-C2D-C3D	-2.02	121.20	124.88
23	H	1017	CLA	CMD-C2D-C3D	-2.02	121.20	124.88
23	b	6022	CLA	C4C-C3C-C2C	-2.02	103.91	106.90
23	c	6029	CLA	C6-C7-C8	-2.02	109.10	115.73
23	b	6020	CLA	CMD-C2D-C3D	-2.02	121.20	124.88
26	K	1051	BCR	C27-C26-C25	-2.02	119.78	122.74
23	b	6017	CLA	CMD-C2D-C3D	-2.02	121.21	124.88
26	b	6048	BCR	C36-C18-C17	-2.02	120.10	122.92
26	K	1051	BCR	C24-C25-C26	-2.02	116.73	121.54
23	c	6031	CLA	CMD-C2D-C3D	-2.01	121.21	124.88
23	B	1024	CLA	CGD-CBD-CAD	-2.01	104.21	110.73
23	B	1020	CLA	CMD-C2D-C3D	-2.01	121.22	124.88
23	c	6028	CLA	CMD-C2D-C3D	-2.01	121.22	124.88
23	B	1012	CLA	CMD-C2D-C3D	-2.01	121.23	124.88
25	D	1042	PQ9	C41-C40-C38	-2.00	106.23	112.85
26	B	1048	BCR	C36-C18-C17	-2.00	120.12	122.92
23	B	1019	CLA	CAC-C3C-C4C	2.00	127.58	124.82
26	T	6046	BCR	C24-C25-C26	2.01	126.33	121.54
23	c	6029	CLA	O2A-CGA-CBA	2.02	117.75	111.92
23	C	1029	CLA	O2A-CGA-CBA	2.02	117.75	111.92
26	T	6046	BCR	C24-C23-C22	2.03	129.27	126.21
23	b	6022	CLA	CMC-C2C-C1C	2.03	128.17	125.05
23	B	1022	CLA	CMC-C2C-C1C	2.04	128.18	125.05
23	b	6014	CLA	CMB-C2B-C3B	2.05	128.61	124.88
23	B	1024	CLA	O2A-CGA-CBA	2.06	117.86	111.92
25	a	6043	PQ9	C40-C38-C37	2.06	125.28	121.10
23	b	6024	CLA	O2A-CGA-CBA	2.06	117.87	111.92
23	B	1014	CLA	CMB-C2B-C3B	2.06	128.64	124.88
26	t	1046	BCR	C24-C25-C26	2.07	126.48	121.54
25	d	6042	PQ9	C11-C2-C1	2.08	118.56	116.88
25	D	1042	PQ9	C40-C41-C42	2.08	118.84	111.87
25	a	6043	PQ9	C39-C38-C40	2.09	118.89	115.29
25	d	6042	PQ9	C15-C13-C12	2.11	125.38	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6014	CLA	CMB-C2B-C1B	2.11	131.71	128.46
23	B	1014	CLA	CMB-C2B-C1B	2.12	131.72	128.46
23	b	6019	CLA	CGD-CBD-CAD	2.14	117.67	110.73
23	B	1019	CLA	CGD-CBD-CAD	2.15	117.69	110.73
25	A	1043	PQ9	C40-C38-C37	2.22	125.62	121.10
25	D	1042	PQ9	C45-C43-C44	2.22	119.61	114.59
23	c	6026	CLA	CAC-C3C-C4C	2.22	127.89	124.82
23	C	1026	CLA	CAC-C3C-C4C	2.23	127.89	124.82
23	b	6022	CLA	CAC-C3C-C2C	2.23	131.31	127.51
23	b	6019	CLA	O2D-CGD-CBD	2.23	115.24	111.28
23	c	6026	CLA	CMC-C2C-C1C	2.23	128.47	125.05
23	B	1022	CLA	CAC-C3C-C2C	2.25	131.34	127.51
23	B	1019	CLA	O2D-CGD-CBD	2.25	115.28	111.28
23	B	1010	CLA	CGD-CBD-CAD	2.26	118.06	110.73
23	C	1026	CLA	CMC-C2C-C1C	2.26	128.52	125.05
23	b	6010	CLA	CGD-CBD-CAD	2.28	118.10	110.73
23	B	1014	CLA	O2A-CGA-CBA	2.32	118.61	111.92
23	c	6034	CLA	O2A-CGA-CBA	2.32	118.62	111.92
23	b	6019	CLA	CAA-C2A-C3A	2.32	119.16	112.81
23	b	6014	CLA	O2A-CGA-CBA	2.32	118.63	111.92
23	B	1019	CLA	CAA-C2A-C3A	2.32	119.17	112.81
23	C	1029	CLA	CMC-C2C-C1C	2.33	128.62	125.05
23	b	6011	CLA	CMC-C2C-C1C	2.33	128.62	125.05
23	c	6029	CLA	CMC-C2C-C1C	2.33	128.63	125.05
23	d	6008	CLA	CMC-C2C-C1C	2.34	128.63	125.05
25	d	6042	PQ9	C25-C23-C22	2.34	125.86	121.10
23	a	6003	CLA	CMC-C2C-C1C	2.34	128.63	125.05
23	B	1011	CLA	CMC-C2C-C1C	2.34	128.64	125.05
23	b	6012	CLA	CMC-C2C-C1C	2.34	128.64	125.05
23	B	1010	CLA	CMC-C2C-C1C	2.34	128.64	125.05
23	B	1021	CLA	CMC-C2C-C1C	2.34	128.64	125.05
23	c	6025	CLA	CMC-C2C-C1C	2.34	128.64	125.05
23	B	1012	CLA	CMC-C2C-C1C	2.35	128.65	125.05
23	b	6021	CLA	CMC-C2C-C1C	2.35	128.65	125.05
23	b	6018	CLA	CMC-C2C-C1C	2.35	128.65	125.05
23	c	6031	CLA	CMC-C2C-C1C	2.35	128.65	125.05
23	A	1003	CLA	CMC-C2C-C1C	2.35	128.65	125.05
23	c	6033	CLA	CMC-C2C-C1C	2.35	128.66	125.05
23	A	1006	CLA	CMC-C2C-C1C	2.35	128.66	125.05
23	C	1032	CLA	CMC-C2C-C1C	2.35	128.66	125.05
23	c	6036	CLA	CMC-C2C-C1C	2.36	128.66	125.05
23	C	1036	CLA	CMC-C2C-C1C	2.36	128.66	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1016	CLA	CMC-C2C-C1C	2.36	128.66	125.05
23	a	6006	CLA	CMC-C2C-C1C	2.36	128.66	125.05
23	C	1033	CLA	CMC-C2C-C1C	2.36	128.66	125.05
23	C	1026	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	D	1005	CLA	CMC-C2C-C1C	2.36	128.66	125.05
23	b	6013	CLA	CMC-C2C-C1C	2.36	128.67	125.05
25	d	6042	PQ9	C36-C35-C33	2.36	120.65	112.85
23	c	6027	CLA	CMC-C2C-C1C	2.36	128.67	125.05
23	b	6010	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	B	1013	CLA	CMC-C2C-C1C	2.36	128.67	125.05
23	c	6030	CLA	CMC-C2C-C1C	2.36	128.67	125.05
23	C	1031	CLA	CMC-C2C-C1C	2.36	128.67	125.05
23	B	1010	CLA	CHB-C4A-NA	2.37	127.78	124.51
23	C	1028	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	d	6005	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	D	1008	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	b	6023	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	B	1018	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	B	1023	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	C	1025	CLA	CMC-C2C-C1C	2.37	128.68	125.05
23	c	6028	CLA	CMC-C2C-C1C	2.37	128.69	125.05
23	c	6037	CLA	CMC-C2C-C1C	2.37	128.69	125.05
23	C	1030	CLA	CMC-C2C-C1C	2.37	128.69	125.05
23	b	6016	CLA	CMC-C2C-C1C	2.37	128.69	125.05
26	C	1054	BCR	C30-C25-C24	2.37	122.40	115.73
26	b	6045	BCR	C23-C24-C25	2.37	133.90	127.25
23	C	1037	CLA	CMC-C2C-C1C	2.38	128.69	125.05
23	c	6032	CLA	CMC-C2C-C1C	2.38	128.69	125.05
23	b	6017	CLA	CMC-C2C-C1C	2.38	128.69	125.05
23	b	6010	CLA	CMC-C2C-C1C	2.38	128.69	125.05
23	B	1020	CLA	CMC-C2C-C1C	2.38	128.69	125.05
23	c	6026	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	C	1034	CLA	CMC-C2C-C1C	2.38	128.70	125.05
23	B	1009	CLA	CMC-C2C-C1C	2.38	128.70	125.05
23	b	6020	CLA	CMC-C2C-C1C	2.38	128.70	125.05
23	C	1027	CLA	CMC-C2C-C1C	2.38	128.70	125.05
26	B	1045	BCR	C23-C24-C25	2.38	133.93	127.25
23	b	6009	CLA	CMC-C2C-C1C	2.39	128.71	125.05
23	H	1017	CLA	CMC-C2C-C1C	2.39	128.71	125.05
23	d	6004	CLA	CMC-C2C-C1C	2.39	128.71	125.05
26	c	6054	BCR	C30-C25-C24	2.39	122.45	115.73
23	c	6035	CLA	CMC-C2C-C1C	2.40	128.72	125.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1035	CLA	CMC-C2C-C1C	2.40	128.73	125.05
23	D	1004	CLA	CMC-C2C-C1C	2.40	128.73	125.05
23	A	1007	CLA	CMC-C2C-C1C	2.43	128.77	125.05
23	a	6007	CLA	CMC-C2C-C1C	2.43	128.77	125.05
23	b	6015	CLA	CMB-C2B-C3B	2.46	129.37	124.88
23	B	1015	CLA	CMB-C2B-C3B	2.48	129.40	124.88
26	K	1051	BCR	C23-C24-C25	2.49	134.21	127.25
26	k	6051	BCR	C23-C24-C25	2.49	134.22	127.25
23	b	6022	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	B	1022	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	c	6026	CLA	CMB-C2B-C3B	2.51	129.45	124.88
23	B	1024	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	C	1026	CLA	CMB-C2B-C3B	2.52	129.46	124.88
23	B	1019	CLA	C4-C3-C5	2.52	119.63	115.29
23	b	6019	CLA	C4-C3-C5	2.52	119.63	115.29
23	b	6024	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	A	1038	PHO	C4-C3-C5	2.54	119.67	115.29
25	A	1043	PQ9	C39-C38-C40	2.54	119.67	115.29
24	d	6038	PHO	C4-C3-C5	2.55	119.69	115.29
26	T	6046	BCR	C1-C6-C7	2.56	122.92	115.73
23	b	6024	CLA	CMB-C2B-C3B	2.56	129.55	124.88
23	B	1024	CLA	CMB-C2B-C3B	2.58	129.57	124.88
26	a	6044	BCR	C37-C22-C23	2.58	122.22	118.10
25	d	6042	PQ9	C14-C13-C15	2.59	119.76	115.29
23	B	1010	CLA	CMB-C2B-C3B	2.60	129.61	124.88
26	A	1044	BCR	C37-C22-C23	2.60	122.25	118.10
26	B	1047	BCR	C30-C25-C24	2.60	123.05	115.73
26	b	6047	BCR	C30-C25-C24	2.61	123.05	115.73
23	b	6010	CLA	CMB-C2B-C3B	2.61	129.64	124.88
23	c	6029	CLA	CMB-C2B-C3B	2.62	129.65	124.88
23	b	6022	CLA	C4-C3-C5	2.62	119.81	115.29
25	d	6042	PQ9	C3-C4-C5	2.63	122.25	118.02
23	C	1029	CLA	CMB-C2B-C3B	2.63	129.67	124.88
23	B	1022	CLA	C4-C3-C5	2.64	119.83	115.29
23	b	6011	CLA	CMB-C2B-C3B	2.64	129.69	124.88
23	C	1030	CLA	CMB-C2B-C3B	2.65	129.71	124.88
23	d	6005	CLA	CAC-C3C-C4C	2.65	128.48	124.82
23	c	6035	CLA	CMB-C2B-C3B	2.65	129.71	124.88
23	A	1007	CLA	C4-C3-C5	2.65	119.87	115.29
23	b	6020	CLA	CMB-C2B-C3B	2.65	129.71	124.88
23	c	6030	CLA	CMB-C2B-C3B	2.66	129.72	124.88
23	a	6007	CLA	C4-C3-C5	2.66	119.88	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1035	CLA	CMB-C2B-C3B	2.67	129.73	124.88
23	b	6016	CLA	CAC-C3C-C4C	2.67	128.50	124.82
23	d	6008	CLA	CMB-C2B-C3B	2.67	129.74	124.88
23	c	6027	CLA	CAC-C3C-C4C	2.67	128.50	124.82
23	B	1011	CLA	CMB-C2B-C3B	2.67	129.75	124.88
23	D	1005	CLA	CMB-C2B-C3B	2.67	129.75	124.88
23	c	6032	CLA	CMB-C2B-C3B	2.67	129.75	124.88
23	C	1032	CLA	CMB-C2B-C3B	2.68	129.75	124.88
23	a	6006	CLA	CMB-C2B-C3B	2.68	129.75	124.88
23	A	1006	CLA	CAC-C3C-C4C	2.68	128.51	124.82
23	C	1037	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	B	1020	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	B	1012	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	c	6037	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	b	6017	CLA	CAC-C3C-C4C	2.68	128.52	124.82
23	c	6035	CLA	CAC-C3C-C4C	2.68	128.52	124.82
23	C	1034	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	D	1008	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	c	6028	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	C	1031	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	C	1025	CLA	CMB-C2B-C3B	2.68	129.76	124.88
23	b	6016	CLA	CMB-C2B-C3B	2.68	129.77	124.88
23	C	1033	CLA	CMB-C2B-C3B	2.68	129.77	124.88
23	c	6028	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	C	1035	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	b	6013	CLA	CMB-C2B-C3B	2.69	129.77	124.88
23	C	1027	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	c	6033	CLA	CMB-C2B-C3B	2.69	129.78	124.88
23	c	6032	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	D	1005	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	b	6014	CLA	C3B-C4B-NB	2.69	112.69	109.21
23	B	1024	CLA	C4-C3-C5	2.69	119.93	115.29
23	c	6027	CLA	CMB-C2B-C3B	2.69	129.78	124.88
23	B	1011	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	B	1014	CLA	C3B-C4B-NB	2.69	112.69	109.21
23	b	6023	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	a	6006	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	B	1013	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	d	6005	CLA	CMB-C2B-C3B	2.69	129.78	124.88
23	c	6031	CLA	CMB-C2B-C3B	2.69	129.78	124.88
23	b	6012	CLA	CAC-C3C-C4C	2.69	128.53	124.82
23	d	6008	CLA	CAC-C3C-C4C	2.69	128.53	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1021	CLA	CMB-C2B-C3B	2.69	129.78	124.88
23	b	6012	CLA	CMB-C2B-C3B	2.69	129.79	124.88
23	c	6025	CLA	CMB-C2B-C3B	2.69	129.79	124.88
23	A	1003	CLA	CMB-C2B-C3B	2.69	129.79	124.88
23	a	6003	CLA	CMB-C2B-C3B	2.69	129.79	124.88
23	b	6018	CLA	CMB-C2B-C3B	2.70	129.79	124.88
23	c	6032	CLA	C4-C3-C5	2.70	119.94	115.29
23	b	6024	CLA	C4-C3-C5	2.70	119.94	115.29
23	a	6003	CLA	C4-C3-C5	2.70	119.94	115.29
23	B	1023	CLA	CMB-C2B-C3B	2.70	129.79	124.88
23	B	1021	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	B	1016	CLA	CMB-C2B-C3B	2.70	129.79	124.88
23	C	1032	CLA	C4-C3-C5	2.70	119.94	115.29
23	b	6021	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	C	1036	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	d	6004	CLA	C4-C3-C5	2.70	119.94	115.29
23	H	1017	CLA	CMB-C2B-C3B	2.70	129.80	124.88
23	C	1027	CLA	CMB-C2B-C3B	2.70	129.80	124.88
23	B	1018	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	C	1032	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	B	1016	CLA	CAC-C3C-C4C	2.70	128.54	124.82
23	b	6019	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	1018	CLA	CMB-C2B-C3B	2.70	129.80	124.88
23	b	6020	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	A	1006	CLA	CMB-C2B-C3B	2.70	129.80	124.88
23	b	6021	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	c	6033	CLA	CAC-C3C-C4C	2.70	128.55	124.82
23	c	6033	CLA	C4-C3-C5	2.70	119.95	115.29
23	b	6020	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	B	1020	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	H	1017	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	D	1004	CLA	CMB-C2B-C3B	2.71	129.81	124.88
23	c	6025	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	b	6011	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	b	6013	CLA	CAC-C3C-C4C	2.71	128.55	124.82
23	b	6017	CLA	CMB-C2B-C3B	2.71	129.81	124.88
23	D	1008	CLA	CAC-C3C-C4C	2.71	128.56	124.82
23	B	1019	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	C	1036	CLA	CMB-C2B-C3B	2.71	129.81	124.88
23	d	6004	CLA	CMB-C2B-C3B	2.71	129.82	124.88
23	C	1028	CLA	CAC-C3C-C4C	2.71	128.56	124.82
23	c	6031	CLA	CAC-C3C-C4C	2.71	128.56	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6004	CLA	CAC-C3C-C4C	2.71	128.56	124.82
23	C	1031	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	B	1012	CLA	CAC-C3C-C4C	2.71	128.56	124.82
26	A	1044	BCR	C23-C24-C25	2.71	134.85	127.25
23	b	6016	CLA	C4-C3-C5	2.71	119.97	115.29
23	B	1013	CLA	CMB-C2B-C3B	2.71	129.82	124.88
26	a	6044	BCR	C23-C24-C25	2.71	134.85	127.25
23	D	1004	CLA	CAC-C3C-C4C	2.71	128.56	124.82
23	A	1003	CLA	C4-C3-C5	2.71	119.97	115.29
23	B	1012	CLA	C4-C3-C5	2.71	119.97	115.29
23	b	6021	CLA	CMB-C2B-C3B	2.71	129.82	124.88
23	d	6005	CLA	C4-C3-C5	2.71	119.97	115.29
23	B	1023	CLA	CAC-C3C-C4C	2.72	128.56	124.82
23	b	6023	CLA	CMB-C2B-C3B	2.72	129.82	124.88
23	A	1003	CLA	CAC-C3C-C4C	2.72	128.57	124.82
23	C	1028	CLA	CMB-C2B-C3B	2.72	129.83	124.88
23	B	1020	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	b	6018	CLA	CAC-C3C-C4C	2.72	128.57	124.82
23	B	1016	CLA	C4-C3-C5	2.72	119.98	115.29
23	b	6012	CLA	C4-C3-C5	2.72	119.98	115.29
23	a	6003	CLA	CAC-C3C-C4C	2.72	128.57	124.82
23	C	1030	CLA	CAC-C3C-C4C	2.72	128.57	124.82
23	C	1025	CLA	CAC-C3C-C4C	2.72	128.57	124.82
23	C	1027	CLA	C4-C3-C5	2.72	119.98	115.29
24	A	1039	PHO	C4-C3-C5	2.72	119.98	115.29
23	D	1005	CLA	C4-C3-C5	2.72	119.98	115.29
23	C	1034	CLA	C4-C3-C5	2.72	119.98	115.29
23	C	1031	CLA	CAC-C3C-C4C	2.72	128.58	124.82
25	D	1042	PQ9	C19-C18-C20	2.72	119.99	115.29
23	b	6023	CLA	C4-C3-C5	2.72	119.99	115.29
23	a	6007	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	B	1016	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	A	1006	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	b	6016	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	C	1034	CLA	CAC-C3C-C4C	2.73	128.58	124.82
23	d	6008	CLA	C4-C3-C5	2.73	119.99	115.29
23	C	1037	CLA	C4-C3-C5	2.73	119.99	115.29
23	b	6011	CLA	C4-C3-C5	2.73	119.99	115.29
23	D	1004	CLA	C4-C3-C5	2.73	119.99	115.29
23	c	6037	CLA	CAC-C3C-C4C	2.73	128.58	124.82
23	A	1006	CLA	C4-C3-C5	2.73	119.99	115.29
23	c	6030	CLA	C4-C3-C5	2.73	119.99	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6031	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	C	1033	CLA	C4-C3-C5	2.73	119.99	115.29
23	B	1023	CLA	C4-C3-C5	2.73	120.00	115.29
24	a	6039	PHO	C4-C3-C5	2.73	120.00	115.29
23	B	1013	CLA	C4-C3-C5	2.73	120.00	115.29
23	C	1030	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	a	6006	CLA	C4-C3-C5	2.73	120.00	115.29
25	D	1042	PQ9	C14-C13-C15	2.73	120.00	115.29
23	B	1020	CLA	C4-C3-C5	2.73	120.00	115.29
23	c	6037	CLA	C4-C3-C5	2.73	120.00	115.29
23	c	6035	CLA	C4-C3-C5	2.73	120.00	115.29
23	c	6030	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	c	6036	CLA	CMB-C2B-C3B	2.73	129.85	124.88
23	C	1028	CLA	C4-C3-C5	2.73	120.00	115.29
23	C	1035	CLA	C4-C3-C5	2.73	120.00	115.29
23	A	1003	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	b	6010	CLA	CAC-C3C-C4C	2.73	128.59	124.82
23	B	1011	CLA	C4-C3-C5	2.73	120.00	115.29
23	C	1034	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	C	1033	CLA	CAC-C3C-C4C	2.73	128.59	124.82
23	b	6013	CLA	C4-C3-C5	2.73	120.00	115.29
26	d	6050	BCR	C23-C24-C25	2.73	134.91	127.25
23	C	1032	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	C	1037	CLA	CAC-C3C-C4C	2.74	128.59	124.82
23	C	1031	CLA	C4-C3-C5	2.74	120.01	115.29
23	C	1030	CLA	C4-C3-C5	2.74	120.01	115.29
23	B	1021	CLA	C4-C3-C5	2.74	120.01	115.29
23	c	6036	CLA	CAC-C3C-C4C	2.74	128.59	124.82
23	H	1017	CLA	C4-C3-C5	2.74	120.01	115.29
23	b	6017	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	B	1013	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	B	1024	CLA	O2D-CGD-CBD	2.74	116.14	111.28
23	D	1008	CLA	C4-C3-C5	2.74	120.02	115.29
23	b	6017	CLA	C4-C3-C5	2.74	120.02	115.29
23	b	6012	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	c	6037	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	c	6030	CLA	CAC-C3C-C4C	2.74	128.60	124.82
23	B	1010	CLA	CAC-C3C-C4C	2.74	128.60	124.82
23	B	1021	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	c	6028	CLA	C4-C3-C5	2.74	120.02	115.29
23	b	6021	CLA	C4-C3-C5	2.74	120.02	115.29
23	H	1017	CLA	CHB-C4A-NA	2.74	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1007	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	b	6020	CLA	C4-C3-C5	2.74	120.02	115.29
23	c	6032	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	a	6003	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	B	1018	CLA	C4-C3-C5	2.75	120.03	115.29
23	b	6024	CLA	O2D-CGD-CBD	2.75	116.15	111.28
23	b	6013	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	a	6006	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	c	6025	CLA	C4-C3-C5	2.75	120.03	115.29
25	D	1042	PQ9	C3-C4-C5	2.75	122.44	118.02
23	C	1037	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	C	1036	CLA	C4-C3-C5	2.75	120.03	115.29
26	D	1050	BCR	C23-C24-C25	2.75	134.96	127.25
23	C	1025	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	C	1025	CLA	C4-C3-C5	2.75	120.04	115.29
23	b	6011	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	C	1035	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	d	6042	PQ9	C39-C38-C40	2.75	120.04	115.29
23	c	6028	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	c	6036	CLA	C4-C3-C5	2.76	120.04	115.29
23	C	1028	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	d	6004	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	B	1023	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	d	6042	PQ9	C35-C33-C32	2.76	126.71	121.10
23	C	1033	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	c	6031	CLA	C4-C3-C5	2.76	120.05	115.29
23	c	6027	CLA	C4-C3-C5	2.76	120.05	115.29
23	b	6020	CLA	O2A-CGA-CBA	2.76	119.91	111.92
23	D	1004	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	b	6018	CLA	C4-C3-C5	2.76	120.06	115.29
23	B	1011	CLA	CHB-C4A-NA	2.76	128.34	124.51
23	c	6036	CLA	CHB-C4A-NA	2.76	128.34	124.51
23	B	1009	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	B	1018	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	B	1020	CLA	O2A-CGA-CBA	2.77	119.92	111.92
23	C	1027	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6035	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	d	6005	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6025	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6033	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	b	6023	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	6031	CLA	O2A-CGA-CBA	2.78	119.95	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	6034	CLA	C4-C3-C5	2.78	120.08	115.29
23	D	1004	CLA	O2A-CGA-CBA	2.78	119.95	111.92
23	D	1005	CLA	O2A-CGA-CBA	2.78	119.95	111.92
23	c	6025	CLA	O2A-CGA-CBA	2.78	119.96	111.92
23	a	6006	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	A	1006	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	C	1031	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	C	1032	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	d	6004	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	d	6005	CLA	O2A-CGA-CBA	2.78	119.97	111.92
23	C	1033	CLA	O2A-CGA-CBA	2.79	119.97	111.92
23	B	1018	CLA	O2A-CGA-CBA	2.79	119.98	111.92
23	B	1012	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	C	1036	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	c	6033	CLA	O2A-CGA-CBA	2.79	119.98	111.92
23	b	6018	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	c	6028	CLA	O2A-CGA-CBA	2.79	119.98	111.92
23	C	1025	CLA	O2A-CGA-CBA	2.79	119.98	111.92
23	D	1008	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	C	1034	CLA	O2A-CGA-CBA	2.79	119.98	111.92
23	b	6009	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	b	6016	CLA	O2A-CGA-CBA	2.79	119.99	111.92
23	c	6032	CLA	O2A-CGA-CBA	2.79	119.99	111.92
24	d	6038	PHO	O2A-CGA-CBA	2.79	119.99	111.92
23	b	6012	CLA	O2A-CGA-CBA	2.79	119.99	111.92
23	D	1005	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	C	1035	CLA	O2A-CGA-CBA	2.79	119.99	111.92
24	A	1038	PHO	O2A-CGA-CBA	2.79	120.00	111.92
23	c	6035	CLA	O2A-CGA-CBA	2.79	120.00	111.92
23	C	1037	CLA	O2A-CGA-CBA	2.79	120.00	111.92
23	C	1030	CLA	O2A-CGA-CBA	2.79	120.00	111.92
23	c	6037	CLA	O2A-CGA-CBA	2.79	120.00	111.92
23	C	1028	CLA	O2A-CGA-CBA	2.80	120.00	111.92
23	C	1029	CLA	C4-C3-C5	2.80	120.11	115.29
23	B	1012	CLA	O2A-CGA-CBA	2.80	120.01	111.92
23	b	6021	CLA	O2A-CGA-CBA	2.80	120.01	111.92
23	C	1027	CLA	O2A-CGA-CBA	2.80	120.01	111.92
23	c	6036	CLA	O2A-CGA-CBA	2.80	120.01	111.92
23	C	1036	CLA	O2A-CGA-CBA	2.80	120.01	111.92
23	B	1023	CLA	O2A-CGA-CBA	2.80	120.02	111.92
23	c	6030	CLA	O2A-CGA-CBA	2.80	120.02	111.92
23	B	1021	CLA	O2A-CGA-CBA	2.80	120.02	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	6008	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	1015	CLA	C4-C3-C5	2.80	120.12	115.29
23	b	6013	CLA	O2A-CGA-CBA	2.80	120.03	111.92
23	A	1003	CLA	O2A-CGA-CBA	2.80	120.03	111.92
23	B	1016	CLA	O2A-CGA-CBA	2.80	120.03	111.92
23	B	1013	CLA	O2A-CGA-CBA	2.80	120.03	111.92
23	b	6023	CLA	O2A-CGA-CBA	2.81	120.03	111.92
23	B	1011	CLA	O2A-CGA-CBA	2.81	120.04	111.92
23	b	6011	CLA	O2A-CGA-CBA	2.81	120.04	111.92
23	b	6009	CLA	CAC-C3C-C4C	2.81	128.69	124.82
23	b	6018	CLA	O2A-CGA-CBA	2.81	120.04	111.92
23	c	6027	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	D	1008	CLA	O2A-CGA-CBA	2.81	120.05	111.92
26	d	6050	BCR	C38-C26-C27	2.81	118.88	113.56
23	b	6017	CLA	O2A-CGA-CBA	2.81	120.05	111.92
23	B	1009	CLA	CAC-C3C-C4C	2.81	128.70	124.82
23	a	6003	CLA	O2A-CGA-CBA	2.81	120.06	111.92
23	c	6029	CLA	C4-C3-C5	2.82	120.14	115.29
23	c	6027	CLA	O2A-CGA-CBA	2.82	120.06	111.92
23	H	1017	CLA	O2A-CGA-CBA	2.82	120.07	111.92
23	b	6015	CLA	C4-C3-C5	2.82	120.16	115.29
23	b	6015	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	d	6008	CLA	O2A-CGA-CBA	2.83	120.09	111.92
30	c	6055	DGD	O1G-C1A-C2A	2.83	120.11	111.92
23	b	6009	CLA	C4-C3-C5	2.84	120.18	115.29
23	B	1015	CLA	CHB-C4A-NA	2.84	128.43	124.51
29	d	6059	MGE	O1G-C1A-C2A	2.84	120.12	111.92
29	d	6062	MGE	O1G-C1A-C2A	2.84	120.13	111.92
26	D	1050	BCR	C38-C26-C27	2.84	118.94	113.56
30	C	1055	DGD	O1G-C1A-C2A	2.84	120.14	111.92
26	b	6048	BCR	C38-C26-C27	2.84	118.94	113.56
26	B	1048	BCR	C38-C26-C27	2.84	118.94	113.56
24	A	1039	PHO	O2A-CGA-CBA	2.85	120.15	111.92
29	J	1059	MGE	O1G-C1A-C2A	2.85	120.15	111.92
29	B	1060	MGE	O1G-C1A-C2A	2.85	120.15	111.92
30	H	1058	DGD	O1G-C1A-C2A	2.85	120.15	111.92
24	a	6039	PHO	O2A-CGA-CBA	2.85	120.16	111.92
29	D	1062	MGE	O1G-C1A-C2A	2.85	120.16	111.92
30	h	6058	DGD	O1G-C1A-C2A	2.85	120.16	111.92
29	L	1061	MGE	O1G-C1A-C2A	2.85	120.17	111.92
30	C	1057	DGD	O1G-C1A-C2A	2.85	120.17	111.92
27	A	1063	LHG	O8-C23-C24	2.85	120.17	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6015	CLA	O2A-CGA-CBA	2.86	120.18	111.92
25	d	6042	PQ9	C40-C41-C42	2.86	121.44	111.87
23	B	1015	CLA	O2A-CGA-CBA	2.86	120.19	111.92
30	c	6057	DGD	O1G-C1A-C2A	2.86	120.19	111.92
23	b	6009	CLA	CMB-C2B-C3B	2.86	130.09	124.88
30	C	1056	DGD	O1G-C1A-C2A	2.86	120.19	111.92
29	d	6061	MGE	O1G-C1A-C2A	2.86	120.19	111.92
29	b	6060	MGE	O1G-C1A-C2A	2.86	120.20	111.92
23	B	1009	CLA	C4-C3-C5	2.86	120.22	115.29
27	a	6063	LHG	O8-C23-C24	2.86	120.20	111.92
30	c	6056	DGD	O1G-C1A-C2A	2.87	120.22	111.92
23	b	6009	CLA	O2A-CGA-CBA	2.87	120.23	111.92
23	B	1009	CLA	CMB-C2B-C3B	2.88	130.12	124.88
23	B	1009	CLA	O2A-CGA-CBA	2.89	120.27	111.92
23	B	1019	CLA	CMB-C2B-C3B	2.89	130.15	124.88
23	b	6019	CLA	CMB-C2B-C3B	2.90	130.16	124.88
23	c	6034	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	Z	1053	BCR	C39-C30-C29	2.91	120.14	108.78
26	z	6053	BCR	C39-C30-C29	2.92	120.16	108.78
26	k	6051	BCR	C33-C5-C4	2.92	119.09	113.56
25	A	1043	PQ9	C3-C4-C5	2.92	122.72	118.02
26	K	1051	BCR	C33-C5-C4	2.93	119.11	113.56
23	A	1007	CLA	CMB-C2B-C3B	2.97	130.29	124.88
23	a	6007	CLA	CMB-C2B-C3B	2.99	130.32	124.88
23	B	1014	CLA	C4-C3-C5	2.99	120.45	115.29
23	b	6014	CLA	C4-C3-C5	3.00	120.45	115.29
25	a	6043	PQ9	C3-C4-C5	3.02	122.88	118.02
25	d	6042	PQ9	C19-C18-C20	3.06	120.56	115.29
23	c	6026	CLA	O2D-CGD-CBD	3.06	116.71	111.28
23	c	6034	CLA	CMB-C2B-C3B	3.07	130.46	124.88
23	C	1026	CLA	O2D-CGD-CBD	3.09	116.75	111.28
23	b	6010	CLA	C4-C3-C5	3.12	120.66	115.29
23	B	1010	CLA	C4-C3-C5	3.12	120.67	115.29
23	C	1029	CLA	O2D-CGD-CBD	3.13	116.84	111.28
23	c	6029	CLA	O2D-CGD-CBD	3.14	116.85	111.28
26	t	1046	BCR	C37-C22-C23	3.16	123.13	118.10
23	A	1007	CLA	O2A-CGA-CBA	3.18	121.11	111.92
23	a	6007	CLA	O2A-CGA-CBA	3.18	121.11	111.92
25	D	1042	PQ9	C36-C35-C33	3.19	123.38	112.85
23	b	6014	CLA	CMC-C2C-C1C	3.19	129.94	125.05
23	B	1014	CLA	CMC-C2C-C1C	3.20	129.96	125.05
26	B	1047	BCR	C33-C5-C4	3.23	119.67	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	6047	BCR	C33-C5-C4	3.23	119.67	113.56
24	a	6039	PHO	C2B-C1B-NB	3.29	114.78	109.79
26	d	6050	BCR	C37-C22-C23	3.29	123.35	118.10
24	A	1039	PHO	C2B-C1B-NB	3.29	114.78	109.79
26	D	1050	BCR	C37-C22-C23	3.29	123.35	118.10
25	D	1042	PQ9	C35-C33-C32	3.30	127.82	121.10
25	d	6042	PQ9	C36-C37-C38	3.32	135.87	127.66
26	T	6046	BCR	C37-C22-C23	3.33	123.40	118.10
26	C	1054	BCR	C33-C5-C4	3.33	119.86	113.56
24	A	1038	PHO	C2B-C1B-NB	3.33	114.84	109.79
26	k	6051	BCR	C38-C26-C27	3.33	119.87	113.56
24	d	6038	PHO	C2B-C1B-NB	3.34	114.85	109.79
26	K	1051	BCR	C38-C26-C27	3.34	119.87	113.56
26	c	6054	BCR	C33-C5-C4	3.34	119.88	113.56
26	a	6044	BCR	C38-C26-C27	3.35	119.91	113.56
23	b	6014	CLA	CHB-C4A-NA	3.36	129.15	124.51
26	A	1044	BCR	C38-C26-C27	3.36	119.92	113.56
26	H	1049	BCR	C38-C26-C27	3.37	119.93	113.56
26	t	1046	BCR	C33-C5-C4	3.37	119.94	113.56
26	h	6049	BCR	C38-C26-C27	3.38	119.95	113.56
26	K	1052	BCR	C38-C26-C27	3.38	119.96	113.56
25	A	1043	PQ9	C21-C20-C18	3.38	124.03	112.85
23	b	6022	CLA	C3B-C4B-NB	3.38	113.59	109.21
23	B	1014	CLA	CHB-C4A-NA	3.39	129.19	124.51
26	k	6052	BCR	C33-C5-C4	3.39	119.97	113.56
26	K	1052	BCR	C33-C5-C4	3.39	119.98	113.56
26	k	6052	BCR	C38-C26-C27	3.40	119.98	113.56
26	b	6045	BCR	C33-C5-C4	3.40	119.99	113.56
26	B	1045	BCR	C33-C5-C4	3.40	119.99	113.56
23	B	1022	CLA	C3B-C4B-NB	3.40	113.61	109.21
26	z	6053	BCR	C38-C26-C27	3.41	120.00	113.56
26	h	6049	BCR	C33-C5-C4	3.42	120.02	113.56
26	H	1049	BCR	C33-C5-C4	3.42	120.02	113.56
26	Z	1053	BCR	C33-C5-C4	3.42	120.03	113.56
26	Z	1053	BCR	C38-C26-C27	3.42	120.03	113.56
26	z	6053	BCR	C33-C5-C4	3.42	120.04	113.56
25	D	1042	PQ9	C36-C37-C38	3.43	136.15	127.66
26	B	1045	BCR	C38-C26-C27	3.44	120.07	113.56
26	b	6045	BCR	C38-C26-C27	3.45	120.09	113.56
26	d	6050	BCR	C33-C5-C4	3.48	120.14	113.56
26	D	1050	BCR	C33-C5-C4	3.49	120.16	113.56
26	A	1044	BCR	C33-C5-C4	3.53	120.25	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	6044	BCR	C33-C5-C4	3.55	120.27	113.56
25	a	6043	PQ9	C21-C20-C18	3.55	124.57	112.85
25	D	1042	PQ9	C11-C2-C1	3.60	119.80	116.88
25	d	6042	PQ9	C40-C38-C37	3.65	128.52	121.10
24	A	1038	PHO	C2D-C1D-ND	3.65	115.32	109.79
24	d	6038	PHO	C2D-C1D-ND	3.67	115.36	109.79
23	a	6007	CLA	O2D-CGD-CBD	3.68	117.81	111.28
23	A	1007	CLA	O2D-CGD-CBD	3.68	117.81	111.28
26	D	1050	BCR	C30-C25-C24	3.69	126.11	115.73
26	d	6050	BCR	C30-C25-C24	3.70	126.12	115.73
23	b	6018	CLA	C3B-C4B-NB	3.72	114.01	109.21
26	b	6048	BCR	C33-C5-C4	3.73	120.62	113.56
23	B	1011	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	b	6011	CLA	C3B-C4B-NB	3.74	114.04	109.21
26	B	1048	BCR	C33-C5-C4	3.75	120.65	113.56
23	B	1021	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	B	1018	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	b	6021	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	C	1028	CLA	C3B-C4B-NB	3.76	114.08	109.21
23	c	6036	CLA	C3B-C4B-NB	3.76	114.08	109.21
26	K	1051	BCR	C37-C22-C23	3.76	124.09	118.10
23	c	6028	CLA	C3B-C4B-NB	3.76	114.08	109.21
23	b	6016	CLA	C3B-C4B-NB	3.77	114.08	109.21
26	k	6051	BCR	C37-C22-C23	3.77	124.10	118.10
23	c	6027	CLA	C3B-C4B-NB	3.77	114.09	109.21
23	B	1016	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	C	1027	CLA	C3B-C4B-NB	3.78	114.09	109.21
23	C	1034	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	d	6004	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	a	6003	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	C	1032	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	D	1004	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	D	1005	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	C	1035	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	c	6031	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	b	6017	CLA	C3B-C4B-NB	3.78	114.10	109.21
23	c	6032	CLA	C3B-C4B-NB	3.79	114.10	109.21
26	A	1044	BCR	C24-C23-C22	3.79	131.90	126.21
23	B	1020	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	C	1036	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	c	6035	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	b	6023	CLA	C3B-C4B-NB	3.79	114.11	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6007	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	H	1017	CLA	C3B-C4B-NB	3.79	114.11	109.21
23	A	1003	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	a	6039	PHO	C2D-C1D-ND	3.80	115.54	109.79
23	B	1013	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	b	6012	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	A	1039	PHO	C2D-C1D-ND	3.80	115.55	109.79
23	d	6005	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	B	1023	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	A	1007	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	c	6037	CLA	C3B-C4B-NB	3.80	114.13	109.21
26	a	6044	BCR	C24-C23-C22	3.81	131.93	126.21
23	b	6020	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	C	1031	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	C	1025	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	c	6029	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	C	1037	CLA	C3B-C4B-NB	3.81	114.14	109.21
23	C	1030	CLA	C3B-C4B-NB	3.81	114.14	109.21
23	C	1029	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	c	6033	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	A	1006	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	D	1008	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	C	1033	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	a	6006	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	b	6015	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	b	6013	CLA	C3B-C4B-NB	3.82	114.15	109.21
23	d	6008	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	c	6030	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	B	1012	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	c	6025	CLA	C3B-C4B-NB	3.84	114.17	109.21
23	B	1015	CLA	C3B-C4B-NB	3.84	114.18	109.21
26	B	1045	BCR	C30-C25-C24	3.91	126.71	115.73
23	B	1010	CLA	C3C-C4C-NC	3.91	115.27	110.43
23	c	6034	CLA	C3B-C4B-NB	3.92	114.28	109.21
23	b	6010	CLA	C3C-C4C-NC	3.92	115.28	110.43
26	b	6045	BCR	C30-C25-C24	3.92	126.74	115.73
23	B	1024	CLA	CMC-C2C-C1C	3.92	131.06	125.05
23	b	6024	CLA	CMC-C2C-C1C	3.93	131.08	125.05
23	B	1009	CLA	C3B-C4B-NB	3.93	114.30	109.21
23	b	6009	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	C	1026	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	c	6026	CLA	C3B-C4B-NB	3.95	114.32	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6010	CLA	C3B-C4B-NB	3.96	114.33	109.21
23	B	1010	CLA	C3B-C4B-NB	3.96	114.33	109.21
26	b	6045	BCR	C37-C22-C23	3.98	124.44	118.10
26	B	1045	BCR	C37-C22-C23	3.99	124.45	118.10
26	k	6051	BCR	C30-C25-C24	4.00	126.97	115.73
26	K	1051	BCR	C30-C25-C24	4.01	126.99	115.73
23	b	6024	CLA	C3C-C4C-NC	4.03	115.42	110.43
23	B	1024	CLA	C3B-C4B-NB	4.04	114.44	109.21
23	B	1024	CLA	C3C-C4C-NC	4.04	115.43	110.43
23	b	6024	CLA	C3B-C4B-NB	4.05	114.44	109.21
26	k	6051	BCR	C24-C23-C22	4.05	132.30	126.21
30	c	6057	DGD	O2G-C1B-C2B	4.06	120.11	111.55
24	A	1038	PHO	O2D-CGD-CBD	4.06	118.48	111.28
26	K	1051	BCR	C24-C23-C22	4.06	132.31	126.21
24	d	6038	PHO	O2D-CGD-CBD	4.06	118.49	111.28
30	C	1057	DGD	O2G-C1B-C2B	4.07	120.13	111.55
29	d	6059	MGE	O2G-C1B-C2B	4.07	120.13	111.55
30	C	1055	DGD	O2G-C1B-C2B	4.07	120.13	111.55
27	a	6063	LHG	O7-C7-C8	4.07	120.14	111.55
30	c	6056	DGD	O2G-C1B-C2B	4.08	120.14	111.55
27	A	1063	LHG	O7-C7-C8	4.08	120.14	111.55
30	c	6055	DGD	O2G-C1B-C2B	4.08	120.14	111.55
30	h	6058	DGD	O2G-C1B-C2B	4.08	120.15	111.55
29	J	1059	MGE	O2G-C1B-C2B	4.08	120.15	111.55
23	c	6029	CLA	C3C-C4C-NC	4.08	115.48	110.43
29	d	6062	MGE	O2G-C1B-C2B	4.08	120.15	111.55
23	C	1029	CLA	C3C-C4C-NC	4.08	115.48	110.43
29	b	6060	MGE	O2G-C1B-C2B	4.09	120.16	111.55
30	C	1056	DGD	O2G-C1B-C2B	4.09	120.16	111.55
29	B	1060	MGE	O2G-C1B-C2B	4.09	120.17	111.55
30	H	1058	DGD	O2G-C1B-C2B	4.09	120.17	111.55
23	B	1022	CLA	C3C-C4C-NC	4.09	115.49	110.43
29	d	6061	MGE	O2G-C1B-C2B	4.10	120.19	111.55
29	L	1061	MGE	O2G-C1B-C2B	4.10	120.19	111.55
23	b	6022	CLA	C3C-C4C-NC	4.10	115.50	110.43
29	D	1062	MGE	O2G-C1B-C2B	4.10	120.20	111.55
25	a	6043	PQ9	C14-C13-C15	4.11	122.38	115.29
23	d	6005	CLA	C3C-C4C-NC	4.14	115.55	110.43
26	C	1054	BCR	C38-C26-C27	4.15	121.41	113.56
23	c	6032	CLA	C3C-C4C-NC	4.16	115.58	110.43
26	c	6054	BCR	C38-C26-C27	4.16	121.44	113.56
23	B	1019	CLA	C3B-C4B-NB	4.16	114.59	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	6013	CLA	C3C-C4C-NC	4.17	115.58	110.43
23	A	1006	CLA	C3C-C4C-NC	4.17	115.59	110.43
23	B	1011	CLA	C3C-C4C-NC	4.17	115.59	110.43
23	D	1005	CLA	C3C-C4C-NC	4.17	115.59	110.43
23	b	6016	CLA	C3C-C4C-NC	4.17	115.59	110.43
23	c	6035	CLA	C3C-C4C-NC	4.18	115.60	110.43
23	b	6019	CLA	C3B-C4B-NB	4.18	114.61	109.21
23	c	6025	CLA	C3C-C4C-NC	4.18	115.60	110.43
24	A	1038	PHO	C4D-C3D-CAD	4.18	112.98	105.39
23	c	6027	CLA	C3C-C4C-NC	4.18	115.61	110.43
23	C	1027	CLA	C3C-C4C-NC	4.18	115.61	110.43
25	D	1042	PQ9	C40-C38-C37	4.19	129.61	121.10
23	b	6020	CLA	C3C-C4C-NC	4.19	115.61	110.43
24	d	6038	PHO	C4D-C3D-CAD	4.19	112.99	105.39
23	c	6037	CLA	C3C-C4C-NC	4.19	115.61	110.43
23	C	1032	CLA	C3C-C4C-NC	4.19	115.61	110.43
23	B	1013	CLA	C3C-C4C-NC	4.19	115.61	110.43
23	B	1016	CLA	C3C-C4C-NC	4.19	115.61	110.43
26	a	6044	BCR	C30-C25-C24	4.19	127.50	115.73
23	c	6028	CLA	C3C-C4C-NC	4.19	115.61	110.43
23	b	6012	CLA	C3C-C4C-NC	4.19	115.61	110.43
23	B	1021	CLA	C3C-C4C-NC	4.19	115.62	110.43
23	b	6021	CLA	C3C-C4C-NC	4.19	115.62	110.43
23	a	6006	CLA	C3C-C4C-NC	4.19	115.62	110.43
23	D	1004	CLA	C3C-C4C-NC	4.19	115.62	110.43
26	A	1044	BCR	C30-C25-C24	4.20	127.53	115.73
23	B	1020	CLA	C3C-C4C-NC	4.20	115.63	110.43
23	C	1035	CLA	C3C-C4C-NC	4.20	115.63	110.43
23	b	6011	CLA	C3C-C4C-NC	4.20	115.63	110.43
23	C	1036	CLA	C3C-C4C-NC	4.20	115.63	110.43
23	a	6003	CLA	C3C-C4C-NC	4.21	115.63	110.43
23	D	1008	CLA	C3C-C4C-NC	4.21	115.63	110.43
23	b	6023	CLA	C3C-C4C-NC	4.21	115.63	110.43
23	B	1023	CLA	C3C-C4C-NC	4.21	115.64	110.43
23	d	6004	CLA	C3C-C4C-NC	4.21	115.64	110.43
23	B	1012	CLA	C3C-C4C-NC	4.21	115.64	110.43
23	C	1028	CLA	C3C-C4C-NC	4.21	115.64	110.43
23	C	1037	CLA	C3C-C4C-NC	4.21	115.64	110.43
23	b	6017	CLA	C3C-C4C-NC	4.22	115.64	110.43
26	B	1045	BCR	C24-C23-C22	4.22	132.55	126.21
23	B	1018	CLA	C3C-C4C-NC	4.22	115.65	110.43
23	c	6036	CLA	C3C-C4C-NC	4.22	115.65	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1031	CLA	C3C-C4C-NC	4.22	115.65	110.43
23	C	1025	CLA	C3C-C4C-NC	4.22	115.66	110.43
23	c	6031	CLA	C3C-C4C-NC	4.23	115.66	110.43
23	d	6008	CLA	C3C-C4C-NC	4.23	115.67	110.43
23	A	1003	CLA	C3C-C4C-NC	4.23	115.67	110.43
23	c	6033	CLA	C3C-C4C-NC	4.23	115.67	110.43
23	c	6030	CLA	C3C-C4C-NC	4.24	115.67	110.43
26	b	6045	BCR	C24-C23-C22	4.24	132.58	126.21
23	C	1030	CLA	C3C-C4C-NC	4.24	115.68	110.43
23	H	1017	CLA	C3C-C4C-NC	4.24	115.68	110.43
23	b	6018	CLA	C3C-C4C-NC	4.24	115.68	110.43
23	C	1033	CLA	C3C-C4C-NC	4.25	115.69	110.43
23	C	1034	CLA	C3C-C4C-NC	4.25	115.69	110.43
23	B	1015	CLA	C3C-C4C-NC	4.29	115.74	110.43
23	b	6015	CLA	C3C-C4C-NC	4.31	115.77	110.43
23	c	6034	CLA	C3C-C4C-NC	4.35	115.81	110.43
26	t	1046	BCR	C38-C26-C27	4.39	121.86	113.56
23	a	6007	CLA	C3C-C4C-NC	4.39	115.86	110.43
26	B	1047	BCR	C38-C26-C27	4.40	121.89	113.56
25	A	1043	PQ9	C14-C13-C15	4.40	122.88	115.29
23	b	6009	CLA	C3C-C4C-NC	4.42	115.89	110.43
26	b	6047	BCR	C38-C26-C27	4.42	121.92	113.56
23	A	1007	CLA	C3C-C4C-NC	4.43	115.92	110.43
23	B	1009	CLA	C3C-C4C-NC	4.44	115.92	110.43
26	D	1050	BCR	C24-C23-C22	4.44	132.89	126.21
26	T	6046	BCR	C38-C26-C27	4.45	121.99	113.56
26	d	6050	BCR	C24-C23-C22	4.46	132.91	126.21
23	C	1026	CLA	O2A-CGA-CBA	4.47	124.85	111.92
23	c	6026	CLA	O2A-CGA-CBA	4.47	124.86	111.92
26	Z	1053	BCR	C7-C8-C9	4.59	133.10	126.21
26	z	6053	BCR	C7-C8-C9	4.59	133.10	126.21
23	B	1014	CLA	C3C-C4C-NC	4.62	116.14	110.43
23	c	6034	CLA	O2D-CGD-CBD	4.63	119.49	111.28
23	b	6014	CLA	C3C-C4C-NC	4.65	116.18	110.43
23	c	6026	CLA	C3C-C4C-NC	4.67	116.20	110.43
23	C	1026	CLA	C3C-C4C-NC	4.69	116.23	110.43
26	T	6046	BCR	C33-C5-C4	4.70	122.46	113.56
24	A	1039	PHO	C4D-C3D-CAD	4.71	113.94	105.39
24	a	6039	PHO	C4D-C3D-CAD	4.73	113.98	105.39
25	A	1043	PQ9	C11-C2-C1	4.74	120.73	116.88
23	B	1015	CLA	O2D-CGD-CBD	4.86	119.90	111.28
23	b	6015	CLA	O2D-CGD-CBD	4.86	119.90	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1012	CLA	O2D-CGD-CBD	4.88	119.93	111.28
23	B	1011	CLA	O2D-CGD-CBD	4.88	119.94	111.28
23	b	6011	CLA	O2D-CGD-CBD	4.88	119.94	111.28
23	b	6012	CLA	O2D-CGD-CBD	4.88	119.94	111.28
23	b	6021	CLA	O2D-CGD-CBD	4.89	119.94	111.28
23	C	1034	CLA	O2D-CGD-CBD	4.89	119.94	111.28
23	C	1037	CLA	O2D-CGD-CBD	4.89	119.94	111.28
23	c	6031	CLA	O2D-CGD-CBD	4.89	119.94	111.28
23	c	6037	CLA	O2D-CGD-CBD	4.89	119.95	111.28
23	C	1025	CLA	O2D-CGD-CBD	4.89	119.95	111.28
23	B	1018	CLA	O2D-CGD-CBD	4.89	119.95	111.28
23	c	6030	CLA	O2D-CGD-CBD	4.89	119.95	111.28
23	c	6032	CLA	O2D-CGD-CBD	4.89	119.96	111.28
23	C	1035	CLA	O2D-CGD-CBD	4.89	119.96	111.28
23	C	1030	CLA	O2D-CGD-CBD	4.90	119.96	111.28
23	c	6033	CLA	O2D-CGD-CBD	4.90	119.96	111.28
23	c	6035	CLA	O2D-CGD-CBD	4.90	119.96	111.28
23	c	6036	CLA	O2D-CGD-CBD	4.90	119.96	111.28
23	C	1031	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	d	6004	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	B	1021	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	A	1006	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	D	1008	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	b	6013	CLA	O2D-CGD-CBD	4.90	119.97	111.28
23	b	6023	CLA	O2D-CGD-CBD	4.90	119.98	111.28
23	C	1032	CLA	O2D-CGD-CBD	4.91	119.98	111.28
23	C	1036	CLA	O2D-CGD-CBD	4.91	119.98	111.28
23	c	6025	CLA	O2D-CGD-CBD	4.91	119.98	111.28
23	B	1023	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	c	6028	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	C	1033	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	d	6008	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	b	6018	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	a	6003	CLA	O2D-CGD-CBD	4.91	119.99	111.28
23	H	1017	CLA	O2D-CGD-CBD	4.92	120.00	111.28
23	b	6017	CLA	O2D-CGD-CBD	4.92	120.00	111.28
23	B	1013	CLA	O2D-CGD-CBD	4.92	120.00	111.28
23	D	1004	CLA	O2D-CGD-CBD	4.92	120.00	111.28
23	C	1028	CLA	O2D-CGD-CBD	4.92	120.00	111.28
23	A	1003	CLA	O2D-CGD-CBD	4.92	120.01	111.28
23	B	1020	CLA	O2D-CGD-CBD	4.92	120.01	111.28
23	d	6005	CLA	O2D-CGD-CBD	4.93	120.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	6006	CLA	O2D-CGD-CBD	4.93	120.02	111.28
23	c	6027	CLA	O2D-CGD-CBD	4.93	120.02	111.28
23	D	1005	CLA	O2D-CGD-CBD	4.93	120.02	111.28
23	C	1027	CLA	O2D-CGD-CBD	4.93	120.03	111.28
23	b	6020	CLA	O2D-CGD-CBD	4.94	120.04	111.28
23	b	6016	CLA	O2D-CGD-CBD	4.94	120.04	111.28
23	B	1016	CLA	O2D-CGD-CBD	4.94	120.05	111.28
26	k	6051	BCR	C20-C19-C18	4.97	140.37	126.42
26	K	1051	BCR	C20-C19-C18	4.98	140.39	126.42
25	a	6043	PQ9	C11-C2-C1	4.99	120.93	116.88
24	A	1039	PHO	O2D-CGD-CBD	5.03	120.20	111.28
24	a	6039	PHO	O2D-CGD-CBD	5.04	120.22	111.28
26	b	6047	BCR	C11-C12-C13	5.14	140.86	126.42
23	b	6024	CLA	CAC-C3C-C4C	5.16	131.93	124.82
23	B	1024	CLA	CAC-C3C-C4C	5.16	131.94	124.82
26	B	1047	BCR	C11-C12-C13	5.16	140.90	126.42
25	A	1043	PQ9	C20-C18-C17	5.18	131.63	121.10
25	a	6043	PQ9	C20-C18-C17	5.29	131.87	121.10
23	b	6019	CLA	C3C-C4C-NC	5.35	117.05	110.43
26	Z	1053	BCR	C39-C30-C25	5.35	118.99	110.31
26	z	6053	BCR	C39-C30-C25	5.36	119.00	110.31
23	B	1019	CLA	C3C-C4C-NC	5.37	117.07	110.43
26	k	6051	BCR	C11-C12-C13	5.39	141.55	126.42
26	K	1051	BCR	C11-C12-C13	5.39	141.55	126.42
26	z	6053	BCR	C29-C30-C25	5.40	118.92	110.48
26	Z	1053	BCR	C29-C30-C25	5.42	118.95	110.48
26	K	1052	BCR	C20-C19-C18	5.63	142.22	126.42
23	b	6015	CLA	C2C-C1C-NC	5.73	116.03	110.09
23	B	1015	CLA	C2C-C1C-NC	5.74	116.03	110.09
23	b	6014	CLA	C2C-C1C-NC	5.89	116.19	110.09
23	a	6007	CLA	C2C-C1C-NC	5.91	116.21	110.09
26	b	6048	BCR	C10-C11-C12	5.91	141.27	123.26
23	A	1007	CLA	C2C-C1C-NC	5.92	116.22	110.09
26	B	1048	BCR	C10-C11-C12	5.92	141.30	123.26
23	B	1014	CLA	C2C-C1C-NC	5.94	116.24	110.09
23	b	6021	CLA	C2C-C1C-NC	5.96	116.26	110.09
23	B	1021	CLA	C2C-C1C-NC	5.98	116.28	110.09
23	c	6031	CLA	C2C-C1C-NC	5.99	116.29	110.09
23	B	1016	CLA	C2C-C1C-NC	5.99	116.30	110.09
23	b	6012	CLA	C2C-C1C-NC	6.00	116.30	110.09
23	B	1012	CLA	C2C-C1C-NC	6.00	116.30	110.09
23	A	1006	CLA	C2C-C1C-NC	6.00	116.30	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	1036	CLA	C2C-C1C-NC	6.00	116.30	110.09
23	c	6033	CLA	C2C-C1C-NC	6.01	116.31	110.09
23	c	6037	CLA	C2C-C1C-NC	6.01	116.31	110.09
23	C	1031	CLA	C2C-C1C-NC	6.01	116.31	110.09
23	D	1005	CLA	C2C-C1C-NC	6.01	116.32	110.09
23	b	6023	CLA	C2C-C1C-NC	6.02	116.32	110.09
23	A	1003	CLA	C2C-C1C-NC	6.02	116.33	110.09
23	C	1037	CLA	C2C-C1C-NC	6.03	116.33	110.09
23	b	6018	CLA	C2C-C1C-NC	6.03	116.34	110.09
23	b	6016	CLA	C2C-C1C-NC	6.03	116.34	110.09
23	C	1033	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	c	6025	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	d	6005	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	b	6020	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	C	1027	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	a	6003	CLA	C2C-C1C-NC	6.04	116.34	110.09
23	d	6008	CLA	C2C-C1C-NC	6.04	116.35	110.09
23	d	6004	CLA	C2C-C1C-NC	6.04	116.35	110.09
23	C	1034	CLA	C2C-C1C-NC	6.04	116.35	110.09
23	C	1025	CLA	C2C-C1C-NC	6.04	116.35	110.09
23	c	6028	CLA	C2C-C1C-NC	6.05	116.35	110.09
23	B	1011	CLA	C2C-C1C-NC	6.05	116.35	110.09
23	a	6006	CLA	C2C-C1C-NC	6.05	116.35	110.09
23	C	1032	CLA	C2C-C1C-NC	6.05	116.35	110.09
23	C	1028	CLA	C2C-C1C-NC	6.05	116.36	110.09
23	B	1023	CLA	C2C-C1C-NC	6.05	116.36	110.09
26	k	6052	BCR	C10-C11-C12	6.05	141.71	123.26
23	B	1020	CLA	C2C-C1C-NC	6.05	116.36	110.09
23	C	1030	CLA	C2C-C1C-NC	6.06	116.36	110.09
23	c	6030	CLA	C2C-C1C-NC	6.06	116.36	110.09
23	D	1004	CLA	C2C-C1C-NC	6.06	116.36	110.09
23	c	6036	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	c	6035	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	D	1008	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	B	1013	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	b	6017	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	B	1018	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	b	6013	CLA	C2C-C1C-NC	6.06	116.37	110.09
23	b	6011	CLA	C2C-C1C-NC	6.07	116.37	110.09
23	H	1017	CLA	C2C-C1C-NC	6.07	116.37	110.09
23	c	6027	CLA	C2C-C1C-NC	6.07	116.37	110.09
26	k	6051	BCR	C10-C11-C12	6.07	141.76	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	1051	BCR	C10-C11-C12	6.07	141.76	123.26
23	C	1035	CLA	C2C-C1C-NC	6.08	116.39	110.09
23	c	6032	CLA	C2C-C1C-NC	6.08	116.39	110.09
23	c	6034	CLA	C2C-C1C-NC	6.09	116.40	110.09
26	b	6045	BCR	C10-C11-C12	6.18	142.08	123.26
26	B	1045	BCR	C10-C11-C12	6.18	142.11	123.26
26	k	6052	BCR	C20-C19-C18	6.22	143.88	126.42
23	C	1029	CLA	C2C-C1C-NC	6.26	116.58	110.09
23	c	6029	CLA	C2C-C1C-NC	6.27	116.58	110.09
23	c	6026	CLA	C2C-C1C-NC	6.27	116.59	110.09
23	C	1026	CLA	C2C-C1C-NC	6.30	116.61	110.09
23	B	1022	CLA	C2C-C1C-NC	6.45	116.77	110.09
23	b	6022	CLA	C2C-C1C-NC	6.46	116.78	110.09
23	B	1010	CLA	C2C-C1C-NC	6.47	116.79	110.09
23	b	6009	CLA	C2C-C1C-NC	6.48	116.80	110.09
23	B	1009	CLA	C2C-C1C-NC	6.48	116.80	110.09
23	b	6010	CLA	C2C-C1C-NC	6.50	116.82	110.09
26	a	6044	BCR	C7-C8-C9	6.54	136.03	126.21
26	A	1044	BCR	C7-C8-C9	6.56	136.07	126.21
26	a	6044	BCR	C20-C19-C18	6.58	144.90	126.42
23	b	6019	CLA	C2C-C1C-NC	6.58	116.90	110.09
26	A	1044	BCR	C20-C19-C18	6.59	144.93	126.42
23	B	1019	CLA	C2C-C1C-NC	6.61	116.93	110.09
26	c	6054	BCR	C11-C12-C13	6.62	145.02	126.42
26	C	1054	BCR	C11-C12-C13	6.62	145.02	126.42
26	b	6045	BCR	C11-C12-C13	6.69	145.22	126.42
26	B	1045	BCR	C11-C12-C13	6.70	145.25	126.42
23	B	1024	CLA	C2C-C1C-NC	6.71	117.04	110.09
23	b	6024	CLA	C2C-C1C-NC	6.72	117.05	110.09
26	h	6049	BCR	C20-C19-C18	6.89	145.77	126.42
26	H	1049	BCR	C20-C19-C18	6.90	145.79	126.42
26	t	1046	BCR	C10-C11-C12	7.20	145.19	123.26
26	T	6046	BCR	C10-C11-C12	7.48	146.04	123.26
26	t	1046	BCR	C20-C19-C18	7.65	147.90	126.42
26	b	6047	BCR	C10-C11-C12	7.80	147.04	123.26
26	B	1047	BCR	C10-C11-C12	7.81	147.05	123.26
26	b	6048	BCR	C16-C15-C14	7.98	140.49	123.46
26	B	1048	BCR	C16-C15-C14	7.98	140.50	123.46
26	K	1052	BCR	C10-C11-C12	8.10	147.94	123.26
26	B	1048	BCR	C20-C19-C18	8.23	149.54	126.42
26	b	6048	BCR	C20-C19-C18	8.24	149.56	126.42
26	C	1054	BCR	C10-C11-C12	8.44	148.99	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	6054	BCR	C10-C11-C12	8.45	149.01	123.26
26	k	6052	BCR	C11-C12-C13	8.47	150.21	126.42
26	C	1054	BCR	C16-C15-C14	8.60	141.81	123.46
26	b	6048	BCR	C11-C12-C13	8.60	150.56	126.42
26	B	1048	BCR	C11-C12-C13	8.61	150.60	126.42
26	c	6054	BCR	C16-C15-C14	8.62	141.87	123.46
26	C	1054	BCR	C20-C19-C18	8.84	151.24	126.42
26	c	6054	BCR	C20-C19-C18	8.84	151.25	126.42
26	b	6045	BCR	C20-C19-C18	8.95	151.57	126.42
26	B	1045	BCR	C20-C19-C18	8.96	151.60	126.42
26	D	1050	BCR	C7-C8-C9	9.02	139.76	126.21
26	K	1052	BCR	C16-C15-C14	9.02	142.71	123.46
26	d	6050	BCR	C7-C8-C9	9.02	139.76	126.21
26	b	6048	BCR	C20-C21-C22	9.29	140.57	127.31
26	B	1048	BCR	C20-C21-C22	9.30	140.59	127.31
26	B	1047	BCR	C16-C17-C18	9.33	140.63	127.31
26	b	6047	BCR	C16-C17-C18	9.34	140.64	127.31
26	C	1054	BCR	C16-C17-C18	9.35	140.65	127.31
26	c	6054	BCR	C16-C17-C18	9.36	140.67	127.31
26	d	6050	BCR	C16-C17-C18	9.60	141.01	127.31
26	D	1050	BCR	C16-C17-C18	9.62	141.03	127.31
23	C	1034	CLA	CED-O2D-CGD	9.67	138.26	115.97
26	T	6046	BCR	C20-C19-C18	9.88	154.16	126.42
26	K	1052	BCR	C11-C12-C13	9.91	154.26	126.42
26	h	6049	BCR	C10-C11-C12	9.94	153.54	123.26
26	H	1049	BCR	C10-C11-C12	9.96	153.61	123.26
26	z	6053	BCR	C20-C21-C22	9.99	141.56	127.31
26	z	6053	BCR	C11-C12-C13	10.04	154.63	126.42
26	H	1049	BCR	C16-C17-C18	10.04	141.64	127.31
26	H	1049	BCR	C20-C21-C22	10.05	141.65	127.31
26	Z	1053	BCR	C11-C12-C13	10.05	154.64	126.42
26	Z	1053	BCR	C20-C21-C22	10.06	141.66	127.31
26	A	1044	BCR	C10-C11-C12	10.06	153.91	123.26
26	h	6049	BCR	C20-C21-C22	10.06	141.67	127.31
26	h	6049	BCR	C16-C17-C18	10.07	141.68	127.31
26	a	6044	BCR	C10-C11-C12	10.07	153.94	123.26
26	z	6053	BCR	C16-C17-C18	10.07	141.68	127.31
26	Z	1053	BCR	C16-C17-C18	10.10	141.73	127.31
26	b	6047	BCR	C20-C21-C22	10.14	141.78	127.31
26	B	1047	BCR	C20-C21-C22	10.15	141.80	127.31
26	b	6047	BCR	C16-C15-C14	10.27	145.39	123.46
26	B	1047	BCR	C16-C15-C14	10.28	145.40	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	6052	BCR	C16-C15-C14	10.32	145.48	123.46
26	k	6052	BCR	C21-C20-C19	10.43	155.03	123.26
26	H	1049	BCR	C21-C20-C19	10.45	155.09	123.26
26	h	6049	BCR	C21-C20-C19	10.46	155.12	123.26
26	K	1052	BCR	C21-C20-C19	11.01	156.80	123.26
26	d	6050	BCR	C20-C19-C18	11.07	157.53	126.42
26	D	1050	BCR	C20-C19-C18	11.08	157.53	126.42
26	t	1046	BCR	C20-C21-C22	11.15	143.22	127.31
26	a	6044	BCR	C11-C12-C13	11.17	157.80	126.42
26	A	1044	BCR	C11-C12-C13	11.18	157.82	126.42
26	K	1052	BCR	C20-C21-C22	11.32	143.47	127.31
26	B	1047	BCR	C20-C19-C18	11.47	158.65	126.42
26	b	6047	BCR	C20-C19-C18	11.49	158.69	126.42
26	Z	1053	BCR	C20-C19-C18	11.52	158.78	126.42
26	z	6053	BCR	C20-C19-C18	11.53	158.80	126.42
26	h	6049	BCR	C7-C8-C9	11.55	143.57	126.21
26	H	1049	BCR	C7-C8-C9	11.56	143.58	126.21
26	B	1045	BCR	C20-C21-C22	11.56	143.81	127.31
26	b	6045	BCR	C20-C21-C22	11.57	143.82	127.31
26	k	6052	BCR	C20-C21-C22	11.64	143.92	127.31
26	B	1045	BCR	C16-C17-C18	11.76	144.09	127.31
26	b	6045	BCR	C16-C17-C18	11.76	144.09	127.31
26	h	6049	BCR	C11-C12-C13	11.92	159.91	126.42
26	H	1049	BCR	C11-C12-C13	11.94	159.96	126.42
26	T	6046	BCR	C16-C17-C18	12.04	144.49	127.31
26	d	6050	BCR	C10-C11-C12	12.37	160.94	123.26
26	D	1050	BCR	C10-C11-C12	12.38	160.98	123.26
26	k	6051	BCR	C20-C21-C22	12.53	145.19	127.31
26	K	1051	BCR	C20-C21-C22	12.54	145.21	127.31
26	B	1045	BCR	C16-C15-C14	13.02	151.25	123.46
26	b	6045	BCR	C16-C15-C14	13.03	151.27	123.46
26	D	1050	BCR	C20-C21-C22	13.73	146.91	127.31
26	d	6050	BCR	C20-C21-C22	13.76	146.95	127.31
26	t	1046	BCR	C21-C20-C19	13.81	165.34	123.26
26	K	1052	BCR	C16-C17-C18	14.07	147.39	127.31
26	z	6053	BCR	C10-C11-C12	14.14	166.35	123.26
26	Z	1053	BCR	C10-C11-C12	14.15	166.38	123.26
26	K	1051	BCR	C16-C15-C14	14.21	153.79	123.46
26	k	6051	BCR	C16-C15-C14	14.22	153.81	123.46
26	A	1044	BCR	C20-C21-C22	14.22	147.61	127.31
26	a	6044	BCR	C20-C21-C22	14.27	147.67	127.31
26	t	1046	BCR	C11-C12-C13	14.52	167.21	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	1050	BCR	C21-C20-C19	14.60	167.76	123.26
26	d	6050	BCR	C21-C20-C19	14.60	167.76	123.26
26	k	6052	BCR	C15-C16-C17	14.83	155.12	123.46
26	k	6052	BCR	C16-C17-C18	14.97	148.68	127.31
26	Z	1053	BCR	C16-C15-C14	15.06	155.60	123.46
26	z	6053	BCR	C16-C15-C14	15.06	155.61	123.46
26	t	1046	BCR	C16-C15-C14	15.08	155.64	123.46
26	a	6044	BCR	C21-C20-C19	15.15	169.41	123.26
26	A	1044	BCR	C21-C20-C19	15.16	169.44	123.26
26	Z	1053	BCR	C21-C20-C19	15.31	169.91	123.26
26	z	6053	BCR	C21-C20-C19	15.34	169.99	123.26
26	C	1054	BCR	C21-C20-C19	15.34	169.99	123.26
26	c	6054	BCR	C21-C20-C19	15.34	170.00	123.26
26	a	6044	BCR	C16-C17-C18	15.36	149.22	127.31
26	A	1044	BCR	C16-C17-C18	15.37	149.25	127.31
26	d	6050	BCR	C16-C15-C14	15.72	157.02	123.46
26	D	1050	BCR	C16-C15-C14	15.73	157.04	123.46
26	a	6044	BCR	C16-C15-C14	16.03	157.68	123.46
26	A	1044	BCR	C16-C15-C14	16.05	157.72	123.46
26	D	1050	BCR	C11-C12-C13	16.28	172.16	126.42
26	d	6050	BCR	C11-C12-C13	16.29	172.17	126.42
26	T	6046	BCR	C11-C12-C13	16.36	172.38	126.42
26	t	1046	BCR	C15-C16-C17	16.61	158.92	123.46
26	b	6048	BCR	C21-C20-C19	16.74	174.25	123.26
26	B	1048	BCR	C21-C20-C19	16.74	174.27	123.26
26	k	6051	BCR	C7-C8-C9	16.75	151.38	126.21
26	K	1051	BCR	C7-C8-C9	16.76	151.39	126.21
26	B	1047	BCR	C21-C20-C19	17.50	176.59	123.26
26	b	6047	BCR	C21-C20-C19	17.52	176.64	123.26
26	T	6046	BCR	C16-C15-C14	17.61	161.05	123.46
26	k	6052	BCR	C7-C8-C9	17.69	152.79	126.21
26	K	1051	BCR	C21-C20-C19	17.75	177.34	123.26
26	k	6051	BCR	C21-C20-C19	17.76	177.37	123.26
26	B	1045	BCR	C21-C20-C19	17.87	177.71	123.26
26	b	6045	BCR	C21-C20-C19	17.87	177.72	123.26
26	K	1052	BCR	C7-C8-C9	18.08	153.37	126.21
25	d	6042	PQ9	C30-C28-C27	18.20	158.12	121.10
26	T	6046	BCR	C21-C20-C19	18.62	180.00	123.26
25	D	1042	PQ9	C30-C28-C27	18.73	159.20	121.10
26	b	6048	BCR	C7-C8-C9	18.98	154.73	126.21
26	B	1048	BCR	C7-C8-C9	19.00	154.76	126.21
26	k	6051	BCR	C16-C17-C18	19.11	154.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	1051	BCR	C16-C17-C18	19.14	154.63	127.31
26	T	6046	BCR	C20-C21-C22	19.22	154.74	127.31
26	c	6054	BCR	C20-C21-C22	20.01	155.86	127.31
26	C	1054	BCR	C20-C21-C22	20.02	155.89	127.31
26	K	1052	BCR	C15-C16-C17	20.38	166.95	123.46
26	t	1046	BCR	C16-C17-C18	20.45	156.49	127.31
25	a	6043	PQ9	C30-C28-C27	20.58	162.97	121.10
26	b	6045	BCR	C7-C8-C9	21.28	158.19	126.21
26	B	1045	BCR	C7-C8-C9	21.29	158.19	126.21
26	T	6046	BCR	C15-C16-C17	21.53	169.41	123.46
26	b	6048	BCR	C16-C17-C18	21.69	158.27	127.31
26	B	1048	BCR	C16-C17-C18	21.70	158.28	127.31
26	d	6050	BCR	C15-C16-C17	21.96	170.33	123.46
26	D	1050	BCR	C15-C16-C17	21.97	170.35	123.46
26	t	1046	BCR	C7-C8-C9	22.05	159.34	126.21
25	A	1043	PQ9	C30-C28-C27	22.65	167.18	121.10
26	B	1048	BCR	C15-C16-C17	23.32	173.25	123.46
26	b	6048	BCR	C15-C16-C17	23.33	173.27	123.46
26	h	6049	BCR	C16-C15-C14	23.56	173.75	123.46
26	H	1049	BCR	C16-C15-C14	23.57	173.78	123.46
26	c	6054	BCR	C15-C16-C17	23.60	173.83	123.46
26	C	1054	BCR	C15-C16-C17	23.62	173.88	123.46
26	B	1047	BCR	C15-C16-C17	23.70	174.06	123.46
26	b	6047	BCR	C15-C16-C17	23.71	174.06	123.46
26	k	6051	BCR	C15-C16-C17	23.79	174.25	123.46
26	K	1051	BCR	C15-C16-C17	23.82	174.31	123.46
26	Z	1053	BCR	C15-C16-C17	24.02	174.73	123.46
26	z	6053	BCR	C15-C16-C17	24.02	174.73	123.46
26	A	1044	BCR	C15-C16-C17	24.08	174.86	123.46
26	a	6044	BCR	C15-C16-C17	24.09	174.89	123.46
26	h	6049	BCR	C15-C16-C17	24.44	175.64	123.46
26	H	1049	BCR	C15-C16-C17	24.45	175.65	123.46
26	b	6045	BCR	C15-C16-C17	25.37	177.62	123.46
26	B	1045	BCR	C15-C16-C17	25.39	177.66	123.46
26	T	6046	BCR	C7-C8-C9	26.80	166.48	126.21
26	c	6054	BCR	C7-C8-C9	27.64	167.74	126.21
26	C	1054	BCR	C7-C8-C9	27.67	167.78	126.21
26	b	6047	BCR	C7-C8-C9	34.13	177.50	126.21
26	B	1047	BCR	C7-C8-C9	34.18	177.56	126.21

All (296) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	6010	CLA	NC
23	b	6010	CLA	ND
23	b	6010	CLA	NA
23	B	1010	CLA	NC
23	B	1010	CLA	ND
23	B	1010	CLA	NA
23	b	6014	CLA	NC
23	b	6014	CLA	ND
23	b	6014	CLA	NA
23	b	6014	CLA	C3A
23	C	1028	CLA	C8
23	C	1028	CLA	NA
23	C	1028	CLA	NC
23	C	1028	CLA	C13
23	C	1028	CLA	ND
23	C	1028	CLA	C3A
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	1037	CLA	CBD
23	C	1037	CLA	C13
23	C	1037	CLA	NC
23	C	1037	CLA	ND
23	C	1037	CLA	NA
23	D	1008	CLA	NC
23	D	1008	CLA	ND
23	D	1008	CLA	NA
23	B	1020	CLA	NC
23	B	1020	CLA	ND
23	B	1020	CLA	NA
23	B	1020	CLA	C3A
24	a	6039	PHO	C13
23	C	1030	CLA	NC
23	C	1030	CLA	ND
23	C	1030	CLA	NA
23	b	6017	CLA	C13
23	b	6017	CLA	NC
23	b	6017	CLA	ND
23	b	6017	CLA	NA
23	b	6022	CLA	CBD
23	b	6022	CLA	C8

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Mol	Chain	Res	Type	Atom
23	b	6022	CLA	NC
23	b	6022	CLA	ND
23	b	6022	CLA	NA
23	A	1006	CLA	NC
23	A	1006	CLA	ND
23	A	1006	CLA	NA
23	B	1021	CLA	C8
23	B	1021	CLA	C13
23	B	1021	CLA	NC
23	B	1021	CLA	ND
23	B	1021	CLA	NA
23	B	1014	CLA	NC
23	B	1014	CLA	ND
23	B	1014	CLA	NA
23	B	1014	CLA	C3A
23	c	6030	CLA	NC
23	c	6030	CLA	ND
23	c	6030	CLA	NA
24	A	1038	PHO	C8
24	A	1038	PHO	C13
23	d	6005	CLA	C8
23	d	6005	CLA	NC
23	d	6005	CLA	ND
23	d	6005	CLA	NA
24	A	1039	PHO	C13
24	d	6038	PHO	C8
24	d	6038	PHO	C13
23	c	6028	CLA	C8
23	c	6028	CLA	NA
23	c	6028	CLA	NC
23	c	6028	CLA	C13
23	c	6028	CLA	ND
23	c	6028	CLA	C3A
23	B	1024	CLA	C13
23	B	1024	CLA	NC
23	B	1024	CLA	ND
23	B	1024	CLA	NA
23	c	6027	CLA	C8
23	c	6027	CLA	NA
23	c	6027	CLA	NC
23	c	6027	CLA	C13
23	c	6027	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	6027	CLA	C3A
23	C	1033	CLA	C8
23	C	1033	CLA	NC
23	C	1033	CLA	ND
23	C	1033	CLA	NA
23	C	1033	CLA	C3A
23	b	6015	CLA	NC
23	b	6015	CLA	ND
23	b	6015	CLA	NA
23	b	6020	CLA	NC
23	b	6020	CLA	ND
23	b	6020	CLA	NA
23	b	6020	CLA	C3A
23	b	6012	CLA	NC
23	b	6012	CLA	ND
23	b	6012	CLA	NA
23	B	1011	CLA	NC
23	B	1011	CLA	ND
23	B	1011	CLA	NA
23	c	6032	CLA	NC
23	c	6032	CLA	ND
23	c	6032	CLA	NA
23	d	6008	CLA	NC
23	d	6008	CLA	ND
23	d	6008	CLA	NA
23	b	6024	CLA	C13
23	b	6024	CLA	NC
23	b	6024	CLA	ND
23	b	6024	CLA	NA
23	b	6021	CLA	C8
23	b	6021	CLA	C13
23	b	6021	CLA	NC
23	b	6021	CLA	ND
23	b	6021	CLA	NA
23	c	6031	CLA	C8
23	c	6031	CLA	NA
23	c	6031	CLA	CBD
23	c	6031	CLA	NC
23	c	6031	CLA	C13
23	c	6031	CLA	ND
23	c	6034	CLA	C2A
23	c	6034	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	6034	CLA	CBD
23	c	6034	CLA	NC
23	c	6034	CLA	C8
23	c	6034	CLA	ND
23	c	6034	CLA	C3A
23	B	1022	CLA	CBD
23	B	1022	CLA	C8
23	B	1022	CLA	NC
23	B	1022	CLA	ND
23	B	1022	CLA	NA
23	b	6023	CLA	CBD
23	b	6023	CLA	C13
23	b	6023	CLA	NC
23	b	6023	CLA	ND
23	b	6023	CLA	NA
23	c	6025	CLA	CBD
23	c	6025	CLA	NC
23	c	6025	CLA	ND
23	c	6025	CLA	NA
23	B	1009	CLA	C8
23	B	1009	CLA	NA
23	B	1009	CLA	CBD
23	B	1009	CLA	NC
23	B	1009	CLA	C13
23	B	1009	CLA	ND
23	A	1003	CLA	NC
23	A	1003	CLA	ND
23	A	1003	CLA	NA
23	b	6011	CLA	NC
23	b	6011	CLA	ND
23	b	6011	CLA	NA
23	a	6006	CLA	NC
23	a	6006	CLA	ND
23	a	6006	CLA	NA
23	c	6037	CLA	CBD
23	c	6037	CLA	C13
23	c	6037	CLA	NC
23	c	6037	CLA	ND
23	c	6037	CLA	NA
23	C	1031	CLA	C8
23	C	1031	CLA	NA
23	C	1031	CLA	CBD

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Mol	Chain	Res	Type	Atom
23	C	1031	CLA	NC
23	C	1031	CLA	C13
23	C	1031	CLA	ND
23	B	1018	CLA	NC
23	B	1018	CLA	ND
23	B	1018	CLA	NA
23	C	1034	CLA	C2A
23	C	1034	CLA	NA
23	C	1034	CLA	CBD
23	C	1034	CLA	NC
23	C	1034	CLA	C8
23	C	1034	CLA	ND
23	C	1034	CLA	C3A
23	C	1026	CLA	C8
23	C	1026	CLA	NC
23	C	1026	CLA	ND
23	C	1026	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	c	6036	CLA	C8
23	c	6036	CLA	C13
23	c	6036	CLA	NC
23	c	6036	CLA	ND
23	c	6036	CLA	NA
23	A	1007	CLA	C13
23	A	1007	CLA	NC
23	A	1007	CLA	ND
23	A	1007	CLA	NA
23	a	6003	CLA	NC
23	a	6003	CLA	ND
23	a	6003	CLA	NA
23	B	1012	CLA	NC
23	B	1012	CLA	ND
23	B	1012	CLA	NA
23	C	1032	CLA	NC
23	C	1032	CLA	ND
23	C	1032	CLA	NA
23	B	1015	CLA	NC
23	B	1015	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	1015	CLA	NA
23	H	1017	CLA	C13
23	H	1017	CLA	NC
23	H	1017	CLA	ND
23	H	1017	CLA	NA
23	a	6007	CLA	C13
23	a	6007	CLA	NC
23	a	6007	CLA	ND
23	a	6007	CLA	NA
23	c	6033	CLA	C8
23	c	6033	CLA	NC
23	c	6033	CLA	ND
23	c	6033	CLA	NA
23	c	6033	CLA	C3A
23	C	1036	CLA	C8
23	C	1036	CLA	C13
23	C	1036	CLA	NC
23	C	1036	CLA	ND
23	C	1036	CLA	NA
23	c	6026	CLA	C8
23	c	6026	CLA	NC
23	c	6026	CLA	ND
23	c	6026	CLA	NA
23	D	1005	CLA	C8
23	D	1005	CLA	NC
23	D	1005	CLA	ND
23	D	1005	CLA	NA
23	b	6018	CLA	NC
23	b	6018	CLA	ND
23	b	6018	CLA	NA
23	b	6013	CLA	NC
23	b	6013	CLA	ND
23	b	6013	CLA	NA
23	d	6004	CLA	NC
23	d	6004	CLA	ND
23	d	6004	CLA	NA
23	C	1035	CLA	NC
23	C	1035	CLA	ND
23	C	1035	CLA	NA
23	b	6019	CLA	C8
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	b	6016	CLA	NC
23	b	6016	CLA	ND
23	b	6016	CLA	NA
23	b	6009	CLA	C8
23	b	6009	CLA	NA
23	b	6009	CLA	CBD
23	b	6009	CLA	NC
23	b	6009	CLA	C13
23	b	6009	CLA	ND
23	C	1025	CLA	CBD
23	C	1025	CLA	NC
23	C	1025	CLA	ND
23	C	1025	CLA	NA
23	B	1023	CLA	CBD
23	B	1023	CLA	C13
23	B	1023	CLA	NC
23	B	1023	CLA	ND
23	B	1023	CLA	NA
23	c	6035	CLA	NC
23	c	6035	CLA	ND
23	c	6035	CLA	NA
23	B	1016	CLA	NC
23	B	1016	CLA	ND
23	B	1016	CLA	NA
23	C	1027	CLA	C8
23	C	1027	CLA	NA
23	C	1027	CLA	NC
23	C	1027	CLA	C13
23	C	1027	CLA	ND
23	C	1027	CLA	C3A
23	B	1019	CLA	C8
23	B	1019	CLA	C13
23	B	1019	CLA	NC
23	B	1019	CLA	ND
23	B	1019	CLA	NA
23	B	1013	CLA	NC
23	B	1013	CLA	ND
23	B	1013	CLA	NA
23	D	1004	CLA	NC
23	D	1004	CLA	ND

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Mol	Chain	Res	Type	Atom
23	D	1004	CLA	NA

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	b	6047	BCR	C17-C16-C15-C14
26	B	1047	BCR	C17-C16-C15-C14
26	B	1048	BCR	C17-C16-C15-C14
26	b	6048	BCR	C17-C16-C15-C14
26	a	6044	BCR	C21-C20-C19-C18
26	A	1044	BCR	C21-C20-C19-C18
29	b	6060	MGE	C3G-O3G-C1D-O6D
29	B	1060	MGE	C3G-O3G-C1D-O6D
26	z	6053	BCR	C21-C20-C19-C18
26	Z	1053	BCR	C21-C20-C19-C18
26	B	1047	BCR	C10-C11-C12-C13
26	b	6047	BCR	C10-C11-C12-C13
26	a	6044	BCR	C10-C11-C12-C13
26	A	1044	BCR	C10-C11-C12-C13
23	b	6011	CLA	CED-O2D-CGD-CBD
23	B	1011	CLA	CED-O2D-CGD-CBD
23	B	1023	CLA	CED-O2D-CGD-CBD
23	b	6023	CLA	CED-O2D-CGD-CBD
23	B	1010	CLA	CED-O2D-CGD-CBD
23	b	6010	CLA	CED-O2D-CGD-CBD
23	B	1012	CLA	CED-O2D-CGD-CBD
23	b	6012	CLA	CED-O2D-CGD-CBD
23	b	6022	CLA	CED-O2D-CGD-CBD
23	B	1022	CLA	CED-O2D-CGD-CBD
23	B	1009	CLA	CED-O2D-CGD-CBD
23	b	6009	CLA	CED-O2D-CGD-CBD
23	a	6007	CLA	CED-O2D-CGD-CBD
23	A	1007	CLA	CED-O2D-CGD-CBD
23	C	1031	CLA	CED-O2D-CGD-CBD
23	c	6031	CLA	CED-O2D-CGD-CBD
24	d	6038	PHO	CED-O2D-CGD-CBD
24	A	1038	PHO	CED-O2D-CGD-CBD

There are no ring outliers.

61 monomers are involved in 2232 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1003	CLA	57	0
23	A	1006	CLA	94	0
23	A	1007	CLA	20	0
24	A	1038	PHO	80	0
24	A	1039	PHO	36	0
25	A	1043	PQ9	7	0
26	A	1044	BCR	25	0
27	A	1063	LHG	58	0
23	B	1009	CLA	49	0
23	B	1010	CLA	45	0
23	B	1011	CLA	107	0
23	B	1012	CLA	65	0
23	B	1013	CLA	84	0
23	B	1014	CLA	79	0
23	B	1015	CLA	29	0
23	B	1016	CLA	61	0
23	B	1018	CLA	21	0
23	B	1019	CLA	88	0
23	B	1020	CLA	74	0
23	B	1021	CLA	72	0
23	B	1022	CLA	67	0
23	B	1023	CLA	82	0
23	B	1024	CLA	40	0
26	B	1045	BCR	30	0
26	B	1047	BCR	25	0
26	B	1048	BCR	36	0
29	B	1060	MGE	47	0
23	C	1025	CLA	54	0
23	C	1026	CLA	32	0
23	C	1027	CLA	51	0
23	C	1028	CLA	32	0
23	C	1029	CLA	45	0
23	C	1030	CLA	31	0
23	C	1031	CLA	63	0
23	C	1032	CLA	56	0
23	C	1033	CLA	67	0
23	C	1034	CLA	86	0
23	C	1035	CLA	21	0
23	C	1036	CLA	52	0
23	C	1037	CLA	27	0
26	C	1054	BCR	26	0
30	C	1055	DGD	34	0
30	C	1056	DGD	57	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	1057	DGD	61	0
23	D	1004	CLA	19	0
23	D	1005	CLA	69	0
23	D	1008	CLA	32	0
25	D	1042	PQ9	32	0
26	D	1050	BCR	62	0
29	D	1062	MGE	23	0
31	E	1040	HEM	10	0
23	H	1017	CLA	60	0
26	H	1049	BCR	53	0
30	H	1058	DGD	32	0
29	J	1059	MGE	34	0
26	K	1051	BCR	43	0
26	K	1052	BCR	47	0
29	L	1061	MGE	33	0
26	T	6046	BCR	18	0
31	V	1041	HEM	10	0
26	Z	1053	BCR	41	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%)	-0.36	5 (1%) 73 62	97, 127, 162, 173	0
1	a	335/344 (97%)	-0.29	5 (1%) 73 62	101, 131, 166, 178	0
2	B	485/488 (99%)	-0.23	9 (1%) 66 54	94, 130, 157, 181	0
2	b	485/488 (99%)	-0.16	13 (2%) 54 42	102, 129, 161, 183	0
3	C	447/447 (100%)	-0.13	10 (2%) 62 49	100, 143, 170, 185	0
3	c	447/447 (100%)	0.06	23 (5%) 28 20	102, 150, 173, 187	0
4	D	340/340 (100%)	-0.18	9 (2%) 56 43	94, 127, 165, 187	0
4	d	340/340 (100%)	-0.21	5 (1%) 73 62	92, 133, 172, 191	0
5	E	82/83 (98%)	0.03	2 (2%) 59 46	117, 156, 184, 186	0
5	e	82/83 (98%)	0.46	8 (9%) 7 6	126, 160, 181, 186	0
6	F	35/44 (79%)	-0.13	4 (11%) 5 4	139, 147, 160, 163	0
6	f	35/44 (79%)	-0.14	3 (8%) 10 8	143, 152, 160, 163	0
7	H	64/64 (100%)	0.24	5 (7%) 13 9	119, 143, 165, 170	0
7	h	64/64 (100%)	0.27	7 (10%) 5 5	120, 143, 164, 169	0
8	I	35/35 (100%)	-0.07	3 (8%) 10 8	127, 137, 166, 173	0
8	i	35/35 (100%)	-0.09	2 (5%) 24 16	124, 141, 175, 176	0
9	J	34/40 (85%)	-0.43	0 100 100	127, 142, 165, 175	0
9	j	34/40 (85%)	0.05	3 (8%) 10 7	131, 146, 172, 174	0
10	K	36/36 (100%)	-0.33	0 100 100	132, 145, 153, 155	0
10	k	36/36 (100%)	0.02	1 (2%) 53 40	140, 151, 162, 164	0
11	L	37/37 (100%)	-0.29	1 (2%) 54 42	102, 123, 178, 184	0
11	l	37/37 (100%)	-0.31	2 (5%) 26 19	110, 130, 181, 188	0
12	M	36/36 (100%)	0.25	6 (16%) 1 1	101, 119, 171, 174	0
12	m	36/36 (100%)	-0.23	2 (5%) 24 17	100, 121, 171, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.06	12 (4%) 29 21	108, 133, 165, 186	0
13	o	242/242 (100%)	-0.00	13 (5%) 26 19	114, 139, 164, 186	0
14	T	30/30 (100%)	-0.40	2 (6%) 18 12	105, 124, 173, 178	0
14	t	30/30 (100%)	-0.43	0 100 100	101, 115, 173, 181	0
15	U	98/98 (100%)	-0.15	3 (3%) 49 36	108, 123, 143, 158	0
15	u	98/98 (100%)	-0.36	0 100 100	112, 128, 143, 167	0
16	V	137/137 (100%)	-0.32	3 (2%) 62 49	104, 131, 160, 170	0
16	v	137/137 (100%)	-0.12	3 (2%) 62 49	114, 145, 165, 176	0
17	X	34/34 (100%)	-0.20	1 (2%) 51 38	148, 155, 164, 170	0
17	x	34/34 (100%)	-0.19	1 (2%) 51 38	151, 159, 169, 175	0
18	Y	28/28 (100%)	-0.19	1 (3%) 42 31	164, 178, 189, 192	0
18	y	28/28 (100%)	-0.24	1 (3%) 42 31	170, 181, 191, 196	0
19	N	0/24	-	-	-	-
19	n	0/24	-	-	-	-
20	Z	62/62 (100%)	-0.17	1 (1%) 72 60	138, 161, 180, 186	0
20	z	62/62 (100%)	0.06	6 (9%) 8 6	144, 164, 184, 187	0
All	All	5194/5298 (98%)	-0.14	175 (3%) 45 33	92, 136, 172, 196	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5142	GLU	6.2
4	d	5228	GLY	5.1
8	i	5035	LYS	5.1
3	c	5034	ALA	5.0
12	M	36	SER	4.8
13	o	5049	ASP	4.5
3	c	5027	ASP	4.2
20	z	5001	MET	4.1
1	a	5011	ALA	4.0
3	c	5249	ILE	3.9
7	h	5022	ALA	3.9
6	f	5012	SER	3.8
6	F	39	ALA	3.8
3	C	34	ALA	3.7
4	d	5230	SER	3.7
18	y	5028	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
4	d	5229	ALA	3.7
9	j	5009	PRO	3.6
16	V	27	ALA	3.6
3	C	147	PHE	3.6
4	d	5233	ARG	3.5
5	e	5018	ARG	3.5
3	c	5035	TRP	3.5
4	D	95	PRO	3.5
13	o	5051	THR	3.4
7	H	15	ASN	3.4
20	Z	1	MET	3.3
9	j	5008	ILE	3.3
3	c	5198	VAL	3.3
13	O	87	GLN	3.3
13	o	5230	VAL	3.3
13	O	59	ASP	3.3
2	b	5181	GLU	3.2
6	f	5013	TYR	3.2
5	E	18	ARG	3.1
3	C	97	TRP	3.1
7	h	5023	PRO	3.1
1	a	5010	SER	3.1
7	h	5056	ASP	3.1
3	c	5184	GLY	3.0
1	a	5075	ASN	3.0
13	o	5048	LEU	3.0
8	I	35	LYS	3.0
20	z	5061	VAL	3.0
3	c	5253	LEU	3.0
2	b	5292	GLY	3.0
13	O	62	GLN	2.9
13	O	61	SER	2.9
1	A	14	TRP	2.9
1	A	232	SER	2.9
2	B	365	SER	2.9
4	D	227	GLU	2.9
5	e	5017	VAL	2.9
6	F	40	MET	2.9
5	e	5026	THR	2.9
13	o	5061	SER	2.8
1	A	12	ASN	2.8
7	H	4	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
13	o	5050	ASP	2.8
16	v	5111	GLU	2.8
13	O	162	ILE	2.8
2	b	5184	PRO	2.8
2	B	379	ALA	2.8
13	o	5229	LYS	2.7
12	M	32	GLN	2.7
3	c	5148	GLY	2.7
3	c	5129	GLY	2.7
5	e	5061	ARG	2.6
20	z	5002	THR	2.6
4	D	233	ARG	2.6
3	c	5128	GLY	2.6
2	b	5081	THR	2.6
3	C	142	GLU	2.6
2	b	5196	VAL	2.6
11	l	5010	VAL	2.6
9	j	5007	ARG	2.6
14	T	28	ARG	2.6
3	c	5036	TRP	2.6
13	O	119	LEU	2.6
6	F	15	ILE	2.5
4	D	228	GLY	2.5
13	o	5063	THR	2.5
2	b	5182	TRP	2.5
5	E	84	LYS	2.5
15	U	92	LEU	2.5
2	B	187	PRO	2.5
2	b	5238	SER	2.5
5	e	5009	PRO	2.5
12	M	5	GLN	2.5
2	b	5121	ARG	2.5
20	z	5060	PHE	2.5
3	c	5238	ILE	2.5
6	F	14	PRO	2.5
12	M	34	LYS	2.5
12	m	5001	MET	2.5
1	A	310	LYS	2.5
4	D	226	GLY	2.5
3	c	5200	THR	2.4
10	k	5011	LEU	2.4
3	c	5199	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
13	o	5092	VAL	2.4
4	D	21	TRP	2.4
13	o	5060	SER	2.4
8	i	5033	LYS	2.4
8	I	34	ARG	2.4
11	l	5001	MET	2.4
2	b	5424	GLY	2.4
3	C	460	ASP	2.4
7	h	5055	LEU	2.4
1	a	5024	THR	2.4
20	z	5030	PRO	2.4
2	b	5351	LEU	2.3
13	O	78	VAL	2.3
4	D	57	SER	2.3
2	b	5185	ASP	2.3
7	h	5021	VAL	2.3
13	O	113	VAL	2.3
3	C	255	THR	2.3
2	B	445	THR	2.3
4	d	5221	THR	2.3
3	C	199	ILE	2.3
2	B	125	ASP	2.3
7	H	26	GLY	2.3
7	H	64	ALA	2.3
18	Y	46	LEU	2.3
16	v	5120	SER	2.3
2	B	165	GLY	2.3
3	c	5281	MET	2.3
4	D	260	ALA	2.3
11	L	1	MET	2.3
13	o	5112	LYS	2.2
4	D	98	GLN	2.2
2	b	5362	SER	2.2
13	O	58	ILE	2.2
17	x	5011	THR	2.2
6	f	5011	VAL	2.2
7	H	16	SER	2.2
15	U	88	VAL	2.2
2	B	164	PRO	2.2
12	M	2	GLU	2.2
1	a	5232	SER	2.2
13	O	136	MET	2.2

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Mol	Chain	Res	Type	RSRZ
13	o	5062	GLN	2.1
2	b	5218	PRO	2.1
8	I	1	MET	2.1
1	A	13	LEU	2.1
3	c	5037	ALA	2.1
3	c	5111	PHE	2.1
13	O	142	ILE	2.1
12	M	35	SER	2.1
16	V	37	PRO	2.1
2	B	126	PRO	2.1
20	z	5004	LEU	2.1
3	C	277	GLY	2.1
5	e	5008	ARG	2.1
13	o	5094	THR	2.1
5	e	5025	ILE	2.1
14	T	30	THR	2.1
3	C	143	TYR	2.0
16	V	29	LEU	2.0
3	C	126	GLY	2.0
7	h	5065	LEU	2.0
7	h	5064	ALA	2.0
3	c	5202	PRO	2.0
17	X	44	ASP	2.0
3	c	5044	ASN	2.0
13	O	39	THR	2.0
5	e	5021	VAL	2.0
12	m	5034	LYS	2.0
2	B	354	LEU	2.0
3	c	5234	VAL	2.0
3	c	5033	PHE	2.0
3	c	5091	HIS	2.0
15	U	38	GLU	2.0
16	v	5113	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	PQ9	a	6043	45/45	0.35	0.40	135,149,185,185	30
27	LHG	a	6063	49/49	0.43	0.75	186,196,200,200	0
26	BCR	c	6054	40/40	0.46	0.60	174,177,183,183	0
26	BCR	H	1049	40/40	0.52	0.55	155,162,188,188	0
23	CLA	c	6027	65/65	0.55	0.61	178,195,198,200	0
26	BCR	b	6047	40/40	0.56	0.53	114,127,145,147	0
26	BCR	K	1052	40/40	0.59	0.43	153,171,178,179	0
26	BCR	k	6052	40/40	0.59	0.35	158,179,200,200	0
26	BCR	a	6044	40/40	0.60	0.74	154,160,163,166	0
26	BCR	z	6053	40/40	0.60	0.76	159,176,186,187	0
27	LHG	A	1063	49/49	0.60	0.54	181,187,194,195	0
25	PQ9	A	1043	45/45	0.62	0.34	138,151,171,171	30
26	BCR	C	1054	40/40	0.63	0.49	158,165,169,170	0
26	BCR	K	1051	40/40	0.67	0.55	175,179,182,183	0
26	BCR	h	6049	40/40	0.68	0.43	156,175,191,192	0
23	CLA	c	6037	65/65	0.68	0.53	184,188,191,200	0
26	BCR	B	1048	40/40	0.68	0.56	148,155,163,163	0
23	CLA	c	6034	65/65	0.69	0.47	87,162,181,181	0
30	DGD	c	6056	66/66	0.69	0.51	170,175,181,183	0
24	PHO	d	6038	64/64	0.70	0.49	136,147,150,150	0
23	CLA	c	6031	65/65	0.70	0.45	173,182,185,186	0
26	BCR	b	6048	40/40	0.71	0.64	141,147,158,159	0
23	CLA	C	1037	65/65	0.71	0.41	180,185,188,200	0
26	BCR	B	1045	40/40	0.71	0.43	146,156,169,170	0
23	CLA	C	1034	65/65	0.72	0.41	134,147,172,174	0
29	MGE	d	6059	48/48	0.73	0.42	164,168,198,200	0
23	CLA	b	6024	65/65	0.73	0.45	172,183,186,187	0
26	BCR	d	6050	40/40	0.73	0.41	149,160,166,167	0
26	BCR	Z	1053	40/40	0.74	0.45	141,166,178,178	0
26	BCR	b	6045	40/40	0.74	0.39	145,156,167,168	0
30	DGD	c	6057	66/66	0.74	0.56	128,149,183,184	0
23	CLA	C	1032	65/65	0.74	0.44	153,166,174,176	0
30	DGD	C	1056	66/66	0.74	0.44	155,171,183,188	0
23	CLA	B	1024	65/65	0.75	0.40	105,177,179,180	0
30	DGD	C	1057	66/66	0.75	0.47	125,140,187,193	0
26	BCR	T	6046	40/40	0.75	0.45	140,149,154,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	6003	65/65	0.75	0.38	121,130,145,193	0
26	BCR	t	1046	40/40	0.75	0.41	144,156,163,163	0
26	BCR	A	1044	40/40	0.75	0.58	147,156,158,159	0
30	DGD	H	1058	66/66	0.76	0.43	131,150,165,166	0
26	BCR	B	1047	40/40	0.76	0.40	101,136,157,157	0
23	CLA	B	1009	65/65	0.76	0.39	119,178,184,185	0
23	CLA	c	6036	65/65	0.77	0.45	177,180,184,200	0
23	CLA	b	6009	65/65	0.77	0.48	160,177,200,200	0
23	CLA	b	6017	65/65	0.78	0.36	118,165,168,200	0
29	MGE	d	6061	48/48	0.78	0.38	141,152,165,169	0
23	CLA	B	1023	65/65	0.78	0.39	155,179,185,200	0
30	DGD	h	6058	66/66	0.78	0.39	140,153,163,170	0
23	CLA	d	6008	65/65	0.78	0.41	172,175,185,200	0
26	BCR	D	1050	40/40	0.79	0.32	149,153,161,162	0
23	CLA	b	6023	65/65	0.79	0.39	149,183,189,190	0
23	CLA	C	1025	65/65	0.79	0.39	131,170,180,200	0
23	CLA	C	1030	65/65	0.79	0.38	92,145,175,176	0
23	CLA	C	1027	65/65	0.79	0.43	167,183,190,200	0
23	CLA	C	1031	65/65	0.79	0.39	164,170,179,200	0
23	CLA	a	6007	65/65	0.79	0.74	143,149,179,183	0
25	PQ9	d	6042	45/45	0.80	0.30	137,146,167,168	0
23	CLA	c	6032	65/65	0.80	0.39	144,175,181,182	0
23	CLA	c	6025	65/65	0.80	0.40	145,170,178,200	0
29	MGE	b	6060	48/48	0.81	0.35	158,178,191,192	0
24	PHO	a	6039	64/64	0.81	0.35	151,165,169,170	0
29	MGE	L	1061	48/48	0.81	0.38	141,144,154,155	0
23	CLA	C	1036	65/65	0.81	0.34	162,166,179,200	0
29	MGE	B	1060	48/48	0.81	0.37	151,170,182,184	0
29	MGE	J	1059	48/48	0.82	0.32	152,158,185,186	0
29	MGE	d	6062	48/48	0.82	0.33	130,155,167,168	0
23	CLA	c	6030	65/65	0.82	0.32	100,154,174,175	0
23	CLA	B	1014	65/65	0.82	0.31	123,169,174,176	0
23	CLA	H	1017	65/65	0.82	0.30	116,169,174,200	0
30	DGD	c	6055	66/66	0.82	0.34	147,153,165,166	0
25	PQ9	D	1042	45/45	0.83	0.29	131,145,154,155	0
23	CLA	b	6014	65/65	0.83	0.28	163,171,179,200	0
28	BR	a	6065	1/1	0.83	0.22	164,164,164,164	0
23	CLA	c	6028	65/65	0.83	0.39	147,157,160,162	0
23	CLA	a	6006	65/65	0.83	0.33	140,145,197,200	0
29	MGE	D	1062	48/48	0.84	0.33	129,148,165,165	0
23	CLA	A	1007	65/65	0.85	0.49	137,141,171,183	0
23	CLA	b	6013	65/65	0.85	0.34	139,154,161,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	D	1008	65/65	0.85	0.35	159,167,182,200	0
23	CLA	B	1013	65/65	0.85	0.32	131,157,165,168	0
31	HEM	e	6040	43/43	0.85	0.42	171,184,185,185	0
30	DGD	C	1055	66/66	0.85	0.34	131,140,147,152	0
23	CLA	c	6029	65/65	0.86	0.29	151,170,173,200	0
23	CLA	c	6035	65/65	0.86	0.30	170,173,177,200	0
23	CLA	B	1015	65/65	0.86	0.29	133,146,153,175	0
23	CLA	c	6026	65/65	0.86	0.35	140,144,157,170	0
23	CLA	b	6012	65/65	0.86	0.34	146,153,159,198	0
23	CLA	A	1003	65/65	0.86	0.32	122,129,147,149	0
24	PHO	A	1038	64/64	0.86	0.32	122,144,147,148	0
23	CLA	b	6016	65/65	0.87	0.35	76,148,153,155	0
23	CLA	B	1010	65/65	0.87	0.30	115,164,166,169	0
26	BCR	k	6051	40/40	0.87	0.37	187,193,197,197	0
23	CLA	b	6021	65/65	0.87	0.32	125,132,157,160	0
23	CLA	B	1020	65/65	0.87	0.28	113,151,177,179	0
23	CLA	B	1018	65/65	0.87	0.34	111,158,165,168	0
23	CLA	A	1006	65/65	0.87	0.34	119,124,190,192	0
23	CLA	C	1028	65/65	0.87	0.33	141,154,159,168	0
23	CLA	C	1029	65/65	0.87	0.30	146,156,159,200	0
23	CLA	b	6015	65/65	0.87	0.29	137,149,155,164	0
23	CLA	C	1033	65/65	0.88	0.28	117,131,162,164	0
23	CLA	B	1022	65/65	0.88	0.28	135,155,159,161	0
23	CLA	B	1016	65/65	0.88	0.30	87,143,150,150	0
23	CLA	D	1004	65/65	0.88	0.32	101,131,139,142	0
23	CLA	B	1012	65/65	0.88	0.34	148,152,159,176	0
23	CLA	c	6033	65/65	0.89	0.31	84,142,180,180	0
23	CLA	C	1035	65/65	0.89	0.26	155,167,173,200	0
23	CLA	b	6022	65/65	0.90	0.25	133,148,156,157	0
23	CLA	b	6019	65/65	0.90	0.26	124,150,155,193	0
24	PHO	A	1039	64/64	0.90	0.29	149,151,160,161	0
23	CLA	B	1019	65/65	0.90	0.23	121,156,158,200	0
23	CLA	C	1026	65/65	0.90	0.26	128,133,146,149	0
23	CLA	b	6011	65/65	0.90	0.35	156,159,165,170	0
23	CLA	d	6004	65/65	0.90	0.27	111,128,134,134	0
23	CLA	b	6020	65/65	0.90	0.28	75,148,170,173	0
23	CLA	d	6005	65/65	0.91	0.34	90,100,117,118	0
23	CLA	b	6010	65/65	0.91	0.32	93,165,169,170	0
31	HEM	E	1040	43/43	0.91	0.45	141,181,194,198	0
23	CLA	b	6018	65/65	0.91	0.34	142,154,162,165	0
23	CLA	B	1021	65/65	0.91	0.26	104,129,142,146	0
28	BR	A	1065	1/1	0.91	0.22	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	D	1005	65/65	0.92	0.29	101,108,116,157	0
31	HEM	V	1041	43/43	0.93	0.32	81,131,132,133	0
23	CLA	B	1011	65/65	0.93	0.34	144,159,161,166	0
31	HEM	v	6041	43/43	0.93	0.28	99,135,139,140	0
28	BR	d	6064	1/1	0.94	0.17	130,130,130,130	0
22	FE2	A	1002	1/1	0.95	0.24	125,125,125,125	0
22	FE2	a	6002	1/1	0.95	0.34	149,149,149,149	0
28	BR	A	1064	1/1	0.96	0.13	113,113,113,113	0
21	OEC	a	6001	5/9	0.98	0.26	87,94,106,107	0
21	OEC	A	1001	5/9	0.99	0.29	79,94,115,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.