



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 05:02 AM GMT

PDB ID : 1S5L
Title : Architecture of the photosynthetic oxygen evolving center
Authors : Ferreira, K.N.; Iverson, T.M.; Maghlaoui, K.; Barber, J.; Iwata, S.
Deposited on : 2004-01-21
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

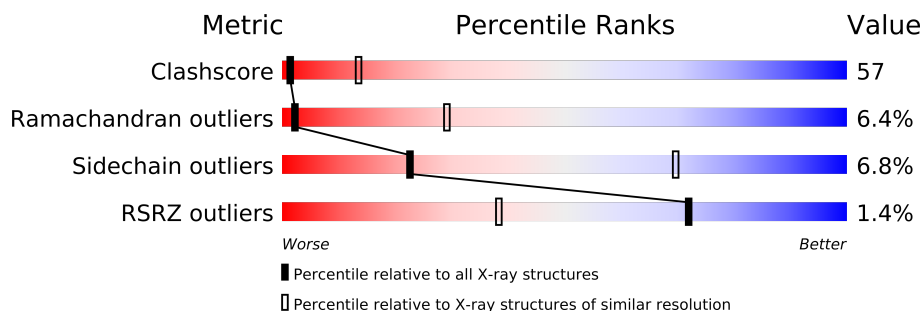
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	473	
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	

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Mol	Chain	Length	Quality of chain
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	246	
13	o	246	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	137	
16	v	137	
17	X	50	
17	x	50	
18	N	37	
18	n	37	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
23	CLA	A	352	-	X
23	CLA	B	511	-	X
23	CLA	B	516	-	X
23	CLA	B	527	-	X
23	CLA	C	480	-	X
23	CLA	C	481	-	X
23	CLA	C	482	-	X
23	CLA	C	485	-	X
23	CLA	C	487	-	X
23	CLA	b	2516	-	X
23	CLA	b	2517	-	X
23	CLA	b	2521	-	X
23	CLA	b	2522	-	X
23	CLA	b	2524	-	X
23	CLA	b	2526	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
23	CLA	c	2478	-	X
23	CLA	c	2483	-	X
23	CLA	c	2486	-	X
23	CLA	c	2487	-	X
26	PL9	A	353	-	X
26	PL9	D	357	-	X
26	PL9	d	2358	-	X
27	LMT	d	2359	-	X
28	BCR	B	528	-	X
28	BCR	B	529	-	X
28	BCR	C	488	-	X
28	BCR	C	489	-	X
28	BCR	F	48	-	X
28	BCR	J	53	-	X
28	BCR	K	50	-	X
28	BCR	b	2527	-	X
28	BCR	b	2528	-	X
28	BCR	c	2488	-	X
28	BCR	c	2489	-	X
28	BCR	d	2360	-	X
28	BCR	k	2050	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45945 atoms, of which 0 are hydrogen and 0 are deuterium.

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	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2616	1714	430	457	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			
2	b	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			
3	c	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INSERTION	UNP Q8DIF8
C	2	LYS	-	INSERTION	UNP Q8DIF8
C	3	THR	-	INSERTION	UNP Q8DIF8
C	4	LEU	-	INSERTION	UNP Q8DIF8
C	5	SER	-	INSERTION	UNP Q8DIF8
C	6	SER	-	INSERTION	UNP Q8DIF8
C	7	GLN	-	INSERTION	UNP Q8DIF8
C	8	LYS	-	INSERTION	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ARG	-	INSERTION	UNP Q8DIF8
C	10	TYR	-	INSERTION	UNP Q8DIF8
C	11	SER	-	INSERTION	UNP Q8DIF8
C	12	PRO	-	INSERTION	UNP Q8DIF8
C	13	VAL	-	INSERTION	UNP Q8DIF8
c	2001	MET	-	INSERTION	UNP Q8DIF8
c	2002	LYS	-	INSERTION	UNP Q8DIF8
c	2003	THR	-	INSERTION	UNP Q8DIF8
c	2004	LEU	-	INSERTION	UNP Q8DIF8
c	2005	SER	-	INSERTION	UNP Q8DIF8
c	2006	SER	-	INSERTION	UNP Q8DIF8
c	2007	GLN	-	INSERTION	UNP Q8DIF8
c	2008	LYS	-	INSERTION	UNP Q8DIF8
c	2009	ARG	-	INSERTION	UNP Q8DIF8
c	2010	TYR	-	INSERTION	UNP Q8DIF8
c	2011	SER	-	INSERTION	UNP Q8DIF8
c	2012	PRO	-	INSERTION	UNP Q8DIF8
c	2013	VAL	-	INSERTION	UNP Q8DIF8

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			
4	d	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			624	411	99	114			
5	e	76	Total	C	N	O	0	0	0
			624	411	99	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called photosystem II PsbH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			
7	h	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

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 M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			
12	m	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			
13	o	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			

- Molecule 14 is a protein called photosystem II PsbT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			
14	t	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	105	Total	C	N	O		0	0	0
			827	521	137	169				
15	u	105	Total	C	N	O		0	0	0
			827	521	137	169				

- 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 PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O	0	0	0
			296	197	47	52			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	x	40	Total	C	N	O	0	0	0
			296	197	47	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	INSERTION	UNP Q9F1R6
X	2	ILE	-	INSERTION	UNP Q9F1R6
X	3	GLN	-	INSERTION	UNP Q9F1R6
X	4	SER	-	INSERTION	UNP Q9F1R6
X	5	ALA	-	INSERTION	UNP Q9F1R6
X	6	SER	-	INSERTION	UNP Q9F1R6
X	7	SER	-	INSERTION	UNP Q9F1R6
X	8	LEU	-	INSERTION	UNP Q9F1R6
X	9	LEU	-	INSERTION	UNP Q9F1R6
X	10	LEU	-	INSERTION	UNP Q9F1R6
x	2001	MET	-	INSERTION	UNP Q9F1R6
x	2002	ILE	-	INSERTION	UNP Q9F1R6
x	2003	GLN	-	INSERTION	UNP Q9F1R6
x	2004	SER	-	INSERTION	UNP Q9F1R6
x	2005	ALA	-	INSERTION	UNP Q9F1R6
x	2006	SER	-	INSERTION	UNP Q9F1R6
x	2007	SER	-	INSERTION	UNP Q9F1R6
x	2008	LEU	-	INSERTION	UNP Q9F1R6
x	2009	LEU	-	INSERTION	UNP Q9F1R6
x	2010	LEU	-	INSERTION	UNP Q9F1R6

- Molecule 18 is a protein called Photosystem II PsbN protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	37	Total	C	N	O	0	0	0
			186	111	37	38			
18	n	37	Total	C	N	O	0	0	0
			186	111	37	38			

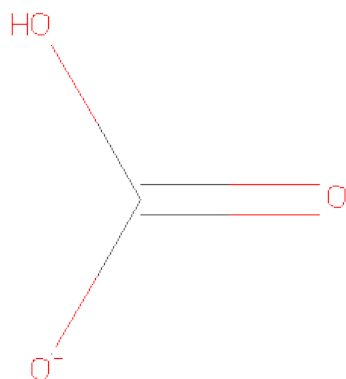
- Molecule 19 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			
19	z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe).

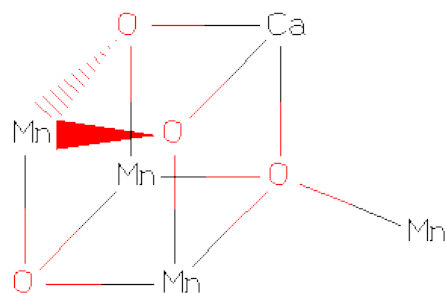
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



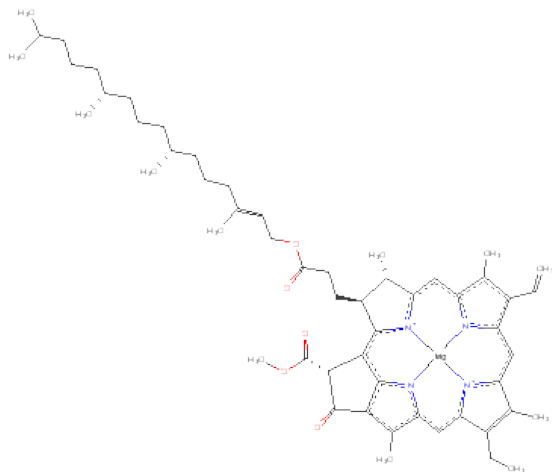
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	1	3		
21	D	1	Total	C	O	0	0
			4	1	3		
21	a	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
22	A	1	9	1	4	4	0	0
22	a	1	9	1	4	4	0	0

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



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

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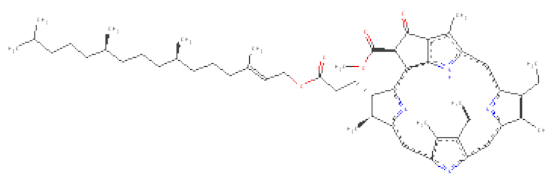
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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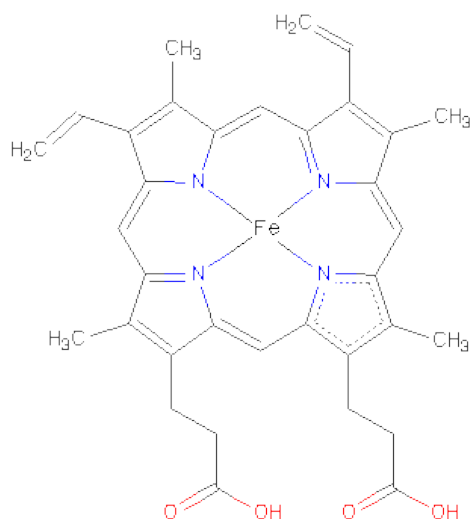
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



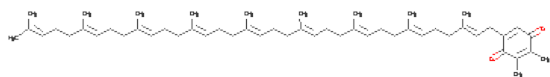
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



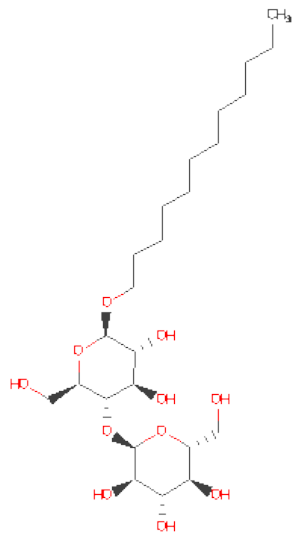
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



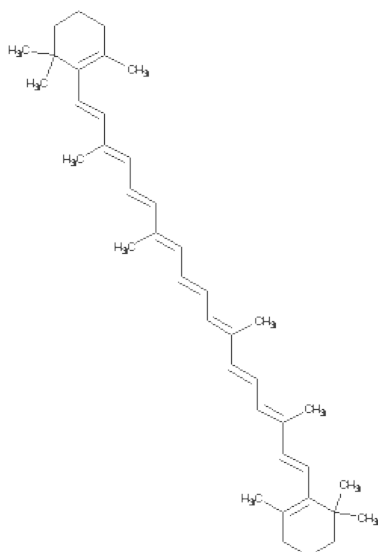
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O	0	0
			45	43	2		
26	A	1	Total	C	O	0	0
			45	43	2		
26	d	1	Total	C	O	0	0
			45	43	2		
26	a	1	Total	C	O	0	0
			45	43	2		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total	C	O	0	0
			35	24	11		
27	d	1	Total	C	O	0	0
			35	24	11		

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	K	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	J	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	d	1	Total	C	0	0
			40	40		
28	c	1	Total	C	0	0
			40	40		
28	k	1	Total	C	0	0
			40	40		

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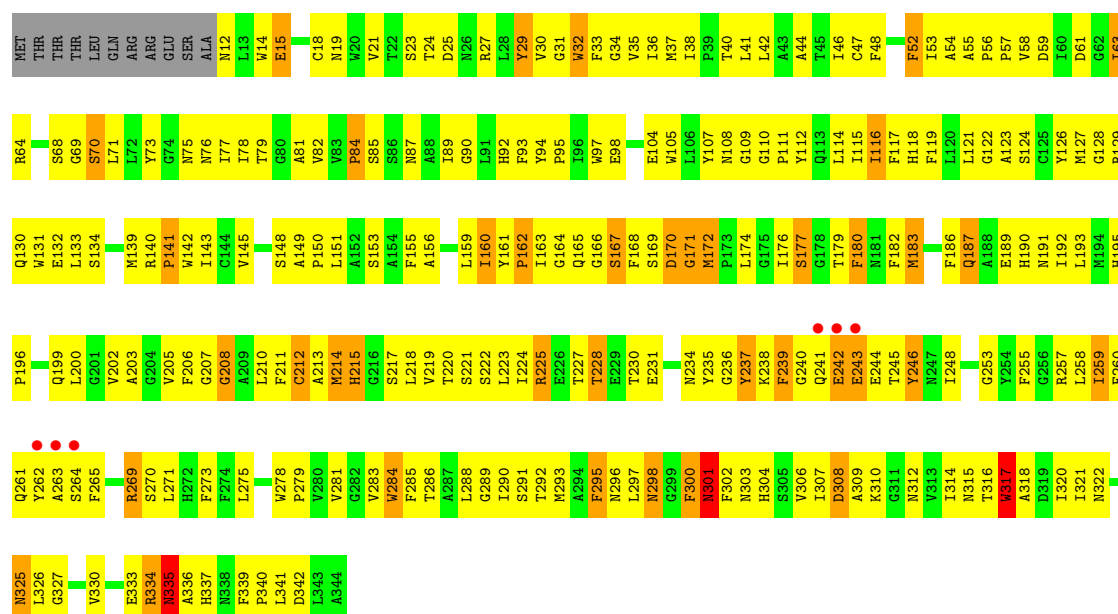
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	j	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0

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

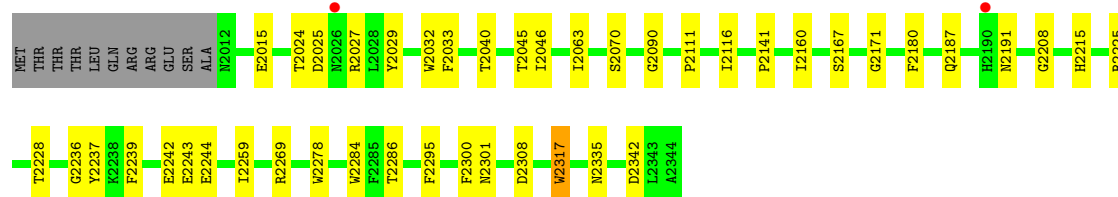
• Molecule 1: Photosystem Q(B) protein

Chain A: 



• Molecule 1: Photosystem Q(B) protein

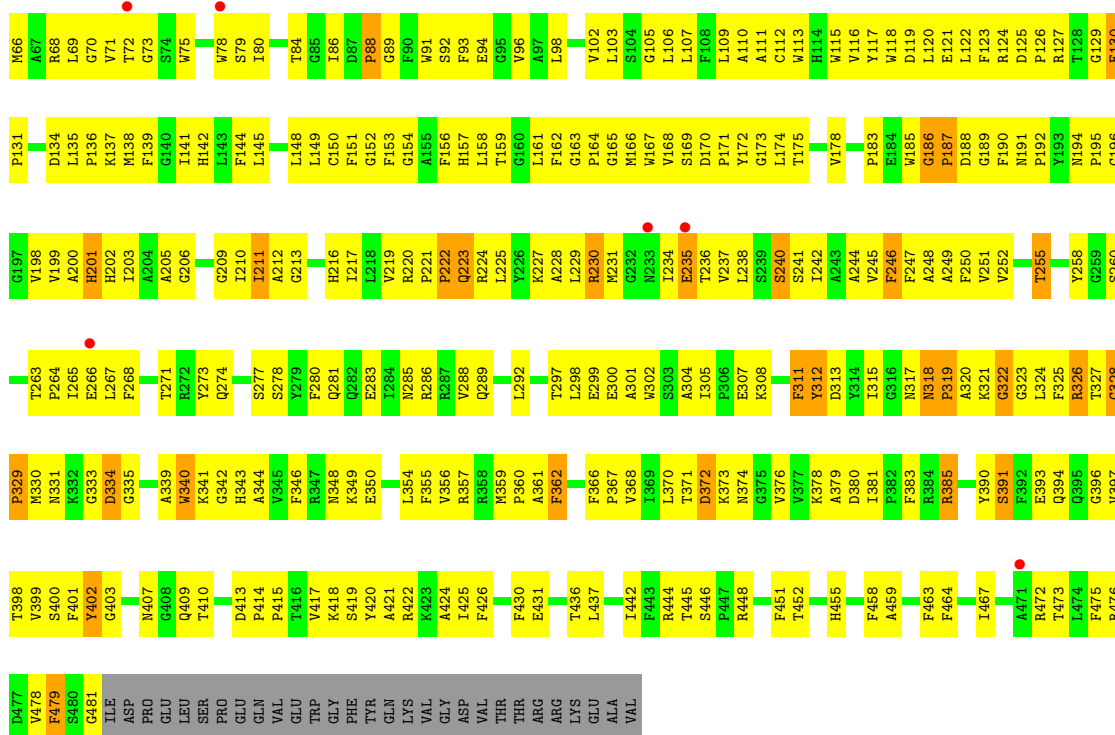
Chain a: 



• Molecule 2: photosystem II core light harvesting protein

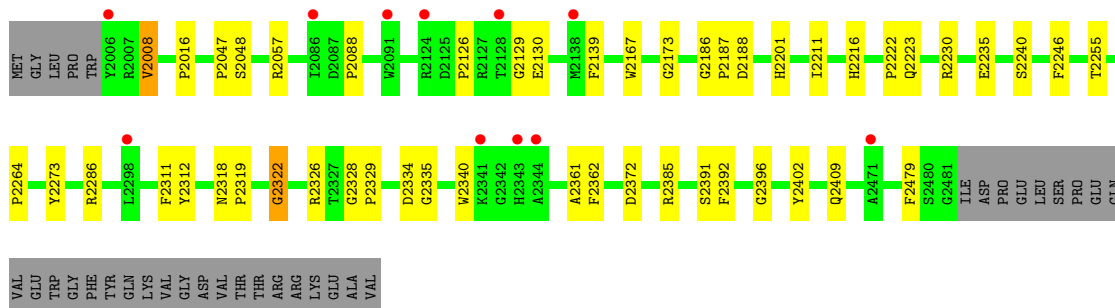
Chain B: 





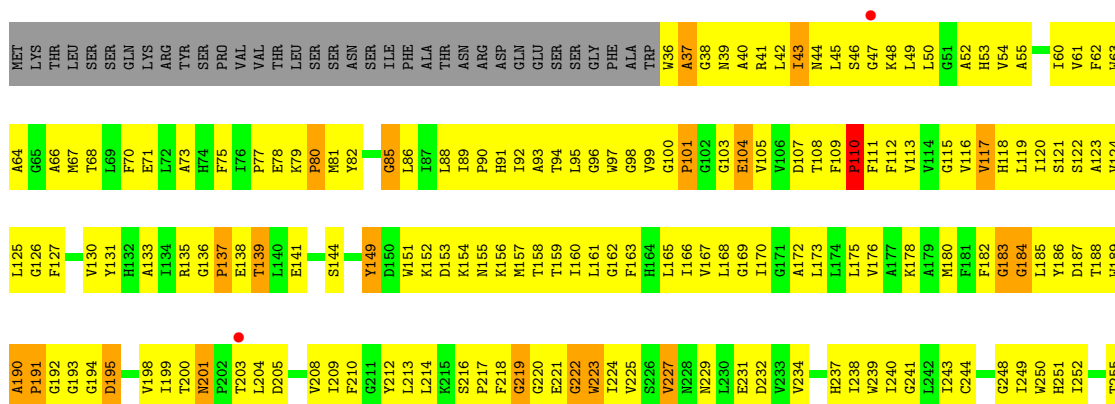
• Molecule 2: photosystem II core light harvesting protein

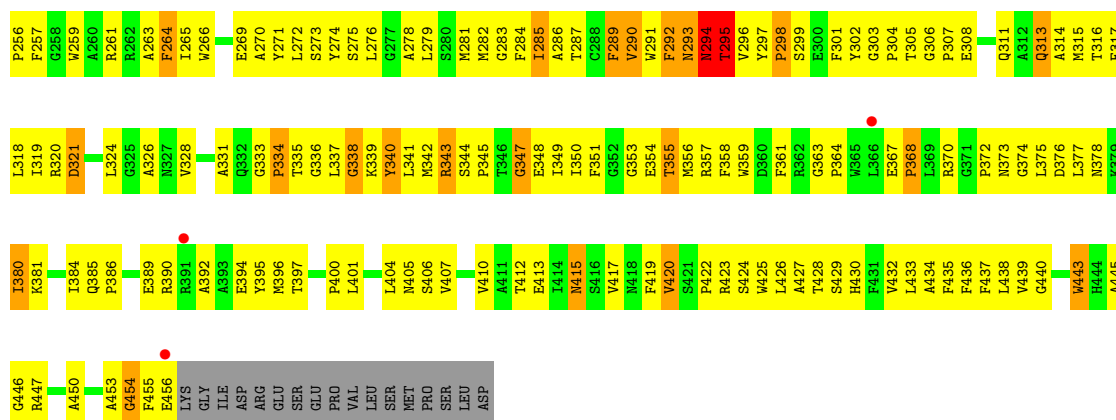
Chain b:



• Molecule 3: photosystem II CP43 protein

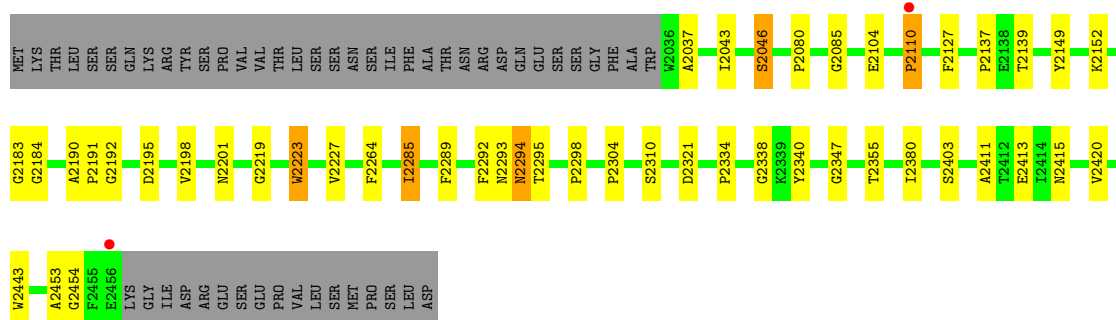
Chain C:





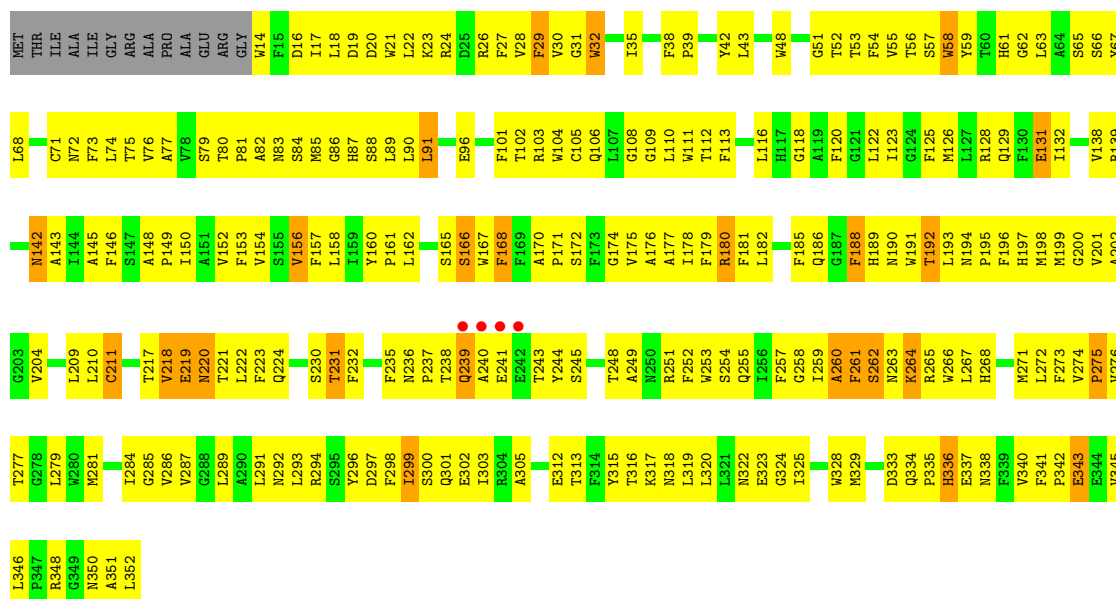
• Molecule 3: photosystem II CP43 protein

Chain c:



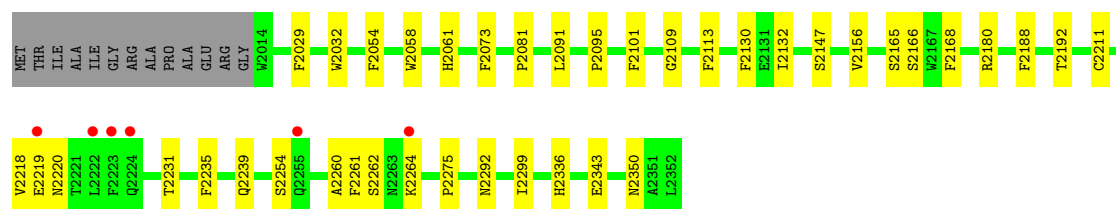
• Molecule 4: photosystem II reaction center D2 protein

Chain D:



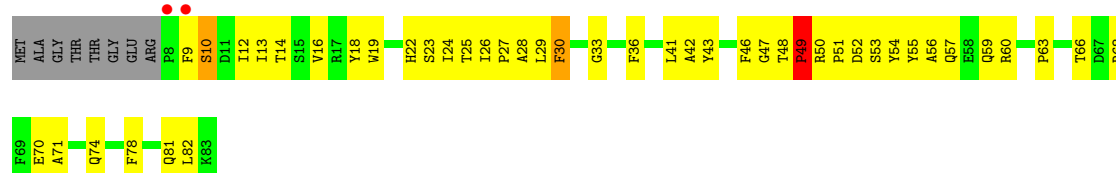
• Molecule 4: photosystem II reaction center D2 protein

Chain d:



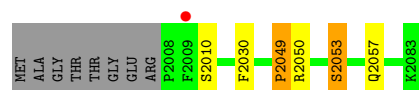
• Molecule 5: Cytochrome b559 alpha subunit

Chain E:



• Molecule 5: Cytochrome b559 alpha subunit

Chain e:



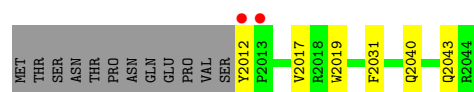
• Molecule 6: Cytochrome b559 beta subunit

Chain F:



• Molecule 6: Cytochrome b559 beta subunit

Chain f:



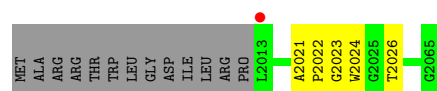
• Molecule 7: photosystem II PsbH protein

Chain H:



• Molecule 7: photosystem II PsbH protein

Chain h:



• Molecule 8: Photosystem II reaction center I protein

Chain I: 



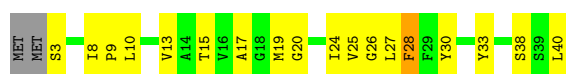
- Molecule 8: Photosystem II reaction center I protein

Chain i: 



- Molecule 9: Photosystem II reaction center J protein

Chain J: 



- Molecule 9: Photosystem II reaction center J protein

Chain j: 



- Molecule 10: Photosystem II reaction center protein K

Chain K: 



- Molecule 10: Photosystem II reaction center protein K

Chain k: 



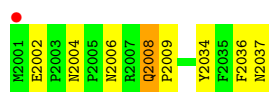
- Molecule 11: Photosystem II reaction center L protein

Chain L: 



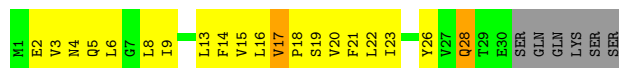
- Molecule 11: Photosystem II reaction center L protein

Chain l: 



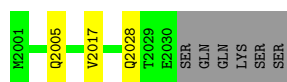
- Molecule 12: Photosystem II reaction center M protein

Chain M:



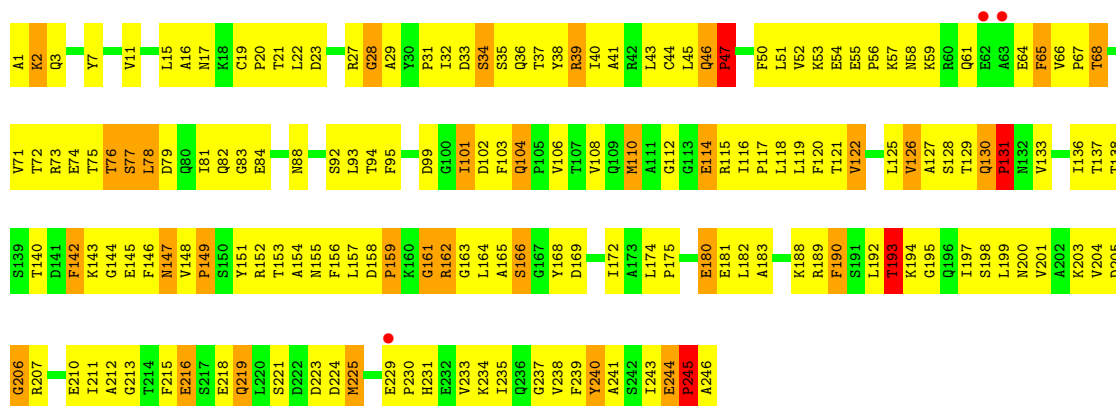
- Molecule 12: Photosystem II reaction center M protein

Chain m:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



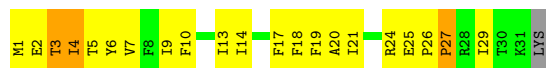
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



- Molecule 14: photosystem II PsbT protein

Chain T:



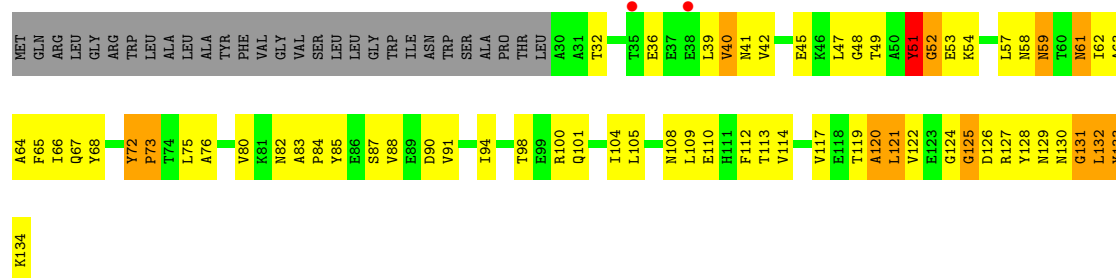
- Molecule 14: photosystem II PsbT protein

Chain t:



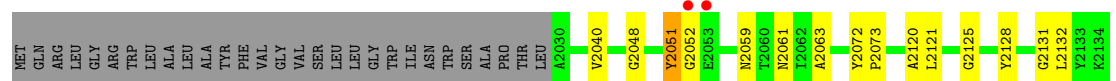
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



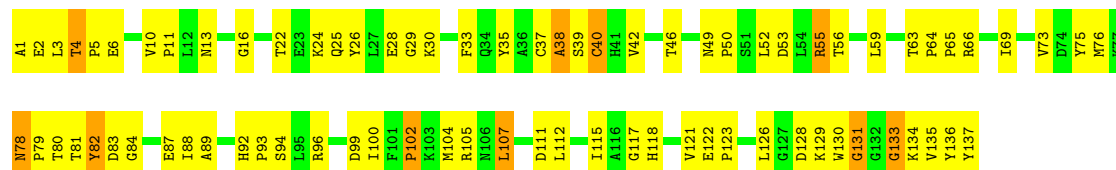
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



- Molecule 16: Cytochrome c-550

Chain V:



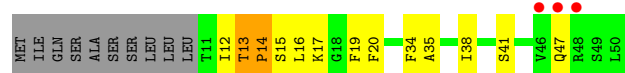
- Molecule 16: Cytochrome c-550

Chain v:



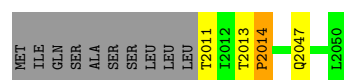
- Molecule 17: photosystem II PsbX protein

Chain X:



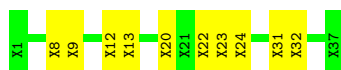
- Molecule 17: photosystem II PsbX protein

Chain x:



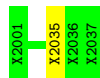
- Molecule 18: Photosystem II PsbN protein

Chain N:



- Molecule 18: Photosystem II PsbN protein

Chain n:



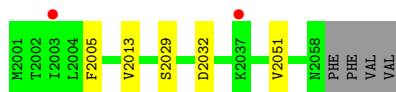
- Molecule 19: Photosystem II reaction center Z protein

Chain Z:



- Molecule 19: Photosystem II reaction center Z protein

Chain z:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 228.85Å 309.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 74.07 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 84.1 (74.07-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.342 0.309 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 105247 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	45945	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, LMT, CLA, PL9, BCT, FE, 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	0.65	0/2702	0.85	2/3685 (0.1%)
1	a	0.62	0/2701	0.83	2/3685 (0.1%)
2	B	0.57	0/3870	0.80	3/5271 (0.1%)
2	b	0.56	0/3870	0.80	4/5271 (0.1%)
3	C	0.60	0/3361	0.81	3/4579 (0.1%)
3	c	0.57	0/3361	0.80	3/4579 (0.1%)
4	D	0.62	0/2797	0.82	1/3813 (0.0%)
4	d	0.62	0/2797	0.83	2/3813 (0.1%)
5	E	0.59	0/643	0.89	1/876 (0.1%)
5	e	0.61	0/643	0.87	1/876 (0.1%)
6	F	0.74	0/278	0.84	0/379
6	f	0.68	0/278	0.84	0/379
7	H	0.58	0/419	0.81	0/570
7	h	0.60	0/419	0.81	0/570
8	I	0.63	0/319	0.73	0/429
8	i	0.61	0/319	0.73	0/429
9	J	0.60	0/278	0.80	0/376
9	j	0.62	0/278	0.84	0/376
10	K	0.66	0/303	0.92	0/416
10	k	0.63	0/303	0.86	0/416
11	L	0.74	1/311 (0.3%)	0.87	0/422
11	l	0.73	1/311 (0.3%)	0.91	0/422
12	M	0.63	0/237	0.77	0/324
12	m	0.70	0/237	0.80	0/324
13	O	0.67	0/1919	0.97	4/2601 (0.2%)
13	o	0.68	0/1919	0.96	3/2601 (0.1%)
14	T	0.71	0/274	0.78	0/370
14	t	0.74	0/274	0.80	0/370
15	U	0.68	0/838	0.91	1/1137 (0.1%)
15	u	0.62	0/838	0.87	0/1137
16	V	0.62	0/1085	0.78	0/1473
16	v	0.56	0/1085	0.77	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.57	0/299	0.72	0/403
17	x	0.61	0/299	0.75	0/403
19	Z	0.54	0/451	0.74	0/617
19	z	0.54	0/451	0.72	0/617
All	All	0.61	2/40767 (0.0%)	0.83	30/55482 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	b	0	1
11	l	0	1
13	O	0	1
15	U	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	2037	ASN	C-OXT	5.21	1.33	1.23
11	L	37	ASN	C-OXT	5.18	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2171	GLY	N-CA-C	-7.28	94.91	113.10
1	A	171	GLY	N-CA-C	-7.27	94.93	113.10
13	O	131	PRO	N-CA-C	6.48	128.95	112.10
1	a	2236	GLY	N-CA-C	6.41	129.12	113.10
4	D	231	THR	N-CA-C	-6.30	93.98	111.00
1	A	236	GLY	N-CA-C	6.29	128.83	113.10
4	d	2231	THR	N-CA-C	-6.18	94.30	111.00
13	o	2131	PRO	N-CA-C	6.08	127.89	112.10
2	B	129	GLY	N-CA-C	-5.90	98.35	113.10
2	b	2129	GLY	N-CA-C	-5.73	98.78	113.10
15	U	121	LEU	CA-CB-CG	-5.67	102.25	115.30
13	o	2193	THR	N-CA-C	5.46	125.75	111.00
13	o	2002	LYS	N-CA-C	5.42	125.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	2335	GLY	N-CA-C	-5.40	99.60	113.10
13	O	193	THR	N-CA-C	5.36	125.47	111.00
3	C	222	GLY	N-CA-C	-5.31	99.83	113.10
2	b	2329	PRO	N-CA-C	-5.25	98.46	112.10
2	B	329	PRO	N-CA-C	-5.23	98.49	112.10
3	c	2294	ASN	N-CA-C	-5.23	96.88	111.00
5	e	2053	SER	N-CA-C	5.22	125.10	111.00
2	B	335	GLY	N-CA-C	-5.19	100.13	113.10
13	O	23	ASP	N-CA-C	5.18	125.00	111.00
3	c	2223	TRP	CA-CB-CG	5.17	123.53	113.70
4	d	2054	PHE	N-CA-C	5.17	124.96	111.00
3	C	347	GLY	N-CA-C	5.12	125.91	113.10
3	C	294	ASN	N-CA-C	-5.11	97.19	111.00
13	O	2	LYS	N-CA-C	5.11	124.80	111.00
2	b	2322	GLY	N-CA-C	5.10	125.84	113.10
3	c	2347	GLY	N-CA-C	5.08	125.80	113.10
5	E	53	SER	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain
2	B	273	TYR	Sidechain
13	O	240	TYR	Sidechain
15	U	133	TYR	Sidechain
15	U	51	TYR	Sidechain
2	b	2273	TYR	Sidechain
11	l	2034	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	451	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	2616	0	2514	0	0
2	B	3739	0	3613	450	0
2	b	3739	0	3613	0	0
3	C	3253	0	3192	532	0
3	c	3253	0	3192	0	0
4	D	2702	0	2605	412	0
4	d	2702	0	2605	0	0
5	E	624	0	613	95	0
5	e	624	0	613	0	0
6	F	269	0	277	43	0
6	f	269	0	277	0	0
7	H	409	0	424	52	0
7	h	409	0	424	0	0
8	I	312	0	329	25	0
8	i	312	0	326	0	0
9	J	272	0	279	43	0
9	j	272	0	279	0	0
10	K	293	0	308	57	0
10	k	293	0	305	0	0
11	L	304	0	316	49	0
11	l	304	0	313	0	0
12	M	234	0	255	32	0
12	m	234	0	252	0	0
13	O	1888	0	1867	274	6
13	o	1888	0	1864	0	0
14	T	265	0	275	41	0
14	t	265	0	272	0	0
15	U	827	0	819	121	0
15	u	827	0	819	0	0
16	V	1064	0	1075	124	0
16	v	1064	0	1070	0	0
17	X	296	0	328	14	0
17	x	296	0	328	0	0
18	N	186	0	40	10	0
18	n	186	0	40	0	6
19	Z	442	0	480	61	0
19	z	442	0	477	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	4	0	0	0	0
21	D	4	0	0	0	0
21	a	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	d	4	0	0	0	0
22	A	9	0	0	1	0
22	a	9	0	0	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	116	0
23	C	910	0	1008	104	0
23	D	130	0	144	18	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	910	0	1008	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	E	43	0	30	16	0
25	V	43	0	30	10	0
25	e	43	0	30	0	0
25	v	43	0	30	0	0
26	A	45	0	61	8	0
26	D	45	0	61	5	0
26	a	45	0	61	0	0
26	d	45	0	61	0	0
27	B	35	0	46	0	0
27	d	35	0	46	0	0
28	B	80	0	112	16	0
28	C	80	0	112	23	0
28	F	40	0	56	3	0
28	J	40	0	56	2	0
28	K	40	0	56	13	0
28	b	80	0	112	0	0
28	c	80	0	112	0	0
28	d	40	0	56	0	0
28	j	40	0	56	0	0
28	k	40	0	56	0	0
All	All	45945	0	45912	2600	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 57.

All (2600) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:V:138:HEM:CMB	25:V:138:HEM:C2B	1.74	1.63
25:V:138:HEM:C2C	25:V:138:HEM:CMC	1.75	1.62
16:V:37:CYS:SG	25:V:138:HEM:HAB	1.57	1.44
5:E:12:ILE:CG2	5:E:18:TYR:HB2	1.44	1.43
5:E:12:ILE:HD12	25:E:84:HEM:O2D	1.31	1.25
6:F:40:GLN:NE2	9:J:27:LEU:HG	1.52	1.24
5:E:12:ILE:HG22	5:E:18:TYR:CB	1.71	1.21
13:O:40:ILE:HG12	13:O:84:GLU:OE1	1.07	1.19
2:B:75:TRP:H	2:B:94:GLU:HG3	1.07	1.18
3:C:158:THR:HG22	3:C:251:HIS:HB3	1.23	1.17
5:E:14:THR:HG22	9:J:8:ILE:HB	1.24	1.16
3:C:158:THR:CG2	3:C:251:HIS:HB3	1.75	1.16
6:F:39:MET:O	6:F:42:ILE:HG22	1.47	1.14
2:B:326:ARG:CD	2:B:327:THR:H	1.61	1.14
13:O:122:VAL:HA	13:O:146:PHE:CE2	1.85	1.12
3:C:308:GLU:HG2	3:C:361:PHE:CE1	1.85	1.10
5:E:60:ARG:HH22	16:V:129:LYS:HE3	1.05	1.10
3:C:455:PHE:HE1	4:D:224:GLN:HA	1.07	1.10
13:O:146:PHE:HB2	13:O:195:GLY:HA3	1.10	1.09
3:C:138:GLU:HG2	3:C:139:THR:H	1.09	1.09
4:D:298:PHE:HA	11:L:37:ASN:HD21	0.93	1.09
4:D:298:PHE:HA	11:L:37:ASN:ND2	1.67	1.09
5:E:14:THR:CG2	9:J:8:ILE:HB	1.83	1.08
1:A:186:PHE:HD2	1:A:192:ILE:HD11	1.05	1.08
3:C:344:SER:HB3	3:C:350:ILE:HD11	1.34	1.08
13:O:130:GLN:HB3	13:O:131:PRO:CD	1.83	1.08
5:E:12:ILE:HG22	5:E:18:TYR:HB2	1.10	1.07
3:C:223:TRP:CD1	3:C:224:ILE:HG13	1.90	1.07
16:V:37:CYS:SG	25:V:138:HEM:CAB	2.41	1.07
15:U:57:LEU:HD21	15:U:112:PHE:HD2	1.02	1.07
5:E:10:SER:HA	5:E:13:ILE:HD12	1.37	1.07
1:A:150:PRO:HB2	23:A:348:CLA:H62	1.38	1.06
15:U:59:ASN:N	15:U:59:ASN:HD22	1.33	1.06
5:E:14:THR:CG2	9:J:8:ILE:HD12	1.85	1.06
13:O:121:THR:HG21	13:O:148:VAL:HG22	1.37	1.06
13:O:40:ILE:CG1	13:O:84:GLU:OE1	2.04	1.05
2:B:326:ARG:HD2	2:B:327:THR:H	0.88	1.05
5:E:60:ARG:NH2	16:V:129:LYS:HE3	1.71	1.05
13:O:47:PRO:HG3	13:O:76:THR:HG21	1.36	1.04
3:C:223:TRP:HD1	3:C:224:ILE:HG13	1.19	1.04
2:B:57:ARG:HD3	2:B:331:ASN:HD21	1.17	1.04
15:U:57:LEU:HD21	15:U:112:PHE:CD2	1.93	1.03
5:E:14:THR:HG21	9:J:8:ILE:CD1	1.89	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:138:MET:HG2	23:B:522:CLA:HBC2	1.37	1.02
2:B:47:PRO:HB3	2:B:78:TRP:CD1	1.94	1.02
3:C:294:ASN:N	3:C:294:ASN:HD22	1.52	1.02
2:B:326:ARG:HD2	2:B:327:THR:N	1.74	1.01
5:E:14:THR:HG21	9:J:8:ILE:HD12	1.38	1.01
13:O:81:ILE:HG22	13:O:82:GLN:H	1.24	1.00
3:C:77:PRO:HA	3:C:104:GLU:OE2	1.59	1.00
1:A:186:PHE:CD2	1:A:192:ILE:HD11	1.95	1.00
3:C:62:PHE:CZ	10:K:19:ILE:HD11	1.95	1.00
15:U:132:LEU:H	15:U:132:LEU:HD23	1.20	1.00
4:D:336:HIS:CD2	4:D:336:HIS:H	1.78	1.00
6:F:40:GLN:OE1	9:J:28:PHE:HA	1.61	0.99
13:O:130:GLN:CB	13:O:131:PRO:HD2	1.91	0.99
3:C:104:GLU:HG2	3:C:105:VAL:HG23	1.40	0.99
5:E:12:ILE:CG2	5:E:18:TYR:CB	2.35	0.99
13:O:106:VAL:HG13	13:O:117:PRO:HG3	1.43	0.99
2:B:222:PRO:HB3	7:H:25:GLY:HA2	1.43	0.98
13:O:193:THR:HG22	13:O:194:LYS:H	1.27	0.98
13:O:39:ARG:HB3	13:O:245:PRO:HG3	1.42	0.98
3:C:343:ARG:HD2	3:C:343:ARG:C	1.84	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.46	0.97
3:C:158:THR:HG22	3:C:251:HIS:CB	1.95	0.97
3:C:455:PHE:CE1	4:D:224:GLN:HA	1.97	0.97
4:D:198:MET:HE1	11:L:30:LEU:HD11	1.46	0.97
3:C:320:ARG:NE	15:U:128:TYR:CE2	2.33	0.96
13:O:47:PRO:HA	13:O:237:GLY:HA3	1.47	0.95
19:Z:19:MET:O	19:Z:23:VAL:HG23	1.65	0.95
2:B:130:GLU:HG2	2:B:131:PRO:HD3	1.48	0.95
4:D:158:LEU:O	4:D:162:LEU:HG	1.66	0.95
23:C:478:CLA:H62	23:C:485:CLA:H12	1.48	0.95
2:B:326:ARG:HH11	2:B:327:THR:CB	1.80	0.95
4:D:88:SER:HB3	5:E:68:ARG:HH21	1.29	0.95
2:B:475:PHE:HB3	2:B:478:VAL:HB	1.46	0.95
15:U:59:ASN:N	15:U:59:ASN:ND2	2.05	0.95
13:O:130:GLN:HB3	13:O:131:PRO:HD2	0.96	0.94
3:C:42:LEU:HG	23:C:486:CLA:HED1	1.49	0.94
5:E:14:THR:HG21	9:J:8:ILE:CG1	1.95	0.94
23:B:521:CLA:HAB	23:B:527:CLA:HED1	1.47	0.94
13:O:81:ILE:HG22	13:O:82:GLN:N	1.80	0.94
2:B:6:TYR:OH	12:M:21:PHE:HZ	1.48	0.93
3:C:326:ALA:HB2	15:U:127:ARG:HD2	1.50	0.93
16:V:133:GLY:O	16:V:137:TYR:HB2	1.69	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:U:72:TYR:CD2	15:U:73:PRO:N	2.36	0.93
3:C:71:GLU:OE1	3:C:86:LEU:HB3	1.69	0.93
3:C:320:ARG:HE	15:U:128:TYR:HE2	1.08	0.93
1:A:225:ARG:HB3	2:B:481:GLY:C	1.88	0.93
15:U:59:ASN:HD22	15:U:59:ASN:H	0.99	0.93
13:O:44:CYS:HB3	13:O:240:TYR:HB3	1.51	0.93
3:C:271:TYR:HA	3:C:274:TYR:CD1	2.04	0.93
3:C:308:GLU:OE2	3:C:361:PHE:HZ	1.52	0.92
3:C:157:MET:HE2	3:C:160:ILE:HD12	1.50	0.92
4:D:319:LEU:HA	4:D:322:ASN:HD22	1.34	0.92
4:D:52:THR:HG22	4:D:67:TYR:HE1	1.35	0.91
3:C:344:SER:HB3	3:C:350:ILE:CD1	1.99	0.91
3:C:62:PHE:HZ	10:K:19:ILE:HD11	1.32	0.91
6:F:40:GLN:HE22	9:J:27:LEU:C	1.74	0.91
28:C:488:BCR:H312	19:Z:9:LEU:HD11	1.50	0.91
4:D:68:LEU:HA	6:F:39:MET:HE1	1.52	0.90
2:B:57:ARG:HD3	2:B:331:ASN:ND2	1.85	0.90
1:A:237:TYR:CZ	1:A:245:THR:HG23	2.06	0.90
1:A:317:TRP:HA	4:D:63:LEU:HD13	1.54	0.90
13:O:43:LEU:HD12	13:O:240:TYR:O	1.72	0.90
2:B:56:TRP:CZ3	2:B:266:GLU:HA	2.07	0.90
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.54	0.89
5:E:12:ILE:HG21	5:E:18:TYR:HB2	1.53	0.89
5:E:14:THR:HG22	9:J:8:ILE:CB	2.02	0.89
3:C:138:GLU:HG2	3:C:139:THR:N	1.87	0.89
1:A:300:PHE:HB3	1:A:302:PHE:HE1	1.36	0.89
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.51	0.89
2:B:318:ASN:HD22	2:B:319:PRO:N	1.70	0.89
16:V:4:THR:HG22	16:V:5:PRO:HD2	1.53	0.89
16:V:37:CYS:HG	25:V:138:HEM:CAB	1.84	0.89
13:O:104:GLN:OE1	13:O:104:GLN:N	2.05	0.89
16:V:46:THR:HG22	16:V:49:ASN:H	1.38	0.89
3:C:43:ILE:HG13	3:C:44:ASN:H	1.36	0.89
1:A:307:ILE:CG1	1:A:314:ILE:HD11	2.03	0.88
1:A:89:ILE:HG12	13:O:73:ARG:NH2	1.88	0.88
3:C:55:ALA:HB1	28:C:488:BCR:H373	1.55	0.88
1:A:239:PHE:HZ	4:D:223:PHE:HZ	1.22	0.88
2:B:56:TRP:HZ3	2:B:266:GLU:HA	1.38	0.88
19:Z:33:TRP:HE3	19:Z:37:LYS:HD3	1.37	0.88
2:B:322:GLY:HA2	2:B:325:PHE:CE1	2.08	0.88
1:A:334:ARG:HH11	4:D:320:LEU:HD11	1.38	0.88
1:A:286:THR:HG22	23:A:348:CLA:O1D	1.73	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:71:CYS:HB2	4:D:76:VAL:HG23	1.55	0.87
13:O:146:PHE:HB2	13:O:195:GLY:CA	2.01	0.87
3:C:307:PRO:HB3	3:C:358:PHE:CD2	2.09	0.87
3:C:116:VAL:HG13	28:C:488:BCR:H332	1.57	0.87
13:O:164:LEU:HD23	15:U:42:VAL:HG13	1.56	0.87
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.38	0.87
3:C:305:THR:HA	3:C:423:ARG:NH1	1.90	0.87
13:O:163:GLY:HA2	13:O:188:LYS:HG3	1.57	0.87
4:D:198:MET:CE	11:L:30:LEU:HD11	2.03	0.87
13:O:155:ASN:HD22	15:U:129:ASN:ND2	1.72	0.87
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.56	0.87
13:O:140:THR:HB	13:O:201:VAL:H	1.40	0.87
1:A:230:THR:HG22	1:A:231:GLU:H	1.39	0.87
13:O:146:PHE:CB	13:O:195:GLY:HA3	2.01	0.86
19:Z:51:VAL:HG12	19:Z:52:LEU:HD23	1.53	0.86
3:C:285:ILE:HA	23:C:487:CLA:HMB2	1.56	0.86
2:B:326:ARG:HD3	28:B:529:BCR:H402	1.56	0.86
11:L:7:ARG:C	11:L:9:PRO:HD3	1.96	0.86
2:B:9:HIS:HB2	23:B:523:CLA:HBA2	1.55	0.86
13:O:155:ASN:ND2	15:U:129:ASN:ND2	2.23	0.86
13:O:140:THR:HG21	13:O:201:VAL:O	1.74	0.86
5:E:60:ARG:HH22	16:V:129:LYS:CE	1.87	0.86
1:A:57:PRO:HG2	13:O:115:ARG:NH1	1.91	0.86
5:E:14:THR:CG2	9:J:8:ILE:CB	2.53	0.86
3:C:269:GLU:OE2	3:C:447:ARG:HG2	1.75	0.86
16:V:75:TYR:HE2	16:V:80:THR:H	1.22	0.86
1:A:214:MET:CE	1:A:214:MET:HA	2.05	0.86
2:B:120:LEU:HD23	2:B:130:GLU:HA	1.58	0.85
7:H:39:VAL:O	7:H:43:ILE:HG13	1.76	0.85
1:A:142:TRP:NE1	3:C:443:TRP:CH2	2.45	0.85
11:L:31:PHE:HB3	11:L:35:PHE:HE1	1.40	0.85
2:B:280:PHE:CE1	2:B:312:TYR:HB3	2.12	0.85
16:V:55:ARG:HH21	16:V:131:GLY:HA3	1.39	0.85
3:C:305:THR:H	3:C:308:GLU:HG3	1.41	0.85
1:A:223:LEU:HD22	1:A:245:THR:HG22	1.57	0.85
23:B:518:CLA:H141	23:B:524:CLA:HMA2	1.59	0.85
1:A:307:ILE:HG13	1:A:314:ILE:HD11	1.58	0.85
4:D:197:HIS:O	4:D:201:VAL:HG23	1.76	0.85
1:A:29:TYR:HD2	1:A:133:LEU:CD1	1.90	0.85
13:O:47:PRO:HG3	13:O:76:THR:CG2	2.06	0.85
2:B:122:LEU:HD12	23:B:525:CLA:HMA2	1.57	0.85
12:M:19:SER:O	12:M:23:ILE:HG12	1.77	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.12	0.84
3:C:282:MET:HA	3:C:285:ILE:HG13	1.57	0.84
3:C:257:PHE:O	3:C:261:ARG:HG3	1.77	0.84
4:D:90:LEU:HD11	4:D:96:GLU:OE1	1.78	0.84
13:O:126:VAL:O	13:O:144:GLY:HA3	1.78	0.84
13:O:43:LEU:CD1	13:O:241:ALA:HB2	2.08	0.84
2:B:318:ASN:HD22	2:B:318:ASN:C	1.79	0.84
2:B:357:ARG:HH22	4:D:337:GLU:HB3	1.41	0.83
2:B:339:ALA:HB3	2:B:430:PHE:HD1	1.43	0.83
2:B:322:GLY:HA2	2:B:325:PHE:CD1	2.13	0.83
1:A:334:ARG:NH1	4:D:320:LEU:HD11	1.93	0.83
5:E:14:THR:CG2	9:J:8:ILE:CG1	2.56	0.83
3:C:294:ASN:N	3:C:294:ASN:ND2	2.21	0.83
1:A:221:SER:HA	4:D:139:ARG:HB2	1.60	0.83
1:A:243:GLU:HA	4:D:240:ALA:HB1	1.58	0.83
23:B:512:CLA:H191	23:B:520:CLA:H151	1.61	0.83
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.43	0.83
3:C:279:LEU:HB3	23:C:481:CLA:HBC1	1.59	0.83
10:K:25:ALA:HB1	28:K:50:BCR:H19C	1.60	0.82
2:B:339:ALA:HB3	2:B:430:PHE:CD1	2.14	0.82
4:D:174:GLY:O	4:D:178:ILE:HG12	1.80	0.82
3:C:55:ALA:HB1	28:C:488:BCR:C37	2.09	0.82
23:A:350:CLA:HED1	4:D:175:VAL:HG13	1.61	0.82
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.14	0.82
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.14	0.82
2:B:212:ALA:HB2	23:B:511:CLA:HMC3	1.62	0.82
5:E:12:ILE:HD12	25:E:84:HEM:CGD	2.09	0.82
4:D:195:PRO:HA	4:D:198:MET:HE2	1.59	0.82
1:A:306:VAL:HG22	1:A:307:ILE:H	1.42	0.82
1:A:330:VAL:CG1	4:D:348:ARG:HG3	2.10	0.82
4:D:195:PRO:HA	4:D:198:MET:CE	2.09	0.82
3:C:203:THR:HG22	3:C:208:VAL:HG11	1.62	0.82
15:U:91:VAL:O	15:U:94:ILE:HG13	1.80	0.82
16:V:80:THR:HG23	16:V:84:GLY:HA2	1.62	0.81
4:D:71:CYS:HB2	4:D:76:VAL:CG2	2.09	0.81
3:C:292:PHE:N	3:C:292:PHE:HD2	1.78	0.81
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.62	0.81
16:V:56:THR:HA	16:V:59:LEU:HD12	1.60	0.81
4:D:102:THR:HG22	4:D:106:GLN:HE21	1.43	0.81
1:A:301:ASN:HD21	3:C:407:VAL:CG2	1.93	0.81
2:B:413:ASP:HB3	2:B:415:PRO:HD2	1.60	0.81
13:O:95:PHE:CB	13:O:127:ALA:HB3	2.10	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:81:ILE:CG2	13:O:82:GLN:H	1.94	0.81
13:O:39:ARG:CB	13:O:245:PRO:HG3	2.10	0.81
1:A:326:LEU:HD13	3:C:412:THR:HG21	1.60	0.81
1:A:92:HIS:HD2	3:C:219:GLY:HA3	1.44	0.81
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.62	0.81
13:O:40:ILE:HG22	13:O:41:ALA:H	1.46	0.81
13:O:40:ILE:HG12	13:O:84:GLU:CD	2.02	0.81
3:C:295:THR:O	3:C:298:PRO:HD3	1.79	0.80
2:B:222:PRO:HB3	7:H:25:GLY:CA	2.11	0.80
2:B:248:ALA:HA	23:B:517:CLA:H42	1.62	0.80
9:J:40:LEU:HD23	16:V:30:LYS:HE2	1.61	0.80
2:B:170:ASP:OD1	2:B:175:THR:HG22	1.81	0.80
3:C:199:ILE:HD12	3:C:234:VAL:HG21	1.62	0.80
3:C:120:ILE:O	3:C:124:VAL:HG23	1.82	0.80
3:C:212:TYR:O	3:C:223:TRP:HB2	1.81	0.80
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.62	0.80
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.17	0.80
2:B:302:TRP:O	2:B:341:LYS:HE3	1.81	0.80
3:C:126:GLY:O	3:C:130:VAL:HG23	1.80	0.80
2:B:75:TRP:N	2:B:94:GLU:HG3	1.93	0.80
2:B:136:PRO:HD3	2:B:231:MET:HE1	1.64	0.80
3:C:308:GLU:HG2	3:C:361:PHE:HE1	1.42	0.80
19:Z:8:ALA:O	19:Z:11:ALA:HB3	1.82	0.80
4:D:138:VAL:HG12	4:D:139:ARG:N	1.97	0.80
2:B:478:VAL:HG11	4:D:139:ARG:HA	1.64	0.80
4:D:190:ASN:HB2	4:D:296:TYR:HD1	1.44	0.80
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.64	0.80
1:A:29:TYR:HD1	1:A:29:TYR:C	1.85	0.79
3:C:405:ASN:HB2	3:C:407:VAL:HG23	1.62	0.79
1:A:246:TYR:CE1	1:A:248:ILE:HG12	2.17	0.79
13:O:122:VAL:HA	13:O:146:PHE:HE2	1.47	0.79
16:V:4:THR:HG22	16:V:5:PRO:CD	2.12	0.79
11:L:12:LEU:HD11	11:L:16:SER:HB3	1.64	0.79
4:D:336:HIS:H	4:D:336:HIS:HD2	1.28	0.79
1:A:210:LEU:HD12	1:A:210:LEU:O	1.82	0.79
3:C:334:PRO:HA	13:O:153:THR:HB	1.65	0.79
5:E:56:ALA:HB2	5:E:82:LEU:HD23	1.62	0.79
23:B:512:CLA:H193	23:B:523:CLA:H102	1.62	0.79
3:C:292:PHE:CD2	3:C:292:PHE:N	2.50	0.79
15:U:132:LEU:N	15:U:132:LEU:HD23	1.96	0.79
5:E:14:THR:CG2	9:J:8:ILE:CD1	2.54	0.79
3:C:285:ILE:HA	23:C:487:CLA:CMB	2.11	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:79:PRO:HB2	16:V:88:ILE:CG1	2.13	0.79
3:C:264:PHE:HD2	3:C:264:PHE:N	1.81	0.79
1:A:14:TRP:CZ3	1:A:18:CYS:SG	2.76	0.79
1:A:239:PHE:HZ	4:D:223:PHE:CZ	2.01	0.79
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.65	0.79
1:A:296:ASN:CG	3:C:401:LEU:HD23	2.04	0.78
3:C:273:SER:HB3	3:C:445:ALA:HB2	1.66	0.78
13:O:140:THR:HB	13:O:201:VAL:HG23	1.64	0.78
2:B:264:PRO:HG3	2:B:267:LEU:HD12	1.64	0.78
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.18	0.78
13:O:75:THR:HG22	13:O:103:PHE:HD2	1.47	0.78
10:K:16:LEU:HB3	10:K:17:PRO:CD	2.13	0.78
8:I:27:ASP:HB2	8:I:28:PRO:CD	2.13	0.78
23:A:350:CLA:H121	26:A:353:PL9:H162	1.66	0.78
2:B:221:PRO:HG3	2:B:225:LEU:HD12	1.64	0.78
1:A:239:PHE:CE1	4:D:245:SER:HA	2.19	0.78
1:A:253:GLY:O	1:A:257:ARG:HG2	1.83	0.78
4:D:236:ASN:OD1	4:D:239:GLN:HB2	1.83	0.78
3:C:86:LEU:HD13	3:C:89:ILE:HD12	1.64	0.78
1:A:301:ASN:ND2	3:C:407:VAL:HG21	1.99	0.78
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.18	0.77
5:E:22:HIS:HA	5:E:25:THR:HB	1.64	0.77
3:C:347:GLY:HA3	13:O:17:ASN:OD1	1.85	0.77
4:D:298:PHE:CA	11:L:37:ASN:HD21	1.87	0.77
2:B:145:LEU:HD13	23:B:522:CLA:HMB1	1.65	0.77
4:D:176:ALA:HA	4:D:179:PHE:HD1	1.48	0.77
6:F:36:ILE:HA	6:F:39:MET:HG3	1.67	0.77
10:K:2:LEU:N	10:K:3:PRO:HD3	1.98	0.77
23:B:522:CLA:H171	23:B:525:CLA:CMD	2.14	0.77
5:E:12:ILE:HG22	5:E:18:TYR:CG	2.20	0.77
3:C:320:ARG:HH12	16:V:50:PRO:HD2	1.46	0.77
2:B:327:THR:HG22	2:B:329:PRO:HD3	1.67	0.77
2:B:478:VAL:CG1	4:D:139:ARG:HA	2.15	0.77
16:V:37:CYS:HG	25:V:138:HEM:HAB	1.37	0.77
16:V:79:PRO:HB2	16:V:88:ILE:HG12	1.67	0.77
1:A:63:ILE:HD11	1:A:336:ALA:HB2	1.67	0.77
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.67	0.77
3:C:320:ARG:NH1	16:V:50:PRO:HD2	1.99	0.77
2:B:326:ARG:CD	2:B:327:THR:N	2.41	0.76
26:D:357:PL9:H38	14:T:18:PHE:HB2	1.66	0.76
1:A:306:VAL:HG22	1:A:307:ILE:N	1.99	0.76
2:B:326:ARG:NH1	2:B:327:THR:OG1	2.17	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:113:TRP:HB3	23:B:525:CLA:HED1	1.67	0.76
8:I:7:THR:O	8:I:11:VAL:HG23	1.85	0.76
2:B:142:HIS:CE1	23:B:524:CLA:H142	2.21	0.76
1:A:295:PHE:HB3	3:C:291:TRP:CZ3	2.20	0.76
1:A:301:ASN:HD21	3:C:407:VAL:HG21	1.48	0.76
4:D:323:GLU:HG2	13:O:168:TYR:OH	1.86	0.76
1:A:142:TRP:HE1	3:C:443:TRP:HH2	1.33	0.76
3:C:175:LEU:HD11	23:C:479:CLA:HED3	1.67	0.76
1:A:29:TYR:HD1	1:A:30:VAL:N	1.83	0.76
5:E:12:ILE:CD1	25:E:84:HEM:O1A	2.34	0.76
9:J:15:THR:HA	28:K:50:BCR:H372	1.67	0.76
1:A:87:ASN:HD21	3:C:357:ARG:HH11	1.32	0.76
2:B:326:ARG:HH11	2:B:327:THR:HB	1.48	0.75
23:B:522:CLA:H171	23:B:525:CLA:HMD3	1.68	0.75
1:A:148:SER:HB2	1:A:284:TRP:HH2	1.50	0.75
1:A:141:PRO:HG2	3:C:443:TRP:HZ3	1.52	0.75
2:B:118:TRP:CZ2	11:L:3:PRO:HB3	2.21	0.75
1:A:172:MET:HE2	23:A:349:CLA:HMC3	1.69	0.75
23:C:479:CLA:H92	23:C:479:CLA:HAB	1.69	0.75
4:D:31:GLY:HA3	4:D:131:GLU:OE1	1.86	0.75
2:B:305:ILE:O	2:B:305:ILE:HG13	1.86	0.75
3:C:264:PHE:CD2	3:C:264:PHE:N	2.54	0.75
1:A:57:PRO:HB3	1:A:68:SER:HB3	1.68	0.75
2:B:25:MET:HB3	28:B:529:BCR:H332	1.69	0.75
13:O:7:TYR:O	13:O:11:VAL:HG23	1.86	0.75
1:A:56:PRO:HA	1:A:73:TYR:CE1	2.22	0.75
1:A:159:LEU:HD21	23:C:487:CLA:HBD	1.69	0.75
4:D:336:HIS:CD2	4:D:336:HIS:N	2.52	0.75
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.68	0.74
3:C:98:GLY:O	3:C:99:VAL:HG23	1.86	0.74
2:B:187:PRO:O	2:B:190:PHE:N	2.20	0.74
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.69	0.74
4:D:88:SER:CB	5:E:68:ARG:HH21	1.98	0.74
3:C:285:ILE:HG21	23:C:479:CLA:H51	1.69	0.74
3:C:374:GLY:HA2	13:O:7:TYR:CE1	2.22	0.74
11:L:4:ASN:N	11:L:5:PRO:HD3	2.03	0.74
4:D:19:ASP:OD1	4:D:23:LYS:HD2	1.87	0.74
3:C:293:ASN:C	3:C:294:ASN:HD22	1.89	0.74
2:B:172:TYR:CE2	2:B:283:GLU:HB2	2.23	0.74
3:C:308:GLU:HG2	3:C:361:PHE:CZ	2.22	0.74
3:C:363:GLY:O	3:C:367:GLU:HG2	1.87	0.74
2:B:112:CYS:O	2:B:116:VAL:HG23	1.87	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:68:LEU:CA	6:F:39:MET:HE1	2.18	0.74
5:E:9:PHE:O	5:E:10:SER:HB3	1.85	0.74
1:A:29:TYR:CD1	1:A:29:TYR:C	2.59	0.74
4:D:235:PHE:HA	4:D:239:GLN:OE1	1.86	0.74
5:E:43:TYR:CD2	5:E:50:ARG:HG2	2.22	0.74
3:C:229:ASN:HB3	3:C:232:ASP:OD1	1.88	0.74
3:C:350:ILE:HG12	3:C:359:TRP:HB2	1.70	0.74
2:B:63:LEU:HD11	2:B:93:PHE:CE1	2.22	0.74
4:D:71:CYS:HB3	4:D:75:THR:HB	1.68	0.74
4:D:51:GLY:HA2	4:D:55:VAL:HG23	1.69	0.74
5:E:19:TRP:HZ2	9:J:13:VAL:HG22	1.50	0.74
3:C:320:ARG:NE	15:U:128:TYR:HE2	1.79	0.74
4:D:152:VAL:O	4:D:156:VAL:HG23	1.88	0.74
1:A:78:ILE:HD11	11:L:34:TYR:CE1	2.23	0.74
3:C:227:VAL:HG23	3:C:294:ASN:HB3	1.68	0.74
3:C:61:VAL:HG22	23:C:480:CLA:HAC2	1.70	0.74
3:C:41:ARG:HB2	23:C:486:CLA:HED3	1.69	0.74
10:K:19:ILE:HA	10:K:22:LEU:HD12	1.70	0.74
3:C:101:PRO:N	3:C:195:ASP:HB3	2.03	0.73
13:O:43:LEU:HD13	13:O:241:ALA:HB2	1.69	0.73
10:K:2:LEU:H	10:K:3:PRO:HD3	1.51	0.73
2:B:27:THR:O	23:B:518:CLA:HBC1	1.88	0.73
3:C:138:GLU:CG	3:C:139:THR:H	1.96	0.73
4:D:267:LEU:O	4:D:271:MET:HG3	1.87	0.73
4:D:56:THR:HB	5:E:48:THR:HG23	1.71	0.73
1:A:317:TRP:HA	4:D:63:LEU:CD1	2.19	0.73
2:B:357:ARG:NH2	4:D:337:GLU:HB3	2.04	0.73
2:B:368:VAL:HA	2:B:425:ILE:HD11	1.69	0.73
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.69	0.73
14:T:18:PHE:HD2	14:T:19:PHE:CD1	2.07	0.73
3:C:248:GLY:O	3:C:252:ILE:HG13	1.89	0.73
3:C:123:ALA:HB1	19:Z:47:TRP:HH2	1.53	0.73
13:O:50:PHE:HZ	13:O:76:THR:HG23	1.54	0.72
1:A:334:ARG:HH12	13:O:159:PRO:HA	1.53	0.72
1:A:76:ASN:HB3	14:T:2:GLU:OE2	1.90	0.72
4:D:238:THR:O	4:D:240:ALA:N	2.20	0.72
2:B:246:PHE:HE1	2:B:463:PHE:HB2	1.53	0.72
1:A:69:GLY:HA2	1:A:75:ASN:OD1	1.90	0.72
2:B:66:MET:O	2:B:71:VAL:HG23	1.89	0.72
19:Z:41:PHE:HD1	19:Z:41:PHE:H	1.35	0.72
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.71	0.72
1:A:182:PHE:O	1:A:186:PHE:HB2	1.88	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:271:TYR:HA	3:C:274:TYR:HD1	1.50	0.72
2:B:172:TYR:CZ	2:B:283:GLU:HB2	2.25	0.72
2:B:400:SER:OG	2:B:410:THR:HG23	1.88	0.72
4:D:194:ASN:O	4:D:198:MET:HG3	1.88	0.72
2:B:340:TRP:CZ3	2:B:342:GLY:HA3	2.24	0.72
4:D:235:PHE:CD1	4:D:236:ASN:N	2.57	0.72
13:O:162:ARG:O	13:O:162:ARG:HG2	1.90	0.72
3:C:42:LEU:CG	23:C:486:CLA:HED1	2.18	0.72
15:U:132:LEU:H	15:U:132:LEU:CD2	1.96	0.72
4:D:319:LEU:HA	4:D:322:ASN:ND2	2.04	0.72
3:C:42:LEU:HD13	23:C:486:CLA:HMA3	1.70	0.72
15:U:83:ALA:HA	15:U:85:TYR:CE2	2.25	0.72
8:I:15:PHE:HA	8:I:18:LEU:HG	1.72	0.72
13:O:201:VAL:HG13	13:O:211:ILE:HG23	1.71	0.72
5:E:14:THR:HG21	9:J:8:ILE:HG13	1.71	0.72
23:C:477:CLA:CMD	23:C:485:CLA:HAB	2.19	0.72
13:O:223:ASP:HB3	13:O:230:PRO:HG3	1.71	0.72
23:B:518:CLA:C14	23:B:524:CLA:HMA2	2.20	0.71
2:B:68:ARG:HH12	23:B:516:CLA:HED1	1.54	0.71
12:M:18:PRO:O	12:M:22:LEU:HG	1.89	0.71
3:C:343:ARG:HA	3:C:348:GLU:O	1.90	0.71
23:B:520:CLA:HBC3	23:B:523:CLA:H41	1.72	0.71
3:C:99:VAL:HG22	3:C:104:GLU:O	1.90	0.71
1:A:29:TYR:CD2	1:A:133:LEU:CD1	2.72	0.71
1:A:326:LEU:CD1	3:C:412:THR:HG21	2.20	0.71
2:B:248:ALA:O	2:B:252:VAL:HG23	1.89	0.71
13:O:40:ILE:HG22	13:O:41:ALA:N	2.04	0.71
1:A:239:PHE:CZ	4:D:223:PHE:HZ	2.08	0.71
3:C:437:PHE:HA	23:C:483:CLA:CMC	2.19	0.71
1:A:63:ILE:HD11	1:A:336:ALA:CB	2.20	0.71
2:B:17:GLY:O	2:B:20:ILE:HG22	1.89	0.71
3:C:385:GLN:OE1	3:C:386:PRO:HD2	1.91	0.71
2:B:47:PRO:HB3	2:B:78:TRP:HD1	1.51	0.71
3:C:43:ILE:HG13	3:C:44:ASN:N	2.06	0.71
1:A:330:VAL:HG11	4:D:348:ARG:HG3	1.72	0.71
2:B:397:VAL:HG12	2:B:398:THR:N	2.05	0.71
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.72	0.71
4:D:244:TYR:OH	4:D:264:LYS:NZ	2.21	0.71
2:B:318:ASN:C	2:B:318:ASN:ND2	2.44	0.71
1:A:309:ALA:O	16:V:3:LEU:N	2.24	0.71
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.71	0.71
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.54	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:GLU:CA	4:D:240:ALA:HB1	2.21	0.71
1:A:29:TYR:HE1	1:A:31:GLY:CA	2.03	0.71
4:D:190:ASN:CB	4:D:296:TYR:HD1	2.04	0.71
4:D:262:SER:O	4:D:263:ASN:ND2	2.24	0.71
3:C:345:PRO:O	13:O:74:GLU:HB2	1.90	0.71
1:A:159:LEU:HG	1:A:163:ILE:HD11	1.73	0.71
2:B:339:ALA:HB2	2:B:431:GLU:H	1.56	0.71
15:U:73:PRO:HB2	16:V:83:ASP:OD2	1.91	0.71
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.23	0.71
2:B:321:LYS:CE	2:B:325:PHE:HZ	2.04	0.71
2:B:348:ASN:OD1	2:B:349:LYS:N	2.17	0.71
1:A:89:ILE:HG21	1:A:94:TYR:HB2	1.73	0.70
13:O:71:VAL:HG21	13:O:108:VAL:HG23	1.71	0.70
13:O:17:ASN:O	13:O:46:GLN:HG3	1.91	0.70
1:A:214:MET:HE2	1:A:214:MET:HA	1.71	0.70
4:D:221:THR:O	4:D:221:THR:HG22	1.90	0.70
1:A:307:ILE:O	1:A:309:ALA:N	2.23	0.70
3:C:350:ILE:HG21	3:C:359:TRP:HB3	1.73	0.70
1:A:214:MET:HE1	4:D:142:ASN:OD1	1.91	0.70
13:O:164:LEU:O	13:O:165:ALA:HB3	1.89	0.70
3:C:343:ARG:CD	3:C:343:ARG:C	2.59	0.70
4:D:16:ASP:O	4:D:19:ASP:HB3	1.90	0.70
13:O:211:ILE:HB	13:O:241:ALA:HB3	1.73	0.70
1:A:159:LEU:HD11	23:C:487:CLA:OBD	1.92	0.70
10:K:15:VAL:HG11	18:N:13:UNK:CB	2.21	0.70
5:E:52:ASP:O	16:V:1:ALA:HB3	1.90	0.70
13:O:155:ASN:ND2	15:U:129:ASN:HD22	1.88	0.70
3:C:450:ALA:HA	3:C:454:GLY:HA3	1.73	0.70
1:A:142:TRP:NE1	3:C:443:TRP:HH2	1.89	0.70
6:F:31:PHE:O	6:F:31:PHE:HD2	1.74	0.70
3:C:42:LEU:CD1	23:C:486:CLA:HMA3	2.21	0.70
1:A:75:ASN:ND2	1:A:79:THR:HG21	2.05	0.70
12:M:15:VAL:HG12	12:M:16:LEU:HD23	1.73	0.70
7:H:59:VAL:O	7:H:59:VAL:HG12	1.91	0.70
4:D:68:LEU:HA	6:F:39:MET:CE	2.19	0.70
2:B:414:PRO:HG2	2:B:415:PRO:HD3	1.72	0.70
1:A:317:TRP:CA	4:D:63:LEU:HD13	2.22	0.70
4:D:90:LEU:CD1	4:D:96:GLU:HB3	2.21	0.70
4:D:118:GLY:HA3	24:D:355:PHO:H71	1.72	0.69
3:C:121:SER:O	3:C:125:LEU:HG	1.91	0.69
4:D:18:LEU:O	4:D:22:LEU:HB3	1.92	0.69
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.22	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:37:CYS:O	16:V:39:SER:N	2.26	0.69
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.74	0.69
3:C:123:ALA:CB	19:Z:47:TRP:HH2	2.04	0.69
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.26	0.69
2:B:397:VAL:HG12	2:B:398:THR:H	1.56	0.69
16:V:75:TYR:CD2	16:V:79:PRO:HA	2.26	0.69
2:B:41:GLU:OE1	2:B:63:LEU:HB2	1.91	0.69
3:C:305:THR:HA	3:C:423:ARG:HH11	1.56	0.69
13:O:118:LEU:CD1	13:O:233:VAL:HG11	2.23	0.69
2:B:324:LEU:CD1	11:L:34:TYR:HB3	2.22	0.69
10:K:30:TRP:CE3	10:K:31:GLN:NE2	2.60	0.69
1:A:235:TYR:HA	4:D:265:ARG:NH2	2.06	0.69
4:D:186:GLN:HB2	23:D:354:CLA:HBC1	1.73	0.69
4:D:87:HIS:NE2	4:D:166:SER:HA	2.08	0.69
4:D:90:LEU:HD11	4:D:96:GLU:CD	2.13	0.69
16:V:133:GLY:O	16:V:137:TYR:CB	2.41	0.69
1:A:320:ILE:HG22	1:A:320:ILE:O	1.93	0.69
1:A:219:VAL:HG11	4:D:268:HIS:CG	2.28	0.69
13:O:28:GLY:HA3	13:O:137:THR:HG22	1.73	0.69
1:A:161:TYR:HB3	1:A:162:PRO:CD	2.21	0.69
3:C:343:ARG:HD2	3:C:343:ARG:O	1.92	0.69
2:B:30:VAL:HG12	23:B:518:CLA:HHD	1.73	0.69
1:A:281:VAL:HG12	1:A:281:VAL:O	1.91	0.69
3:C:176:VAL:O	3:C:180:MET:HG2	1.93	0.69
13:O:75:THR:HG22	13:O:103:PHE:CD2	2.28	0.69
13:O:47:PRO:CG	13:O:76:THR:HG21	2.20	0.69
3:C:319:ILE:HD13	3:C:389:GLU:HG2	1.74	0.69
13:O:211:ILE:HG22	13:O:212:ALA:N	2.08	0.69
23:B:519:CLA:HMD1	23:B:524:CLA:HAB	1.75	0.69
2:B:57:ARG:HH11	2:B:57:ARG:CG	2.06	0.69
2:B:268:PHE:HB2	2:B:448:ARG:HE	1.56	0.69
13:O:140:THR:CB	13:O:201:VAL:H	2.06	0.68
15:U:62:ILE:HG23	15:U:76:ALA:HB1	1.74	0.68
3:C:158:THR:HG23	3:C:251:HIS:HB3	1.74	0.68
2:B:57:ARG:HH11	2:B:57:ARG:HG3	1.56	0.68
4:D:138:VAL:HG12	4:D:139:ARG:H	1.55	0.68
1:A:29:TYR:HD2	1:A:133:LEU:HD13	1.59	0.68
1:A:76:ASN:HD21	4:D:298:PHE:HE2	1.39	0.68
3:C:203:THR:CG2	3:C:208:VAL:HG11	2.23	0.68
1:A:301:ASN:OD1	3:C:407:VAL:HG21	1.94	0.68
13:O:22:LEU:O	13:O:203:LYS:HD3	1.94	0.68
3:C:116:VAL:HG21	28:C:489:BCR:H323	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:53:THR:HA	4:D:67:TYR:CD1	2.29	0.68
1:A:81:ALA:HB3	1:A:174:LEU:O	1.93	0.68
2:B:145:LEU:HD13	23:B:522:CLA:CMB	2.23	0.68
3:C:443:TRP:CE3	3:C:443:TRP:HA	2.28	0.68
4:D:261:PHE:HA	14:T:24:ARG:HH22	1.59	0.68
13:O:163:GLY:HA3	13:O:188:LYS:HE2	1.76	0.68
2:B:105:GLY:HA2	28:B:528:BCR:H383	1.75	0.68
26:D:357:PL9:H261	14:T:21:ILE:HD11	1.74	0.68
3:C:156:LYS:O	3:C:160:ILE:HG13	1.93	0.68
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.29	0.68
23:C:475:CLA:HBD	28:J:53:BCR:HC21	1.76	0.68
2:B:86:ILE:O	2:B:88:PRO:HD3	1.93	0.68
2:B:124:ARG:HG2	2:B:125:ASP:N	2.07	0.68
4:D:80:THR:HG21	4:D:167:TRP:O	1.94	0.68
2:B:6:TYR:HH	12:M:21:PHE:HZ	0.74	0.68
3:C:275:SER:HB3	23:C:485:CLA:HAA1	1.76	0.68
1:A:61:ASP:HA	1:A:87:ASN:HB2	1.75	0.68
9:J:9:PRO:O	9:J:10:LEU:HD23	1.94	0.68
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.74	0.68
2:B:383:PHE:O	13:O:166:SER:HA	1.93	0.68
10:K:34:VAL:HG12	10:K:34:VAL:O	1.93	0.68
28:C:488:BCR:H341	28:K:50:BCR:HC31	1.76	0.67
7:H:57:VAL:O	7:H:57:VAL:CG1	2.41	0.67
5:E:33:GLY:HA2	6:F:31:PHE:CE2	2.29	0.67
7:H:53:ILE:HG23	17:X:13:THR:OG1	1.94	0.67
2:B:113:TRP:O	2:B:117:TYR:HB2	1.94	0.67
3:C:308:GLU:OE2	3:C:361:PHE:CZ	2.43	0.67
3:C:149:TYR:CD2	3:C:156:LYS:HG3	2.29	0.67
4:D:86:GLY:C	4:D:87:HIS:HD2	1.98	0.67
3:C:108:THR:HG21	10:K:2:LEU:HG	1.76	0.67
2:B:86:ILE:HG22	2:B:86:ILE:O	1.94	0.67
2:B:326:ARG:NH1	2:B:327:THR:CB	2.56	0.67
24:A:351:PHO:NC	4:D:209:LEU:HD12	2.09	0.67
3:C:305:THR:CA	3:C:423:ARG:NH1	2.57	0.67
19:Z:48:ILE:O	19:Z:52:LEU:HG	1.95	0.67
16:V:76:MET:HE3	16:V:115:ILE:HG21	1.76	0.67
3:C:141:GLU:HB3	3:C:144:SER:OG	1.93	0.67
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.76	0.67
1:A:206:PHE:HE1	23:A:348:CLA:HMB1	1.57	0.67
3:C:282:MET:HA	3:C:285:ILE:CG1	2.24	0.67
2:B:266:GLU:HG2	2:B:266:GLU:O	1.93	0.67
3:C:141:GLU:HB2	3:C:144:SER:HB2	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:108:GLY:O	4:D:110:LEU:N	2.27	0.67
1:A:75:ASN:ND2	1:A:79:THR:CG2	2.57	0.67
2:B:135:LEU:HB2	2:B:231:MET:HE3	1.77	0.67
13:O:104:GLN:N	13:O:104:GLN:CD	2.46	0.67
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.09	0.67
13:O:168:TYR:CE1	13:O:172:ILE:HD11	2.29	0.67
13:O:125:LEU:HD12	13:O:145:GLU:O	1.93	0.67
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.24	0.67
5:E:26:ILE:CG1	5:E:27:PRO:HD3	2.25	0.67
2:B:162:PHE:HB3	23:B:515:CLA:HMD3	1.75	0.67
13:O:243:ILE:O	13:O:244:GLU:HB2	1.95	0.67
2:B:324:LEU:HD12	11:L:34:TYR:HB3	1.77	0.67
3:C:291:TRP:HB3	3:C:292:PHE:CD2	2.29	0.67
2:B:414:PRO:CD	2:B:415:PRO:HD3	2.24	0.67
3:C:419:PHE:O	3:C:420:VAL:HG23	1.95	0.67
25:E:84:HEM:HAC	6:F:26:ALA:HB1	1.75	0.67
6:F:40:GLN:HE21	9:J:27:LEU:HG	1.55	0.67
1:A:141:PRO:HG3	3:C:446:GLY:O	1.94	0.67
13:O:164:LEU:H	13:O:188:LYS:HE2	1.60	0.66
4:D:29:PHE:CD2	4:D:29:PHE:C	2.67	0.66
3:C:131:TYR:HE1	3:C:135:ARG:HD3	1.60	0.66
1:A:180:PHE:CE2	4:D:192:THR:HG22	2.31	0.66
1:A:290:ILE:HD11	23:A:348:CLA:CGD	2.25	0.66
14:T:3:THR:O	14:T:5:THR:N	2.28	0.66
23:A:348:CLA:H192	26:D:357:PL9:H252	1.77	0.66
2:B:380:ASP:OD1	2:B:390:TYR:HB2	1.95	0.66
13:O:140:THR:CG2	13:O:201:VAL:HB	2.24	0.66
1:A:255:PHE:HD2	1:A:264:SER:HA	1.60	0.66
3:C:37:ALA:HA	23:C:483:CLA:O1A	1.95	0.66
13:O:164:LEU:CD2	15:U:42:VAL:HG13	2.25	0.66
1:A:222:SER:O	1:A:246:TYR:HB2	1.96	0.66
13:O:102:ASP:OD2	13:O:119:LEU:HD11	1.96	0.66
2:B:58:GLN:O	2:B:329:PRO:CB	2.43	0.66
3:C:450:ALA:HB1	3:C:455:PHE:O	1.96	0.66
16:V:78:ASN:HB2	16:V:96:ARG:HH11	1.60	0.66
15:U:39:LEU:O	15:U:41:ASN:N	2.28	0.66
5:E:12:ILE:HD13	25:E:84:HEM:O1A	1.95	0.66
2:B:58:GLN:O	2:B:329:PRO:HB2	1.94	0.66
3:C:269:GLU:CD	3:C:447:ARG:HG2	2.16	0.66
2:B:6:TYR:OH	23:B:520:CLA:HMD3	1.96	0.66
15:U:88:VAL:HG22	15:U:114:VAL:HG23	1.78	0.66
3:C:443:TRP:HE3	3:C:443:TRP:HA	1.61	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:Z:7:LEU:O	19:Z:11:ALA:HB2	1.95	0.66
5:E:19:TRP:CZ2	9:J:13:VAL:HG22	2.30	0.66
13:O:118:LEU:HD13	13:O:233:VAL:HG11	1.78	0.66
4:D:189:HIS:ND1	4:D:294:ARG:NE	2.43	0.66
3:C:208:VAL:HG13	3:C:209:ILE:N	2.10	0.65
2:B:92:SER:O	2:B:96:VAL:HG23	1.96	0.65
3:C:380:ILE:HG22	3:C:381:LYS:N	2.10	0.65
8:I:18:LEU:N	8:I:18:LEU:HD23	2.10	0.65
1:A:119:PHE:O	1:A:123:ALA:HB2	1.96	0.65
4:D:14:TRP:HA	4:D:17:ILE:HD12	1.78	0.65
13:O:224:ASP:C	13:O:225:MET:HG2	2.16	0.65
1:A:29:TYR:CE1	1:A:31:GLY:N	2.63	0.65
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.30	0.65
3:C:320:ARG:HH12	16:V:50:PRO:CD	2.10	0.65
13:O:158:ASP:HB2	13:O:159:PRO:HD2	1.78	0.65
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.27	0.65
3:C:108:THR:HG23	10:K:2:LEU:HD23	1.79	0.65
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.31	0.65
2:B:84:THR:O	2:B:84:THR:HG22	1.95	0.65
4:D:210:LEU:HD13	4:D:271:MET:HG2	1.79	0.65
7:H:27:THR:N	7:H:28:PRO:HD2	2.10	0.65
13:O:27:ARG:HG3	13:O:29:ALA:HB3	1.77	0.65
15:U:72:TYR:HD2	15:U:73:PRO:N	1.93	0.65
3:C:249:ILE:HA	3:C:252:ILE:HD12	1.78	0.65
1:A:29:TYR:HE1	1:A:31:GLY:N	1.95	0.65
13:O:128:SER:O	13:O:142:PHE:HA	1.96	0.65
3:C:285:ILE:HG23	23:C:487:CLA:HMB1	1.78	0.65
2:B:414:PRO:CG	2:B:415:PRO:HD3	2.26	0.65
8:I:17:LEU:O	8:I:21:PHE:HB2	1.96	0.65
4:D:28:VAL:HB	6:F:17:VAL:HG13	1.79	0.65
2:B:280:PHE:CZ	2:B:312:TYR:HB3	2.32	0.65
3:C:61:VAL:HG22	23:C:480:CLA:CAC	2.25	0.65
10:K:25:ALA:HB1	28:K:50:BCR:C19	2.27	0.65
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.79	0.65
1:A:221:SER:HB3	4:D:138:VAL:HG12	1.78	0.65
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.11	0.65
13:O:152:ARG:NH1	13:O:156:PHE:CZ	2.65	0.65
1:A:97:TRP:HZ3	8:I:8:VAL:HG21	1.62	0.65
2:B:238:LEU:O	2:B:242:ILE:HG13	1.97	0.64
23:B:520:CLA:H161	12:M:17:VAL:HG11	1.79	0.64
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.78	0.64
7:H:49:ASN:OD1	7:H:49:ASN:O	2.15	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:293:ASN:OD1	3:C:297:TYR:O	2.15	0.64
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.78	0.64
1:A:183:MET:HE2	23:A:349:CLA:HMD3	1.79	0.64
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.79	0.64
4:D:52:THR:HG22	4:D:67:TYR:CE1	2.26	0.64
9:J:15:THR:HA	28:K:50:BCR:C37	2.27	0.64
15:U:132:LEU:N	15:U:132:LEU:CD2	2.57	0.64
6:F:40:GLN:NE2	9:J:27:LEU:CG	2.46	0.64
23:B:513:CLA:H91	23:B:516:CLA:HAA1	1.77	0.64
23:B:520:CLA:H161	12:M:17:VAL:CG1	2.27	0.64
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.29	0.64
1:A:285:PHE:O	1:A:288:LEU:HB2	1.97	0.64
13:O:20:PRO:HB2	13:O:240:TYR:CE1	2.33	0.64
10:K:9:PHE:O	10:K:13:VAL:HG23	1.96	0.64
1:A:221:SER:HB3	4:D:138:VAL:CG1	2.27	0.64
11:L:2:GLU:N	11:L:3:PRO:CD	2.61	0.64
13:O:66:VAL:HG13	13:O:67:PRO:HD2	1.80	0.64
6:F:25:LEU:O	6:F:28:PRO:HD2	1.98	0.64
4:D:57:SER:OG	4:D:65:SER:HB2	1.98	0.64
3:C:42:LEU:HG	23:C:486:CLA:CED	2.24	0.64
2:B:478:VAL:HG12	4:D:139:ARG:HG2	1.80	0.64
3:C:319:ILE:CD1	3:C:389:GLU:HG2	2.28	0.64
5:E:59:GLN:HE21	5:E:81:GLN:NE2	1.96	0.64
2:B:138:MET:CG	23:B:522:CLA:HBC2	2.20	0.64
2:B:130:GLU:HG2	2:B:131:PRO:CD	2.26	0.64
2:B:271:THR:OG1	2:B:274:GLN:HG3	1.97	0.64
15:U:39:LEU:C	15:U:41:ASN:H	2.01	0.64
1:A:310:LYS:HB3	1:A:312:ASN:ND2	2.13	0.64
10:K:2:LEU:N	10:K:3:PRO:CD	2.60	0.64
3:C:162:GLY:O	3:C:165:LEU:HB2	1.95	0.64
2:B:73:GLY:O	2:B:92:SER:HB2	1.98	0.64
1:A:159:LEU:HG	1:A:163:ILE:CD1	2.28	0.63
8:I:27:ASP:HB2	8:I:28:PRO:HD3	1.80	0.63
3:C:348:GLU:OE1	3:C:348:GLU:N	2.31	0.63
1:A:281:VAL:HA	1:A:284:TRP:CD1	2.33	0.63
3:C:305:THR:CA	3:C:423:ARG:HH12	2.11	0.63
4:D:263:ASN:O	4:D:265:ARG:N	2.31	0.63
13:O:238:VAL:HG12	13:O:239:PHE:N	2.12	0.63
2:B:221:PRO:HB3	2:B:225:LEU:HB2	1.78	0.63
13:O:39:ARG:CA	13:O:245:PRO:HG3	2.28	0.63
13:O:155:ASN:HD22	15:U:129:ASN:HD21	1.42	0.63
3:C:426:LEU:O	3:C:430:HIS:HB2	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:221:PRO:CG	2:B:225:LEU:HD12	2.29	0.63
2:B:326:ARG:NH1	2:B:327:THR:HB	2.13	0.63
3:C:78:GLU:H	3:C:104:GLU:CD	2.01	0.63
1:A:29:TYR:HD2	1:A:133:LEU:HD12	1.63	0.63
4:D:39:PRO:O	4:D:43:LEU:HG	1.99	0.63
1:A:206:PHE:HE1	23:A:348:CLA:CMB	2.11	0.63
3:C:160:ILE:O	3:C:163:PHE:HB2	1.98	0.63
1:A:63:ILE:HG23	3:C:335:THR:CG2	2.28	0.63
8:I:19:PHE:CZ	8:I:23:PHE:HE1	2.16	0.63
19:Z:46:LEU:O	19:Z:50:LEU:HG	1.99	0.63
3:C:321:ASP:OD1	3:C:321:ASP:N	2.31	0.63
16:V:75:TYR:HE2	16:V:80:THR:N	1.95	0.63
4:D:52:THR:HG23	4:D:76:VAL:HG12	1.81	0.63
4:D:222:LEU:HA	4:D:243:THR:O	1.98	0.63
4:D:253:TRP:HA	4:D:253:TRP:CE3	2.33	0.63
8:I:25:SER:HB2	8:I:28:PRO:HD2	1.80	0.63
2:B:327:THR:OG1	28:B:529:BCR:H401	1.99	0.63
15:U:113:THR:HG22	15:U:114:VAL:N	2.13	0.63
1:A:59:ASP:OD2	1:A:63:ILE:O	2.17	0.63
4:D:42:TYR:CZ	6:F:24:THR:HG23	2.33	0.63
4:D:298:PHE:CA	11:L:37:ASN:ND2	2.54	0.62
3:C:119:LEU:O	3:C:122:SER:OG	2.17	0.62
12:M:8:LEU:HD22	14:T:1:MET:CE	2.29	0.62
5:E:12:ILE:HD11	25:E:84:HEM:O1A	1.99	0.62
16:V:102:PRO:HA	16:V:105:ARG:HG3	1.81	0.62
28:C:489:BCR:H312	19:Z:55:GLY:HA2	1.81	0.62
3:C:120:ILE:HG21	28:C:489:BCR:H353	1.81	0.62
1:A:322:ASN:OD1	3:C:412:THR:HG23	1.99	0.62
3:C:370:ARG:HD3	3:C:375:LEU:CD2	2.29	0.62
1:A:261:GLN:HG3	1:A:262:TYR:N	2.13	0.62
1:A:161:TYR:CE1	1:A:186:PHE:HE1	2.17	0.62
23:A:350:CLA:HED1	4:D:175:VAL:CG1	2.29	0.62
2:B:106:LEU:HD22	23:B:522:CLA:H143	1.80	0.62
2:B:234:ILE:O	2:B:236:THR:N	2.32	0.62
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.67	0.62
4:D:56:THR:HG23	4:D:56:THR:O	1.98	0.62
2:B:225:LEU:HD13	2:B:231:MET:SD	2.38	0.62
23:B:520:CLA:HAA2	23:B:520:CLA:HBD	1.81	0.62
3:C:70:PHE:O	3:C:73:ALA:HB3	1.99	0.62
1:A:180:PHE:HE2	4:D:192:THR:O	1.82	0.62
1:A:239:PHE:HE1	4:D:245:SER:HA	1.61	0.62
10:K:15:VAL:HG21	18:N:9:UNK:O	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:309:ALA:HB1	16:V:1:ALA:O	2.00	0.62
19:Z:37:LYS:O	19:Z:41:PHE:CD1	2.52	0.62
13:O:162:ARG:O	13:O:162:ARG:CG	2.48	0.62
2:B:323:GLY:HA2	4:D:293:LEU:HG	1.81	0.62
3:C:320:ARG:NH1	16:V:49:ASN:HA	2.15	0.62
4:D:186:GLN:HA	4:D:186:GLN:NE2	2.14	0.62
10:K:10:ASP:HB3	10:K:11:PRO:HD3	1.81	0.62
13:O:168:TYR:CD1	13:O:172:ILE:HD11	2.35	0.62
3:C:216:SER:O	3:C:221:GLU:O	2.18	0.62
5:E:12:ILE:HD13	25:E:84:HEM:CGA	2.30	0.62
1:A:180:PHE:HD1	1:A:180:PHE:H	1.47	0.62
15:U:57:LEU:CD2	15:U:112:PHE:HD2	1.95	0.62
13:O:11:VAL:O	13:O:11:VAL:HG12	2.00	0.62
2:B:69:LEU:HD12	23:B:518:CLA:HBA2	1.82	0.62
2:B:29:LEU:HB3	28:B:528:BCR:H351	1.82	0.62
28:B:528:BCR:H331	28:B:528:BCR:HC8	1.82	0.62
16:V:129:LYS:CE	16:V:135:VAL:HG23	2.30	0.62
3:C:120:ILE:CG2	28:C:489:BCR:H353	2.30	0.62
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.81	0.62
5:E:56:ALA:O	5:E:57:GLN:C	2.37	0.62
4:D:180:ARG:C	4:D:180:ARG:HD3	2.21	0.62
23:B:524:CLA:H13	23:B:524:CLA:OBD	2.00	0.61
5:E:9:PHE:O	5:E:10:SER:CB	2.47	0.61
19:Z:44:SER:O	19:Z:48:ILE:HG22	2.00	0.61
1:A:237:TYR:CE2	1:A:245:THR:HA	2.35	0.61
7:H:53:ILE:HG23	17:X:13:THR:HG1	1.65	0.61
3:C:103:GLY:O	3:C:104:GLU:C	2.39	0.61
3:C:38:GLY:HA2	3:C:41:ARG:HE	1.64	0.61
3:C:405:ASN:HB2	3:C:407:VAL:CG2	2.30	0.61
13:O:53:LYS:HE2	13:O:234:LYS:HB2	1.82	0.61
4:D:91:LEU:HD23	4:D:91:LEU:N	2.14	0.61
3:C:225:VAL:HB	23:C:487:CLA:HMC3	1.81	0.61
28:C:489:BCR:H341	19:Z:51:VAL:HG13	1.82	0.61
1:A:89:ILE:HD12	1:A:108:ASN:HB3	1.83	0.61
13:O:50:PHE:HZ	13:O:76:THR:CG2	2.13	0.61
5:E:12:ILE:CG1	25:E:84:HEM:O2D	2.47	0.61
15:U:59:ASN:H	15:U:59:ASN:ND2	1.80	0.61
13:O:102:ASP:O	13:O:103:PHE:CD1	2.53	0.61
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.31	0.61
13:O:163:GLY:CA	13:O:188:LYS:HE2	2.30	0.61
4:D:108:GLY:C	4:D:110:LEU:H	2.02	0.61
14:T:4:ILE:HG13	14:T:5:THR:N	2.15	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:LEU:CD1	1:A:118:HIS:CE1	2.84	0.61
2:B:135:LEU:HD23	2:B:138:MET:SD	2.40	0.61
3:C:285:ILE:HG12	23:C:487:CLA:HMB2	1.82	0.61
28:C:489:BCR:C34	19:Z:51:VAL:HG13	2.31	0.61
13:O:94:THR:HA	13:O:127:ALA:O	2.01	0.61
13:O:40:ILE:CG2	13:O:41:ALA:H	2.14	0.61
3:C:282:MET:HA	3:C:285:ILE:HB	1.83	0.61
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.81	0.61
3:C:265:ILE:HG22	3:C:266:TRP:H	1.66	0.61
1:A:296:ASN:OD1	3:C:401:LEU:HD23	2.00	0.61
2:B:271:THR:HG22	2:B:448:ARG:NH1	2.15	0.61
1:A:301:ASN:CG	3:C:407:VAL:HG21	2.19	0.61
15:U:82:ASN:O	15:U:85:TYR:HE2	1.84	0.61
15:U:127:ARG:O	15:U:128:TYR:HD1	1.82	0.61
1:A:149:ALA:HA	1:A:284:TRP:CZ3	2.36	0.61
4:D:157:PHE:O	4:D:158:LEU:HD23	2.00	0.61
4:D:171:PRO:HG3	4:D:181:PHE:CE1	2.36	0.61
3:C:227:VAL:HG23	3:C:227:VAL:O	2.00	0.61
3:C:36:TRP:O	3:C:38:GLY:N	2.31	0.61
4:D:22:LEU:HD21	4:D:32:TRP:CE3	2.35	0.61
13:O:92:SER:HB2	13:O:129:THR:O	2.01	0.61
13:O:137:THR:O	13:O:140:THR:HG23	2.01	0.61
25:E:84:HEM:C4A	6:F:19:TRP:HH2	2.18	0.61
3:C:39:ASN:HA	3:C:42:LEU:HD12	1.82	0.61
1:A:224:ILE:HG21	1:A:227:THR:OG1	2.01	0.61
1:A:306:VAL:CG2	1:A:307:ILE:H	2.13	0.61
3:C:333:GLY:O	3:C:335:THR:N	2.34	0.61
4:D:18:LEU:HA	17:X:41:SER:OG	2.01	0.61
13:O:112:GLY:C	13:O:114:GLU:H	2.03	0.61
16:V:75:TYR:HE1	25:V:138:HEM:C2A	2.19	0.60
1:A:180:PHE:CD2	4:D:192:THR:HB	2.37	0.60
3:C:272:LEU:O	3:C:276:LEU:HB2	2.00	0.60
4:D:83:ASN:O	4:D:83:ASN:ND2	2.34	0.60
1:A:322:ASN:O	1:A:326:LEU:HB2	2.00	0.60
13:O:95:PHE:HB2	13:O:127:ALA:HB3	1.81	0.60
13:O:28:GLY:HA3	13:O:137:THR:CG2	2.30	0.60
1:A:187:GLN:HG3	1:A:193:LEU:HG	1.83	0.60
2:B:57:ARG:CG	2:B:57:ARG:NH1	2.64	0.60
2:B:98:LEU:O	2:B:102:VAL:HG23	2.01	0.60
3:C:433:LEU:O	3:C:437:PHE:HB2	2.02	0.60
23:C:486:CLA:H61	28:C:488:BCR:H393	1.83	0.60
2:B:321:LYS:HE3	2:B:325:PHE:HZ	1.66	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:PRO:HG2	4:D:211:CYS:HB3	1.81	0.60
2:B:7:ARG:HA	23:B:523:CLA:O1A	2.01	0.60
10:K:6:TYR:O	10:K:8:ILE:N	2.34	0.60
4:D:253:TRP:HE3	4:D:253:TRP:HA	1.67	0.60
4:D:77:ALA:CB	4:D:174:GLY:HA3	2.31	0.60
3:C:95:LEU:HD21	23:C:479:CLA:OBD	2.01	0.60
3:C:275:SER:CB	23:C:485:CLA:HAA1	2.30	0.60
1:A:223:LEU:HD22	1:A:245:THR:CG2	2.30	0.60
4:D:138:VAL:CG1	4:D:139:ARG:N	2.65	0.60
11:L:23:LEU:O	11:L:27:LEU:HB2	2.01	0.60
4:D:196:PHE:HD1	4:D:285:GLY:HA2	1.66	0.60
2:B:399:VAL:HG23	2:B:417:VAL:HG13	1.83	0.60
4:D:188:PHE:CD1	4:D:188:PHE:N	2.69	0.60
2:B:123:PHE:CG	2:B:123:PHE:O	2.54	0.60
2:B:229:LEU:O	2:B:230:ARG:C	2.40	0.60
2:B:142:HIS:ND1	23:B:524:CLA:H142	2.16	0.60
3:C:95:LEU:HA	3:C:185:LEU:HD12	1.84	0.60
3:C:78:GLU:HA	3:C:78:GLU:OE1	2.01	0.60
23:C:486:CLA:H42	10:K:30:TRP:NE1	2.17	0.60
7:H:30:MET:O	7:H:33:PHE:N	2.35	0.60
13:O:95:PHE:HB3	13:O:127:ALA:CB	2.31	0.60
1:A:261:GLN:HG3	1:A:262:TYR:H	1.66	0.60
23:C:474:CLA:H8	23:C:477:CLA:H143	1.84	0.60
13:O:88:ASN:ND2	13:O:92:SER:OG	2.34	0.60
1:A:321:ILE:O	1:A:325:ASN:ND2	2.34	0.60
2:B:191:ASN:HB2	2:B:192:PRO:HD2	1.83	0.60
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.83	0.60
1:A:104:GLU:OE2	13:O:73:ARG:HD3	2.02	0.60
2:B:372:ASP:OD2	2:B:376:VAL:HG23	2.02	0.60
16:V:38:ALA:O	16:V:42:VAL:HG23	2.01	0.60
3:C:297:TYR:CD2	3:C:302:TYR:HE1	2.19	0.60
2:B:321:LYS:CE	2:B:325:PHE:CZ	2.84	0.60
11:L:8:GLN:N	11:L:9:PRO:HD3	2.17	0.60
4:D:261:PHE:HD1	4:D:266:TRP:CD1	2.19	0.60
17:X:12:ILE:HG22	17:X:16:LEU:HD13	1.82	0.60
5:E:12:ILE:HG23	5:E:18:TYR:HB2	1.70	0.60
4:D:58:TRP:HA	4:D:62:GLY:H	1.67	0.60
11:L:1:MET:C	11:L:3:PRO:HD2	2.23	0.60
11:L:36:PHE:O	12:M:3:VAL:HG23	2.01	0.60
7:H:28:PRO:O	7:H:32:VAL:HG23	2.02	0.60
5:E:59:GLN:HE21	5:E:81:GLN:HE22	1.50	0.60
2:B:355:PHE:CE1	2:B:373:LYS:HB3	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:240:ILE:HG22	3:C:244:CYS:SG	2.42	0.59
16:V:118:HIS:CD2	16:V:122:GLU:OE1	2.55	0.59
3:C:62:PHE:CZ	10:K:19:ILE:CD1	2.81	0.59
5:E:26:ILE:HG12	5:E:27:PRO:HD3	1.84	0.59
1:A:57:PRO:HG2	13:O:115:ARG:HH11	1.67	0.59
1:A:281:VAL:CG1	1:A:281:VAL:O	2.50	0.59
2:B:235:GLU:HB3	2:B:473:THR:OG1	2.02	0.59
2:B:190:PHE:CE1	23:B:527:CLA:HED3	2.38	0.59
13:O:27:ARG:C	13:O:29:ALA:H	2.04	0.59
3:C:349:ILE:C	3:C:350:ILE:HG13	2.22	0.59
10:K:6:TYR:O	10:K:7:ALA:C	2.41	0.59
13:O:194:LYS:HG3	13:O:194:LYS:O	2.01	0.59
4:D:101:PHE:CE2	4:D:105:CYS:SG	2.95	0.59
3:C:169:GLY:O	3:C:173:LEU:HG	2.02	0.59
6:F:40:GLN:HE22	9:J:27:LEU:HG	1.58	0.59
1:A:281:VAL:HG22	1:A:284:TRP:HD1	1.67	0.59
23:C:486:CLA:H172	19:Z:23:VAL:HG21	1.84	0.59
2:B:171:PRO:CG	7:H:62:LYS:HA	2.33	0.59
3:C:299:SER:HB2	3:C:303:GLY:O	2.02	0.59
16:V:69:ILE:O	16:V:73:VAL:HG23	2.01	0.59
2:B:12:LEU:HD11	2:B:18:ARG:C	2.23	0.59
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.84	0.59
13:O:233:VAL:HG12	13:O:234:LYS:N	2.17	0.59
3:C:141:GLU:HB2	3:C:144:SER:CB	2.32	0.59
2:B:380:ASP:OD1	2:B:390:TYR:CB	2.50	0.59
16:V:117:GLY:O	16:V:121:VAL:HG23	2.03	0.59
4:D:66:SER:HA	4:D:76:VAL:HG13	1.85	0.59
3:C:223:TRP:CD1	3:C:224:ILE:N	2.71	0.59
16:V:55:ARG:HG3	16:V:56:THR:N	2.16	0.59
2:B:174:LEU:HG	2:B:174:LEU:O	2.01	0.59
2:B:302:TRP:O	2:B:305:ILE:HG12	2.02	0.59
19:Z:47:TRP:CD1	19:Z:47:TRP:C	2.76	0.59
2:B:321:LYS:HE2	2:B:325:PHE:CZ	2.37	0.59
13:O:164:LEU:O	13:O:165:ALA:CB	2.51	0.59
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.37	0.59
4:D:235:PHE:CG	4:D:236:ASN:N	2.70	0.59
3:C:374:GLY:HA2	13:O:7:TYR:HE1	1.65	0.59
7:H:53:ILE:HG22	17:X:15:SER:HB2	1.85	0.59
1:A:265:PHE:HB2	1:A:271:LEU:HD21	1.85	0.59
15:U:32:THR:O	15:U:36:GLU:HG3	2.03	0.59
2:B:225:LEU:O	2:B:231:MET:HG2	2.03	0.59
3:C:284:PHE:HD1	3:C:434:ALA:HB1	1.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:437:PHE:HA	23:C:483:CLA:HMC3	1.84	0.59
10:K:15:VAL:HG12	10:K:15:VAL:O	2.02	0.59
2:B:301:ALA:O	2:B:304:ALA:HB3	2.02	0.59
3:C:429:SER:O	3:C:432:VAL:HB	2.03	0.59
3:C:239:TRP:O	3:C:243:ILE:HG13	2.03	0.58
5:E:30:PHE:HD2	5:E:30:PHE:O	1.84	0.58
2:B:136:PRO:HD3	2:B:231:MET:CE	2.32	0.58
2:B:46:ASP:HB3	2:B:58:GLN:OE1	2.03	0.58
4:D:88:SER:OG	5:E:68:ARG:NE	2.36	0.58
2:B:340:TRP:CD1	2:B:340:TRP:N	2.71	0.58
2:B:171:PRO:HG3	7:H:62:LYS:HA	1.86	0.58
2:B:223:GLN:HG3	2:B:227:LYS:HE3	1.85	0.58
4:D:27:PHE:HB3	6:F:17:VAL:HG11	1.84	0.58
2:B:234:ILE:HG21	23:B:513:CLA:HAC1	1.85	0.58
3:C:62:PHE:CE1	3:C:119:LEU:HD11	2.39	0.58
1:A:307:ILE:HG13	1:A:314:ILE:CD1	2.30	0.58
13:O:156:PHE:O	13:O:188:LYS:NZ	2.36	0.58
1:A:29:TYR:CD2	1:A:133:LEU:HD12	2.37	0.58
13:O:221:SER:OG	13:O:231:HIS:N	2.36	0.58
8:I:19:PHE:CE1	8:I:23:PHE:HE1	2.21	0.58
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.31	0.58
1:A:210:LEU:HD13	24:D:355:PHO:ND	2.18	0.58
3:C:77:PRO:O	3:C:78:GLU:HB2	2.03	0.58
3:C:266:TRP:HA	3:C:271:TYR:HE2	1.68	0.58
4:D:32:TRP:N	4:D:131:GLU:OE2	2.35	0.58
3:C:373:ASN:OD1	13:O:16:ALA:HA	2.03	0.58
16:V:63:THR:HB	16:V:83:ASP:O	2.03	0.58
3:C:293:ASN:OD1	3:C:423:ARG:NH2	2.37	0.58
3:C:71:GLU:HB3	3:C:89:ILE:HD11	1.85	0.58
4:D:29:PHE:HE2	4:D:31:GLY:CA	2.16	0.58
4:D:267:LEU:O	4:D:271:MET:HE2	2.03	0.58
1:A:98:GLU:HG3	1:A:98:GLU:O	2.02	0.58
13:O:215:PHE:O	13:O:216:GLU:HB2	2.02	0.58
28:B:529:BCR:H311	28:B:529:BCR:H342	1.86	0.58
3:C:271:TYR:HA	3:C:274:TYR:CE1	2.39	0.58
3:C:113:VAL:O	3:C:117:VAL:HG23	2.03	0.58
13:O:215:PHE:HB3	13:O:237:GLY:H	1.69	0.58
13:O:40:ILE:HG23	13:O:84:GLU:OE2	2.04	0.58
2:B:150:CYS:HB2	23:B:517:CLA:HMC3	1.84	0.58
4:D:35:ILE:O	4:D:39:PRO:HD2	2.03	0.58
3:C:63:TRP:CE2	3:C:67:MET:HG3	2.39	0.58
23:C:477:CLA:H142	23:C:477:CLA:H101	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:ARG:HH11	4:D:320:LEU:CD1	2.13	0.58
17:X:34:PHE:O	17:X:38:ILE:HG13	2.04	0.58
16:V:75:TYR:CE2	16:V:79:PRO:HA	2.39	0.58
13:O:39:ARG:HA	13:O:245:PRO:HG3	1.85	0.58
3:C:243:ILE:O	23:C:474:CLA:HMC1	2.03	0.58
14:T:3:THR:O	14:T:6:TYR:N	2.33	0.58
23:B:521:CLA:CAB	23:B:527:CLA:HED1	2.27	0.58
3:C:63:TRP:CZ2	3:C:67:MET:HG3	2.39	0.58
3:C:123:ALA:HB1	19:Z:47:TRP:CH2	2.37	0.58
1:A:14:TRP:HH2	8:I:25:SER:HB3	1.68	0.58
4:D:28:VAL:H	6:F:17:VAL:HG11	1.69	0.57
1:A:78:ILE:O	1:A:177:SER:HB2	2.03	0.57
23:B:520:CLA:HAA2	23:B:520:CLA:CBD	2.33	0.57
11:L:27:LEU:HD23	12:M:14:PHE:CE2	2.39	0.57
13:O:53:LYS:HG2	13:O:65:PHE:CD2	2.39	0.57
16:V:76:MET:O	16:V:94:SER:HA	2.04	0.57
3:C:188:THR:O	3:C:188:THR:HG22	2.03	0.57
1:A:228:THR:HG22	1:A:228:THR:O	2.04	0.57
3:C:344:SER:O	3:C:347:GLY:N	2.32	0.57
13:O:215:PHE:HB3	13:O:237:GLY:N	2.19	0.57
16:V:38:ALA:O	16:V:42:VAL:CG2	2.52	0.57
23:B:518:CLA:H142	23:B:524:CLA:HBA1	1.86	0.57
3:C:286:ALA:O	3:C:289:PHE:HB3	2.03	0.57
3:C:305:THR:O	3:C:308:GLU:HB2	2.04	0.57
3:C:94:THR:C	3:C:96:GLY:H	2.07	0.57
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.39	0.57
10:K:11:PRO:HB3	18:N:9:UNK:CB	2.34	0.57
8:I:5:LYS:O	8:I:9:TYR:HD1	1.86	0.57
13:O:200:ASN:O	13:O:213:GLY:HA3	2.04	0.57
3:C:436:PHE:O	3:C:439:VAL:HB	2.04	0.57
6:F:14:ILE:HG13	6:F:14:ILE:O	2.03	0.57
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.19	0.57
1:A:89:ILE:HD13	1:A:94:TYR:CG	2.39	0.57
1:A:218:LEU:CD2	4:D:142:ASN:HD22	2.16	0.57
1:A:286:THR:CG2	23:A:348:CLA:O1D	2.50	0.57
1:A:141:PRO:HG3	3:C:446:GLY:C	2.24	0.57
10:K:24:LEU:O	10:K:27:ALA:HB3	2.04	0.57
3:C:318:LEU:HD22	3:C:328:VAL:HG21	1.87	0.57
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.86	0.57
12:M:8:LEU:HD22	14:T:1:MET:HE3	1.85	0.57
19:Z:12:LEU:HD12	19:Z:12:LEU:O	2.04	0.57
1:A:161:TYR:CE2	1:A:165:GLN:HG3	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:ALA:HB1	26:A:353:PL9:H151	1.86	0.57
1:A:69:GLY:O	1:A:81:ALA:HA	2.04	0.57
3:C:291:TRP:HB3	3:C:292:PHE:CE2	2.39	0.57
1:A:142:TRP:CD1	3:C:443:TRP:CH2	2.92	0.57
1:A:341:LEU:HD21	15:U:134:LYS:NZ	2.19	0.57
2:B:192:PRO:HG3	7:H:48:TYR:CE1	2.40	0.57
1:A:15:GLU:O	1:A:19:ASN:ND2	2.38	0.57
4:D:72:ASN:OD1	4:D:74:LEU:HB2	2.03	0.57
14:T:9:ILE:HG22	14:T:9:ILE:O	2.05	0.57
15:U:75:LEU:HD21	15:U:101:GLN:HE21	1.69	0.57
1:A:142:TRP:HB2	4:D:220:ASN:HB2	1.86	0.57
3:C:155:ASN:HB3	3:C:255:THR:OG1	2.05	0.57
4:D:261:PHE:CD1	4:D:266:TRP:CD1	2.93	0.57
14:T:24:ARG:HG2	14:T:25:GLU:N	2.19	0.57
4:D:68:LEU:N	6:F:39:MET:HE1	2.20	0.57
2:B:45:PHE:CE2	2:B:78:TRP:CZ2	2.92	0.57
23:B:524:CLA:O1A	23:B:524:CLA:H2	2.04	0.57
4:D:122:LEU:HD21	23:D:354:CLA:C9	2.35	0.57
2:B:479:PHE:C	2:B:479:PHE:HD2	2.07	0.57
1:A:143:ILE:HD13	4:D:253:TRP:CH2	2.40	0.57
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.03	0.57
1:A:316:THR:O	1:A:318:ALA:N	2.37	0.57
2:B:250:PHE:CD1	2:B:459:ALA:HB1	2.40	0.57
2:B:247:PHE:CE1	23:B:521:CLA:H72	2.40	0.57
4:D:168:PHE:HD2	4:D:168:PHE:C	2.08	0.57
2:B:479:PHE:C	2:B:479:PHE:CD2	2.78	0.57
2:B:414:PRO:N	2:B:415:PRO:CD	2.67	0.57
4:D:110:LEU:O	4:D:113:PHE:HB3	2.05	0.57
3:C:284:PHE:O	3:C:285:ILE:C	2.42	0.57
3:C:292:PHE:HE1	23:C:487:CLA:HBC3	1.69	0.57
3:C:42:LEU:CD2	23:C:486:CLA:HED1	2.35	0.57
16:V:22:THR:H	16:V:25:GLN:NE2	2.03	0.57
13:O:78:LEU:O	13:O:79:ASP:OD1	2.23	0.57
3:C:282:MET:CA	3:C:285:ILE:HG13	2.32	0.57
1:A:335:ASN:HD22	1:A:335:ASN:C	2.08	0.57
2:B:414:PRO:N	2:B:415:PRO:HD3	2.20	0.57
13:O:102:ASP:O	13:O:103:PHE:HD1	1.85	0.57
4:D:52:THR:O	4:D:67:TYR:HD1	1.88	0.57
4:D:86:GLY:C	4:D:87:HIS:CD2	2.78	0.57
13:O:39:ARG:HA	13:O:245:PRO:CB	2.35	0.57
3:C:155:ASN:OD1	3:C:156:LYS:HG2	2.04	0.57
4:D:29:PHE:C	4:D:29:PHE:HD2	2.08	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:10:THR:O	2:B:13:ILE:HG22	2.04	0.57
15:U:40:VAL:HG12	15:U:40:VAL:O	2.05	0.57
3:C:314:ALA:HB3	3:C:351:PHE:CD1	2.40	0.56
3:C:417:VAL:HG21	16:V:42:VAL:HG22	1.86	0.56
3:C:326:ALA:CB	15:U:127:ARG:HD2	2.31	0.56
2:B:414:PRO:O	2:B:418:LYS:HG3	2.04	0.56
1:A:29:TYR:CD1	1:A:30:VAL:N	2.69	0.56
3:C:412:THR:HG22	16:V:136:TYR:HE2	1.69	0.56
13:O:53:LYS:CE	13:O:234:LYS:HB2	2.35	0.56
3:C:141:GLU:CB	3:C:144:SER:OG	2.53	0.56
13:O:66:VAL:CG1	13:O:67:PRO:HD2	2.35	0.56
17:X:12:ILE:HA	17:X:16:LEU:HD12	1.87	0.56
1:A:114:LEU:HD11	1:A:118:HIS:CE1	2.39	0.56
1:A:214:MET:HE3	1:A:214:MET:HA	1.83	0.56
1:A:52:PHE:CE1	1:A:81:ALA:HB2	2.40	0.56
23:B:512:CLA:H203	23:B:523:CLA:H192	1.87	0.56
4:D:186:GLN:HE21	4:D:186:GLN:HA	1.69	0.56
1:A:237:TYR:CD1	1:A:237:TYR:N	2.73	0.56
4:D:138:VAL:CG1	4:D:139:ARG:H	2.17	0.56
4:D:329:MET:O	4:D:329:MET:HG2	2.05	0.56
2:B:348:ASN:CG	2:B:349:LYS:H	2.07	0.56
3:C:324:LEU:HD21	15:U:72:TYR:OH	2.05	0.56
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.87	0.56
2:B:458:PHE:CE1	23:B:516:CLA:HBB1	2.41	0.56
3:C:88:LEU:O	3:C:91:HIS:HB2	2.05	0.56
23:C:476:CLA:H12	23:C:483:CLA:H2	1.86	0.56
11:L:7:ARG:O	11:L:9:PRO:HD3	2.05	0.56
4:D:261:PHE:HA	14:T:24:ARG:NH2	2.20	0.56
23:B:511:CLA:HMD1	7:H:26:THR:HB	1.86	0.56
3:C:229:ASN:OD1	3:C:231:GLU:HG3	2.05	0.56
7:H:53:ILE:HG23	7:H:53:ILE:O	2.04	0.56
13:O:149:PRO:HA	13:O:192:LEU:HD12	1.86	0.56
13:O:43:LEU:HD12	13:O:241:ALA:HB2	1.87	0.56
3:C:281:MET:O	3:C:284:PHE:HB2	2.05	0.56
4:D:231:THR:HG22	4:D:232:PHE:N	2.20	0.56
1:A:110:GLY:O	1:A:111:PRO:C	2.43	0.56
3:C:284:PHE:CD1	3:C:434:ALA:HB1	2.41	0.56
16:V:129:LYS:NZ	16:V:135:VAL:CG2	2.69	0.56
1:A:133:LEU:HD23	4:D:252:PHE:CD1	2.41	0.56
14:T:24:ARG:HG2	14:T:25:GLU:H	1.70	0.56
2:B:372:ASP:OD2	2:B:374:ASN:HB2	2.03	0.56
1:A:195:HIS:O	1:A:199:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:350:ILE:CG2	3:C:359:TRP:HB3	2.35	0.56
1:A:114:LEU:CD1	1:A:118:HIS:HE1	2.19	0.56
4:D:87:HIS:CD2	4:D:166:SER:HA	2.41	0.56
1:A:330:VAL:HG13	4:D:348:ARG:HG3	1.87	0.56
11:L:12:LEU:HD11	11:L:16:SER:CB	2.34	0.56
13:O:192:LEU:HD22	15:U:119:THR:HG23	1.88	0.56
2:B:394:GLN:NE2	15:U:52:GLY:HA3	2.21	0.56
3:C:279:LEU:HB3	23:C:481:CLA:CBC	2.35	0.56
2:B:371:THR:HG22	2:B:372:ASP:O	2.05	0.56
16:V:22:THR:H	16:V:25:GLN:HE21	1.52	0.56
1:A:93:PHE:CZ	23:A:352:CLA:HBA1	2.41	0.56
7:H:47:ILE:HG12	7:H:52:LEU:HD23	1.87	0.56
2:B:41:GLU:HG2	2:B:60:MET:SD	2.45	0.56
4:D:32:TRP:HA	4:D:32:TRP:CE3	2.41	0.56
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.36	0.56
1:A:281:VAL:HG22	1:A:284:TRP:CD1	2.41	0.56
3:C:61:VAL:HG11	3:C:121:SER:HB2	1.88	0.56
10:K:16:LEU:HB3	10:K:17:PRO:HD3	1.88	0.56
1:A:205:VAL:HG12	4:D:204:VAL:HG12	1.87	0.56
23:B:519:CLA:H142	23:D:356:CLA:H42	1.88	0.56
4:D:87:HIS:CD2	4:D:87:HIS:N	2.73	0.56
13:O:118:LEU:CD1	13:O:233:VAL:HG21	2.35	0.56
5:E:59:GLN:NE2	5:E:81:GLN:NE2	2.54	0.56
1:A:95:PRO:HD2	1:A:98:GLU:HB3	1.87	0.56
13:O:32:ILE:C	13:O:34:SER:H	2.10	0.56
1:A:316:THR:O	1:A:317:TRP:C	2.43	0.55
4:D:168:PHE:CD2	4:D:168:PHE:C	2.79	0.55
10:K:30:TRP:CZ3	10:K:31:GLN:NE2	2.74	0.55
4:D:257:PHE:CZ	26:D:357:PL9:H253	2.41	0.55
1:A:159:LEU:CG	1:A:163:ILE:HD11	2.36	0.55
3:C:101:PRO:CA	3:C:195:ASP:HB3	2.36	0.55
11:L:2:GLU:N	11:L:3:PRO:HD2	2.21	0.55
4:D:302:GLU:O	4:D:305:ALA:HB3	2.06	0.55
3:C:331:ALA:O	3:C:338:GLY:HA2	2.05	0.55
4:D:118:GLY:CA	24:D:355:PHO:H71	2.37	0.55
1:A:221:SER:CA	4:D:139:ARG:HB2	2.33	0.55
3:C:173:LEU:HA	3:C:176:VAL:HG23	1.88	0.55
1:A:142:TRP:HH2	1:A:273:PHE:HE1	1.54	0.55
3:C:342:MET:HE3	3:C:353:GLY:H	1.70	0.55
1:A:139:MET:HE2	4:D:248:THR:CG2	2.36	0.55
13:O:68:THR:HA	13:O:110:MET:HE1	1.87	0.55
4:D:59:TYR:HE1	5:E:49:PRO:HG2	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:326:ARG:HD3	28:B:529:BCR:C40	2.31	0.55
3:C:285:ILE:HG12	23:C:487:CLA:CMB	2.37	0.55
3:C:294:ASN:O	3:C:296:VAL:N	2.40	0.55
4:D:198:MET:HE1	11:L:30:LEU:CD1	2.30	0.55
2:B:418:LYS:HZ1	15:U:45:GLU:CD	2.10	0.55
16:V:55:ARG:O	16:V:59:LEU:HG	2.07	0.55
23:B:511:CLA:HBC3	7:H:33:PHE:CD2	2.42	0.55
1:A:12:ASN:O	1:A:15:GLU:HG3	2.06	0.55
2:B:12:LEU:HG	2:B:19:LEU:HB2	1.87	0.55
15:U:88:VAL:CG2	15:U:114:VAL:HG23	2.36	0.55
13:O:153:THR:HG22	13:O:154:ALA:N	2.22	0.55
1:A:325:ASN:N	1:A:325:ASN:HD22	2.05	0.55
1:A:297:LEU:HD22	3:C:428:THR:HG21	1.87	0.55
13:O:19:CYS:HB3	13:O:240:TYR:HB2	1.89	0.55
2:B:12:LEU:HD21	2:B:19:LEU:HA	1.88	0.55
2:B:6:TYR:N	2:B:6:TYR:CD2	2.75	0.55
7:H:21:ALA:HB3	7:H:22:PRO:CD	2.37	0.55
1:A:224:ILE:HG22	1:A:224:ILE:O	2.06	0.55
3:C:187:ASP:O	3:C:194:GLY:O	2.25	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.88	0.55
3:C:158:THR:O	3:C:161:LEU:HB3	2.07	0.55
2:B:47:PRO:HA	2:B:78:TRP:HE1	1.72	0.55
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.41	0.55
3:C:98:GLY:O	3:C:105:VAL:HG13	2.07	0.55
3:C:116:VAL:HG13	28:C:488:BCR:C33	2.33	0.55
23:C:478:CLA:C9	23:C:482:CLA:HAA1	2.36	0.55
3:C:447:ARG:O	3:C:447:ARG:HG3	2.06	0.55
1:A:301:ASN:HD21	3:C:407:VAL:HG23	1.71	0.55
13:O:32:ILE:C	13:O:34:SER:N	2.59	0.55
1:A:180:PHE:CD2	4:D:192:THR:CG2	2.90	0.55
15:U:57:LEU:HD11	15:U:112:PHE:HB3	1.89	0.55
23:C:478:CLA:H162	23:C:482:CLA:HMD2	1.89	0.55
1:A:224:ILE:HD11	1:A:243:GLU:HG3	1.89	0.55
4:D:29:PHE:HE2	4:D:31:GLY:HA3	1.72	0.55
2:B:356:VAL:HG23	2:B:370:LEU:HD23	1.89	0.55
2:B:327:THR:C	2:B:329:PRO:HD3	2.27	0.55
12:M:17:VAL:HG12	12:M:18:PRO:N	2.22	0.55
15:U:124:GLY:O	15:U:125:GLY:C	2.46	0.55
2:B:153:PHE:N	23:B:515:CLA:HMC3	2.22	0.55
16:V:66:ARG:HH11	16:V:66:ARG:HG3	1.72	0.55
2:B:231:MET:HE2	2:B:231:MET:O	2.07	0.54
1:A:291:SER:O	1:A:295:PHE:CE1	2.59	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:90:PRO:HB2	3:C:302:TYR:HE2	1.72	0.54
2:B:342:GLY:HA2	2:B:403:GLY:HA3	1.89	0.54
1:A:14:TRP:CH2	8:I:25:SER:HB3	2.42	0.54
13:O:211:ILE:CG2	13:O:212:ALA:N	2.70	0.54
4:D:71:CYS:HB3	4:D:75:THR:CB	2.38	0.54
10:K:19:ILE:HG13	10:K:20:PRO:HD3	1.89	0.54
2:B:302:TRP:CZ3	2:B:343:HIS:HB2	2.43	0.54
3:C:182:PHE:O	3:C:184:GLY:N	2.41	0.54
15:U:51:TYR:O	15:U:53:GLU:N	2.40	0.54
2:B:458:PHE:CD1	23:B:516:CLA:HMC3	2.42	0.54
2:B:6:TYR:OH	12:M:21:PHE:CZ	2.35	0.54
1:A:142:TRP:N	4:D:220:ASN:OD1	2.40	0.54
10:K:9:PHE:O	10:K:10:ASP:C	2.44	0.54
19:Z:17:PHE:O	19:Z:21:ILE:HG13	2.06	0.54
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
1:A:334:ARG:O	1:A:335:ASN:ND2	2.40	0.54
2:B:212:ALA:CB	23:B:511:CLA:HMC3	2.36	0.54
13:O:22:LEU:O	13:O:203:LYS:CD	2.55	0.54
1:A:97:TRP:CE3	8:I:5:LYS:HA	2.43	0.54
16:V:92:HIS:ND1	16:V:93:PRO:HD2	2.22	0.54
2:B:159:THR:O	2:B:159:THR:HG22	2.07	0.54
4:D:30:VAL:HG22	4:D:38:PHE:HE1	1.71	0.54
13:O:140:THR:HG21	13:O:201:VAL:HB	1.88	0.54
13:O:243:ILE:HG22	13:O:244:GLU:N	2.22	0.54
1:A:278:TRP:HE1	23:A:350:CLA:H42	1.73	0.54
2:B:45:PHE:HE1	2:B:55:MET:HA	1.72	0.54
3:C:36:TRP:C	3:C:38:GLY:H	2.10	0.54
4:D:90:LEU:HD13	4:D:96:GLU:HB3	1.87	0.54
1:A:303:ASN:C	1:A:304:HIS:HD1	2.10	0.54
3:C:199:ILE:CD1	3:C:234:VAL:HG21	2.33	0.54
3:C:200:THR:C	3:C:201:ASN:HD22	2.10	0.54
2:B:372:ASP:CG	2:B:373:LYS:N	2.60	0.54
2:B:15:ASP:OD1	2:B:15:ASP:C	2.45	0.54
2:B:321:LYS:HE2	2:B:325:PHE:HZ	1.71	0.54
2:B:225:LEU:C	2:B:231:MET:HG2	2.28	0.54
1:A:180:PHE:HD2	4:D:192:THR:HB	1.72	0.54
3:C:88:LEU:O	3:C:91:HIS:N	2.40	0.54
1:A:302:PHE:N	1:A:302:PHE:CD1	2.75	0.54
1:A:133:LEU:HD21	4:D:252:PHE:HA	1.90	0.54
1:A:63:ILE:HG23	3:C:335:THR:HG21	1.89	0.54
4:D:29:PHE:HD2	4:D:29:PHE:O	1.91	0.54
2:B:371:THR:HG22	2:B:372:ASP:N	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:402:TYR:HD1	2:B:402:TYR:N	2.06	0.54
6:F:19:TRP:CH2	6:F:23:HIS:NE2	2.76	0.54
4:D:52:THR:O	4:D:76:VAL:HG11	2.08	0.54
2:B:110:ALA:O	2:B:113:TRP:N	2.37	0.54
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.43	0.54
4:D:336:HIS:N	4:D:336:HIS:HD2	1.99	0.54
19:Z:37:LYS:O	19:Z:41:PHE:HD1	1.90	0.54
1:A:258:LEU:O	4:D:128:ARG:NH2	2.40	0.54
1:A:89:ILE:CG2	1:A:94:TYR:HB2	2.38	0.54
2:B:183:PRO:HD3	2:B:199:VAL:HG11	1.90	0.54
4:D:182:LEU:HA	23:D:354:CLA:HMD2	1.90	0.54
28:C:489:BCR:C31	19:Z:55:GLY:HA2	2.37	0.54
13:O:193:THR:HG22	13:O:194:LYS:N	2.11	0.54
1:A:243:GLU:HA	4:D:240:ALA:CB	2.34	0.54
4:D:221:THR:O	4:D:221:THR:CG2	2.56	0.54
4:D:281:MET:O	4:D:284:ILE:N	2.40	0.54
2:B:134:ASP:OD2	2:B:220:ARG:NH2	2.40	0.54
3:C:285:ILE:O	23:C:487:CLA:HBB1	2.07	0.54
4:D:83:ASN:HB3	4:D:336:HIS:ND1	2.23	0.54
1:A:320:ILE:O	1:A:320:ILE:CG2	2.55	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.76	0.54
7:H:57:VAL:HG12	7:H:57:VAL:O	2.07	0.54
2:B:153:PHE:O	2:B:158:LEU:HG	2.07	0.54
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.07	0.54
15:U:72:TYR:HD2	15:U:73:PRO:CD	2.20	0.54
1:A:114:LEU:HD12	1:A:118:HIS:CE1	2.43	0.54
23:A:349:CLA:H51	24:A:351:PHO:HMB3	1.89	0.54
4:D:156:VAL:CG1	4:D:171:PRO:HG2	2.38	0.54
3:C:151:TRP:C	3:C:153:ASP:H	2.10	0.54
2:B:209:GLY:HA3	23:B:518:CLA:H201	1.90	0.53
2:B:21:ALA:O	2:B:24:LEU:HB2	2.08	0.53
4:D:152:VAL:HG13	23:D:354:CLA:CED	2.38	0.53
3:C:324:LEU:HD12	15:U:128:TYR:CZ	2.43	0.53
15:U:73:PRO:HG2	16:V:83:ASP:CG	2.28	0.53
3:C:417:VAL:HG22	16:V:38:ALA:HB1	1.90	0.53
5:E:68:ARG:HH12	7:H:50:SER:HB3	1.72	0.53
4:D:96:GLU:CD	5:E:68:ARG:O	2.46	0.53
4:D:319:LEU:CA	4:D:322:ASN:HD22	2.14	0.53
13:O:152:ARG:HD2	13:O:156:PHE:CD2	2.43	0.53
16:V:22:THR:N	16:V:25:GLN:HE21	2.06	0.53
19:Z:36:SER:HA	19:Z:39:LEU:HD12	1.89	0.53
2:B:137:LYS:O	2:B:141:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:B:513:CLA:H18	23:B:524:CLA:CGA	2.38	0.53
23:B:518:CLA:C14	23:B:524:CLA:HBA1	2.38	0.53
2:B:6:TYR:CE1	2:B:8:VAL:HG21	2.42	0.53
4:D:179:PHE:HA	4:D:182:LEU:CD1	2.38	0.53
3:C:88:LEU:HD22	23:C:480:CLA:CGD	2.39	0.53
3:C:437:PHE:HA	23:C:483:CLA:HMC1	1.90	0.53
3:C:55:ALA:HB1	28:C:488:BCR:H371	1.90	0.53
4:D:195:PRO:O	4:D:198:MET:HB2	2.09	0.53
13:O:133:VAL:HG12	13:O:133:VAL:O	2.07	0.53
13:O:79:ASP:HA	13:O:101:ILE:HG21	1.91	0.53
1:A:213:ALA:O	1:A:217:SER:HB2	2.08	0.53
2:B:234:ILE:CG2	23:B:524:CLA:H193	2.38	0.53
4:D:83:ASN:CB	4:D:336:HIS:HD1	2.22	0.53
3:C:165:LEU:HD21	23:C:474:CLA:CBB	2.38	0.53
4:D:201:VAL:O	4:D:201:VAL:HG12	2.09	0.53
1:A:292:THR:HG23	3:C:428:THR:HG23	1.91	0.53
3:C:316:THR:HG21	3:C:396:MET:HE1	1.91	0.53
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.91	0.53
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.89	0.53
23:C:477:CLA:HMD1	23:C:485:CLA:HAB	1.91	0.53
2:B:174:LEU:HD22	2:B:308:LYS:HZ2	1.74	0.53
2:B:321:LYS:HE3	2:B:325:PHE:CZ	2.43	0.53
3:C:318:LEU:HD22	3:C:328:VAL:CG2	2.38	0.53
15:U:75:LEU:HD21	15:U:101:GLN:NE2	2.24	0.53
16:V:40:CYS:SG	25:V:138:HEM:CAC	2.97	0.53
2:B:313:ASP:O	2:B:313:ASP:OD1	2.26	0.53
3:C:176:VAL:HG13	3:C:234:VAL:HG13	1.91	0.53
5:E:26:ILE:HG13	5:E:27:PRO:HD3	1.89	0.53
15:U:72:TYR:CG	15:U:73:PRO:N	2.74	0.53
3:C:291:TRP:O	3:C:305:THR:HG23	2.08	0.53
16:V:122:GLU:HB3	16:V:123:PRO:CD	2.39	0.53
16:V:100:ILE:C	16:V:102:PRO:HD3	2.29	0.53
2:B:308:LYS:HE2	2:B:312:TYR:CE2	2.43	0.53
3:C:384:ILE:O	3:C:384:ILE:HG23	2.06	0.53
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.33	0.53
16:V:52:LEU:HD23	25:V:138:HEM:HAD2	1.90	0.53
2:B:62:VAL:HG11	23:B:518:CLA:HED3	1.91	0.53
14:T:10:PHE:CE2	14:T:14:ILE:HD11	2.43	0.53
2:B:479:PHE:O	4:D:139:ARG:NH2	2.29	0.53
2:B:263:THR:HG22	2:B:263:THR:O	2.09	0.53
1:A:306:VAL:CG2	1:A:307:ILE:N	2.69	0.53
1:A:29:TYR:HE1	1:A:31:GLY:HA3	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:GLY:O	1:A:34:GLY:N	2.38	0.53
2:B:340:TRP:CE3	2:B:342:GLY:HA3	2.44	0.53
2:B:381:ILE:O	2:B:381:ILE:HG22	2.09	0.53
1:A:307:ILE:C	1:A:309:ALA:N	2.62	0.53
16:V:78:ASN:ND2	16:V:87:GLU:OE2	2.42	0.53
13:O:110:MET:H	13:O:110:MET:HE2	1.73	0.53
2:B:236:THR:O	2:B:240:SER:HB3	2.09	0.53
2:B:458:PHE:CG	23:B:516:CLA:HMC3	2.44	0.53
3:C:112:PHE:O	3:C:116:VAL:HG23	2.09	0.53
1:A:23:SER:OG	1:A:24:THR:N	2.41	0.53
6:F:30:ILE:O	6:F:30:ILE:HG22	2.09	0.53
3:C:222:GLY:O	3:C:223:TRP:C	2.47	0.52
19:Z:37:LYS:HA	19:Z:40:ILE:HD12	1.91	0.52
2:B:344:ALA:HB2	2:B:401:PHE:HE1	1.74	0.52
2:B:421:ALA:O	2:B:424:ALA:HB3	2.08	0.52
10:K:16:LEU:HB3	10:K:17:PRO:HD2	1.90	0.52
1:A:63:ILE:CD1	1:A:336:ALA:HB2	2.38	0.52
5:E:48:THR:O	5:E:49:PRO:O	2.27	0.52
1:A:217:SER:OG	4:D:142:ASN:HA	2.09	0.52
3:C:292:PHE:CE1	23:C:487:CLA:HBC3	2.43	0.52
7:H:22:PRO:O	7:H:23:GLY:O	2.26	0.52
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.44	0.52
4:D:108:GLY:C	4:D:110:LEU:N	2.60	0.52
2:B:46:ASP:OD1	2:B:48:SER:OG	2.19	0.52
2:B:103:LEU:HD21	23:B:518:CLA:HMC3	1.91	0.52
1:A:218:LEU:HD23	4:D:142:ASN:HD22	1.74	0.52
14:T:18:PHE:HD2	14:T:19:PHE:HD1	1.56	0.52
1:A:223:LEU:O	1:A:225:ARG:HG3	2.09	0.52
2:B:328:GLY:HA3	23:B:514:CLA:O1A	2.10	0.52
1:A:189:GLU:CD	22:A:347:OEC:O1	2.37	0.52
23:D:356:CLA:H12	7:H:42:LEU:HD21	1.91	0.52
10:K:19:ILE:CG1	10:K:20:PRO:HD3	2.39	0.52
4:D:83:ASN:OD1	4:D:336:HIS:ND1	2.39	0.52
3:C:201:ASN:O	3:C:201:ASN:ND2	2.41	0.52
1:A:246:TYR:HE1	1:A:248:ILE:HG12	1.74	0.52
5:E:43:TYR:O	5:E:47:GLY:N	2.42	0.52
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.52
13:O:201:VAL:CG1	13:O:211:ILE:HG23	2.37	0.52
1:A:52:PHE:O	1:A:52:PHE:CD2	2.63	0.52
2:B:62:VAL:CG1	23:B:518:CLA:HED3	2.40	0.52
4:D:268:HIS:O	4:D:271:MET:HB2	2.10	0.52
7:H:51:THR:HG22	7:H:51:THR:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:110:ALA:O	2:B:111:ALA:C	2.46	0.52
4:D:87:HIS:HA	4:D:167:TRP:NE1	2.25	0.52
1:A:295:PHE:CD1	1:A:295:PHE:N	2.76	0.52
1:A:53:ILE:O	1:A:53:ILE:HG22	2.10	0.52
2:B:247:PHE:O	2:B:251:VAL:HG23	2.09	0.52
2:B:110:ALA:HA	23:B:522:CLA:H203	1.90	0.52
4:D:286:VAL:HG21	23:D:354:CLA:HED2	1.92	0.52
23:B:520:CLA:H201	12:M:18:PRO:HB3	1.92	0.52
3:C:278:ALA:O	3:C:282:MET:HG3	2.09	0.52
3:C:122:SER:O	28:C:488:BCR:H363	2.09	0.52
3:C:167:VAL:CG2	23:C:482:CLA:HMB2	2.39	0.52
1:A:303:ASN:O	1:A:304:HIS:ND1	2.40	0.52
19:Z:5:PHE:CZ	19:Z:54:VAL:HG13	2.45	0.52
8:I:31:ASN:O	8:I:31:ASN:CG	2.48	0.52
15:U:62:ILE:O	15:U:64:ALA:N	2.42	0.52
1:A:153:SER:OG	23:A:348:CLA:HED1	2.09	0.52
4:D:122:LEU:HD21	23:D:354:CLA:H92	1.92	0.52
14:T:18:PHE:CD2	14:T:19:PHE:CD1	2.95	0.52
13:O:122:VAL:HA	13:O:146:PHE:CD2	2.43	0.52
3:C:289:PHE:HD2	3:C:289:PHE:O	1.92	0.52
4:D:83:ASN:HB3	4:D:336:HIS:HD1	1.75	0.52
13:O:38:TYR:O	13:O:245:PRO:HB2	2.09	0.52
3:C:264:PHE:CZ	23:C:474:CLA:CGA	2.92	0.52
13:O:52:VAL:HG11	13:O:116:ILE:HD13	1.91	0.52
3:C:131:TYR:HE1	3:C:135:ARG:CD	2.23	0.52
3:C:316:THR:HG21	3:C:396:MET:CE	2.39	0.52
8:I:32:PRO:HG2	8:I:35:LYS:O	2.09	0.52
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.45	0.52
1:A:340:PRO:O	4:D:352:LEU:HD23	2.10	0.52
3:C:350:ILE:HG22	3:C:351:PHE:O	2.10	0.52
13:O:17:ASN:ND2	13:O:77:SER:OG	2.43	0.52
16:V:79:PRO:HG3	16:V:88:ILE:C	2.30	0.52
1:A:260:PHE:O	1:A:263:ALA:HB3	2.09	0.52
13:O:233:VAL:CG1	13:O:234:LYS:N	2.72	0.52
1:A:337:HIS:CE1	4:D:352:LEU:HD12	2.44	0.51
23:B:521:CLA:H112	23:D:356:CLA:H92	1.92	0.51
3:C:390:ARG:NH1	16:V:100:ILE:CG2	2.73	0.51
23:C:486:CLA:H42	10:K:30:TRP:HE1	1.74	0.51
2:B:451:PHE:CD1	2:B:451:PHE:C	2.84	0.51
7:H:21:ALA:CB	7:H:22:PRO:CD	2.87	0.51
3:C:340:TYR:CD1	3:C:340:TYR:N	2.77	0.51
2:B:393:GLU:N	2:B:393:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.68	0.51
3:C:138:GLU:O	3:C:139:THR:HB	2.09	0.51
4:D:318:ASN:O	4:D:322:ASN:ND2	2.44	0.51
7:H:37:PHE:O	7:H:40:PHE:HB3	2.11	0.51
13:O:93:LEU:O	13:O:128:SER:HA	2.11	0.51
12:M:5:GLN:O	12:M:5:GLN:HG3	2.10	0.51
3:C:354:GLU:C	3:C:356:MET:H	2.13	0.51
2:B:250:PHE:CE1	2:B:459:ALA:HB1	2.45	0.51
4:D:220:ASN:ND2	4:D:220:ASN:O	2.44	0.51
1:A:307:ILE:HG22	1:A:309:ALA:CB	2.40	0.51
11:L:27:LEU:HD23	12:M:14:PHE:HE2	1.75	0.51
2:B:246:PHE:C	2:B:246:PHE:CD2	2.83	0.51
2:B:168:VAL:HG12	2:B:169:SER:N	2.24	0.51
16:V:63:THR:CG2	16:V:83:ASP:O	2.59	0.51
1:A:70:SER:O	1:A:75:ASN:HB2	2.10	0.51
4:D:80:THR:HG22	4:D:81:PRO:HD2	1.92	0.51
4:D:90:LEU:HD11	4:D:96:GLU:HB3	1.90	0.51
13:O:164:LEU:HG	13:O:188:LYS:HB2	1.93	0.51
1:A:131:TRP:O	1:A:134:SER:HB2	2.10	0.51
2:B:164:PRO:HB3	23:B:515:CLA:HED2	1.93	0.51
3:C:68:THR:HB	3:C:115:GLY:HA2	1.93	0.51
13:O:1:ALA:O	13:O:2:LYS:HB2	2.10	0.51
3:C:343:ARG:HB3	13:O:78:LEU:CD1	2.40	0.51
1:A:162:PRO:HG3	1:A:171:GLY:HA2	1.93	0.51
23:B:519:CLA:HMD1	23:B:524:CLA:CAB	2.40	0.51
4:D:258:GLY:O	14:T:21:ILE:HG23	2.10	0.51
3:C:105:VAL:HG12	3:C:107:ASP:O	2.10	0.51
5:E:68:ARG:HH12	7:H:50:SER:CB	2.24	0.51
2:B:318:ASN:O	2:B:320:ALA:N	2.43	0.51
13:O:152:ARG:HD2	13:O:156:PHE:CE2	2.46	0.51
5:E:26:ILE:HA	5:E:29:LEU:HD12	1.93	0.51
4:D:58:TRP:HB3	4:D:63:LEU:O	2.10	0.51
6:F:36:ILE:CA	6:F:39:MET:HG3	2.40	0.51
23:B:521:CLA:H172	23:D:356:CLA:H72	1.92	0.51
2:B:308:LYS:HE2	2:B:312:TYR:CZ	2.46	0.51
19:Z:41:PHE:CD1	19:Z:41:PHE:N	2.73	0.51
13:O:188:LYS:HD2	13:O:225:MET:HG3	1.93	0.51
2:B:340:TRP:CZ3	2:B:342:GLY:CA	2.92	0.51
16:V:64:PRO:HD2	16:V:66:ARG:HH22	1.76	0.51
1:A:333:GLU:OE1	3:C:354:GLU:OE2	2.29	0.51
3:C:166:ILE:O	3:C:170:ILE:HG13	2.10	0.51
4:D:175:VAL:HG12	4:D:179:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:T:3:THR:O	14:T:4:ILE:C	2.48	0.51
2:B:452:THR:HG22	4:D:291:LEU:HD11	1.92	0.51
1:A:176:ILE:O	1:A:179:THR:HB	2.11	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
1:A:116:ILE:HG22	1:A:117:PHE:N	2.25	0.51
3:C:343:ARG:NH1	3:C:345:PRO:HD3	2.25	0.51
25:E:84:HEM:C4A	6:F:19:TRP:CH2	2.99	0.51
4:D:52:THR:O	4:D:67:TYR:CD1	2.64	0.51
16:V:30:LYS:HG2	16:V:118:HIS:CD2	2.46	0.51
4:D:298:PHE:O	4:D:299:ILE:C	2.49	0.51
19:Z:23:VAL:O	19:Z:27:TYR:CD1	2.64	0.51
3:C:318:LEU:HD21	3:C:340:TYR:CB	2.40	0.51
4:D:261:PHE:CD2	14:T:24:ARG:NH2	2.79	0.51
13:O:27:ARG:O	13:O:29:ALA:N	2.44	0.51
4:D:71:CYS:HB2	4:D:76:VAL:HG22	1.89	0.51
2:B:62:VAL:HG13	23:B:518:CLA:O1D	2.11	0.51
4:D:199:MET:O	4:D:202:ALA:HB3	2.11	0.51
2:B:321:LYS:NZ	4:D:297:ASP:OD2	2.42	0.51
14:T:20:ALA:O	14:T:24:ARG:HB2	2.11	0.51
11:L:4:ASN:N	11:L:5:PRO:CD	2.72	0.51
2:B:402:TYR:N	2:B:402:TYR:CD1	2.78	0.51
4:D:82:ALA:H	4:D:85:MET:CE	2.24	0.51
16:V:33:PHE:CD2	16:V:37:CYS:SG	3.04	0.50
1:A:210:LEU:HD13	24:D:355:PHO:C1D	2.40	0.50
23:A:348:CLA:CAB	23:A:350:CLA:HMD2	2.41	0.50
3:C:37:ALA:HA	23:C:483:CLA:HBA1	1.92	0.50
16:V:133:GLY:O	16:V:137:TYR:CA	2.59	0.50
2:B:420:TYR:O	2:B:424:ALA:N	2.44	0.50
4:D:54:PHE:HB3	5:E:46:PHE:CD1	2.46	0.50
1:A:126:TYR:O	1:A:130:GLN:HG3	2.11	0.50
1:A:57:PRO:CB	1:A:68:SER:HB3	2.37	0.50
1:A:316:THR:HB	4:D:75:THR:CG2	2.40	0.50
1:A:317:TRP:N	4:D:63:LEU:HD13	2.26	0.50
3:C:123:ALA:CB	19:Z:47:TRP:CH2	2.91	0.50
2:B:340:TRP:CH2	2:B:342:GLY:HA3	2.45	0.50
3:C:301:PHE:N	3:C:301:PHE:CD2	2.79	0.50
1:A:316:THR:HB	4:D:75:THR:HG21	1.93	0.50
1:A:183:MET:CE	23:A:349:CLA:HMD3	2.41	0.50
3:C:305:THR:H	3:C:308:GLU:CG	2.19	0.50
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.46	0.50
13:O:54:GLU:OE1	13:O:231:HIS:CD2	2.64	0.50
3:C:420:VAL:HG12	3:C:425:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:64:PRO:O	16:V:66:ARG:NH1	2.44	0.50
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.94	0.50
13:O:41:ALA:N	13:O:83:GLY:O	2.43	0.50
1:A:177:SER:O	1:A:180:PHE:HB2	2.12	0.50
13:O:121:THR:HG21	13:O:148:VAL:CG2	2.26	0.50
1:A:237:TYR:CE2	1:A:245:THR:HG23	2.46	0.50
15:U:42:VAL:HG12	15:U:45:GLU:H	1.76	0.50
2:B:418:LYS:NZ	15:U:45:GLU:OE2	2.45	0.50
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.42	0.50
15:U:85:TYR:N	15:U:85:TYR:CD2	2.75	0.50
3:C:377:LEU:HD21	13:O:99:ASP:CG	2.32	0.50
3:C:350:ILE:HG22	3:C:351:PHE:N	2.27	0.50
1:A:148:SER:HB2	1:A:284:TRP:CH2	2.37	0.50
1:A:278:TRP:CB	1:A:279:PRO:HD3	2.35	0.50
1:A:334:ARG:NH1	13:O:159:PRO:HA	2.25	0.50
8:I:6:ILE:O	8:I:10:ILE:HG13	2.11	0.50
6:F:31:PHE:HD2	6:F:31:PHE:C	2.15	0.50
3:C:183:GLY:O	3:C:184:GLY:O	2.30	0.50
1:A:200:LEU:O	1:A:203:ALA:HB3	2.11	0.50
6:F:40:GLN:OE1	9:J:28:PHE:CD2	2.65	0.50
1:A:180:PHE:N	1:A:180:PHE:CD1	2.77	0.50
1:A:78:ILE:HD13	11:L:34:TYR:OH	2.10	0.50
15:U:105:LEU:O	15:U:109:LEU:N	2.41	0.50
15:U:108:ASN:O	15:U:109:LEU:C	2.50	0.50
15:U:54:LYS:HD2	15:U:113:THR:OG1	2.11	0.50
1:A:237:TYR:CD2	1:A:241:GLN:OE1	2.65	0.50
13:O:120:PHE:HE1	13:O:235:ILE:HG21	1.77	0.50
16:V:37:CYS:O	16:V:38:ALA:C	2.50	0.50
16:V:75:TYR:CE2	16:V:80:THR:N	2.70	0.50
2:B:136:PRO:CD	2:B:231:MET:HE1	2.40	0.50
2:B:240:SER:OG	2:B:241:SER:N	2.44	0.50
2:B:29:LEU:HD11	28:B:529:BCR:H331	1.94	0.50
4:D:200:GLY:O	4:D:204:VAL:HG23	2.11	0.50
3:C:287:THR:O	3:C:290:VAL:HB	2.11	0.50
3:C:302:TYR:O	3:C:422:PRO:HD2	2.12	0.50
23:C:487:CLA:HBC2	23:C:487:CLA:HHD	1.94	0.50
4:D:222:LEU:HD22	4:D:243:THR:HB	1.93	0.50
11:L:6:ASN:HD22	11:L:6:ASN:H	1.59	0.50
4:D:261:PHE:HD2	14:T:24:ARG:NH2	2.10	0.50
13:O:168:TYR:CZ	13:O:172:ILE:HD11	2.46	0.50
1:A:95:PRO:HG2	1:A:98:GLU:CB	2.41	0.50
1:A:24:THR:CB	4:D:251:ARG:NH2	2.74	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:Z:5:PHE:CE2	19:Z:54:VAL:HG13	2.47	0.50
6:F:40:GLN:OE1	9:J:28:PHE:HD2	1.95	0.50
1:A:320:ILE:HG21	4:D:333:ASP:OD2	2.12	0.50
2:B:206:GLY:O	2:B:210:ILE:HG13	2.11	0.50
13:O:54:GLU:CD	13:O:231:HIS:CE1	2.85	0.50
1:A:89:ILE:HD13	1:A:94:TYR:CD2	2.46	0.50
13:O:238:VAL:CG1	13:O:239:PHE:N	2.75	0.50
15:U:72:TYR:HD2	15:U:73:PRO:HG3	1.77	0.50
1:A:150:PRO:O	1:A:153:SER:HB3	2.12	0.50
13:O:39:ARG:HA	13:O:245:PRO:HB3	1.92	0.50
1:A:300:PHE:CB	1:A:302:PHE:HE1	2.16	0.50
15:U:84:PRO:C	15:U:85:TYR:CD2	2.85	0.50
4:D:24:ARG:HB3	4:D:26:ARG:HE	1.77	0.50
2:B:205:ALA:O	23:B:518:CLA:H191	2.12	0.49
23:C:487:CLA:H51	23:C:487:CLA:H102	1.94	0.49
3:C:98:GLY:O	3:C:99:VAL:CG2	2.58	0.49
4:D:198:MET:HE3	11:L:30:LEU:HD11	1.90	0.49
13:O:189:ARG:NE	15:U:39:LEU:HD23	2.27	0.49
1:A:183:MET:HB3	23:A:348:CLA:HBC2	1.94	0.49
2:B:244:ALA:O	2:B:247:PHE:HB3	2.11	0.49
23:A:348:CLA:HBB1	23:D:354:CLA:NC	2.27	0.49
3:C:91:HIS:O	3:C:94:THR:HB	2.11	0.49
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.94	0.49
23:C:486:CLA:H192	19:Z:19:MET:HG2	1.94	0.49
6:F:31:PHE:CD2	6:F:31:PHE:C	2.83	0.49
7:H:24:TRP:CE3	7:H:24:TRP:HA	2.46	0.49
3:C:349:ILE:O	3:C:350:ILE:HG13	2.13	0.49
3:C:345:PRO:HB3	13:O:73:ARG:CZ	2.41	0.49
16:V:33:PHE:HD2	16:V:37:CYS:SG	2.34	0.49
4:D:56:THR:CG2	4:D:56:THR:O	2.60	0.49
3:C:278:ALA:HB1	23:C:479:CLA:H142	1.94	0.49
3:C:88:LEU:O	3:C:89:ILE:C	2.50	0.49
1:A:308:ASP:O	1:A:309:ALA:C	2.50	0.49
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.42	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
2:B:194:ASN:C	2:B:196:GLY:N	2.66	0.49
16:V:63:THR:HB	16:V:83:ASP:C	2.32	0.49
1:A:215:HIS:HA	26:A:353:PL9:O1	2.12	0.49
3:C:291:TRP:HB3	3:C:292:PHE:HD2	1.74	0.49
3:C:149:TYR:CG	3:C:156:LYS:HG3	2.47	0.49
2:B:472:ARG:NE	2:B:479:PHE:HE1	2.11	0.49
3:C:337:LEU:HA	13:O:104:GLN:HE21	1.75	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:118:LEU:CD2	13:O:233:VAL:HG21	2.43	0.49
5:E:26:ILE:HG13	5:E:27:PRO:CD	2.42	0.49
2:B:297:THR:O	2:B:298:LEU:C	2.48	0.49
5:E:48:THR:HG22	5:E:48:THR:O	2.13	0.49
2:B:12:LEU:CD2	2:B:19:LEU:HD12	2.43	0.49
3:C:450:ALA:HA	3:C:454:GLY:CA	2.42	0.49
28:K:50:BCR:H333	19:Z:17:PHE:HA	1.94	0.49
2:B:260:SER:H	2:B:263:THR:HB	1.77	0.49
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.12	0.49
1:A:75:ASN:HD22	1:A:79:THR:HG21	1.77	0.49
2:B:61:PHE:O	2:B:64:PRO:HD2	2.12	0.49
3:C:286:ALA:HA	3:C:289:PHE:HB3	1.95	0.49
3:C:285:ILE:CA	23:C:487:CLA:HMB2	2.35	0.49
3:C:138:GLU:CG	3:C:139:THR:N	2.61	0.49
13:O:50:PHE:O	13:O:68:THR:OG1	2.31	0.49
6:F:17:VAL:O	6:F:18:ARG:C	2.50	0.49
2:B:234:ILE:HG23	23:B:513:CLA:HMD2	1.95	0.49
2:B:326:ARG:HG2	12:M:4:ASN:HD22	1.78	0.49
3:C:297:TYR:O	3:C:298:PRO:C	2.51	0.49
3:C:52:ALA:HB1	23:C:486:CLA:HMB3	1.95	0.49
2:B:311:PHE:O	2:B:313:ASP:N	2.45	0.49
11:L:12:LEU:CD1	11:L:16:SER:HB3	2.39	0.49
3:C:66:ALA:HB1	10:K:17:PRO:HB3	1.95	0.49
13:O:65:PHE:CD1	13:O:65:PHE:N	2.81	0.49
15:U:75:LEU:CD2	15:U:101:GLN:HE21	2.25	0.49
2:B:451:PHE:CZ	2:B:455:HIS:ND1	2.80	0.49
1:A:166:GLY:O	1:A:167:SER:HB3	2.13	0.49
5:E:12:ILE:HD12	25:E:84:HEM:CBD	2.42	0.49
2:B:45:PHE:CE2	2:B:46:ASP:O	2.66	0.49
3:C:99:VAL:CG1	3:C:100:GLY:N	2.74	0.49
3:C:109:PHE:CZ	28:C:489:BCR:HC32	2.47	0.49
4:D:195:PRO:CA	4:D:198:MET:HE2	2.38	0.49
2:B:422:ARG:NH2	13:O:169:ASP:HB3	2.28	0.49
2:B:397:VAL:CG1	2:B:398:THR:N	2.76	0.49
2:B:156:PHE:HA	2:B:161:LEU:HB2	1.93	0.49
4:D:188:PHE:HD1	4:D:188:PHE:N	2.10	0.49
5:E:63:PRO:HB3	5:E:78:PHE:CD2	2.47	0.49
1:A:124:SER:O	1:A:127:MET:HB3	2.12	0.49
2:B:24:LEU:HD12	2:B:111:ALA:HA	1.93	0.49
2:B:6:TYR:CE1	2:B:8:VAL:CG2	2.96	0.49
2:B:78:TRP:HZ3	2:B:93:PHE:CE1	2.30	0.49
2:B:326:ARG:HG2	12:M:4:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:128:ASP:HB3	16:V:134:LYS:HG3	1.95	0.49
2:B:305:ILE:O	2:B:341:LYS:HD2	2.12	0.49
8:I:27:ASP:N	8:I:27:ASP:OD1	2.46	0.49
4:D:18:LEU:HD12	17:X:41:SER:OG	2.12	0.49
19:Z:53:VAL:O	19:Z:57:LEU:HG	2.13	0.49
1:A:255:PHE:CE2	26:A:353:PL9:H152	2.48	0.49
3:C:296:VAL:O	3:C:298:PRO:HD2	2.13	0.49
3:C:71:GLU:C	3:C:73:ALA:H	2.15	0.49
1:A:243:GLU:N	4:D:240:ALA:HB1	2.28	0.49
1:A:301:ASN:O	1:A:301:ASN:CG	2.51	0.49
3:C:97:TRP:HA	3:C:97:TRP:CE3	2.48	0.49
11:L:10:VAL:O	12:M:28:GLN:NE2	2.46	0.49
15:U:47:LEU:C	15:U:49:THR:H	2.16	0.49
3:C:304:PRO:HB3	3:C:395:TYR:CG	2.48	0.49
4:D:20:ASP:O	4:D:21:TRP:C	2.50	0.49
12:M:9:ILE:O	12:M:13:LEU:HG	2.13	0.49
6:F:43:GLN:HG2	6:F:44:ARG:HG2	1.94	0.49
2:B:360:PRO:C	2:B:362:PHE:H	2.16	0.49
2:B:31:ALA:N	23:B:518:CLA:HBC3	2.28	0.48
2:B:62:VAL:O	2:B:63:LEU:C	2.51	0.48
4:D:158:LEU:O	4:D:161:PRO:HD2	2.13	0.48
7:H:23:GLY:C	7:H:25:GLY:N	2.66	0.48
13:O:38:TYR:O	13:O:245:PRO:CG	2.61	0.48
4:D:315:TYR:CE2	4:D:319:LEU:HD11	2.48	0.48
4:D:196:PHE:HD1	4:D:285:GLY:CA	2.25	0.48
9:J:24:ILE:O	9:J:27:LEU:HB3	2.12	0.48
23:B:512:CLA:O2A	23:B:512:CLA:H2A	2.13	0.48
3:C:282:MET:O	3:C:285:ILE:HB	2.13	0.48
23:C:486:CLA:CHB	28:C:488:BCR:H402	2.43	0.48
2:B:475:PHE:O	2:B:476:ARG:C	2.51	0.48
4:D:333:ASP:OD1	4:D:333:ASP:O	2.31	0.48
3:C:186:TYR:CD2	3:C:186:TYR:C	2.86	0.48
1:A:107:TYR:HD1	13:O:115:ARG:CZ	2.26	0.48
1:A:89:ILE:CG1	13:O:73:ARG:NH2	2.71	0.48
15:U:72:TYR:HD2	15:U:73:PRO:CG	2.26	0.48
6:F:22:VAL:O	6:F:26:ALA:HB3	2.13	0.48
6:F:39:MET:O	6:F:41:PHE:N	2.46	0.48
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.48	0.48
3:C:153:ASP:OD1	3:C:155:ASN:OD1	2.30	0.48
1:A:242:GLU:O	4:D:241:GLU:HA	2.12	0.48
3:C:208:VAL:CG1	3:C:209:ILE:N	2.77	0.48
4:D:236:ASN:HB2	4:D:237:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:LEU:HD13	1:A:285:PHE:HD1	1.75	0.48
2:B:84:THR:O	2:B:84:THR:CG2	2.61	0.48
4:D:112:THR:HG22	4:D:116:LEU:CD1	2.43	0.48
3:C:347:GLY:O	13:O:16:ALA:HB3	2.13	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CA	2.96	0.48
15:U:76:ALA:O	15:U:80:VAL:HG23	2.14	0.48
3:C:320:ARG:HH11	16:V:49:ASN:HA	1.78	0.48
1:A:211:PHE:CE2	1:A:278:TRP:CD1	3.02	0.48
4:D:154:VAL:HG13	4:D:158:LEU:HD12	1.94	0.48
3:C:71:GLU:C	3:C:73:ALA:N	2.67	0.48
10:K:19:ILE:HD12	28:K:50:BCR:H342	1.95	0.48
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.43	0.48
4:D:343:GLU:OE2	16:V:134:LYS:NZ	2.40	0.48
16:V:133:GLY:O	16:V:137:TYR:N	2.47	0.48
1:A:307:ILE:C	1:A:309:ALA:H	2.16	0.48
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.43	0.48
3:C:316:THR:OG1	3:C:392:ALA:HB1	2.14	0.48
4:D:84:SER:HB2	5:E:66:THR:O	2.13	0.48
13:O:45:LEU:HD11	13:O:215:PHE:CE1	2.48	0.48
23:B:519:CLA:C14	23:D:356:CLA:H11	2.43	0.48
3:C:293:ASN:CG	3:C:423:ARG:NH2	2.67	0.48
2:B:57:ARG:HA	2:B:330:MET:HG3	1.96	0.48
3:C:109:PHE:O	3:C:111:PHE:N	2.47	0.48
3:C:40:ALA:O	3:C:43:ILE:HG23	2.12	0.48
16:V:33:PHE:CD2	16:V:37:CYS:HB2	2.48	0.48
1:A:259:ILE:HD13	26:A:353:PL9:H172	1.95	0.48
23:C:479:CLA:HAB	23:C:479:CLA:C9	2.41	0.48
1:A:224:ILE:CG2	1:A:227:THR:OG1	2.61	0.48
2:B:302:TRP:C	2:B:304:ALA:H	2.17	0.48
3:C:367:GLU:O	3:C:370:ARG:N	2.37	0.48
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.96	0.48
15:U:61:ASN:CB	15:U:126:ASP:O	2.62	0.48
1:A:129:ARG:NH2	4:D:255:GLN:O	2.46	0.48
16:V:13:ASN:C	16:V:13:ASN:OD1	2.51	0.48
15:U:65:PHE:HD1	15:U:76:ALA:HB1	1.78	0.48
16:V:46:THR:HG22	16:V:49:ASN:N	2.19	0.48
16:V:63:THR:O	16:V:80:THR:HG21	2.14	0.48
1:A:180:PHE:HE2	4:D:192:THR:C	2.17	0.48
1:A:284:TRP:HA	1:A:284:TRP:CE3	2.49	0.48
2:B:71:VAL:O	2:B:93:PHE:HE2	1.96	0.48
4:D:129:GLN:HE21	4:D:142:ASN:HB3	1.78	0.48
7:H:29:LEU:O	7:H:33:PHE:HD1	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:372:ASP:HB3	2:B:376:VAL:HB	1.95	0.48
2:B:360:PRO:O	2:B:362:PHE:N	2.46	0.48
6:F:20:VAL:O	6:F:21:ALA:C	2.52	0.48
3:C:372:PRO:O	3:C:373:ASN:HB2	2.14	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CD	2.96	0.48
1:A:150:PRO:O	1:A:153:SER:N	2.47	0.48
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.48	0.48
2:B:199:VAL:O	2:B:203:ILE:HG13	2.13	0.48
2:B:63:LEU:HB3	2:B:64:PRO:CD	2.38	0.48
3:C:289:PHE:CE2	3:C:294:ASN:OD1	2.67	0.48
3:C:294:ASN:O	3:C:295:THR:C	2.50	0.48
13:O:161:GLY:O	13:O:168:TYR:N	2.43	0.48
13:O:71:VAL:CG2	13:O:108:VAL:HG23	2.39	0.48
2:B:91:TRP:CB	23:B:515:CLA:H43	2.44	0.48
1:A:119:PHE:O	1:A:123:ALA:CB	2.62	0.48
13:O:32:ILE:O	13:O:35:SER:N	2.45	0.48
15:U:61:ASN:HB3	15:U:126:ASP:O	2.14	0.48
10:K:26:LEU:HD21	18:N:20:UNK:CB	2.43	0.48
13:O:137:THR:HG23	13:O:138:THR:N	2.29	0.48
13:O:45:LEU:HB3	13:O:79:ASP:HB2	1.96	0.48
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.48	0.48
3:C:282:MET:HA	3:C:285:ILE:CB	2.44	0.48
3:C:282:MET:HE2	23:C:479:CLA:H41	1.95	0.48
8:I:27:ASP:HB2	8:I:28:PRO:HD2	1.94	0.48
15:U:47:LEU:O	15:U:49:THR:N	2.46	0.48
8:I:31:ASN:O	8:I:31:ASN:OD1	2.31	0.48
2:B:235:GLU:HA	2:B:235:GLU:OE1	2.14	0.48
2:B:237:VAL:HG22	23:B:524:CLA:HBC2	1.96	0.48
4:D:152:VAL:CG1	23:D:354:CLA:H43	2.44	0.48
3:C:305:THR:N	3:C:308:GLU:HG3	2.21	0.48
3:C:64:ALA:HB3	3:C:118:HIS:HB3	1.95	0.48
2:B:57:ARG:NH2	2:B:334:ASP:OD2	2.45	0.48
1:A:238:LYS:O	1:A:240:GLY:N	2.47	0.48
1:A:242:GLU:O	1:A:244:GLU:N	2.47	0.48
1:A:307:ILE:HD13	5:E:54:TYR:HB2	1.95	0.48
2:B:385:ARG:HG3	13:O:165:ALA:HA	1.95	0.48
6:F:27:VAL:N	6:F:28:PRO:CD	2.77	0.48
16:V:25:GLN:O	16:V:26:TYR:C	2.52	0.48
15:U:66:ILE:O	15:U:66:ILE:HG22	2.13	0.48
1:A:104:GLU:HG2	1:A:105:TRP:N	2.29	0.47
13:O:46:GLN:O	13:O:238:VAL:O	2.31	0.47
16:V:79:PRO:HG3	16:V:89:ALA:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:284:TRP:HE3	1:A:284:TRP:HA	1.79	0.47
2:B:12:LEU:HG	2:B:19:LEU:CD1	2.43	0.47
10:K:35:GLY:O	10:K:36:PHE:HB2	2.13	0.47
4:D:90:LEU:HD11	4:D:96:GLU:CB	2.44	0.47
2:B:328:GLY:HA2	2:B:444:ARG:HD3	1.95	0.47
4:D:191:TRP:HE1	4:D:197:HIS:CD2	2.31	0.47
3:C:208:VAL:HG13	3:C:209:ILE:H	1.79	0.47
3:C:370:ARG:HD3	3:C:375:LEU:HD23	1.94	0.47
2:B:148:LEU:O	2:B:151:PHE:HB3	2.13	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
1:A:205:VAL:CG1	4:D:204:VAL:HG12	2.44	0.47
1:A:75:ASN:HD21	4:D:313:THR:HG21	1.79	0.47
2:B:247:PHE:HE1	23:B:521:CLA:H72	1.77	0.47
2:B:326:ARG:C	28:B:529:BCR:H292	2.34	0.47
4:D:178:ILE:O	4:D:182:LEU:HG	2.14	0.47
4:D:243:THR:HG22	4:D:243:THR:O	2.13	0.47
4:D:83:ASN:CB	4:D:336:HIS:ND1	2.77	0.47
13:O:164:LEU:N	13:O:188:LYS:HE2	2.29	0.47
3:C:339:LYS:HB2	3:C:340:TYR:CE1	2.49	0.47
2:B:394:GLN:CD	15:U:52:GLY:HA3	2.34	0.47
3:C:376:ASP:OD1	3:C:378:ASN:HB2	2.14	0.47
1:A:283:VAL:O	1:A:284:TRP:C	2.52	0.47
4:D:80:THR:CG2	4:D:168:PHE:HA	2.43	0.47
23:A:348:CLA:H191	14:T:17:PHE:CZ	2.49	0.47
13:O:193:THR:CG2	13:O:194:LYS:H	2.05	0.47
16:V:53:ASP:OD1	16:V:55:ARG:HB3	2.14	0.47
4:D:348:ARG:NH1	15:U:133:TYR:CE1	2.82	0.47
15:U:61:ASN:HB3	15:U:130:ASN:ND2	2.28	0.47
1:A:42:LEU:O	1:A:46:ILE:HG12	2.14	0.47
6:F:19:TRP:CZ3	6:F:23:HIS:CE1	3.03	0.47
19:Z:19:MET:HE1	19:Z:43:GLY:HA3	1.97	0.47
1:A:225:ARG:CB	2:B:481:GLY:C	2.72	0.47
4:D:337:GLU:O	4:D:338:ASN:HB2	2.14	0.47
1:A:301:ASN:HB2	1:A:303:ASN:HD21	1.79	0.47
3:C:199:ILE:HD12	3:C:234:VAL:CG2	2.39	0.47
17:X:12:ILE:O	17:X:12:ILE:HG13	2.15	0.47
2:B:198:VAL:O	2:B:201:HIS:HB3	2.14	0.47
1:A:161:TYR:CE1	1:A:186:PHE:CE1	3.00	0.47
1:A:202:VAL:HG21	23:A:350:CLA:OBD	2.15	0.47
1:A:180:PHE:CE2	4:D:192:THR:CG2	2.97	0.47
15:U:58:ASN:C	15:U:59:ASN:HD22	2.08	0.47
13:O:81:ILE:CG2	13:O:82:GLN:N	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:213:LEU:HD21	23:C:474:CLA:H171	1.97	0.47
3:C:249:ILE:O	3:C:252:ILE:HB	2.15	0.47
23:C:478:CLA:H91	23:C:482:CLA:HAA1	1.96	0.47
2:B:264:PRO:HG2	2:B:267:LEU:HB2	1.96	0.47
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.14	0.47
23:B:514:CLA:H202	11:L:27:LEU:HD11	1.96	0.47
13:O:27:ARG:C	13:O:29:ALA:N	2.68	0.47
3:C:392:ALA:O	3:C:396:MET:HB3	2.15	0.47
5:E:74:GLN:O	5:E:78:PHE:CD1	2.67	0.47
13:O:211:ILE:HG22	13:O:212:ALA:H	1.79	0.47
15:U:73:PRO:HG2	16:V:83:ASP:OD1	2.13	0.47
3:C:154:LYS:O	3:C:158:THR:OG1	2.15	0.47
1:A:315:ASN:HB2	4:D:63:LEU:HD23	1.95	0.47
1:A:44:ALA:CB	24:A:351:PHO:H91	2.44	0.47
2:B:464:PHE:HD2	23:B:523:CLA:HAC2	1.79	0.47
15:U:112:PHE:N	15:U:112:PHE:CD1	2.82	0.47
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.97	0.47
1:A:139:MET:HE2	4:D:248:THR:HG21	1.96	0.47
7:H:24:TRP:HA	7:H:24:TRP:HE3	1.78	0.47
5:E:25:THR:HG21	25:E:84:HEM:C4B	2.50	0.47
4:D:71:CYS:HB3	4:D:75:THR:CG2	2.45	0.47
23:B:519:CLA:CBB	4:D:123:ILE:HG12	2.44	0.47
1:A:52:PHE:CD1	1:A:81:ALA:HB2	2.50	0.47
2:B:124:ARG:CG	2:B:125:ASP:N	2.76	0.47
12:M:21:PHE:CD2	12:M:22:LEU:HD23	2.50	0.47
3:C:79:LYS:O	3:C:80:PRO:C	2.53	0.47
23:C:476:CLA:HED3	23:C:483:CLA:H71	1.96	0.47
10:K:31:GLN:HB3	10:K:36:PHE:HD2	1.80	0.47
13:O:39:ARG:HA	13:O:245:PRO:CG	2.44	0.47
1:A:143:ILE:HG21	4:D:253:TRP:HH2	1.80	0.47
2:B:252:VAL:O	2:B:255:THR:HB	2.15	0.47
13:O:118:LEU:HD13	13:O:233:VAL:HG21	1.96	0.47
7:H:54:LEU:HB2	7:H:57:VAL:HB	1.97	0.47
17:X:13:THR:O	17:X:15:SER:N	2.47	0.47
4:D:291:LEU:O	4:D:293:LEU:N	2.48	0.47
15:U:66:ILE:HG23	16:V:82:TYR:CE2	2.49	0.47
13:O:147:ASN:HA	13:O:147:ASN:HD22	1.43	0.47
1:A:210:LEU:HD12	1:A:210:LEU:C	2.36	0.47
2:B:187:PRO:HA	2:B:190:PHE:HB2	1.95	0.47
4:D:153:PHE:CZ	24:D:355:PHO:H92	2.50	0.47
3:C:227:VAL:HG23	3:C:294:ASN:CB	2.42	0.47
3:C:39:ASN:HB2	23:C:483:CLA:HBA2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:11:VAL:HG13	11:L:6:ASN:CB	2.45	0.47
3:C:97:TRP:CZ3	3:C:178:LYS:HE3	2.50	0.47
5:E:23:SER:O	5:E:27:PRO:HG2	2.15	0.47
1:A:261:GLN:CG	1:A:262:TYR:H	2.28	0.47
3:C:343:ARG:HB3	13:O:78:LEU:HD12	1.97	0.47
3:C:320:ARG:HG2	15:U:128:TYR:HE2	1.80	0.47
15:U:72:TYR:CB	15:U:73:PRO:CD	2.91	0.47
9:J:27:LEU:O	9:J:30:TYR:N	2.48	0.47
5:E:14:THR:CB	9:J:8:ILE:HD12	2.43	0.47
1:A:186:PHE:CD2	1:A:192:ILE:CD1	2.85	0.47
2:B:250:PHE:HB3	23:B:521:CLA:H142	1.96	0.47
3:C:305:THR:O	3:C:306:GLY:C	2.52	0.47
23:C:476:CLA:HBD	23:C:486:CLA:CBB	2.45	0.47
19:Z:37:LYS:O	19:Z:41:PHE:CE1	2.68	0.47
13:O:158:ASP:CB	13:O:159:PRO:CD	2.92	0.47
2:B:153:PHE:O	2:B:157:HIS:HB3	2.14	0.47
1:A:271:LEU:O	1:A:275:LEU:HG	2.15	0.47
18:N:31:UNK:HA	19:Z:30:PRO:CG	2.45	0.47
4:D:52:THR:HG23	4:D:76:VAL:CG1	2.44	0.47
2:B:26:HIS:HB2	23:B:513:CLA:HMB2	1.96	0.47
1:A:291:SER:O	1:A:295:PHE:HE1	1.98	0.47
4:D:83:ASN:CG	4:D:336:HIS:HD1	2.16	0.47
13:O:152:ARG:HD2	13:O:156:PHE:CG	2.50	0.47
2:B:340:TRP:HH2	2:B:401:PHE:CD1	2.33	0.47
13:O:54:GLU:OE1	13:O:231:HIS:NE2	2.48	0.47
2:B:390:TYR:O	2:B:391:SER:O	2.33	0.47
7:H:27:THR:N	7:H:28:PRO:CD	2.78	0.47
2:B:224:ARG:O	2:B:228:ALA:HB3	2.15	0.47
13:O:210:GLU:HA	13:O:210:GLU:OE1	2.15	0.47
5:E:70:GLU:O	5:E:71:ALA:C	2.52	0.47
2:B:183:PRO:HB2	2:B:200:ALA:HB2	1.96	0.46
23:B:519:CLA:HBB2	4:D:123:ILE:HG12	1.97	0.46
2:B:45:PHE:CE2	2:B:78:TRP:HZ2	2.32	0.46
13:O:122:VAL:HG12	13:O:122:VAL:O	2.15	0.46
1:A:36:ILE:HD13	23:C:487:CLA:H141	1.97	0.46
16:V:126:LEU:O	16:V:129:LYS:HG3	2.15	0.46
7:H:21:ALA:HB3	7:H:22:PRO:HD2	1.97	0.46
3:C:337:LEU:HA	13:O:104:GLN:NE2	2.29	0.46
2:B:401:PHE:HZ	2:B:420:TYR:CD2	2.34	0.46
2:B:467:ILE:HD13	4:D:126:MET:CE	2.45	0.46
4:D:188:PHE:H	4:D:188:PHE:HD1	1.63	0.46
2:B:234:ILE:O	2:B:235:GLU:C	2.53	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:25:MET:HB3	28:B:529:BCR:C33	2.42	0.46
3:C:292:PHE:H	3:C:292:PHE:HD2	1.56	0.46
23:C:480:CLA:H42	23:C:481:CLA:HBD	1.98	0.46
1:A:230:THR:HG22	1:A:231:GLU:N	2.18	0.46
3:C:412:THR:O	3:C:412:THR:HG22	2.14	0.46
11:L:12:LEU:CD1	11:L:16:SER:CB	2.93	0.46
1:A:288:LEU:O	1:A:289:GLY:C	2.54	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.97	0.46
13:O:180:GLU:HG3	13:O:181:GLU:H	1.80	0.46
2:B:119:ASP:HB3	2:B:121:GLU:HG3	1.97	0.46
28:B:529:BCR:H393	28:B:529:BCR:H371	1.97	0.46
23:C:477:CLA:HMD3	23:C:485:CLA:HAB	1.96	0.46
1:A:31:GLY:O	1:A:33:PHE:N	2.48	0.46
13:O:114:GLU:OE2	13:O:231:HIS:NE2	2.47	0.46
13:O:32:ILE:O	13:O:34:SER:N	2.48	0.46
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.50	0.46
1:A:211:PHE:HE2	1:A:278:TRP:CD1	2.33	0.46
23:B:518:CLA:H61	23:B:518:CLA:H41	1.79	0.46
9:J:19:MET:SD	28:K:50:BCR:H361	2.55	0.46
4:D:325:ILE:O	4:D:329:MET:HB3	2.14	0.46
3:C:108:THR:CG2	10:K:2:LEU:HD23	2.44	0.46
4:D:72:ASN:OD1	4:D:74:LEU:CB	2.63	0.46
15:U:100:ARG:HG3	15:U:104:ILE:HD11	1.98	0.46
3:C:93:ALA:HB3	3:C:301:PHE:CE1	2.51	0.46
2:B:297:THR:O	2:B:300:GLU:N	2.49	0.46
13:O:137:THR:CG2	13:O:138:THR:N	2.77	0.46
16:V:33:PHE:CD2	16:V:37:CYS:CB	2.99	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD1	2.38	0.46
28:K:50:BCR:HC42	19:Z:17:PHE:CD1	2.49	0.46
1:A:33:PHE:CD1	1:A:128:GLY:C	2.89	0.46
3:C:200:THR:O	3:C:201:ASN:ND2	2.32	0.46
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.15	0.46
2:B:163:GLY:O	2:B:165:GLY:N	2.46	0.46
2:B:185:TRP:O	2:B:186:GLY:O	2.33	0.46
3:C:347:GLY:O	13:O:16:ALA:CB	2.64	0.46
13:O:46:GLN:HB3	13:O:46:GLN:HE21	1.50	0.46
1:A:75:ASN:ND2	1:A:79:THR:HG22	2.31	0.46
3:C:281:MET:O	3:C:285:ILE:HG13	2.16	0.46
3:C:71:GLU:O	3:C:75:PHE:HB2	2.15	0.46
3:C:73:ALA:O	10:K:1:LYS:HA	2.14	0.46
3:C:100:GLY:O	3:C:101:PRO:C	2.53	0.46
1:A:261:GLN:CG	1:A:262:TYR:N	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:53:ASN:ND2	2:B:58:GLN:OE1	2.49	0.46
3:C:293:ASN:HD22	3:C:293:ASN:N	2.12	0.46
10:K:10:ASP:N	10:K:11:PRO:CD	2.79	0.46
4:D:238:THR:C	4:D:240:ALA:N	2.68	0.46
2:B:307:GLU:O	2:B:308:LYS:C	2.48	0.46
1:A:312:ASN:HB3	5:E:55:TYR:CE1	2.51	0.46
3:C:335:THR:O	3:C:335:THR:HG22	2.16	0.46
4:D:267:LEU:C	4:D:271:MET:HE2	2.35	0.46
4:D:110:LEU:O	4:D:113:PHE:N	2.49	0.46
13:O:238:VAL:HG12	13:O:239:PHE:H	1.78	0.46
16:V:81:THR:O	16:V:83:ASP:N	2.49	0.46
13:O:40:ILE:CG2	13:O:41:ALA:N	2.72	0.46
2:B:234:ILE:HG13	23:B:524:CLA:H191	1.97	0.46
2:B:55:MET:HE1	2:B:80:ILE:HD13	1.97	0.46
4:D:87:HIS:HE1	4:D:162:LEU:HA	1.80	0.46
4:D:165:SER:O	4:D:166:SER:HB3	2.16	0.46
3:C:286:ALA:HA	3:C:289:PHE:CB	2.46	0.46
3:C:99:VAL:HG12	3:C:100:GLY:O	2.15	0.46
2:B:222:PRO:CB	7:H:25:GLY:HA2	2.30	0.46
4:D:329:MET:O	4:D:333:ASP:HB2	2.15	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.46
1:A:109:GLY:O	1:A:110:GLY:C	2.53	0.46
13:O:40:ILE:O	13:O:243:ILE:HG23	2.16	0.46
2:B:19:LEU:HD21	23:B:524:CLA:H192	1.97	0.46
1:A:218:LEU:CD2	4:D:142:ASN:ND2	2.79	0.46
14:T:7:VAL:O	14:T:10:PHE:HB3	2.16	0.46
3:C:95:LEU:HD11	23:C:480:CLA:HBA2	1.97	0.46
1:A:141:PRO:HG2	3:C:443:TRP:CZ3	2.41	0.46
19:Z:48:ILE:HG12	19:Z:48:ILE:O	2.15	0.46
13:O:152:ARG:NH1	13:O:156:PHE:CE2	2.84	0.46
3:C:406:SER:OG	23:C:475:CLA:O1A	2.34	0.46
16:V:78:ASN:HB2	16:V:96:ARG:NH1	2.28	0.46
11:L:28:ALA:O	11:L:29:LEU:C	2.53	0.46
13:O:28:GLY:HA2	13:O:204:VAL:HB	1.96	0.46
11:L:24:ILE:HD13	12:M:18:PRO:HB2	1.97	0.46
3:C:48:LYS:NZ	23:C:486:CLA:HBA1	2.31	0.46
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.98	0.46
5:E:43:TYR:CE2	5:E:50:ARG:HG2	2.51	0.46
15:U:39:LEU:C	15:U:41:ASN:N	2.68	0.46
2:B:346:PHE:O	2:B:354:LEU:HB2	2.16	0.46
13:O:136:ILE:HG22	13:O:204:VAL:HG21	1.98	0.45
1:A:159:LEU:CD2	1:A:163:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:390:ARG:NH1	16:V:100:ILE:HG23	2.31	0.45
3:C:210:PHE:O	3:C:213:LEU:HB2	2.16	0.45
2:B:479:PHE:C	2:B:481:GLY:N	2.69	0.45
2:B:280:PHE:O	2:B:281:GLN:C	2.55	0.45
13:O:53:LYS:HB3	13:O:64:GLU:O	2.16	0.45
7:H:53:ILE:HG22	17:X:15:SER:CB	2.45	0.45
18:N:22:UNK:C	18:N:24:UNK:N	2.75	0.45
1:A:112:TYR:CZ	1:A:116:ILE:HD11	2.51	0.45
3:C:341:LEU:HD22	3:C:349:ILE:HG22	1.97	0.45
1:A:169:SER:O	1:A:170:ASP:HB2	2.16	0.45
1:A:172:MET:HE2	23:A:349:CLA:CMC	2.44	0.45
2:B:249:ALA:CB	2:B:459:ALA:HB2	2.47	0.45
23:B:521:CLA:HAB	23:B:527:CLA:CED	2.31	0.45
2:B:19:LEU:HD21	23:B:524:CLA:C19	2.46	0.45
3:C:285:ILE:HD12	23:C:479:CLA:H71	1.98	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG21	2.32	0.45
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.99	0.45
1:A:320:ILE:HD13	4:D:333:ASP:HA	1.98	0.45
16:V:66:ARG:NH1	16:V:66:ARG:HG3	2.31	0.45
15:U:72:TYR:O	15:U:76:ALA:HB3	2.16	0.45
28:B:529:BCR:H361	28:B:529:BCR:H20C	1.66	0.45
4:D:65:SER:OG	4:D:77:ALA:O	2.31	0.45
14:T:17:PHE:O	14:T:18:PHE:C	2.55	0.45
1:A:155:PHE:O	1:A:159:LEU:N	2.41	0.45
11:L:37:ASN:OXT	11:L:37:ASN:ND2	2.50	0.45
19:Z:51:VAL:HG12	19:Z:52:LEU:CD2	2.36	0.45
3:C:151:TRP:C	3:C:153:ASP:N	2.70	0.45
2:B:171:PRO:HD3	7:H:64:LEU:HD11	1.98	0.45
1:A:117:PHE:O	1:A:121:LEU:HG	2.16	0.45
23:A:350:CLA:H121	26:A:353:PL9:C16	2.43	0.45
16:V:30:LYS:HG2	16:V:118:HIS:NE2	2.32	0.45
28:C:488:BCR:C21	10:K:23:PHE:HE2	2.29	0.45
3:C:169:GLY:O	3:C:173:LEU:CD1	2.65	0.45
1:A:14:TRP:CH2	1:A:18:CYS:SG	3.09	0.45
2:B:194:ASN:O	2:B:196:GLY:N	2.50	0.45
19:Z:2:THR:O	19:Z:6:GLN:HG3	2.17	0.45
3:C:313:GLN:O	3:C:317:PHE:HD1	2.00	0.45
13:O:110:MET:CE	13:O:110:MET:H	2.28	0.45
5:E:25:THR:HG21	25:E:84:HEM:C3B	2.51	0.45
1:A:52:PHE:O	1:A:52:PHE:HD2	1.98	0.45
4:D:279:LEU:N	4:D:279:LEU:HD23	2.32	0.45
1:A:303:ASN:HB2	3:C:415:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:ILE:HD11	1:A:336:ALA:HB1	1.99	0.45
3:C:178:LYS:O	3:C:178:LYS:CG	2.64	0.45
3:C:435:PHE:O	3:C:436:PHE:C	2.55	0.45
15:U:100:ARG:O	15:U:101:GLN:C	2.55	0.45
2:B:219:VAL:HG12	2:B:220:ARG:N	2.32	0.45
3:C:456:GLU:C	4:D:230:SER:CB	2.85	0.45
5:E:25:THR:HG23	25:E:84:HEM:HAB	1.98	0.45
2:B:113:TRP:HB3	23:B:525:CLA:CED	2.41	0.45
2:B:12:LEU:HG	2:B:19:LEU:HD13	1.97	0.45
14:T:18:PHE:HD2	14:T:19:PHE:CE1	2.35	0.45
10:K:9:PHE:HE2	19:Z:13:VAL:HG21	1.81	0.45
13:O:38:TYR:O	13:O:245:PRO:CB	2.65	0.45
23:C:477:CLA:HAA2	23:C:477:CLA:HBD	1.97	0.45
3:C:336:GLY:O	13:O:104:GLN:HG2	2.17	0.45
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.49	0.45
3:C:229:ASN:HD21	3:C:231:GLU:HB2	1.82	0.45
2:B:422:ARG:H	2:B:422:ARG:HG3	1.57	0.45
16:V:111:ASP:O	16:V:115:ILE:HG13	2.16	0.45
8:I:5:LYS:HG3	8:I:9:TYR:HE1	1.82	0.45
4:D:231:THR:HG22	4:D:232:PHE:H	1.81	0.45
14:T:29:ILE:O	14:T:29:ILE:HG22	2.16	0.45
3:C:297:TYR:CG	3:C:302:TYR:HE1	2.35	0.45
15:U:58:ASN:HB2	15:U:59:ASN:ND2	2.32	0.45
19:Z:19:MET:CE	19:Z:43:GLY:HA3	2.47	0.45
1:A:224:ILE:HD11	1:A:243:GLU:CG	2.47	0.45
1:A:300:PHE:CD2	3:C:404:LEU:HB2	2.52	0.45
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.97	0.45
2:B:152:GLY:C	23:B:515:CLA:HMC3	2.37	0.45
12:M:8:LEU:HD22	14:T:1:MET:HE1	1.98	0.45
1:A:289:GLY:O	1:A:293:MET:HG3	2.16	0.45
2:B:194:ASN:C	2:B:196:GLY:H	2.20	0.45
1:A:193:LEU:HB3	4:D:179:PHE:CD2	2.52	0.45
2:B:135:LEU:O	2:B:138:MET:N	2.50	0.45
4:D:129:GLN:NE2	4:D:142:ASN:HB3	2.32	0.45
3:C:63:TRP:CZ3	3:C:88:LEU:HD11	2.52	0.45
3:C:80:PRO:O	3:C:81:MET:C	2.53	0.45
15:U:113:THR:CG2	15:U:114:VAL:N	2.78	0.45
3:C:276:LEU:HD23	3:C:440:GLY:O	2.17	0.45
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.99	0.45
2:B:315:ILE:HD13	2:B:359:MET:CE	2.47	0.45
28:B:529:BCR:H403	12:M:6:LEU:HD12	1.99	0.45
3:C:294:ASN:C	3:C:296:VAL:N	2.70	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:271:THR:HG22	2:B:448:ARG:HH11	1.82	0.45
16:V:5:PRO:O	16:V:6:GLU:C	2.55	0.45
2:B:302:TRP:CE3	2:B:343:HIS:HB2	2.52	0.45
2:B:302:TRP:CH2	2:B:343:HIS:CG	3.05	0.45
13:O:163:GLY:HA3	13:O:188:LYS:CE	2.45	0.45
4:D:19:ASP:O	4:D:23:LYS:HG3	2.16	0.45
3:C:395:TYR:O	3:C:396:MET:C	2.55	0.45
2:B:451:PHE:CD1	2:B:451:PHE:O	2.69	0.45
14:T:26:PRO:HA	14:T:27:PRO:HD3	1.83	0.45
1:A:161:TYR:O	1:A:162:PRO:C	2.54	0.45
1:A:307:ILE:HG12	1:A:314:ILE:HD11	1.92	0.45
19:Z:33:TRP:CE3	19:Z:37:LYS:HD3	2.30	0.45
3:C:205:ASP:O	3:C:208:VAL:HG12	2.17	0.45
1:A:87:ASN:HD21	3:C:357:ARG:NH1	2.08	0.45
1:A:235:TYR:HA	4:D:265:ARG:HH22	1.77	0.45
2:B:156:PHE:HB2	23:B:515:CLA:HAC1	1.99	0.45
16:V:64:PRO:HB2	16:V:65:PRO:HD2	1.98	0.45
1:A:38:ILE:O	1:A:42:LEU:HG	2.17	0.45
13:O:140:THR:HG22	13:O:201:VAL:HB	1.98	0.44
5:E:25:THR:O	5:E:28:ALA:HB3	2.16	0.44
9:J:8:ILE:HA	9:J:9:PRO:HD3	1.82	0.44
1:A:192:ILE:O	1:A:193:LEU:C	2.55	0.44
2:B:234:ILE:O	2:B:237:VAL:N	2.43	0.44
1:A:295:PHE:HB3	3:C:291:TRP:CH2	2.53	0.44
3:C:105:VAL:CG1	3:C:107:ASP:O	2.65	0.44
3:C:339:LYS:NZ	15:U:125:GLY:HA3	2.32	0.44
5:E:56:ALA:CB	5:E:82:LEU:HD23	2.38	0.44
16:V:25:GLN:O	16:V:28:GLU:N	2.51	0.44
2:B:258:TYR:N	2:B:258:TYR:CD2	2.85	0.44
13:O:68:THR:HA	13:O:110:MET:CE	2.47	0.44
23:A:350:CLA:HMA1	24:D:355:PHO:C20	2.47	0.44
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.83	0.44
5:E:10:SER:HA	5:E:13:ILE:CD1	2.27	0.44
1:A:224:ILE:HG13	1:A:245:THR:O	2.18	0.44
8:I:7:THR:HA	8:I:10:ILE:HD12	1.98	0.44
4:D:89:LEU:CB	4:D:91:LEU:HD21	2.47	0.44
1:A:95:PRO:CG	1:A:98:GLU:HB2	2.48	0.44
3:C:435:PHE:O	3:C:438:LEU:N	2.48	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
13:O:211:ILE:CG2	13:O:212:ALA:H	2.29	0.44
4:D:68:LEU:HD23	5:E:48:THR:HB	1.99	0.44
2:B:190:PHE:CE1	23:B:527:CLA:CED	3.01	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:156:VAL:O	4:D:161:PRO:HD3	2.17	0.44
3:C:296:VAL:HG21	23:C:479:CLA:HMA2	1.99	0.44
4:D:300:SER:N	11:L:37:ASN:OD1	2.51	0.44
10:K:27:ALA:O	10:K:31:GLN:HG2	2.18	0.44
1:A:29:TYR:CE1	1:A:31:GLY:CA	2.93	0.44
13:O:153:THR:CG2	13:O:154:ALA:N	2.81	0.44
4:D:281:MET:HE1	4:D:284:ILE:HD12	1.99	0.44
3:C:376:ASP:OD1	3:C:378:ASN:N	2.50	0.44
2:B:31:ALA:HB2	23:B:518:CLA:CBC	2.47	0.44
3:C:220:GLY:H	23:C:487:CLA:HBC1	1.82	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
4:D:102:THR:HG23	5:E:46:PHE:C	2.38	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HA	1.98	0.44
13:O:218:GLU:HG3	13:O:233:VAL:O	2.17	0.44
13:O:55:GLU:HG2	13:O:64:GLU:HG3	2.00	0.44
4:D:91:LEU:CD2	4:D:91:LEU:N	2.73	0.44
3:C:311:GLN:NE2	3:C:355:THR:O	2.50	0.44
3:C:136:GLY:HA2	3:C:137:PRO:HD3	1.77	0.44
2:B:436:THR:O	2:B:437:LEU:HD23	2.17	0.44
1:A:104:GLU:O	1:A:105:TRP:C	2.56	0.44
16:V:79:PRO:HG3	16:V:89:ALA:HA	1.99	0.44
9:J:25:VAL:O	9:J:26:GLY:C	2.54	0.44
3:C:286:ALA:O	3:C:290:VAL:N	2.49	0.44
3:C:50:LEU:HD23	23:C:482:CLA:HMD3	2.00	0.44
4:D:88:SER:CB	5:E:68:ARG:NH2	2.74	0.44
1:A:238:LYS:O	1:A:239:PHE:C	2.55	0.44
2:B:478:VAL:O	2:B:481:GLY:N	2.47	0.44
4:D:296:TYR:O	4:D:296:TYR:CG	2.70	0.44
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.52	0.44
2:B:397:VAL:CG1	2:B:398:THR:H	2.28	0.44
13:O:55:GLU:HB3	13:O:61:GLN:NE2	2.32	0.44
2:B:370:LEU:HD12	2:B:379:ALA:HB3	1.99	0.44
16:V:92:HIS:CE1	16:V:93:PRO:HD2	2.52	0.44
14:T:13:ILE:HG22	14:T:13:ILE:O	2.17	0.44
2:B:12:LEU:HD21	2:B:22:ALA:CB	2.48	0.44
4:D:158:LEU:C	4:D:161:PRO:HD2	2.37	0.44
11:L:24:ILE:HD11	12:M:18:PRO:HB2	2.00	0.44
3:C:287:THR:HG23	3:C:427:ALA:HA	1.99	0.44
3:C:85:GLY:C	3:C:86:LEU:HD23	2.37	0.44
3:C:270:ALA:O	3:C:274:TYR:CE1	2.71	0.44
1:A:230:THR:CG2	1:A:231:GLU:H	2.20	0.44
1:A:330:VAL:HG12	4:D:348:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:U:133:TYR:O	15:U:134:LYS:OXT	2.36	0.44
1:A:97:TRP:CZ3	8:I:8:VAL:HG21	2.49	0.44
4:D:42:TYR:CZ	6:F:24:THR:CG2	3.00	0.44
19:Z:39:LEU:HG	19:Z:39:LEU:H	1.39	0.44
1:A:269:ARG:HD3	1:A:270:SER:N	2.32	0.44
1:A:107:TYR:HD1	13:O:115:ARG:NH1	2.16	0.44
15:U:62:ILE:CG2	15:U:76:ALA:HB1	2.47	0.44
1:A:149:ALA:CA	1:A:284:TRP:CZ3	3.00	0.44
1:A:213:ALA:O	1:A:217:SER:CB	2.65	0.44
4:D:57:SER:CB	4:D:79:SER:HB2	2.48	0.44
1:A:78:ILE:CD1	11:L:34:TYR:CE1	2.99	0.44
3:C:217:PRO:HA	3:C:222:GLY:HA2	2.00	0.44
23:C:476:CLA:H61	23:C:483:CLA:H72	1.99	0.44
10:K:6:TYR:CD1	10:K:6:TYR:N	2.86	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HB3	2.52	0.44
19:Z:5:PHE:HD2	19:Z:5:PHE:O	2.01	0.44
3:C:93:ALA:CB	3:C:301:PHE:CE1	3.01	0.44
2:B:350:GLU:N	2:B:350:GLU:OE1	2.50	0.44
4:D:28:VAL:HG12	4:D:28:VAL:O	2.17	0.44
1:A:315:ASN:O	4:D:63:LEU:HD22	2.16	0.44
3:C:201:ASN:CG	3:C:201:ASN:O	2.57	0.44
13:O:33:ASP:O	13:O:36:GLN:HB2	2.17	0.44
4:D:350:ASN:HD22	4:D:351:ALA:N	2.16	0.44
4:D:350:ASN:ND2	4:D:351:ALA:N	2.65	0.44
3:C:317:PHE:O	3:C:321:ASP:OD1	2.36	0.44
26:A:353:PL9:H23	26:A:353:PL9:H271	1.42	0.44
2:B:200:ALA:C	23:B:521:CLA:HBB1	2.38	0.44
23:B:519:CLA:H142	23:D:356:CLA:H11	1.99	0.44
4:D:161:PRO:HG3	4:D:170:ALA:CB	2.46	0.44
3:C:89:ILE:HB	3:C:90:PRO:CD	2.44	0.44
3:C:157:MET:HE2	3:C:160:ILE:CD1	2.34	0.44
3:C:274:TYR:HB3	23:C:485:CLA:C3B	2.48	0.44
5:E:68:ARG:NH1	7:H:50:SER:O	2.50	0.44
4:D:146:PHE:O	4:D:149:PRO:HD2	2.18	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
4:D:101:PHE:O	4:D:102:THR:C	2.56	0.44
1:A:54:ALA:O	1:A:55:ALA:C	2.55	0.44
4:D:110:LEU:O	4:D:111:TRP:C	2.55	0.44
3:C:299:SER:O	3:C:303:GLY:O	2.36	0.44
15:U:75:LEU:CD2	15:U:101:GLN:NE2	2.81	0.44
13:O:31:PRO:HB2	13:O:33:ASP:H	1.83	0.44
13:O:190:PHE:CE1	15:U:120:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:40:GLN:NE2	9:J:27:LEU:O	2.48	0.43
1:A:187:GLN:HE21	1:A:187:GLN:HB3	1.50	0.43
1:A:41:LEU:HD13	24:A:351:PHO:C2	2.48	0.43
3:C:243:ILE:HG22	23:C:474:CLA:HMC1	2.00	0.43
2:B:264:PRO:HD2	2:B:268:PHE:HE1	1.83	0.43
1:A:341:LEU:HD21	15:U:134:LYS:HZ2	1.81	0.43
1:A:326:LEU:HD13	3:C:412:THR:CG2	2.39	0.43
5:E:33:GLY:O	5:E:36:PHE:N	2.48	0.43
15:U:47:LEU:HB3	15:U:51:TYR:HD1	1.83	0.43
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.18	0.43
2:B:360:PRO:C	2:B:362:PHE:N	2.71	0.43
3:C:350:ILE:CG2	3:C:351:PHE:N	2.81	0.43
2:B:234:ILE:HG21	23:B:524:CLA:H193	2.00	0.43
12:M:16:LEU:O	12:M:17:VAL:C	2.53	0.43
15:U:88:VAL:HG12	15:U:109:LEU:CD1	2.48	0.43
16:V:134:LYS:C	16:V:137:TYR:H	2.22	0.43
4:D:101:PHE:O	4:D:104:TRP:N	2.52	0.43
13:O:32:ILE:HA	13:O:133:VAL:HG11	2.00	0.43
3:C:189:TRP:O	3:C:190:ALA:O	2.36	0.43
13:O:182:LEU:O	13:O:183:ALA:C	2.55	0.43
13:O:243:ILE:CG2	13:O:244:GLU:N	2.81	0.43
2:B:18:ARG:NH1	2:B:115:TRP:O	2.50	0.43
4:D:178:ILE:O	4:D:181:PHE:HB3	2.19	0.43
1:A:160:ILE:H	1:A:160:ILE:HG13	1.66	0.43
3:C:48:LYS:HD3	3:C:133:ALA:O	2.18	0.43
5:E:55:TYR:O	16:V:1:ALA:HB2	2.17	0.43
2:B:418:LYS:O	2:B:419:SER:C	2.55	0.43
7:H:59:VAL:O	7:H:59:VAL:CG1	2.64	0.43
2:B:156:PHE:CD1	2:B:156:PHE:N	2.86	0.43
2:B:91:TRP:HB3	23:B:515:CLA:H43	2.00	0.43
3:C:187:ASP:OD1	3:C:189:TRP:N	2.51	0.43
16:V:35:TYR:O	16:V:35:TYR:CD2	2.71	0.43
5:E:22:HIS:C	5:E:24:ILE:N	2.70	0.43
5:E:24:ILE:O	5:E:24:ILE:HG22	2.18	0.43
12:M:20:VAL:O	12:M:21:PHE:C	2.55	0.43
1:A:159:LEU:O	1:A:160:ILE:C	2.56	0.43
10:K:9:PHE:N	10:K:9:PHE:CD1	2.86	0.43
2:B:302:TRP:C	2:B:304:ALA:N	2.71	0.43
7:H:57:VAL:O	7:H:57:VAL:HG13	2.17	0.43
5:E:30:PHE:C	5:E:30:PHE:CD2	2.91	0.43
3:C:191:PRO:O	3:C:193:GLY:N	2.48	0.43
3:C:394:GLU:O	3:C:397:THR:HB	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:57:LYS:O	13:O:57:LYS:HG3	2.18	0.43
1:A:339:PHE:CE1	3:C:314:ALA:HA	2.53	0.43
1:A:162:PRO:CG	1:A:171:GLY:HA2	2.48	0.43
4:D:181:PHE:O	4:D:182:LEU:C	2.57	0.43
23:D:356:CLA:H12	7:H:42:LEU:CD2	2.48	0.43
3:C:94:THR:C	3:C:96:GLY:N	2.71	0.43
3:C:223:TRP:HD1	3:C:224:ILE:N	2.14	0.43
4:D:218:VAL:O	4:D:220:ASN:N	2.52	0.43
19:Z:13:VAL:HG13	19:Z:17:PHE:CE1	2.54	0.43
3:C:155:ASN:O	3:C:159:THR:OG1	2.27	0.43
3:C:167:VAL:CG1	23:C:482:CLA:H11	2.48	0.43
2:B:479:PHE:C	2:B:481:GLY:H	2.21	0.43
4:D:189:HIS:CE1	4:D:294:ARG:HH21	2.36	0.43
19:Z:42:LEU:O	19:Z:46:LEU:HB2	2.18	0.43
13:O:34:SER:O	13:O:35:SER:C	2.57	0.43
13:O:34:SER:C	13:O:36:GLN:N	2.69	0.43
4:D:273:PHE:O	4:D:277:THR:HB	2.17	0.43
2:B:234:ILE:HG23	23:B:524:CLA:H193	2.01	0.43
2:B:63:LEU:HD12	2:B:63:LEU:HA	1.87	0.43
4:D:195:PRO:HA	4:D:198:MET:HE3	1.95	0.43
4:D:195:PRO:O	4:D:199:MET:HG3	2.19	0.43
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.18	0.43
2:B:311:PHE:C	2:B:313:ASP:N	2.71	0.43
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.84	0.43
6:F:32:PHE:CE1	28:F:48:BCR:H14C	2.54	0.43
2:B:354:LEU:CD2	2:B:378:LYS:HG3	2.48	0.43
23:A:350:CLA:HMD3	4:D:182:LEU:HD11	2.01	0.43
2:B:327:THR:O	2:B:329:PRO:HD3	2.18	0.43
1:A:295:PHE:O	3:C:291:TRP:CH2	2.72	0.43
10:K:31:GLN:HB3	10:K:36:PHE:CD2	2.54	0.43
2:B:252:VAL:HG22	23:B:517:CLA:O1A	2.19	0.43
4:D:22:LEU:CD2	4:D:32:TRP:CE3	3.01	0.43
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.33	0.43
16:V:22:THR:N	16:V:25:GLN:NE2	2.65	0.43
2:B:297:THR:HB	2:B:299:GLU:OE1	2.18	0.43
1:A:290:ILE:HD11	23:A:348:CLA:OBD	2.19	0.43
23:A:350:CLA:HMA1	24:D:355:PHO:H201	2.00	0.43
14:T:10:PHE:HE2	14:T:14:ILE:HD11	1.83	0.43
19:Z:7:LEU:O	19:Z:11:ALA:CB	2.63	0.43
3:C:256:PRO:HA	23:C:474:CLA:HED3	2.01	0.43
13:O:58:ASN:O	13:O:59:LYS:HB2	2.19	0.43
2:B:265:ILE:C	2:B:267:LEU:H	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:L:6:ASN:N	11:L:6:ASN:HD22	2.15	0.43
13:O:126:VAL:O	13:O:126:VAL:HG12	2.18	0.43
1:A:301:ASN:HD22	1:A:301:ASN:N	2.16	0.43
1:A:234:ASN:C	4:D:265:ARG:HH12	2.22	0.43
10:K:34:VAL:CG1	10:K:34:VAL:O	2.64	0.43
14:T:1:MET:C	14:T:3:THR:N	2.68	0.43
3:C:377:LEU:HD21	13:O:99:ASP:OD2	2.18	0.43
3:C:355:THR:OG1	3:C:355:THR:O	2.37	0.43
2:B:135:LEU:N	2:B:136:PRO:HD2	2.33	0.43
2:B:237:VAL:CG2	23:B:524:CLA:HBC2	2.49	0.43
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.53	0.43
2:B:149:LEU:O	2:B:150:CYS:C	2.56	0.43
2:B:88:PRO:O	2:B:89:GLY:C	2.57	0.43
7:H:49:ASN:CG	7:H:49:ASN:O	2.57	0.43
1:A:196:PRO:HA	1:A:199:GLN:HB2	2.01	0.43
4:D:21:TRP:O	4:D:26:ARG:NH2	2.40	0.43
16:V:112:LEU:HA	16:V:112:LEU:HD23	1.80	0.43
1:A:104:GLU:O	1:A:107:TYR:N	2.41	0.43
1:A:89:ILE:HD13	1:A:94:TYR:CD1	2.54	0.43
5:E:48:THR:O	5:E:49:PRO:C	2.57	0.43
1:A:168:PHE:O	1:A:169:SER:C	2.57	0.43
2:B:6:TYR:HE1	2:B:8:VAL:HG21	1.83	0.43
4:D:204:VAL:HG21	23:D:354:CLA:HMA1	2.01	0.43
4:D:55:VAL:O	4:D:65:SER:HB3	2.18	0.43
16:V:100:ILE:O	16:V:102:PRO:HD3	2.19	0.43
23:C:484:CLA:C4B	28:C:489:BCR:H393	2.48	0.43
10:K:8:ILE:H	10:K:8:ILE:HG13	1.68	0.43
13:O:152:ARG:HD2	13:O:156:PHE:CZ	2.54	0.43
5:E:33:GLY:O	5:E:36:PHE:HB3	2.18	0.43
16:V:35:TYR:C	16:V:35:TYR:CD2	2.92	0.43
15:U:87:SER:HB3	15:U:90:ASP:OD1	2.19	0.43
4:D:328:TRP:CE2	4:D:346:LEU:HD13	2.54	0.43
16:V:79:PRO:CB	16:V:88:ILE:HG12	2.44	0.42
23:B:522:CLA:H171	23:B:525:CLA:HMD1	1.99	0.42
15:U:58:ASN:C	15:U:59:ASN:ND2	2.70	0.42
10:K:10:ASP:O	10:K:11:PRO:C	2.58	0.42
3:C:274:TYR:CE2	23:C:477:CLA:HED3	2.53	0.42
11:L:6:ASN:OD1	11:L:8:GLN:HG2	2.19	0.42
2:B:368:VAL:HG22	2:B:425:ILE:HD12	2.01	0.42
13:O:33:ASP:O	13:O:37:THR:N	2.50	0.42
18:N:31:UNK:HA	19:Z:30:PRO:HG2	2.01	0.42
16:V:104:MET:HE3	16:V:107:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:43:LEU:HD11	13:O:239:PHE:CD1	2.53	0.42
25:E:84:HEM:O1D	6:F:18:ARG:NE	2.48	0.42
1:A:150:PRO:O	1:A:151:LEU:C	2.55	0.42
13:O:122:VAL:O	13:O:125:LEU:HB2	2.19	0.42
2:B:331:ASN:C	2:B:333:GLY:H	2.21	0.42
3:C:116:VAL:HG11	28:C:489:BCR:H321	2.00	0.42
3:C:276:LEU:HD13	23:C:483:CLA:HBB1	2.01	0.42
10:K:30:TRP:HE3	10:K:31:GLN:HE21	1.65	0.42
4:D:221:THR:HG22	4:D:245:SER:H	1.84	0.42
13:O:54:GLU:OE1	13:O:114:GLU:OE1	2.37	0.42
2:B:323:GLY:N	4:D:294:ARG:O	2.49	0.42
4:D:350:ASN:O	4:D:351:ALA:HB3	2.19	0.42
9:J:3:SER:N	18:N:32:UNK:CB	2.82	0.42
5:E:14:THR:HG22	9:J:8:ILE:CD1	2.44	0.42
5:E:14:THR:HG22	9:J:8:ILE:HD12	1.88	0.42
2:B:327:THR:O	2:B:329:PRO:N	2.53	0.42
4:D:170:ALA:O	4:D:171:PRO:C	2.56	0.42
1:A:142:TRP:HH2	1:A:273:PHE:CE1	2.34	0.42
3:C:204:LEU:HD12	3:C:239:TRP:HE1	1.84	0.42
13:O:104:GLN:HB3	13:O:151:TYR:HE1	1.85	0.42
1:A:307:ILE:HG22	1:A:309:ALA:HB3	2.00	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.02	0.42
3:C:108:THR:HG21	10:K:2:LEU:CG	2.47	0.42
3:C:315:MET:O	3:C:319:ILE:HG13	2.18	0.42
5:E:30:PHE:HD2	5:E:30:PHE:C	2.23	0.42
15:U:51:TYR:HB3	15:U:52:GLY:H	1.34	0.42
15:U:130:ASN:O	15:U:131:GLY:C	2.57	0.42
4:D:316:THR:O	4:D:317:LYS:C	2.58	0.42
1:A:57:PRO:CA	1:A:68:SER:HB3	2.49	0.42
3:C:324:LEU:HD23	3:C:324:LEU:HA	1.77	0.42
16:V:37:CYS:HB2	16:V:38:ALA:H	1.71	0.42
23:B:524:CLA:O1D	23:B:524:CLA:H93	2.20	0.42
3:C:81:MET:HE2	3:C:90:PRO:HG3	2.02	0.42
3:C:139:THR:HG23	3:C:139:THR:O	2.19	0.42
3:C:443:TRP:CA	3:C:443:TRP:CE3	3.00	0.42
3:C:168:LEU:HD21	23:C:478:CLA:H72	2.02	0.42
3:C:213:LEU:HD11	23:C:474:CLA:H171	2.01	0.42
3:C:159:THR:HA	3:C:252:ILE:HA	2.01	0.42
1:A:64:ARG:O	13:O:152:ARG:NH2	2.50	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.01	0.42
4:D:126:MET:SD	4:D:143:ALA:O	2.77	0.42
13:O:229:GLU:HA	13:O:230:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ILE:HD11	14:T:6:TYR:CD2	2.54	0.42
1:A:139:MET:CE	4:D:248:THR:CG2	2.97	0.42
4:D:273:PHE:O	4:D:277:THR:CB	2.67	0.42
17:X:17:LYS:O	17:X:20:PHE:N	2.52	0.42
8:I:13:THR:O	8:I:16:VAL:HB	2.19	0.42
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.49	0.42
2:B:245:VAL:HG22	23:B:513:CLA:H172	2.02	0.42
15:U:108:ASN:O	15:U:110:GLU:N	2.53	0.42
3:C:48:LYS:HZ2	23:C:486:CLA:HBA1	1.83	0.42
9:J:15:THR:CA	28:K:50:BCR:H372	2.45	0.42
4:D:249:ALA:O	4:D:252:PHE:HB3	2.20	0.42
1:A:55:ALA:HA	1:A:56:PRO:HD3	1.92	0.42
3:C:97:TRP:CE3	3:C:178:LYS:CE	3.02	0.42
6:F:32:PHE:CD1	28:F:48:BCR:H14C	2.54	0.42
1:A:297:LEU:CD2	3:C:428:THR:HG21	2.50	0.42
2:B:168:VAL:CG1	2:B:169:SER:N	2.83	0.42
4:D:20:ASP:O	4:D:24:ARG:N	2.52	0.42
2:B:49:ASP:HA	2:B:50:PRO:HD3	1.87	0.42
25:V:138:HEM:HMC1	25:V:138:HEM:HBC2	2.02	0.42
1:A:180:PHE:CE2	4:D:192:THR:O	2.68	0.42
1:A:76:ASN:CB	14:T:2:GLU:OE2	2.64	0.42
1:A:142:TRP:CH2	1:A:273:PHE:HE1	2.35	0.42
3:C:37:ALA:O	3:C:38:GLY:C	2.57	0.42
9:J:15:THR:HG23	28:K:50:BCR:H372	2.01	0.42
19:Z:47:TRP:HE1	19:Z:51:VAL:HG23	1.85	0.42
1:A:31:GLY:HA3	1:A:132:GLU:OE2	2.19	0.42
10:K:16:LEU:O	10:K:18:VAL:N	2.52	0.42
2:B:277:SER:O	2:B:278:SER:C	2.57	0.42
2:B:35:GLY:O	2:B:39:LEU:HG	2.19	0.42
2:B:106:LEU:HB3	23:B:522:CLA:H121	2.02	0.42
23:B:523:CLA:HAA2	23:B:523:CLA:HBD	2.01	0.42
1:A:160:ILE:O	1:A:164:GLY:N	2.46	0.42
16:V:29:GLY:HA3	16:V:118:HIS:HB2	2.02	0.42
3:C:38:GLY:HA3	23:C:486:CLA:C1D	2.50	0.42
4:D:146:PHE:O	4:D:150:ILE:HG13	2.20	0.42
2:B:340:TRP:CE3	2:B:342:GLY:CA	3.02	0.42
23:B:511:CLA:H102	7:H:37:PHE:CD1	2.55	0.42
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.02	0.42
7:H:51:THR:CG2	7:H:51:THR:O	2.68	0.42
4:D:116:LEU:O	4:D:120:PHE:HD1	2.03	0.42
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.42
1:A:339:PHE:HB3	3:C:313:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:81:THR:HB	16:V:83:ASP:OD1	2.19	0.42
9:J:30:TYR:O	9:J:33:TYR:HB2	2.20	0.42
4:D:186:GLN:NE2	4:D:192:THR:OG1	2.53	0.42
4:D:80:THR:CG2	4:D:81:PRO:HD2	2.49	0.42
3:C:60:ILE:O	23:C:480:CLA:HMD3	2.20	0.42
1:A:142:TRP:O	1:A:145:VAL:N	2.49	0.42
9:J:19:MET:HG2	28:K:50:BCR:H361	2.01	0.42
3:C:210:PHE:O	3:C:214:LEU:HG	2.20	0.42
1:A:63:ILE:HG23	3:C:335:THR:HG23	1.99	0.42
1:A:73:TYR:CD2	1:A:73:TYR:N	2.88	0.42
2:B:463:PHE:CZ	2:B:467:ILE:HD11	2.54	0.42
23:C:475:CLA:H51	28:J:53:BCR:H342	2.01	0.42
11:L:36:PHE:C	12:M:3:VAL:HG23	2.40	0.42
2:B:399:VAL:CG2	2:B:417:VAL:HG13	2.49	0.42
4:D:30:VAL:HG22	4:D:38:PHE:CE1	2.53	0.42
4:D:281:MET:O	4:D:284:ILE:HB	2.19	0.42
2:B:451:PHE:CZ	2:B:455:HIS:CE1	3.08	0.42
15:U:67:GLN:O	15:U:68:TYR:CD2	2.73	0.42
9:J:17:ALA:O	9:J:20:GLY:N	2.53	0.42
2:B:366:PHE:HA	2:B:367:PRO:HD3	1.71	0.42
23:B:512:CLA:OBD	23:B:520:CLA:HHC	2.20	0.42
23:B:516:CLA:H111	23:B:522:CLA:H42	2.00	0.42
14:T:18:PHE:CD2	14:T:19:PHE:CE1	3.08	0.42
3:C:307:PRO:O	3:C:308:GLU:C	2.57	0.42
3:C:289:PHE:CD1	23:C:487:CLA:HBB2	2.55	0.42
19:Z:9:LEU:HD12	19:Z:9:LEU:HA	1.83	0.42
3:C:259:TRP:HZ3	23:C:474:CLA:O2A	2.03	0.42
5:E:68:ARG:NH1	7:H:50:SER:HB3	2.34	0.42
2:B:56:TRP:HH2	2:B:312:TYR:HE2	1.67	0.42
2:B:325:PHE:O	2:B:328:GLY:N	2.52	0.42
1:A:21:VAL:HG13	1:A:30:VAL:O	2.19	0.42
3:C:173:LEU:HA	3:C:176:VAL:CG2	2.49	0.42
3:C:425:TRP:CE2	23:C:475:CLA:HBA2	2.54	0.42
13:O:198:SER:O	13:O:199:LEU:HD23	2.20	0.42
4:D:43:LEU:HD22	28:F:48:BCR:H323	2.02	0.42
2:B:223:GLN:HG2	2:B:227:LYS:HG3	2.01	0.42
1:A:327:GLY:HA3	4:D:324:GLY:O	2.20	0.42
1:A:315:ASN:C	4:D:63:LEU:HD22	2.39	0.42
4:D:67:TYR:C	6:F:39:MET:HE1	2.40	0.42
1:A:214:MET:HG2	26:A:353:PL9:HC8	2.02	0.42
2:B:19:LEU:HD23	23:B:524:CLA:H201	2.02	0.42
26:D:357:PL9:H38	14:T:18:PHE:CB	2.44	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:172:ALA:N	23:C:479:CLA:HAC1	2.35	0.42
4:D:90:LEU:HD11	4:D:96:GLU:CG	2.49	0.42
2:B:264:PRO:O	2:B:448:ARG:NH2	2.52	0.42
4:D:103:ARG:C	4:D:105:CYS:N	2.72	0.42
4:D:291:LEU:C	4:D:293:LEU:N	2.73	0.42
13:O:142:PHE:O	13:O:143:LYS:HG2	2.19	0.42
7:H:47:ILE:CG1	7:H:52:LEU:HD23	2.50	0.42
2:B:72:THR:HG22	2:B:79:SER:HB2	2.02	0.42
1:A:89:ILE:HG21	1:A:94:TYR:CB	2.46	0.41
13:O:101:ILE:HG22	13:O:102:ASP:N	2.35	0.41
13:O:75:THR:O	13:O:76:THR:C	2.57	0.41
4:D:48:TRP:CE3	24:D:355:PHO:H161	2.55	0.41
1:A:291:SER:O	1:A:295:PHE:CD1	2.73	0.41
1:A:141:PRO:O	3:C:443:TRP:CZ3	2.73	0.41
3:C:273:SER:CB	3:C:445:ALA:HB2	2.44	0.41
1:A:220:THR:O	1:A:223:LEU:HG	2.20	0.41
3:C:339:LYS:HE2	15:U:129:ASN:OD1	2.19	0.41
10:K:16:LEU:CB	10:K:17:PRO:CD	2.85	0.41
13:O:118:LEU:HD22	13:O:233:VAL:HG21	2.01	0.41
4:D:189:HIS:CE1	4:D:294:ARG:HE	2.38	0.41
4:D:301:GLN:O	4:D:302:GLU:C	2.58	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41
2:B:145:LEU:CD1	23:B:522:CLA:HAB	2.49	0.41
23:B:516:CLA:HAA2	23:B:516:CLA:HBD	2.02	0.41
16:V:129:LYS:NZ	16:V:135:VAL:HG23	2.35	0.41
3:C:49:LEU:O	3:C:52:ALA:N	2.53	0.41
9:J:19:MET:CG	28:K:50:BCR:H361	2.50	0.41
19:Z:52:LEU:O	19:Z:56:VAL:HG23	2.21	0.41
23:C:474:CLA:HBB2	23:C:485:CLA:HED1	2.01	0.41
3:C:339:LYS:HB2	3:C:340:TYR:CD1	2.54	0.41
3:C:199:ILE:HG22	3:C:200:THR:N	2.35	0.41
13:O:197:ILE:HG12	13:O:198:SER:N	2.35	0.41
14:T:9:ILE:CG2	14:T:9:ILE:O	2.68	0.41
13:O:207:ARG:O	13:O:210:GLU:OE2	2.38	0.41
5:E:41:LEU:O	5:E:42:ALA:C	2.59	0.41
1:A:337:HIS:ND1	4:D:352:LEU:HD12	2.35	0.41
15:U:62:ILE:HG12	15:U:80:VAL:HG21	2.02	0.41
16:V:63:THR:HG21	16:V:83:ASP:O	2.19	0.41
2:B:235:GLU:O	2:B:238:LEU:HB3	2.21	0.41
2:B:46:ASP:HA	2:B:47:PRO:HD3	1.68	0.41
3:C:89:ILE:O	3:C:92:ILE:N	2.53	0.41
3:C:195:ASP:OD1	3:C:195:ASP:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:78:GLU:HG3	16:V:105:ARG:NH1	2.35	0.41
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.37	0.41
11:L:31:PHE:O	11:L:32:SER:C	2.57	0.41
1:A:143:ILE:HD12	4:D:252:PHE:CE2	2.56	0.41
3:C:412:THR:HG22	16:V:136:TYR:CE2	2.52	0.41
2:B:175:THR:HG23	2:B:175:THR:O	2.21	0.41
8:I:27:ASP:CB	8:I:28:PRO:CD	2.88	0.41
2:B:372:ASP:OD1	2:B:373:LYS:N	2.53	0.41
17:X:34:PHE:O	17:X:35:ALA:C	2.58	0.41
16:V:22:THR:OG1	16:V:25:GLN:HG3	2.20	0.41
11:L:14:ARG:HA	12:M:26:TYR:CE1	2.55	0.41
1:A:339:PHE:CB	3:C:313:GLN:OE1	2.68	0.41
3:C:320:ARG:NE	15:U:128:TYR:CZ	2.77	0.41
1:A:160:ILE:HG21	1:A:291:SER:OG	2.20	0.41
4:D:199:MET:O	4:D:202:ALA:N	2.51	0.41
23:C:474:CLA:H122	23:C:485:CLA:H13	2.03	0.41
3:C:218:PHE:O	3:C:219:GLY:C	2.58	0.41
15:U:84:PRO:C	15:U:85:TYR:HD2	2.22	0.41
4:D:259:ILE:O	4:D:260:ALA:HB2	2.20	0.41
3:C:321:ASP:CG	15:U:128:TYR:CD2	2.94	0.41
16:V:79:PRO:CB	16:V:88:ILE:CG1	2.93	0.41
1:A:210:LEU:O	1:A:214:MET:HB2	2.20	0.41
3:C:222:GLY:O	3:C:223:TRP:O	2.38	0.41
3:C:98:GLY:C	3:C:99:VAL:HG23	2.41	0.41
1:A:140:ARG:HB2	4:D:220:ASN:CG	2.41	0.41
10:K:6:TYR:H	10:K:6:TYR:HD1	1.67	0.41
19:Z:47:TRP:CD1	19:Z:51:VAL:HG23	2.55	0.41
2:B:265:ILE:O	2:B:267:LEU:N	2.54	0.41
1:A:307:ILE:O	1:A:308:ASP:C	2.58	0.41
4:D:29:PHE:CD2	4:D:29:PHE:O	2.72	0.41
2:B:467:ILE:HD13	4:D:126:MET:HE3	2.01	0.41
18:N:22:UNK:O	18:N:23:UNK:C	2.68	0.41
14:T:27:PRO:HG2	14:T:27:PRO:O	2.21	0.41
4:D:342:PRO:HG2	4:D:345:VAL:CG2	2.51	0.41
2:B:288:VAL:O	2:B:292:LEU:HB2	2.21	0.41
1:A:58:VAL:HG13	1:A:107:TYR:O	2.21	0.41
3:C:320:ARG:HG2	15:U:128:TYR:CE2	2.56	0.41
3:C:343:ARG:HD3	3:C:344:SER:C	2.40	0.41
13:O:76:THR:HB	13:O:77:SER:H	1.29	0.41
1:A:207:GLY:HA3	1:A:278:TRP:CD1	2.56	0.41
14:T:14:ILE:O	14:T:17:PHE:HB2	2.21	0.41
3:C:90:PRO:CB	3:C:302:TYR:HE2	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:22:PRO:HG2	7:H:23:GLY:H	1.85	0.41
2:B:308:LYS:HE2	2:B:312:TYR:OH	2.20	0.41
7:H:43:ILE:HG12	17:X:19:PHE:CZ	2.56	0.41
3:C:190:ALA:HA	3:C:191:PRO:HA	1.49	0.41
13:O:157:LEU:HD23	13:O:157:LEU:HA	1.79	0.41
1:A:149:ALA:HA	1:A:284:TRP:CE3	2.56	0.41
23:B:513:CLA:H18	23:B:524:CLA:O1A	2.20	0.41
1:A:159:LEU:HD21	1:A:163:ILE:HD11	2.03	0.41
3:C:281:MET:C	3:C:285:ILE:HG13	2.41	0.41
3:C:443:TRP:CD1	23:C:483:CLA:HMD3	2.56	0.41
3:C:54:VAL:O	3:C:54:VAL:HG12	2.21	0.41
4:D:322:ASN:O	4:D:325:ILE:N	2.53	0.41
4:D:217:THR:OG1	4:D:253:TRP:HZ2	2.03	0.41
2:B:339:ALA:HB1	2:B:340:TRP:HD1	1.86	0.41
13:O:71:VAL:HG21	13:O:108:VAL:CG2	2.46	0.41
1:A:95:PRO:HG2	1:A:98:GLU:HB2	2.02	0.41
3:C:395:TYR:N	3:C:395:TYR:CD2	2.87	0.41
19:Z:31:GLN:O	19:Z:32:ASP:C	2.59	0.41
3:C:45:LEU:O	3:C:47:GLY:N	2.54	0.41
3:C:82:TYR:C	3:C:82:TYR:CD1	2.94	0.41
13:O:15:LEU:O	13:O:16:ALA:C	2.59	0.41
4:D:58:TRP:HA	4:D:62:GLY:N	2.32	0.41
1:A:40:THR:CG2	1:A:118:HIS:O	2.69	0.41
2:B:12:LEU:HD11	2:B:19:LEU:N	2.36	0.41
2:B:135:LEU:HB2	2:B:231:MET:CE	2.47	0.41
3:C:175:LEU:HD23	3:C:237:HIS:CD2	2.55	0.41
15:U:113:THR:HG22	15:U:114:VAL:H	1.82	0.41
15:U:57:LEU:HD23	15:U:57:LEU:HA	1.78	0.41
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.21	0.41
4:D:218:VAL:O	4:D:219:GLU:C	2.59	0.41
3:C:273:SER:HB2	23:C:477:CLA:HED1	2.02	0.41
3:C:275:SER:OG	23:C:485:CLA:HAA1	2.21	0.41
3:C:53:HIS:ND1	23:C:478:CLA:H141	2.35	0.41
2:B:385:ARG:HG3	13:O:165:ALA:C	2.41	0.41
1:A:341:LEU:HD21	15:U:134:LYS:HZ3	1.86	0.41
5:E:19:TRP:HZ2	9:J:13:VAL:CG2	2.27	0.41
2:B:315:ILE:HD13	2:B:359:MET:HE2	2.02	0.41
13:O:118:LEU:HD22	13:O:221:SER:HA	2.01	0.41
2:B:288:VAL:O	2:B:292:LEU:CB	2.68	0.41
1:A:208:GLY:O	1:A:212:CYS:HB2	2.20	0.41
15:U:65:PHE:CD1	15:U:76:ALA:CB	3.04	0.41
9:J:25:VAL:O	9:J:28:PHE:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:PHE:HD1	1:A:180:PHE:N	2.12	0.41
1:A:41:LEU:HD21	1:A:122:GLY:C	2.40	0.41
2:B:187:PRO:O	2:B:189:GLY:N	2.53	0.41
2:B:12:LEU:HG	2:B:19:LEU:CB	2.51	0.41
2:B:9:HIS:HE1	23:B:512:CLA:HED1	1.86	0.41
23:B:520:CLA:H51	28:B:529:BCR:H313	2.02	0.41
4:D:156:VAL:HG23	23:D:354:CLA:HED1	2.03	0.41
4:D:51:GLY:HA2	4:D:55:VAL:CG2	2.46	0.41
3:C:290:VAL:HG12	3:C:291:TRP:N	2.35	0.41
3:C:172:ALA:N	23:C:479:CLA:CAC	2.84	0.41
3:C:101:PRO:HA	3:C:195:ASP:HB3	2.02	0.41
3:C:62:PHE:CD2	10:K:20:PRO:HG3	2.56	0.41
28:C:488:BCR:C20	10:K:23:PHE:HE2	2.33	0.41
19:Z:47:TRP:NE1	19:Z:51:VAL:HG23	2.36	0.41
3:C:249:ILE:HG13	3:C:250:TRP:N	2.36	0.41
3:C:263:ALA:HB3	3:C:264:PHE:CD2	2.55	0.41
2:B:472:ARG:O	2:B:472:ARG:HG2	2.19	0.41
1:A:309:ALA:HB1	16:V:2:GLU:HA	2.03	0.41
23:B:514:CLA:H61	23:B:514:CLA:H41	1.93	0.41
2:B:33:TRP:HE1	23:B:514:CLA:HBC2	1.86	0.41
13:O:224:ASP:O	13:O:224:ASP:OD1	2.38	0.41
2:B:340:TRP:CZ3	2:B:407:ASN:HB3	2.55	0.41
7:H:29:LEU:HD12	7:H:29:LEU:HA	1.79	0.41
15:U:100:ARG:O	15:U:104:ILE:HG13	2.21	0.41
1:A:24:THR:OG1	4:D:251:ARG:NH2	2.53	0.41
13:O:205:ASP:O	13:O:206:GLY:C	2.58	0.41
4:D:125:PHE:CD2	4:D:125:PHE:O	2.74	0.41
2:B:135:LEU:O	2:B:137:LYS:N	2.54	0.41
2:B:9:HIS:CE1	23:B:512:CLA:HED1	2.55	0.41
23:B:516:CLA:H41	23:B:516:CLA:H61	1.94	0.41
3:C:81:MET:HE1	3:C:90:PRO:N	2.35	0.41
1:A:225:ARG:HG3	1:A:225:ARG:H	1.19	0.41
2:B:265:ILE:HG21	2:B:312:TYR:CE1	2.55	0.41
4:D:32:TRP:HA	4:D:32:TRP:HE3	1.82	0.41
1:A:325:ASN:H	1:A:325:ASN:HD22	1.69	0.41
2:B:201:HIS:CD2	2:B:202:HIS:N	2.89	0.41
4:D:341:PHE:HA	4:D:342:PRO:HD2	1.73	0.41
2:B:166:MET:CE	2:B:195:PRO:HB3	2.51	0.41
13:O:238:VAL:CG1	13:O:239:PHE:H	2.33	0.40
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.65	0.40
2:B:12:LEU:HD23	2:B:19:LEU:HD12	2.02	0.40
2:B:249:ALA:HB3	2:B:459:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:47:PRO:HA	2:B:78:TRP:NE1	2.36	0.40
7:H:42:LEU:HA	7:H:42:LEU:HD23	1.72	0.40
3:C:291:TRP:HZ3	3:C:424:SER:HA	1.86	0.40
19:Z:13:VAL:HG13	19:Z:17:PHE:HE1	1.86	0.40
2:B:271:THR:CG2	2:B:448:ARG:NH1	2.82	0.40
2:B:321:LYS:CG	2:B:322:GLY:N	2.84	0.40
2:B:325:PHE:CZ	4:D:297:ASP:OD2	2.74	0.40
13:O:152:ARG:HD2	13:O:156:PHE:CD1	2.56	0.40
2:B:211:ILE:HG22	2:B:212:ALA:N	2.36	0.40
1:A:53:ILE:O	1:A:53:ILE:CG2	2.69	0.40
5:E:50:ARG:HB3	5:E:51:PRO:HD2	2.03	0.40
2:B:91:TRP:CD1	23:B:515:CLA:H51	2.55	0.40
14:T:3:THR:C	14:T:5:THR:N	2.74	0.40
15:U:61:ASN:HB3	15:U:130:ASN:HD22	1.85	0.40
18:N:8:UNK:O	18:N:12:UNK:N	2.54	0.40
1:A:32:TRP:HA	1:A:35:VAL:CG2	2.51	0.40
2:B:445:THR:HG22	2:B:446:SER:N	2.35	0.40
4:D:303:ILE:HD13	12:M:2:GLU:OE1	2.21	0.40
7:H:38:LEU:HD23	7:H:38:LEU:HA	1.87	0.40
15:U:65:PHE:HD1	15:U:76:ALA:CB	2.34	0.40
1:A:183:MET:HA	23:A:348:CLA:HMD2	2.03	0.40
1:A:174:LEU:HD13	24:A:351:PHO:H143	2.02	0.40
1:A:41:LEU:HD21	1:A:122:GLY:HA3	2.04	0.40
1:A:40:THR:HG22	1:A:41:LEU:N	2.36	0.40
2:B:109:LEU:O	2:B:113:TRP:HE3	2.03	0.40
2:B:327:THR:N	28:B:529:BCR:H292	2.36	0.40
2:B:124:ARG:HG3	23:B:525:CLA:H43	2.03	0.40
3:C:297:TYR:HB3	3:C:302:TYR:HD1	1.86	0.40
3:C:305:THR:CB	3:C:308:GLU:HG3	2.51	0.40
23:C:479:CLA:CMD	23:C:481:CLA:H111	2.52	0.40
3:C:42:LEU:O	3:C:43:ILE:C	2.59	0.40
2:B:267:LEU:HA	2:B:267:LEU:HD23	1.95	0.40
1:A:131:TRP:O	1:A:134:SER:N	2.54	0.40
4:D:287:VAL:O	4:D:287:VAL:HG12	2.20	0.40
1:A:110:GLY:O	1:A:112:TYR:N	2.54	0.40
13:O:137:THR:O	13:O:140:THR:CG2	2.67	0.40
4:D:68:LEU:HA	4:D:68:LEU:HD12	1.84	0.40
1:A:52:PHE:CD1	1:A:81:ALA:CB	3.04	0.40
2:B:122:LEU:HB3	2:B:123:PHE:H	1.63	0.40
3:C:308:GLU:CG	3:C:361:PHE:CZ	2.98	0.40
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.86	0.40
15:U:108:ASN:C	15:U:112:PHE:HE1	2.25	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:19:ILE:O	10:K:23:PHE:HD1	2.05	0.40
28:C:489:BCR:H342	19:Z:51:VAL:HG13	2.03	0.40
3:C:271:TYR:N	3:C:271:TYR:CD2	2.90	0.40
1:A:239:PHE:C	1:A:241:GLN:N	2.73	0.40
3:C:176:VAL:HG11	3:C:238:ILE:HG12	2.04	0.40
13:O:168:TYR:CE1	13:O:172:ILE:CD1	3.01	0.40
3:C:425:TRP:NE1	23:C:475:CLA:HBA2	2.36	0.40
13:O:201:VAL:HG11	13:O:204:VAL:CG2	2.51	0.40
16:V:75:TYR:HD2	16:V:79:PRO:HA	1.82	0.40
16:V:81:THR:O	16:V:84:GLY:N	2.54	0.40
16:V:63:THR:CB	16:V:83:ASP:O	2.67	0.40
5:E:12:ILE:HB	25:E:84:HEM:HAD2	2.02	0.40
4:D:66:SER:O	4:D:71:CYS:SG	2.74	0.40
1:A:255:PHE:CD2	1:A:264:SER:HA	2.47	0.40
1:A:44:ALA:HB1	24:A:351:PHO:H91	2.02	0.40
3:C:240:ILE:HG13	23:C:479:CLA:HBB1	2.03	0.40
2:B:333:GLY:HA2	2:B:442:ILE:O	2.22	0.40
3:C:112:PHE:HE2	10:K:6:TYR:CZ	2.39	0.40
1:A:301:ASN:OD1	3:C:407:VAL:HG11	2.20	0.40
11:L:36:PHE:CE2	12:M:8:LEU:N	2.90	0.40
13:O:27:ARG:HG3	13:O:29:ALA:CB	2.48	0.40
16:V:24:LYS:HE2	16:V:28:GLU:OE2	2.21	0.40
3:C:189:TRP:O	3:C:190:ALA:C	2.59	0.40
2:B:258:TYR:N	2:B:258:TYR:HD2	2.19	0.40
1:A:48:PHE:HB2	1:A:115:ILE:HD13	2.03	0.40
16:V:10:VAL:HA	16:V:11:PRO:HD3	1.98	0.40
13:O:72:THR:HG22	13:O:75:THR:OG1	2.21	0.40
3:C:343:ARG:CB	13:O:78:LEU:CD1	2.99	0.40
2:B:225:LEU:HD23	2:B:229:LEU:HD12	2.03	0.40
23:D:356:CLA:H151	23:D:356:CLA:H112	1.92	0.40
19:Z:9:LEU:C	19:Z:11:ALA:N	2.73	0.40
3:C:162:GLY:HA3	3:C:248:GLY:O	2.21	0.40
1:A:243:GLU:O	1:A:244:GLU:HB2	2.22	0.40
4:D:190:ASN:ND2	4:D:193:LEU:CD1	2.85	0.40
2:B:346:PHE:CE2	2:B:399:VAL:HG22	2.57	0.40
13:O:120:PHE:HA	13:O:219:GLN:HE22	1.86	0.40
1:A:46:ILE:O	1:A:47:CYS:C	2.59	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:246:ALA:C	18:n:2035:UNK:O[2_555]	1.76	0.44
13:O:246:ALA:N	18:n:2035:UNK:O[2_555]	1.97	0.23
13:O:246:ALA:O	18:n:2035:UNK:O[2_555]	2.07	0.13
13:O:246:ALA:O	18:n:2035:UNK:CB[2_555]	2.15	0.05
13:O:246:ALA:N	18:n:2035:UNK:C[2_555]	2.17	0.03
13:O:246:ALA:CA	18:n:2035:UNK:O[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	331/344 (96%)	251 (76%)	58 (18%)	22 (7%)	2	28
1	a	331/344 (96%)	253 (76%)	56 (17%)	22 (7%)	2	28
2	B	474/510 (93%)	367 (77%)	84 (18%)	23 (5%)	3	37
2	b	474/510 (93%)	367 (77%)	83 (18%)	24 (5%)	3	36
3	C	419/473 (89%)	326 (78%)	60 (14%)	33 (8%)	1	22
3	c	419/473 (89%)	326 (78%)	62 (15%)	31 (7%)	2	24
4	D	337/352 (96%)	274 (81%)	49 (14%)	14 (4%)	4	43
4	d	337/352 (96%)	270 (80%)	51 (15%)	16 (5%)	4	39
5	E	74/84 (88%)	62 (84%)	10 (14%)	2 (3%)	8	56
5	e	74/84 (88%)	57 (77%)	14 (19%)	3 (4%)	4	44
6	F	31/45 (69%)	23 (74%)	5 (16%)	3 (10%)	1	16
6	f	31/45 (69%)	22 (71%)	6 (19%)	3 (10%)	1	16
7	H	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	32
7	h	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	32
8	I	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	8	55
8	i	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	3	34
9	J	36/40 (90%)	32 (89%)	3 (8%)	1 (3%)	8	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	36/40 (90%)	30 (83%)	4 (11%)	2 (6%)	3	34
10	K	35/37 (95%)	27 (77%)	2 (6%)	6 (17%)	0	4
10	k	35/37 (95%)	26 (74%)	3 (9%)	6 (17%)	0	4
11	L	35/37 (95%)	28 (80%)	3 (9%)	4 (11%)	1	12
11	l	35/37 (95%)	27 (77%)	5 (14%)	3 (9%)	1	19
12	M	28/36 (78%)	22 (79%)	5 (18%)	1 (4%)	5	49
12	m	28/36 (78%)	22 (79%)	4 (14%)	2 (7%)	2	25
13	O	244/246 (99%)	180 (74%)	44 (18%)	20 (8%)	1	21
13	o	244/246 (99%)	179 (73%)	45 (18%)	20 (8%)	1	21
14	T	29/32 (91%)	23 (79%)	3 (10%)	3 (10%)	1	14
14	t	29/32 (91%)	22 (76%)	5 (17%)	2 (7%)	2	27
15	U	103/134 (77%)	78 (76%)	14 (14%)	11 (11%)	1	13
15	u	103/134 (77%)	81 (79%)	11 (11%)	11 (11%)	1	13
16	V	135/137 (98%)	111 (82%)	16 (12%)	8 (6%)	2	32
16	v	135/137 (98%)	106 (78%)	22 (16%)	7 (5%)	3	35
17	X	38/50 (76%)	36 (95%)	1 (3%)	1 (3%)	8	57
17	x	38/50 (76%)	35 (92%)	2 (5%)	1 (3%)	8	57
19	Z	56/62 (90%)	39 (70%)	15 (27%)	2 (4%)	5	49
19	z	56/62 (90%)	40 (71%)	13 (23%)	3 (5%)	3	35
All	All	4984/5446 (92%)	3864 (78%)	801 (16%)	319 (6%)	2	29

All (319) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLY
1	A	228	THR
1	A	242	GLU
1	A	308	ASP
2	B	88	PRO
2	B	126	PRO
2	B	173	GLY
2	B	235	GLU
2	B	326	ARG
2	B	391	SER
3	C	37	ALA

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Mol	Chain	Res	Type
3	C	104	GLU
3	C	137	PRO
3	C	184	GLY
3	C	190	ALA
3	C	192	GLY
3	C	227	VAL
3	C	285	ILE
4	D	218	VAL
4	D	264	LYS
5	E	49	PRO
6	F	17	VAL
7	H	21	ALA
10	K	7	ALA
10	K	8	ILE
11	L	8	GLN
11	L	9	PRO
13	O	76	THR
13	O	77	SER
13	O	101	ILE
13	O	130	GLN
13	O	245	PRO
15	U	40	VAL
15	U	52	GLY
15	U	72	TYR
16	V	38	ALA
17	X	14	PRO
1	a	2090	GLY
1	a	2141	PRO
1	a	2228	THR
2	b	2088	PRO
2	b	2126	PRO
2	b	2173	GLY
2	b	2235	GLU
2	b	2326	ARG
2	b	2391	SER
3	c	2037	ALA
3	c	2104	GLU
3	c	2184	GLY
3	c	2190	ALA
3	c	2191	PRO
3	c	2192	GLY
3	c	2285	ILE

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Mol	Chain	Res	Type
4	d	2218	VAL
4	d	2264	LYS
5	e	2049	PRO
6	f	2017	VAL
7	h	2021	ALA
10	k	2007	ALA
10	k	2008	ILE
11	l	2009	PRO
13	o	2076	THR
13	o	2077	SER
13	o	2130	GLN
13	o	2245	PRO
15	u	2040	VAL
15	u	2051	TYR
15	u	2052	GLY
15	u	2072	TYR
16	v	2038	ALA
17	x	2014	PRO
1	A	32	TRP
1	A	141	PRO
1	A	160	ILE
1	A	225	ARG
1	A	239	PHE
1	A	243	GLU
1	A	317	TRP
1	A	335	ASN
2	B	186	GLY
2	B	201	HIS
2	B	230	ARG
2	B	328	GLY
2	B	396	GLY
3	C	43	ILE
3	C	183	GLY
3	C	219	GLY
3	C	295	THR
3	C	453	ALA
4	D	109	GLY
4	D	156	VAL
4	D	219	GLU
4	D	292	ASN
5	E	10	SER
6	F	40	GLN

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Mol	Chain	Res	Type
7	H	23	GLY
10	K	11	PRO
10	K	17	PRO
13	O	56	PRO
13	O	131	PRO
13	O	206	GLY
13	O	216	GLU
14	T	4	ILE
15	U	48	GLY
15	U	51	TYR
15	U	63	ALA
15	U	73	PRO
15	U	120	ALA
15	U	121	LEU
15	U	125	GLY
15	U	131	GLY
16	V	82	TYR
19	Z	32	ASP
1	a	2032	TRP
1	a	2160	ILE
1	a	2225	ARG
1	a	2239	PHE
1	a	2242	GLU
1	a	2243	GLU
1	a	2308	ASP
2	b	2186	GLY
2	b	2201	HIS
2	b	2230	ARG
2	b	2328	GLY
2	b	2396	GLY
3	c	2137	PRO
3	c	2183	GLY
3	c	2219	GLY
3	c	2227	VAL
3	c	2295	THR
3	c	2453	ALA
4	d	2109	GLY
4	d	2219	GLU
4	d	2292	ASN
4	d	2299	ILE
5	e	2010	SER
6	f	2040	GLN

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Mol	Chain	Res	Type
7	h	2023	GLY
10	k	2011	PRO
11	l	2008	GLN
13	o	2056	PRO
13	o	2078	LEU
13	o	2101	ILE
13	o	2161	GLY
13	o	2206	GLY
14	t	2004	ILE
15	u	2048	GLY
15	u	2063	ALA
15	u	2073	PRO
15	u	2120	ALA
15	u	2121	LEU
15	u	2131	GLY
16	v	2082	TYR
1	A	215	HIS
2	B	187	PRO
2	B	222	PRO
2	B	223	GLN
2	B	312	TYR
2	B	319	PRO
2	B	361	ALA
3	C	80	PRO
3	C	110	PRO
3	C	191	PRO
3	C	223	TRP
3	C	334	PRO
3	C	355	THR
3	C	415	ASN
3	C	454	GLY
4	D	260	ALA
4	D	299	ILE
7	H	22	PRO
9	J	28	PHE
13	O	28	GLY
13	O	78	LEU
13	O	149	PRO
13	O	161	GLY
16	V	16	GLY
16	V	99	ASP
1	a	2191	ASN

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Mol	Chain	Res	Type
1	a	2259	ILE
1	a	2317	TRP
2	b	2187	PRO
2	b	2222	PRO
2	b	2223	GLN
2	b	2319	PRO
2	b	2361	ALA
3	c	2110	PRO
3	c	2152	LYS
3	c	2223	TRP
3	c	2355	THR
3	c	2413	GLU
3	c	2415	ASN
4	d	2239	GLN
4	d	2260	ALA
4	d	2343	GLU
6	f	2019	TRP
7	h	2022	PRO
9	j	2028	PHE
10	k	2017	PRO
13	o	2131	PRO
13	o	2149	PRO
13	o	2180	GLU
13	o	2216	GLU
15	u	2125	GLY
16	v	2016	GLY
19	z	2032	ASP
1	A	167	SER
1	A	191	ASN
1	A	208	GLY
1	A	259	ILE
1	A	300	PHE
1	A	301	ASN
1	A	334	ARG
3	C	46	SER
3	C	85	GLY
3	C	152	LYS
3	C	195	ASP
3	C	298	PRO
3	C	420	VAL
4	D	132	ILE
4	D	166	SER

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Mol	Chain	Res	Type
4	D	239	GLN
4	D	343	GLU
13	O	114	GLU
14	T	27	PRO
16	V	133	GLY
19	Z	29	SER
1	a	2167	SER
1	a	2208	GLY
1	a	2215	HIS
1	a	2300	PHE
1	a	2301	ASN
2	b	2188	ASP
2	b	2312	TYR
3	c	2043	ILE
3	c	2334	PRO
3	c	2411	ALA
3	c	2420	VAL
4	d	2166	SER
13	o	2047	PRO
13	o	2114	GLU
14	t	2027	PRO
16	v	2021	LEU
16	v	2102	PRO
16	v	2131	GLY
2	B	188	ASP
3	C	413	GLU
4	D	131	GLU
6	F	19	TRP
8	I	32	PRO
10	K	16	LEU
13	O	47	PRO
13	O	180	GLU
16	V	102	PRO
16	V	107	LEU
16	V	131	GLY
1	a	2116	ILE
1	a	2244	GLU
2	b	2047	PRO
3	c	2046	SER
3	c	2080	PRO
3	c	2454	GLY
4	d	2101	PHE

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Mol	Chain	Res	Type
5	e	2057	GLN
10	k	2016	LEU
12	m	2005	GLN
13	o	2028	GLY
16	v	2133	GLY
19	z	2029	SER
1	A	116	ILE
2	B	47	PRO
3	C	380	ILE
11	L	2	GLU
14	T	3	THR
3	c	2085	GLY
3	c	2195	ASP
3	c	2298	PRO
3	c	2338	GLY
4	d	2113	PHE
4	d	2132	ILE
11	l	2002	GLU
12	m	2017	VAL
13	o	2175	PRO
1	A	63	ILE
2	B	16	PRO
3	C	101	PRO
3	C	117	VAL
13	O	159	PRO
13	O	244	GLU
1	a	2046	ILE
1	a	2063	ILE
2	b	2264	PRO
13	o	2159	PRO
2	B	211	ILE
2	B	322	GLY
3	C	338	GLY
13	O	122	VAL
2	b	2016	PRO
2	b	2211	ILE
2	b	2322	GLY
13	o	2122	VAL
10	K	2	LEU
11	L	4	ASN
2	b	2008	VAL
9	j	2016	VAL

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Mol	Chain	Res	Type
2	B	8	VAL
3	C	410	VAL
4	D	275	PRO
12	M	17	VAL
3	c	2380	ILE
4	d	2156	VAL
8	i	2008	VAL
8	i	2032	PRO
10	k	2002	LEU
13	o	2244	GLU
13	O	175	PRO
4	d	2095	PRO
4	d	2275	PRO
19	z	2013	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	244 (90%)	26 (10%)	12	51
1	a	270/280 (96%)	249 (92%)	21 (8%)	18	63
2	B	377/407 (93%)	355 (94%)	22 (6%)	28	75
2	b	377/407 (93%)	355 (94%)	22 (6%)	28	75
3	C	326/374 (87%)	306 (94%)	20 (6%)	26	73
3	c	326/374 (87%)	307 (94%)	19 (6%)	28	75
4	D	275/283 (97%)	257 (94%)	18 (6%)	24	71
4	d	275/283 (97%)	253 (92%)	22 (8%)	17	61
5	E	68/73 (93%)	65 (96%)	3 (4%)	39	83
5	e	68/73 (93%)	64 (94%)	4 (6%)	28	75
6	F	27/39 (69%)	25 (93%)	2 (7%)	20	66
6	f	27/39 (69%)	24 (89%)	3 (11%)	9	42
7	H	44/55 (80%)	41 (93%)	3 (7%)	22	70
7	h	44/55 (80%)	42 (96%)	2 (4%)	38	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	35/35 (100%)	31 (89%)	4 (11%)	8	40
8	i	35/35 (100%)	33 (94%)	2 (6%)	29	76
9	J	26/28 (93%)	25 (96%)	1 (4%)	44	85
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	23	70
10	k	30/30 (100%)	30 (100%)	0	100	100
11	L	35/35 (100%)	31 (89%)	4 (11%)	8	40
11	l	35/35 (100%)	31 (89%)	4 (11%)	8	40
12	M	27/33 (82%)	26 (96%)	1 (4%)	45	86
12	m	27/33 (82%)	26 (96%)	1 (4%)	45	86
13	O	208/208 (100%)	187 (90%)	21 (10%)	11	48
13	o	208/208 (100%)	190 (91%)	18 (9%)	15	57
14	T	28/29 (97%)	28 (100%)	0	100	100
14	t	28/29 (97%)	28 (100%)	0	100	100
15	U	89/112 (80%)	85 (96%)	4 (4%)	38	83
15	u	89/112 (80%)	84 (94%)	5 (6%)	30	76
16	V	117/117 (100%)	112 (96%)	5 (4%)	40	84
16	v	117/117 (100%)	112 (96%)	5 (4%)	40	84
17	X	33/42 (79%)	30 (91%)	3 (9%)	14	54
17	x	33/42 (79%)	29 (88%)	4 (12%)	7	36
19	Z	48/52 (92%)	42 (88%)	6 (12%)	7	35
19	z	48/52 (92%)	46 (96%)	2 (4%)	40	84
All	All	4126/4464 (92%)	3847 (93%)	279 (7%)	22	70

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	25	ASP
1	A	27	ARG
1	A	29	TYR
1	A	52	PHE
1	A	70	SER
1	A	84	PRO

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Mol	Chain	Res	Type
1	A	162	PRO
1	A	170	ASP
1	A	172	MET
1	A	177	SER
1	A	180	PHE
1	A	183	MET
1	A	187	GLN
1	A	212	CYS
1	A	214	MET
1	A	237	TYR
1	A	269	ARG
1	A	284	TRP
1	A	295	PHE
1	A	298	ASN
1	A	301	ASN
1	A	317	TRP
1	A	325	ASN
1	A	335	ASN
1	A	342	ASP
2	B	8	VAL
2	B	48	SER
2	B	57	ARG
2	B	130	GLU
2	B	139	PHE
2	B	167	TRP
2	B	216	HIS
2	B	240	SER
2	B	246	PHE
2	B	255	THR
2	B	285	ASN
2	B	286	ARG
2	B	311	PHE
2	B	318	ASN
2	B	334	ASP
2	B	340	TRP
2	B	362	PHE
2	B	372	ASP
2	B	385	ARG
2	B	402	TYR
2	B	409	GLN
2	B	479	PHE
3	C	110	PRO

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Mol	Chain	Res	Type
3	C	127	PHE
3	C	139	THR
3	C	149	TYR
3	C	198	VAL
3	C	201	ASN
3	C	264	PHE
3	C	289	PHE
3	C	290	VAL
3	C	292	PHE
3	C	293	ASN
3	C	294	ASN
3	C	295	THR
3	C	313	GLN
3	C	321	ASP
3	C	340	TYR
3	C	343	ARG
3	C	368	PRO
3	C	400	PRO
3	C	443	TRP
4	D	29	PHE
4	D	32	TRP
4	D	58	TRP
4	D	61	HIS
4	D	73	PHE
4	D	91	LEU
4	D	142	ASN
4	D	168	PHE
4	D	180	ARG
4	D	188	PHE
4	D	192	THR
4	D	211	CYS
4	D	220	ASN
4	D	254	SER
4	D	261	PHE
4	D	262	SER
4	D	336	HIS
4	D	340	VAL
5	E	16	VAL
5	E	30	PHE
5	E	49	PRO
6	F	12	TYR
6	F	31	PHE

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Mol	Chain	Res	Type
7	H	26	THR
7	H	48	TYR
7	H	57	VAL
8	I	16	VAL
8	I	18	LEU
8	I	27	ASP
8	I	30	ARG
9	J	38	SER
10	K	6	TYR
10	K	36	PHE
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
11	L	36	PHE
12	M	28	GLN
13	O	3	GLN
13	O	21	THR
13	O	34	SER
13	O	39	ARG
13	O	46	GLN
13	O	47	PRO
13	O	65	PHE
13	O	68	THR
13	O	104	GLN
13	O	110	MET
13	O	126	VAL
13	O	142	PHE
13	O	147	ASN
13	O	162	ARG
13	O	166	SER
13	O	174	LEU
13	O	190	PHE
13	O	193	THR
13	O	219	GLN
13	O	225	MET
13	O	245	PRO
15	U	51	TYR
15	U	59	ASN
15	U	61	ASN
15	U	132	LEU
16	V	4	THR
16	V	40	CYS

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Mol	Chain	Res	Type
16	V	55	ARG
16	V	78	ASN
16	V	130	TRP
17	X	13	THR
17	X	14	PRO
17	X	47	GLN
19	Z	5	PHE
19	Z	32	ASP
19	Z	34	ASP
19	Z	41	PHE
19	Z	42	LEU
19	Z	51	VAL
1	a	2015	GLU
1	a	2024	THR
1	a	2025	ASP
1	a	2027	ARG
1	a	2029	TYR
1	a	2033	PHE
1	a	2040	THR
1	a	2045	THR
1	a	2070	SER
1	a	2111	PRO
1	a	2180	PHE
1	a	2187	GLN
1	a	2237	TYR
1	a	2269	ARG
1	a	2278	TRP
1	a	2284	TRP
1	a	2286	THR
1	a	2295	PHE
1	a	2317	TRP
1	a	2335	ASN
1	a	2342	ASP
2	b	2008	VAL
2	b	2048	SER
2	b	2057	ARG
2	b	2130	GLU
2	b	2139	PHE
2	b	2167	TRP
2	b	2216	HIS
2	b	2240	SER
2	b	2246	PHE

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Mol	Chain	Res	Type
2	b	2255	THR
2	b	2286	ARG
2	b	2311	PHE
2	b	2318	ASN
2	b	2334	ASP
2	b	2340	TRP
2	b	2362	PHE
2	b	2372	ASP
2	b	2385	ARG
2	b	2392	PHE
2	b	2402	TYR
2	b	2409	GLN
2	b	2479	PHE
3	c	2046	SER
3	c	2110	PRO
3	c	2127	PHE
3	c	2139	THR
3	c	2149	TYR
3	c	2198	VAL
3	c	2201	ASN
3	c	2264	PHE
3	c	2285	ILE
3	c	2289	PHE
3	c	2292	PHE
3	c	2293	ASN
3	c	2294	ASN
3	c	2304	PRO
3	c	2310	SER
3	c	2321	ASP
3	c	2340	TYR
3	c	2403	SER
3	c	2443	TRP
4	d	2029	PHE
4	d	2032	TRP
4	d	2058	TRP
4	d	2061	HIS
4	d	2073	PHE
4	d	2081	PRO
4	d	2091	LEU
4	d	2130	PHE
4	d	2147	SER
4	d	2165	SER

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Mol	Chain	Res	Type
4	d	2168	PHE
4	d	2180	ARG
4	d	2188	PHE
4	d	2192	THR
4	d	2211	CYS
4	d	2220	ASN
4	d	2235	PHE
4	d	2254	SER
4	d	2261	PHE
4	d	2262	SER
4	d	2336	HIS
4	d	2350	ASN
5	e	2030	PHE
5	e	2049	PRO
5	e	2050	ARG
5	e	2053	SER
6	f	2012	TYR
6	f	2031	PHE
6	f	2043	GLN
7	h	2024	TRP
7	h	2026	THR
8	i	2027	ASP
8	i	2030	ARG
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
11	l	2036	PHE
12	m	2028	GLN
13	o	2005	LEU
13	o	2006	THR
13	o	2021	THR
13	o	2039	ARG
13	o	2047	PRO
13	o	2060	ARG
13	o	2068	THR
13	o	2103	PHE
13	o	2104	GLN
13	o	2110	MET
13	o	2147	ASN
13	o	2159	PRO
13	o	2166	SER
13	o	2174	LEU

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Mol	Chain	Res	Type
13	o	2193	THR
13	o	2225	MET
13	o	2239	PHE
13	o	2245	PRO
15	u	2051	TYR
15	u	2059	ASN
15	u	2061	ASN
15	u	2128	TYR
15	u	2132	LEU
16	v	2004	THR
16	v	2040	CYS
16	v	2050	PRO
16	v	2055	ARG
16	v	2093	PRO
17	x	2011	THR
17	x	2013	THR
17	x	2014	PRO
17	x	2047	GLN
19	z	2005	PHE
19	z	2051	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	199	GLN
1	A	296	ASN
1	A	301	ASN
1	A	303	ASN
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
2	B	233	ASN
2	B	285	ASN
2	B	318	ASN
2	B	331	ASN
2	B	374	ASN
2	B	395	GLN

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Mol	Chain	Res	Type
2	B	438	ASN
3	C	39	ASN
3	C	201	ASN
3	C	294	ASN
3	C	311	GLN
3	C	378	ASN
4	D	83	ASN
4	D	87	HIS
4	D	106	GLN
4	D	129	GLN
4	D	164	GLN
4	D	186	GLN
4	D	255	GLN
4	D	263	ASN
4	D	322	ASN
4	D	338	ASN
4	D	350	ASN
5	E	81	GLN
6	F	40	GLN
6	F	43	GLN
10	K	31	GLN
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
12	M	4	ASN
12	M	28	GLN
13	O	36	GLN
13	O	46	GLN
13	O	61	GLN
13	O	124	ASN
13	O	132	ASN
13	O	147	ASN
13	O	155	ASN
13	O	200	ASN
13	O	219	GLN
15	U	59	ASN
15	U	61	ASN
15	U	82	ASN
15	U	130	ASN
16	V	25	GLN
19	Z	6	GLN
1	a	2019	ASN

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Mol	Chain	Res	Type
1	a	2092	HIS
1	a	2165	GLN
1	a	2187	GLN
1	a	2199	GLN
1	a	2296	ASN
1	a	2301	ASN
1	a	2303	ASN
1	a	2322	ASN
1	a	2325	ASN
1	a	2335	ASN
2	b	2285	ASN
2	b	2318	ASN
2	b	2331	ASN
2	b	2343	HIS
2	b	2374	ASN
2	b	2395	GLN
2	b	2438	ASN
3	c	2039	ASN
3	c	2201	ASN
3	c	2294	ASN
3	c	2322	GLN
3	c	2405	ASN
4	d	2083	ASN
4	d	2087	HIS
4	d	2129	GLN
4	d	2142	ASN
4	d	2164	GLN
4	d	2186	GLN
4	d	2190	ASN
4	d	2250	ASN
4	d	2255	GLN
4	d	2263	ASN
4	d	2322	ASN
4	d	2338	ASN
4	d	2350	ASN
6	f	2040	GLN
6	f	2043	GLN
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
12	m	2004	ASN
12	m	2028	GLN

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Mol	Chain	Res	Type
13	o	2036	GLN
13	o	2046	GLN
13	o	2061	GLN
13	o	2124	ASN
13	o	2147	ASN
13	o	2155	ASN
13	o	2236	GLN
15	u	2059	ASN
15	u	2061	ASN
15	u	2108	ASN
15	u	2111	HIS
15	u	2130	ASN
16	v	2078	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 108 ligands modelled in this entry, 2 are monoatomic - leaving 106 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	BCT	A	346	22	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	OEC	A	347	1,3,21	7,13,13	20.40	7 (100%)	0,27,27	0.00	-
23	CLA	A	348	1	73,73,73	1.49	13 (17%)	95,113,113	1.67	21 (22%)
23	CLA	A	349	-	73,73,73	1.46	12 (16%)	95,113,113	1.90	24 (25%)
23	CLA	A	350	-	73,73,73	1.45	10 (13%)	95,113,113	1.57	19 (20%)
24	PHO	A	351	-	69,69,69	2.11	9 (13%)	91,99,99	1.55	14 (15%)
23	CLA	A	352	1	73,73,73	1.59	12 (16%)	95,113,113	1.58	19 (20%)
26	PL9	A	353	-	45,45,55	2.56	20 (44%)	55,57,69	2.49	20 (36%)
23	CLA	B	511	2	73,73,73	1.59	20 (27%)	95,113,113	1.80	26 (27%)
23	CLA	B	512	2	73,73,73	1.61	12 (16%)	95,113,113	1.62	19 (20%)
23	CLA	B	513	2	73,73,73	1.66	12 (16%)	95,113,113	1.83	27 (28%)
23	CLA	B	514	-	73,73,73	1.52	14 (19%)	95,113,113	1.77	24 (25%)
23	CLA	B	515	2	73,73,73	1.51	13 (17%)	95,113,113	1.75	25 (26%)
23	CLA	B	516	2	73,73,73	1.76	17 (23%)	95,113,113	1.74	19 (20%)
23	CLA	B	517	2	73,73,73	1.40	13 (17%)	95,113,113	1.67	22 (23%)
23	CLA	B	518	2	73,73,73	1.43	13 (17%)	95,113,113	1.75	20 (21%)
23	CLA	B	519	2	73,73,73	1.61	16 (21%)	95,113,113	2.08	22 (23%)
23	CLA	B	520	2	73,73,73	1.62	17 (23%)	95,113,113	2.15	20 (21%)
23	CLA	B	521	2	73,73,73	1.52	14 (19%)	95,113,113	1.43	15 (15%)
23	CLA	B	522	2	73,73,73	1.44	13 (17%)	95,113,113	1.62	22 (23%)
23	CLA	B	523	2	73,73,73	1.53	15 (20%)	95,113,113	1.73	21 (22%)
23	CLA	B	524	-	73,73,73	1.39	10 (13%)	95,113,113	1.76	21 (22%)
23	CLA	B	525	2	73,73,73	1.66	13 (17%)	95,113,113	1.60	18 (18%)
27	LMT	B	526	-	36,36,36	1.29	4 (11%)	47,47,47	1.80	8 (17%)
23	CLA	B	527	-	73,73,73	1.81	17 (23%)	95,113,113	1.79	23 (24%)
28	BCR	B	528	-	41,41,41	1.96	6 (14%)	56,56,56	2.16	19 (33%)
28	BCR	B	529	-	41,41,41	2.04	10 (24%)	56,56,56	2.24	22 (39%)
23	CLA	C	474	3	73,73,73	1.51	12 (16%)	95,113,113	1.71	24 (25%)
23	CLA	C	475	-	73,73,73	1.71	21 (28%)	95,113,113	1.72	22 (23%)
23	CLA	C	476	3	73,73,73	1.54	11 (15%)	95,113,113	1.55	20 (21%)
23	CLA	C	477	3	73,73,73	1.66	16 (21%)	95,113,113	2.01	22 (23%)
23	CLA	C	478	3	73,73,73	1.48	15 (20%)	95,113,113	1.76	21 (22%)
23	CLA	C	479	3	73,73,73	1.56	12 (16%)	95,113,113	1.81	27 (28%)
23	CLA	C	480	3	73,73,73	1.44	12 (16%)	95,113,113	1.52	18 (18%)
23	CLA	C	481	3	73,73,73	1.48	13 (17%)	95,113,113	1.82	20 (21%)
23	CLA	C	482	3	73,73,73	1.62	14 (19%)	95,113,113	1.63	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	483	3	73,73,73	1.66	15 (20%)	95,113,113	1.80	22 (23%)
23	CLA	C	484	3	73,73,73	1.74	14 (19%)	95,113,113	1.56	20 (21%)
23	CLA	C	485	-	73,73,73	1.48	12 (16%)	95,113,113	1.65	26 (27%)
23	CLA	C	486	3	73,73,73	1.62	15 (20%)	95,113,113	1.68	21 (22%)
23	CLA	C	487	-	73,73,73	1.50	11 (15%)	95,113,113	1.65	24 (25%)
28	BCR	C	488	-	41,41,41	1.78	10 (24%)	56,56,56	1.95	19 (33%)
28	BCR	C	489	-	41,41,41	1.70	7 (17%)	56,56,56	1.92	17 (30%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	73,73,73	1.57	10 (13%)	95,113,113	1.79	16 (16%)
24	PHO	D	355	-	69,69,69	1.77	7 (10%)	91,99,99	1.67	20 (21%)
23	CLA	D	356	4	73,73,73	1.61	15 (20%)	95,113,113	1.51	18 (18%)
26	PL9	D	357	-	45,45,55	2.46	18 (40%)	55,57,69	1.93	13 (23%)
25	HEM	E	84	5,6	49,50,50	3.90	27 (55%)	46,82,82	2.27	14 (30%)
28	BCR	F	48	-	41,41,41	1.94	8 (19%)	56,56,56	2.47	22 (39%)
28	BCR	J	53	-	41,41,41	1.87	7 (17%)	56,56,56	2.08	21 (37%)
28	BCR	K	50	-	41,41,41	2.06	18 (43%)	56,56,56	1.88	16 (28%)
25	HEM	V	138	16	49,50,50	7.90	39 (79%)	46,82,82	3.37	19 (41%)
21	BCT	a	2346	22	0,3,3	0.00	-	0,3,3	0.00	-
22	OEC	a	2347	1,3,21	7,13,13	20.12	7 (100%)	0,27,27	0.00	-
23	CLA	a	2348	1	73,73,73	1.56	12 (16%)	95,113,113	1.65	21 (22%)
23	CLA	a	2349	-	73,73,73	1.52	11 (15%)	95,113,113	1.55	18 (18%)
24	PHO	a	2350	-	69,69,69	1.95	10 (14%)	91,99,99	1.57	16 (17%)
23	CLA	a	2351	1	73,73,73	1.63	13 (17%)	95,113,113	1.59	21 (22%)
26	PL9	a	2352	-	45,45,55	2.56	19 (42%)	55,57,69	2.52	19 (34%)
23	CLA	b	2511	2	73,73,73	1.64	17 (23%)	95,113,113	1.83	26 (27%)
23	CLA	b	2512	2	73,73,73	1.51	11 (15%)	95,113,113	1.66	19 (20%)
23	CLA	b	2513	2	73,73,73	1.63	12 (16%)	95,113,113	1.83	26 (27%)
23	CLA	b	2514	-	73,73,73	1.52	11 (15%)	95,113,113	1.79	23 (24%)
23	CLA	b	2515	2	73,73,73	1.54	12 (16%)	95,113,113	1.75	24 (25%)
23	CLA	b	2516	2	73,73,73	1.74	18 (24%)	95,113,113	1.74	20 (21%)
23	CLA	b	2517	2	73,73,73	1.41	12 (16%)	95,113,113	1.66	21 (22%)
23	CLA	b	2518	2	73,73,73	1.47	15 (20%)	95,113,113	1.72	20 (21%)
23	CLA	b	2519	2	73,73,73	1.65	14 (19%)	95,113,113	2.09	23 (24%)
23	CLA	b	2520	2	73,73,73	1.66	17 (23%)	95,113,113	2.17	19 (20%)
23	CLA	b	2521	2	73,73,73	1.55	11 (15%)	95,113,113	1.43	15 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	2522	2	73,73,73	1.47	11 (15%)	95,113,113	1.60	21 (22%)
23	CLA	b	2523	2	73,73,73	1.50	19 (26%)	95,113,113	1.72	20 (21%)
23	CLA	b	2524	-	73,73,73	1.43	12 (16%)	95,113,113	1.77	23 (24%)
23	CLA	b	2525	2	73,73,73	1.65	14 (19%)	95,113,113	1.60	19 (20%)
23	CLA	b	2526	-	73,73,73	1.76	14 (19%)	95,113,113	1.79	22 (23%)
28	BCR	b	2527	-	41,41,41	1.86	7 (17%)	56,56,56	2.17	20 (35%)
28	BCR	b	2528	-	41,41,41	2.01	9 (21%)	56,56,56	2.17	21 (37%)
23	CLA	c	2474	3	73,73,73	1.44	12 (16%)	95,113,113	1.67	23 (24%)
23	CLA	c	2475	-	73,73,73	1.70	20 (27%)	95,113,113	1.71	20 (21%)
23	CLA	c	2476	3	73,73,73	1.62	15 (20%)	95,113,113	1.55	19 (20%)
23	CLA	c	2477	3	73,73,73	1.65	14 (19%)	95,113,113	2.01	23 (24%)
23	CLA	c	2478	3	73,73,73	1.48	14 (19%)	95,113,113	1.76	23 (24%)
23	CLA	c	2479	3	73,73,73	1.59	15 (20%)	95,113,113	1.82	26 (27%)
23	CLA	c	2480	3	73,73,73	1.53	14 (19%)	95,113,113	1.52	18 (18%)
23	CLA	c	2481	3	73,73,73	1.51	14 (19%)	95,113,113	1.81	20 (21%)
23	CLA	c	2482	3	73,73,73	1.60	14 (19%)	95,113,113	1.59	19 (20%)
23	CLA	c	2483	3	73,73,73	1.61	14 (19%)	95,113,113	1.79	22 (23%)
23	CLA	c	2484	3	73,73,73	1.61	11 (15%)	95,113,113	1.55	19 (20%)
23	CLA	c	2485	-	73,73,73	1.57	15 (20%)	95,113,113	1.64	27 (28%)
23	CLA	c	2486	3	73,73,73	1.57	14 (19%)	95,113,113	1.67	22 (23%)
23	CLA	c	2487	-	73,73,73	1.50	14 (19%)	95,113,113	1.66	25 (26%)
28	BCR	c	2488	-	41,41,41	1.93	11 (26%)	56,56,56	1.94	20 (35%)
28	BCR	c	2489	-	41,41,41	1.89	9 (21%)	56,56,56	1.94	17 (30%)
21	BCT	d	2353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	2354	4	73,73,73	1.58	11 (15%)	95,113,113	1.77	17 (17%)
23	CLA	d	2355	-	73,73,73	1.45	12 (16%)	95,113,113	1.84	22 (23%)
24	PHO	d	2356	-	69,69,69	1.98	8 (11%)	91,99,99	1.65	19 (20%)
23	CLA	d	2357	4	73,73,73	1.67	15 (20%)	95,113,113	1.51	17 (17%)
26	PL9	d	2358	-	45,45,55	2.54	19 (42%)	55,57,69	1.93	13 (23%)
27	LMT	d	2359	-	36,36,36	1.29	4 (11%)	47,47,47	1.79	8 (17%)
28	BCR	d	2360	-	41,41,41	1.95	8 (19%)	56,56,56	2.42	22 (39%)
25	HEM	e	2084	5,6	49,50,50	3.41	28 (57%)	46,82,82	1.93	11 (23%)
28	BCR	j	2053	-	41,41,41	2.11	9 (21%)	56,56,56	2.09	20 (35%)
28	BCR	k	2050	-	41,41,41	2.10	18 (43%)	56,56,56	1.85	17 (30%)
25	HEM	v	2138	16	49,50,50	3.65	26 (53%)	46,82,82	2.69	18 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCT	A	346	22	-	0/0/0/0	0/0/0/0
22	OEC	A	347	1,3,21	-	0/0/54/54	0/0/5/5
23	CLA	A	348	1	-	0/37/135/135	0/0/9/9
23	CLA	A	349	-	-	0/37/135/135	0/0/9/9
23	CLA	A	350	-	-	0/37/135/135	0/0/9/9
24	PHO	A	351	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	A	352	1	-	0/37/135/135	0/0/9/9
26	PL9	A	353	-	-	0/41/61/73	0/1/1/1
23	CLA	B	511	2	-	0/37/135/135	0/0/9/9
23	CLA	B	512	2	-	0/37/135/135	0/0/9/9
23	CLA	B	513	2	-	0/37/135/135	0/0/9/9
23	CLA	B	514	-	-	0/37/135/135	0/0/9/9
23	CLA	B	515	2	-	0/37/135/135	0/0/9/9
23	CLA	B	516	2	-	0/37/135/135	0/0/9/9
23	CLA	B	517	2	-	0/37/135/135	0/0/9/9
23	CLA	B	518	2	-	0/37/135/135	0/0/9/9
23	CLA	B	519	2	-	0/37/135/135	0/0/9/9
23	CLA	B	520	2	-	0/37/135/135	0/0/9/9
23	CLA	B	521	2	-	0/37/135/135	0/0/9/9
23	CLA	B	522	2	-	0/37/135/135	0/0/9/9
23	CLA	B	523	2	-	0/37/135/135	0/0/9/9
23	CLA	B	524	-	-	0/37/135/135	0/0/9/9
23	CLA	B	525	2	-	0/37/135/135	0/0/9/9
27	LMT	B	526	-	-	0/21/61/61	0/2/2/2
23	CLA	B	527	-	-	0/37/135/135	0/0/9/9
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
23	CLA	C	474	3	-	0/37/135/135	0/0/9/9
23	CLA	C	475	-	-	0/37/135/135	0/0/9/9
23	CLA	C	476	3	-	0/37/135/135	0/0/9/9
23	CLA	C	477	3	-	0/37/135/135	0/0/9/9
23	CLA	C	478	3	-	0/37/135/135	0/0/9/9
23	CLA	C	479	3	-	0/37/135/135	0/0/9/9
23	CLA	C	480	3	-	0/37/135/135	0/0/9/9
23	CLA	C	481	3	-	0/37/135/135	0/0/9/9
23	CLA	C	482	3	-	0/37/135/135	0/0/9/9
23	CLA	C	483	3	-	0/37/135/135	0/0/9/9
23	CLA	C	484	3	-	0/37/135/135	0/0/9/9
23	CLA	C	485	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	486	3	-	0/37/135/135	0/0/9/9
23	CLA	C	487	-	-	0/37/135/135	0/0/9/9
28	BCR	C	488	-	-	0/29/63/63	0/2/2/2
28	BCR	C	489	-	-	0/29/63/63	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	-	0/37/135/135	0/0/9/9
24	PHO	D	355	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	D	356	4	-	0/37/135/135	0/0/9/9
26	PL9	D	357	-	-	0/41/61/73	0/1/1/1
25	HEM	E	84	5,6	-	0/14/114/114	0/0/8/8
28	BCR	F	48	-	-	0/29/63/63	0/2/2/2
28	BCR	J	53	-	-	0/29/63/63	0/2/2/2
28	BCR	K	50	-	-	0/29/63/63	0/2/2/2
25	HEM	V	138	16	-	0/14/114/114	0/0/8/8
21	BCT	a	2346	22	-	0/0/0/0	0/0/0/0
22	OEC	a	2347	1,3,21	-	0/0/54/54	0/0/5/5
23	CLA	a	2348	1	-	0/37/135/135	0/0/9/9
23	CLA	a	2349	-	-	0/37/135/135	0/0/9/9
24	PHO	a	2350	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	a	2351	1	-	0/37/135/135	0/0/9/9
26	PL9	a	2352	-	-	0/41/61/73	0/1/1/1
23	CLA	b	2511	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2512	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2513	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2514	-	-	0/37/135/135	0/0/9/9
23	CLA	b	2515	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2516	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2517	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2518	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2519	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2520	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2521	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2522	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2523	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2524	-	-	0/37/135/135	0/0/9/9
23	CLA	b	2525	2	-	0/37/135/135	0/0/9/9
23	CLA	b	2526	-	-	0/37/135/135	0/0/9/9
28	BCR	b	2527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	2528	-	-	0/29/63/63	0/2/2/2
23	CLA	c	2474	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2475	-	-	0/37/135/135	0/0/9/9
23	CLA	c	2476	3	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	2477	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2478	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2479	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2480	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2481	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2482	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2483	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2484	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2485	-	-	0/37/135/135	0/0/9/9
23	CLA	c	2486	3	-	0/37/135/135	0/0/9/9
23	CLA	c	2487	-	-	0/37/135/135	0/0/9/9
28	BCR	c	2488	-	-	0/29/63/63	0/2/2/2
28	BCR	c	2489	-	-	0/29/63/63	0/2/2/2
21	BCT	d	2353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	2354	4	-	0/37/135/135	0/0/9/9
23	CLA	d	2355	-	-	0/37/135/135	0/0/9/9
24	PHO	d	2356	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	d	2357	4	-	0/37/135/135	0/0/9/9
26	PL9	d	2358	-	-	0/41/61/73	0/1/1/1
27	LMT	d	2359	-	-	0/21/61/61	0/2/2/2
28	BCR	d	2360	-	-	0/29/63/63	0/2/2/2
25	HEM	e	2084	5,6	-	0/14/114/114	0/0/8/8
28	BCR	j	2053	-	-	0/29/63/63	0/2/2/2
28	BCR	k	2050	-	-	0/29/63/63	0/2/2/2
25	HEM	v	2138	16	-	0/14/114/114	0/0/8/8

All (1377) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	138	HEM	C3D-C4D	36.81	1.53	1.44
22	A	347	OEC	O1-MN2	-25.52	1.77	2.02
22	a	2347	OEC	O1-MN2	-25.10	1.77	2.02
22	A	347	OEC	O2-MN3	-22.24	1.80	2.02
22	A	347	OEC	O3-MN3	-21.60	1.81	2.02
22	a	2347	OEC	O3-MN3	-21.59	1.81	2.02
22	a	2347	OEC	O2-MN1	-20.31	1.82	2.02
22	A	347	OEC	O2-MN2	-20.31	1.82	2.02
22	a	2347	OEC	O2-MN3	-20.09	1.82	2.02
22	A	347	OEC	O2-MN1	-20.00	1.82	2.02
22	a	2347	OEC	O2-MN2	-19.47	1.83	2.02
22	a	2347	OEC	O3-MN1	-17.03	1.85	2.02
22	A	347	OEC	O3-MN1	-16.10	1.86	2.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2347	OEC	O1-MN1	-15.86	1.86	2.02
22	A	347	OEC	O1-MN1	-15.10	1.87	2.02
25	V	138	HEM	C3B-C4B	13.94	1.61	1.44
24	d	2356	PHO	CHC-C1C	12.86	1.44	1.35
24	A	351	PHO	CHC-C1C	12.74	1.43	1.35
25	v	2138	HEM	C3D-C4D	-12.50	1.41	1.44
25	E	84	HEM	C3D-C4D	12.06	1.47	1.44
25	V	138	HEM	C1C-NC	11.65	1.54	1.38
25	V	138	HEM	C4A-NA	10.88	1.57	1.36
25	E	84	HEM	C2D-C1D	10.67	1.47	1.44
24	a	2350	PHO	CHC-C1C	10.57	1.42	1.35
24	D	355	PHO	CHC-C1C	10.37	1.42	1.35
25	V	138	HEM	C1A-NA	9.95	1.55	1.36
25	V	138	HEM	CMC-C2C	9.09	1.75	1.47
25	V	138	HEM	CHB-C1B	8.96	1.48	1.35
25	V	138	HEM	CMB-C2B	8.77	1.74	1.47
25	V	138	HEM	C1D-ND	8.72	1.58	1.37
25	V	138	HEM	C4B-NB	8.29	1.57	1.37
25	e	2084	HEM	C4A-C3A	8.26	1.50	1.40
25	V	138	HEM	CHD-C4C	8.21	1.52	1.36
25	v	2138	HEM	C2D-C1D	8.19	1.46	1.44
25	E	84	HEM	C2B-C1B	-8.13	1.42	1.44
25	V	138	HEM	C1B-NB	8.04	1.56	1.39
25	V	138	HEM	C4C-NC	8.01	1.49	1.38
25	v	2138	HEM	CHB-C1B	7.70	1.46	1.35
25	e	2084	HEM	CHB-C1B	7.51	1.46	1.35
28	j	2053	BCR	C30-C25	7.29	1.64	1.53
26	a	2352	PL9	C7-C3	7.17	1.57	1.51
25	V	138	HEM	CMA-C3A	7.02	1.66	1.51
25	V	138	HEM	C2D-C1D	7.02	1.46	1.44
25	V	138	HEM	C1A-CHA	6.89	1.58	1.39
25	E	84	HEM	C4A-C3A	6.82	1.48	1.40
25	V	138	HEM	CMD-C2D	6.82	1.68	1.47
25	e	2084	HEM	C2D-C1D	6.81	1.46	1.44
25	V	138	HEM	CHA-C4D	-6.74	1.26	1.35
28	F	48	BCR	C30-C25	6.70	1.63	1.53
26	A	353	PL9	C7-C3	6.63	1.57	1.51
23	B	527	CLA	C1B-C2B	6.63	1.48	1.40
25	v	2138	HEM	C1C-NC	6.58	1.47	1.38
23	C	484	CLA	C1B-C2B	6.57	1.48	1.40
23	d	2357	CLA	C1B-C2B	6.54	1.48	1.40
23	b	2526	CLA	C1B-C2B	6.48	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	525	CLA	C3B-CAB	-6.45	1.43	1.49
23	a	2351	CLA	C1B-C2B	6.38	1.48	1.40
23	A	352	CLA	C1B-C2B	6.29	1.48	1.40
23	B	512	CLA	C1B-C2B	6.24	1.48	1.40
23	D	356	CLA	C1B-C2B	6.21	1.47	1.40
23	c	2476	CLA	C1B-C2B	6.20	1.47	1.40
28	J	53	BCR	C30-C25	6.20	1.62	1.53
25	V	138	HEM	C3B-C2B	6.20	1.54	1.43
25	v	2138	HEM	C1A-NA	6.13	1.48	1.36
24	A	351	PHO	C1D-CHD	6.13	1.42	1.35
23	B	513	CLA	C1B-C2B	6.07	1.47	1.40
23	b	2511	CLA	C3B-C4B	6.03	1.50	1.40
25	v	2138	HEM	CMC-C2C	5.91	1.65	1.47
23	C	476	CLA	C1B-C2B	5.89	1.47	1.40
25	E	84	HEM	CHD-C4C	5.88	1.47	1.36
28	B	529	BCR	C30-C25	5.87	1.62	1.53
23	c	2479	CLA	C1B-C2B	5.83	1.47	1.40
28	B	528	BCR	C30-C25	5.81	1.62	1.53
23	b	2525	CLA	C3B-CAB	-5.79	1.43	1.49
23	c	2480	CLA	C1B-C2B	5.78	1.47	1.40
24	a	2350	PHO	C1D-CHD	5.77	1.41	1.35
26	d	2358	PL9	C7-C3	5.76	1.56	1.51
23	a	2349	CLA	C1B-C2B	5.75	1.47	1.40
23	c	2483	CLA	C1B-C2B	5.73	1.47	1.40
25	V	138	HEM	C2A-C3A	5.73	1.54	1.37
24	a	2350	PHO	C3B-C4B	5.71	1.49	1.40
28	b	2528	BCR	C30-C25	5.71	1.62	1.53
26	D	357	PL9	C7-C3	5.69	1.56	1.51
28	d	2360	BCR	C30-C25	5.67	1.61	1.53
23	C	484	CLA	C3B-C4B	5.65	1.49	1.40
25	v	2138	HEM	CMB-C2B	5.61	1.64	1.47
28	B	529	BCR	C26-C25	5.59	1.43	1.34
23	c	2477	CLA	C1B-C2B	5.57	1.47	1.40
23	C	482	CLA	C1B-C2B	5.54	1.47	1.40
23	b	2513	CLA	C1B-C2B	5.53	1.47	1.40
23	c	2482	CLA	C1B-C2B	5.50	1.47	1.40
23	c	2484	CLA	C1B-C2B	5.50	1.47	1.40
23	d	2354	CLA	C1B-C2B	5.48	1.47	1.40
23	C	483	CLA	C1B-C2B	5.48	1.47	1.40
23	b	2521	CLA	C1B-C2B	5.41	1.46	1.40
28	C	489	BCR	C30-C25	5.41	1.61	1.53
23	C	479	CLA	C1B-C2B	5.40	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2526	CLA	C3B-C4B	5.40	1.48	1.40
25	V	138	HEM	C4D-ND	5.40	1.51	1.39
28	c	2489	BCR	C30-C25	5.38	1.61	1.53
28	j	2053	BCR	C26-C25	5.35	1.42	1.34
23	C	481	CLA	C1B-C2B	5.34	1.46	1.40
23	B	516	CLA	C1B-C2B	5.34	1.46	1.40
23	B	527	CLA	C3B-C4B	5.34	1.48	1.40
28	b	2527	BCR	C5-C6	5.32	1.42	1.34
23	a	2348	CLA	C3B-C4B	5.30	1.48	1.40
25	v	2138	HEM	CMD-C2D	5.30	1.64	1.47
25	e	2084	HEM	C3D-C4D	5.28	1.45	1.44
23	c	2481	CLA	C1B-C2B	5.26	1.46	1.40
28	j	2053	BCR	C5-C6	5.25	1.42	1.34
25	v	2138	HEM	C3B-CAB	5.25	1.57	1.40
23	b	2512	CLA	C1B-C2B	5.20	1.46	1.40
26	d	2358	PL9	C53-C6	-5.20	1.39	1.51
23	b	2520	CLA	C3B-C4B	5.19	1.48	1.40
23	D	354	CLA	C3B-C4B	5.18	1.48	1.40
23	b	2516	CLA	C1B-C2B	5.18	1.46	1.40
28	B	528	BCR	C26-C25	5.15	1.42	1.34
23	B	512	CLA	C3B-C4B	5.14	1.48	1.40
23	b	2519	CLA	C1C-NC	-5.14	1.34	1.38
26	D	357	PL9	C53-C6	-5.08	1.40	1.51
26	d	2358	PL9	C52-C5	-5.07	1.40	1.51
24	D	355	PHO	C3B-C4B	5.07	1.48	1.40
23	B	514	CLA	C3B-C4B	5.06	1.48	1.40
23	B	513	CLA	CAA-C2A	5.05	1.63	1.54
25	e	2084	HEM	CMB-C2B	5.02	1.63	1.47
26	D	357	PL9	C31-C29	4.98	1.63	1.51
23	b	2525	CLA	C1B-C2B	4.98	1.46	1.40
23	c	2484	CLA	C3B-C4B	4.97	1.48	1.40
23	d	2354	CLA	C3B-C4B	4.97	1.48	1.40
23	c	2477	CLA	C3B-C4B	4.95	1.48	1.40
25	e	2084	HEM	C3C-CAC	4.94	1.56	1.40
23	C	474	CLA	C1C-NC	-4.93	1.34	1.38
25	e	2084	HEM	C3B-C4B	4.93	1.50	1.44
23	c	2487	CLA	MG-NA	4.92	2.21	2.07
28	b	2528	BCR	C26-C25	4.92	1.42	1.34
23	B	511	CLA	C3B-C4B	4.92	1.48	1.40
25	V	138	HEM	C3C-C2C	4.92	1.52	1.43
24	A	351	PHO	C3B-C4B	4.92	1.48	1.40
23	B	521	CLA	C3B-C4B	4.91	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	E	84	HEM	CHA-C4D	4.90	1.42	1.35
28	B	528	BCR	C5-C6	4.90	1.42	1.34
23	B	523	CLA	C3B-C4B	4.88	1.48	1.40
26	d	2358	PL9	C23-C24	4.87	1.42	1.32
26	a	2352	PL9	C53-C6	-4.86	1.40	1.51
25	E	84	HEM	CMB-C2B	4.85	1.62	1.47
23	B	520	CLA	C1B-C2B	4.85	1.46	1.40
23	C	477	CLA	C3B-C4B	4.85	1.48	1.40
23	A	348	CLA	C3B-C4B	4.84	1.48	1.40
23	B	525	CLA	C1B-C2B	4.83	1.46	1.40
26	a	2352	PL9	C22-C23	-4.83	1.36	1.50
28	c	2488	BCR	C1-C6	4.83	1.60	1.53
23	C	486	CLA	C1B-C2B	4.83	1.46	1.40
25	E	84	HEM	CMA-C3A	4.82	1.61	1.51
23	C	483	CLA	C3B-C4B	4.82	1.48	1.40
23	C	477	CLA	C1B-C2B	4.80	1.46	1.40
23	b	2520	CLA	C1B-C2B	4.79	1.46	1.40
23	b	2514	CLA	C3B-C4B	4.78	1.47	1.40
23	b	2522	CLA	C1C-NC	-4.78	1.34	1.38
23	B	519	CLA	C3B-C4B	4.78	1.47	1.40
26	A	353	PL9	C33-C34	4.78	1.42	1.32
26	d	2358	PL9	C18-C19	4.78	1.42	1.32
23	C	479	CLA	C3B-C4B	4.77	1.47	1.40
25	e	2084	HEM	C3B-CAB	4.77	1.55	1.40
23	d	2357	CLA	C3B-C4B	4.77	1.47	1.40
23	a	2349	CLA	C3B-C4B	4.77	1.47	1.40
23	a	2351	CLA	C3B-C4B	4.77	1.47	1.40
25	E	84	HEM	C1A-C2A	4.77	1.51	1.43
23	B	515	CLA	C3B-C4B	4.75	1.47	1.40
23	B	527	CLA	C4B-NB	4.75	1.40	1.34
23	D	356	CLA	C3B-C4B	4.74	1.47	1.40
23	c	2485	CLA	C3B-CAB	-4.73	1.44	1.49
23	b	2519	CLA	C3B-C4B	4.73	1.47	1.40
26	A	353	PL9	C52-C5	-4.73	1.40	1.51
23	C	480	CLA	C1B-C2B	4.72	1.46	1.40
26	A	353	PL9	C22-C23	-4.71	1.36	1.50
23	c	2479	CLA	C3B-C4B	4.71	1.47	1.40
28	b	2527	BCR	C26-C25	4.70	1.41	1.34
28	b	2527	BCR	C30-C25	4.70	1.60	1.53
23	B	516	CLA	C3B-C4B	4.70	1.47	1.40
23	c	2485	CLA	C1B-C2B	4.70	1.46	1.40
23	b	2521	CLA	C3B-C4B	4.70	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	354	CLA	C1B-C2B	4.69	1.46	1.40
23	C	474	CLA	C1B-C2B	4.69	1.46	1.40
28	J	53	BCR	C5-C6	4.68	1.41	1.34
28	k	2050	BCR	C17-C18	-4.67	1.29	1.35
23	B	522	CLA	C3B-C4B	4.67	1.47	1.40
23	C	477	CLA	C1C-NC	-4.66	1.34	1.38
28	K	50	BCR	C17-C18	-4.65	1.29	1.35
26	a	2352	PL9	C28-C29	4.65	1.42	1.32
23	c	2481	CLA	C3B-C4B	4.64	1.47	1.40
23	B	520	CLA	C3B-C4B	4.64	1.47	1.40
23	C	474	CLA	C3B-C4B	4.64	1.47	1.40
23	B	518	CLA	C3B-C4B	4.63	1.47	1.40
23	C	478	CLA	C3B-C4B	4.62	1.47	1.40
23	a	2348	CLA	C1B-C2B	4.62	1.45	1.40
23	C	487	CLA	MG-NA	4.62	2.20	2.07
26	A	353	PL9	C53-C6	-4.62	1.41	1.51
28	d	2360	BCR	C5-C6	4.62	1.41	1.34
25	E	84	HEM	C1A-NA	4.61	1.45	1.36
23	B	513	CLA	C3B-C4B	4.60	1.47	1.40
23	B	521	CLA	C1B-C2B	4.60	1.45	1.40
23	A	350	CLA	C1B-C2B	4.59	1.45	1.40
23	A	352	CLA	C3B-C4B	4.58	1.47	1.40
23	b	2515	CLA	C3B-C4B	4.57	1.47	1.40
23	b	2513	CLA	CAA-C2A	4.55	1.62	1.54
23	c	2486	CLA	C3B-C4B	4.53	1.47	1.40
25	V	138	HEM	FE-NA	4.53	2.11	1.92
23	c	2480	CLA	C3B-C4B	4.52	1.47	1.40
28	c	2489	BCR	C1-C6	4.51	1.60	1.53
23	c	2478	CLA	C3B-C4B	4.50	1.47	1.40
23	C	486	CLA	C3B-C4B	4.48	1.47	1.40
23	C	485	CLA	C3B-CAB	-4.48	1.45	1.49
23	c	2474	CLA	C1B-C2B	4.48	1.45	1.40
26	A	353	PL9	C38-C39	4.48	1.43	1.34
23	b	2523	CLA	C3B-C4B	4.47	1.47	1.40
26	D	357	PL9	C18-C19	4.47	1.42	1.32
23	b	2524	CLA	C1B-C2B	4.46	1.45	1.40
25	e	2084	HEM	C1C-NC	4.45	1.44	1.38
23	c	2483	CLA	C3B-C4B	4.45	1.47	1.40
25	e	2084	HEM	C3D-C2D	-4.45	1.36	1.43
23	b	2517	CLA	C3B-C4B	4.44	1.47	1.40
23	C	484	CLA	C4B-NB	4.43	1.40	1.34
23	b	2513	CLA	C3B-C4B	4.43	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	480	CLA	C3B-C4B	4.43	1.47	1.40
28	d	2360	BCR	C26-C25	4.43	1.41	1.34
23	c	2476	CLA	C3B-C4B	4.43	1.47	1.40
26	a	2352	PL9	C52-C5	-4.41	1.41	1.51
23	b	2511	CLA	C1B-C2B	4.41	1.45	1.40
23	b	2522	CLA	C3B-C4B	4.40	1.47	1.40
23	C	476	CLA	C3B-C4B	4.39	1.47	1.40
25	V	138	HEM	C3B-CAB	4.39	1.54	1.40
26	D	357	PL9	C52-C5	-4.38	1.41	1.51
25	v	2138	HEM	CHD-C4C	4.38	1.44	1.36
23	b	2516	CLA	C2-C3	4.38	1.41	1.32
23	C	483	CLA	C1C-NC	-4.37	1.35	1.38
23	C	482	CLA	C3B-C4B	4.35	1.47	1.40
25	e	2084	HEM	CMD-C2D	4.34	1.60	1.47
25	V	138	HEM	C4A-C3A	4.33	1.45	1.40
26	A	353	PL9	C28-C29	4.33	1.41	1.32
23	c	2474	CLA	C3B-C4B	4.32	1.47	1.40
23	b	2526	CLA	C4B-NB	4.31	1.39	1.34
23	A	349	CLA	C1B-C2B	4.31	1.45	1.40
25	V	138	HEM	O1A-CGA	4.31	1.37	1.22
23	c	2475	CLA	C1B-C2B	4.31	1.45	1.40
23	C	486	CLA	MG-NA	4.30	2.19	2.07
25	V	138	HEM	O2D-CGD	-4.30	1.14	1.30
28	F	48	BCR	C26-C25	4.29	1.41	1.34
23	c	2486	CLA	C1B-C2B	4.28	1.45	1.40
25	e	2084	HEM	CBB-CAB	4.28	1.53	1.28
26	d	2358	PL9	C31-C29	4.27	1.61	1.51
25	e	2084	HEM	C1A-NA	4.27	1.44	1.36
23	C	481	CLA	C3B-C4B	4.26	1.47	1.40
25	E	84	HEM	C3B-CAB	4.26	1.53	1.40
23	d	2355	CLA	C3B-C4B	4.25	1.47	1.40
23	c	2475	CLA	C2-C3	4.25	1.41	1.32
23	b	2512	CLA	C3B-C4B	4.24	1.47	1.40
28	c	2488	BCR	C30-C25	4.24	1.59	1.53
23	d	2355	CLA	C1C-NC	-4.22	1.35	1.38
23	B	519	CLA	C1B-C2B	4.22	1.45	1.40
25	E	84	HEM	CBB-CAB	4.20	1.53	1.28
23	D	354	CLA	MG-NA	4.19	2.19	2.07
23	B	522	CLA	C1C-NC	-4.19	1.35	1.38
23	A	349	CLA	C3B-C4B	4.19	1.46	1.40
24	d	2356	PHO	C3B-C4B	4.18	1.46	1.40
25	e	2084	HEM	C4C-NC	4.18	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	E	84	HEM	C3C-CAC	4.18	1.53	1.40
25	E	84	HEM	CMC-C2C	4.17	1.60	1.47
28	F	48	BCR	C1-C6	4.17	1.59	1.53
28	b	2528	BCR	C2-C1	4.16	1.64	1.54
23	A	348	CLA	C1B-C2B	4.16	1.45	1.40
23	C	475	CLA	C2-C3	4.16	1.41	1.32
23	C	475	CLA	CAA-C2A	4.13	1.61	1.54
25	e	2084	HEM	CHC-C1C	4.13	1.44	1.36
23	b	2526	CLA	MG-NA	4.13	2.19	2.07
25	E	84	HEM	CMD-C2D	4.12	1.60	1.47
28	J	53	BCR	C26-C25	4.12	1.40	1.34
23	d	2355	CLA	C1B-C2B	4.10	1.45	1.40
23	B	527	CLA	MG-NA	4.10	2.19	2.07
26	D	357	PL9	C23-C24	4.10	1.41	1.32
23	d	2354	CLA	MG-NA	4.07	2.19	2.07
23	b	2518	CLA	C3B-C4B	4.06	1.46	1.40
23	b	2516	CLA	CAA-C2A	4.05	1.61	1.54
23	B	515	CLA	C1C-NC	-4.05	1.35	1.38
25	E	84	HEM	C4C-NC	4.02	1.43	1.38
23	b	2513	CLA	C1C-NC	-4.02	1.35	1.38
23	C	485	CLA	C1B-C2B	4.02	1.45	1.40
23	B	514	CLA	C1C-NC	-4.01	1.35	1.38
26	a	2352	PL9	C38-C39	4.00	1.42	1.34
23	b	2514	CLA	C1C-NC	-4.00	1.35	1.38
26	a	2352	PL9	C13-C14	4.00	1.41	1.32
23	A	350	CLA	C3B-C4B	3.99	1.46	1.40
23	B	520	CLA	CAA-CBA	-3.99	1.39	1.52
23	b	2519	CLA	C1B-C2B	3.99	1.45	1.40
24	A	351	PHO	C1B-CHB	-3.99	1.30	1.35
23	C	479	CLA	C1C-NC	-3.99	1.35	1.38
25	V	138	HEM	CBB-CAB	3.98	1.52	1.28
26	d	2358	PL9	C33-C34	3.97	1.41	1.32
23	B	518	CLA	C1B-C2B	3.97	1.45	1.40
23	B	517	CLA	C3B-C4B	3.96	1.46	1.40
28	C	488	BCR	C30-C25	3.96	1.59	1.53
28	d	2360	BCR	C1-C6	3.95	1.59	1.53
23	b	2516	CLA	C3B-C4B	3.95	1.46	1.40
28	B	529	BCR	C2-C1	3.94	1.64	1.54
26	A	353	PL9	C13-C14	3.93	1.40	1.32
24	d	2356	PHO	C1D-CHD	3.91	1.39	1.35
23	B	511	CLA	C1B-C2B	3.91	1.45	1.40
23	B	523	CLA	C1B-C2B	3.91	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	2354	CLA	C4B-NB	3.90	1.39	1.34
23	a	2348	CLA	MG-NA	3.89	2.18	2.07
24	D	355	PHO	C1D-CHD	3.89	1.39	1.35
23	C	475	CLA	C3B-C4B	3.89	1.46	1.40
25	e	2084	HEM	C4A-NA	3.89	1.44	1.36
23	c	2475	CLA	C3B-C4B	3.88	1.46	1.40
23	c	2482	CLA	C3B-C4B	3.87	1.46	1.40
23	c	2486	CLA	MG-NA	3.86	2.18	2.07
23	C	487	CLA	CAA-C2A	3.86	1.61	1.54
23	b	2520	CLA	CAA-CBA	-3.85	1.39	1.52
28	c	2488	BCR	C29-C30	3.85	1.64	1.54
28	d	2360	BCR	C29-C30	3.84	1.63	1.54
23	C	487	CLA	C4C-C3C	3.83	1.52	1.45
25	E	84	HEM	CBC-CAC	3.83	1.51	1.28
23	b	2523	CLA	C1B-C2B	3.83	1.44	1.40
28	k	2050	BCR	C1-C6	3.82	1.59	1.53
23	C	478	CLA	C1C-NC	-3.81	1.35	1.38
23	B	516	CLA	C2-C3	3.81	1.40	1.32
23	B	523	CLA	CAA-CBA	-3.81	1.40	1.52
23	b	2513	CLA	C1A-NA	3.81	1.40	1.32
28	c	2489	BCR	C29-C30	3.80	1.63	1.54
23	b	2523	CLA	CAA-CBA	-3.80	1.40	1.52
26	D	357	PL9	C28-C29	3.80	1.40	1.32
23	b	2518	CLA	C3D-CAD	-3.79	1.39	1.47
23	b	2515	CLA	C1C-NC	-3.79	1.35	1.38
25	e	2084	HEM	CBC-CAC	3.78	1.50	1.28
28	c	2489	BCR	C26-C25	3.78	1.40	1.34
23	B	525	CLA	C1C-NC	-3.78	1.35	1.38
23	c	2475	CLA	CAA-C2A	3.77	1.60	1.54
23	c	2482	CLA	C4B-NB	3.77	1.39	1.34
28	F	48	BCR	C5-C6	3.77	1.40	1.34
23	C	482	CLA	CAA-C2A	3.76	1.60	1.54
23	B	527	CLA	C1A-NA	3.76	1.40	1.32
23	b	2520	CLA	C1C-NC	-3.75	1.35	1.38
23	c	2486	CLA	C1A-NA	3.75	1.40	1.32
23	B	516	CLA	C1C-NC	-3.74	1.35	1.38
23	C	475	CLA	C1B-C2B	3.72	1.44	1.40
26	A	353	PL9	C23-C24	3.71	1.40	1.32
23	c	2476	CLA	MG-NA	3.71	2.18	2.07
23	B	512	CLA	C4B-NB	3.71	1.39	1.34
23	b	2514	CLA	C1B-CHB	-3.70	1.29	1.39
28	C	488	BCR	C29-C30	3.70	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2487	CLA	CAA-C2A	3.69	1.60	1.54
26	d	2358	PL9	C13-C14	3.69	1.40	1.32
25	V	138	HEM	C3D-C2D	3.69	1.50	1.43
23	C	486	CLA	C1A-NA	3.68	1.40	1.32
23	c	2482	CLA	MG-NA	3.68	2.18	2.07
23	C	482	CLA	MG-NA	3.68	2.18	2.07
25	e	2084	HEM	CHD-C4C	3.68	1.43	1.36
23	b	2526	CLA	C1A-NA	3.67	1.40	1.32
28	c	2488	BCR	C26-C25	3.67	1.40	1.34
23	B	521	CLA	C4B-NB	3.67	1.39	1.34
24	a	2350	PHO	C1B-CHB	-3.66	1.31	1.35
25	e	2084	HEM	C1B-NB	3.65	1.47	1.39
23	B	517	CLA	C1C-NC	-3.64	1.35	1.38
23	b	2513	CLA	C4A-NA	-3.64	1.31	1.39
23	c	2477	CLA	MG-NA	3.63	2.18	2.07
23	B	516	CLA	MG-NA	3.64	2.18	2.07
28	b	2527	BCR	C2-C1	3.63	1.63	1.54
28	K	50	BCR	C23-C22	-3.62	1.37	1.45
23	c	2487	CLA	C4C-C3C	3.62	1.51	1.45
26	d	2358	PL9	C28-C29	3.61	1.40	1.32
23	b	2524	CLA	C3B-C4B	3.60	1.45	1.40
23	c	2482	CLA	CAA-C2A	3.59	1.60	1.54
28	C	488	BCR	C1-C6	3.58	1.58	1.53
28	b	2527	BCR	C29-C30	3.58	1.63	1.54
23	C	477	CLA	MG-NA	3.58	2.17	2.07
26	a	2352	PL9	C33-C34	3.58	1.40	1.32
23	C	479	CLA	C1A-NA	3.57	1.40	1.32
26	D	357	PL9	C33-C34	3.57	1.40	1.32
23	c	2477	CLA	CAA-CBA	-3.57	1.40	1.52
23	B	524	CLA	C1B-C2B	3.57	1.44	1.40
23	C	477	CLA	C4B-NB	3.56	1.39	1.34
28	d	2360	BCR	C2-C1	3.56	1.63	1.54
23	C	487	CLA	C1C-NC	-3.56	1.35	1.38
23	B	519	CLA	O2A-CGA	3.56	1.44	1.33
28	k	2050	BCR	C19-C18	-3.56	1.38	1.45
23	B	514	CLA	CAA-CBA	-3.56	1.40	1.52
23	B	524	CLA	C3B-C4B	3.56	1.45	1.40
28	k	2050	BCR	C23-C22	-3.56	1.38	1.45
26	a	2352	PL9	C23-C24	3.56	1.40	1.32
28	j	2053	BCR	C2-C1	3.55	1.63	1.54
23	b	2514	CLA	CAA-CBA	-3.55	1.40	1.52
28	c	2489	BCR	C5-C6	3.54	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2479	CLA	CAA-CBA	-3.53	1.41	1.52
23	b	2519	CLA	O2A-CGA	3.54	1.44	1.33
23	C	475	CLA	C3B-CAB	-3.53	1.46	1.49
23	d	2354	CLA	C1A-NA	3.52	1.40	1.32
23	B	514	CLA	C1B-CHB	-3.52	1.30	1.39
23	B	513	CLA	C4B-NB	3.52	1.39	1.34
28	C	489	BCR	C29-C30	3.52	1.63	1.54
23	c	2485	CLA	C4A-NA	-3.51	1.31	1.39
28	B	528	BCR	C29-C30	3.51	1.63	1.54
28	b	2528	BCR	C1-C6	3.51	1.58	1.53
23	B	524	CLA	C1C-NC	-3.51	1.35	1.38
23	c	2479	CLA	C1A-NA	3.51	1.40	1.32
25	E	84	HEM	C1C-NC	3.51	1.43	1.38
23	b	2521	CLA	MG-NA	3.50	2.17	2.07
27	B	526	LMT	C3B-C2B	-3.50	1.43	1.52
23	b	2518	CLA	C1B-C2B	3.50	1.44	1.40
28	J	53	BCR	C29-C30	3.49	1.63	1.54
23	b	2522	CLA	C1B-C2B	3.49	1.44	1.40
23	b	2517	CLA	C1B-C2B	3.49	1.44	1.40
23	D	354	CLA	C1C-NC	-3.48	1.35	1.38
28	j	2053	BCR	C29-C30	3.48	1.63	1.54
28	c	2488	BCR	C2-C1	3.48	1.63	1.54
23	c	2478	CLA	C1A-NA	3.47	1.39	1.32
23	c	2487	CLA	C1A-NA	3.47	1.39	1.32
23	A	349	CLA	C1C-NC	-3.47	1.35	1.38
23	b	2515	CLA	C3D-CAD	-3.47	1.40	1.47
23	C	487	CLA	C1A-NA	3.47	1.39	1.32
23	C	482	CLA	C4B-NB	3.47	1.38	1.34
23	c	2486	CLA	C1C-NC	-3.46	1.35	1.38
23	C	485	CLA	C4A-NA	-3.46	1.31	1.39
28	K	50	BCR	C19-C18	-3.45	1.38	1.45
23	C	484	CLA	MG-NA	3.45	2.17	2.07
25	v	2138	HEM	CBB-CAB	3.44	1.48	1.28
23	b	2515	CLA	C1B-C2B	3.44	1.44	1.40
28	b	2528	BCR	C29-C30	3.43	1.62	1.54
23	b	2512	CLA	C4B-NB	3.43	1.38	1.34
23	c	2484	CLA	C4B-NB	3.42	1.38	1.34
23	a	2349	CLA	MG-NA	3.42	2.17	2.07
28	C	489	BCR	C26-C25	3.41	1.39	1.34
23	C	481	CLA	MG-NA	3.41	2.17	2.07
28	k	2050	BCR	C26-C25	3.41	1.39	1.34
23	b	2525	CLA	C4A-NA	-3.41	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	486	CLA	CAA-C2A	3.41	1.60	1.54
23	c	2477	CLA	C1B-NB	3.40	1.38	1.34
23	B	525	CLA	C4A-NA	-3.40	1.31	1.39
23	d	2357	CLA	C4A-NA	-3.40	1.31	1.39
23	B	524	CLA	C4A-NA	-3.39	1.31	1.39
28	B	528	BCR	C2-C1	3.39	1.62	1.54
23	b	2525	CLA	C1A-NA	3.39	1.39	1.32
23	b	2512	CLA	C4A-NA	-3.39	1.31	1.39
28	C	488	BCR	C2-C1	3.38	1.62	1.54
23	d	2357	CLA	C1C-NC	-3.37	1.35	1.38
25	v	2138	HEM	C1A-CHA	3.37	1.49	1.39
23	A	348	CLA	MG-NA	3.37	2.17	2.07
23	c	2485	CLA	C4B-NB	3.37	1.38	1.34
28	B	529	BCR	C24-C23	3.36	1.42	1.32
25	v	2138	HEM	O1A-CGA	3.35	1.34	1.22
23	A	350	CLA	MG-NA	3.35	2.17	2.07
23	D	356	CLA	C4A-NA	-3.35	1.32	1.39
28	B	529	BCR	C1-C6	3.35	1.58	1.53
23	b	2525	CLA	C3B-C4B	3.35	1.45	1.40
23	C	480	CLA	MG-NA	3.34	2.17	2.07
23	a	2348	CLA	C4A-NA	-3.34	1.32	1.39
23	b	2520	CLA	C2-C3	3.33	1.39	1.32
23	a	2351	CLA	C4A-NA	-3.33	1.32	1.39
28	K	50	BCR	C30-C25	3.32	1.58	1.53
23	c	2487	CLA	MG-NC	3.31	2.17	2.07
23	c	2481	CLA	MG-NA	3.31	2.17	2.07
23	c	2481	CLA	C4B-NB	3.31	1.38	1.34
23	c	2485	CLA	C3B-C4B	3.30	1.45	1.40
23	b	2522	CLA	MG-NA	3.30	2.17	2.07
23	B	513	CLA	C1A-NA	3.30	1.39	1.32
23	C	485	CLA	C3B-C4B	3.29	1.45	1.40
28	F	48	BCR	C2-C1	3.29	1.62	1.54
23	c	2484	CLA	MG-NA	3.29	2.17	2.07
23	B	515	CLA	C1B-C2B	3.29	1.44	1.40
23	A	348	CLA	C3B-C2B	-3.29	1.35	1.41
23	C	481	CLA	C4B-NB	3.29	1.38	1.34
23	A	352	CLA	C4A-NA	-3.28	1.32	1.39
23	a	2351	CLA	C4B-NB	3.28	1.38	1.34
23	c	2477	CLA	C1C-NC	-3.28	1.35	1.38
28	c	2488	BCR	C5-C6	3.28	1.39	1.34
28	k	2050	BCR	C29-C30	3.27	1.62	1.54
23	C	477	CLA	CAA-CBA	-3.27	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2516	CLA	MG-NA	3.27	2.16	2.07
23	B	515	CLA	MG-NA	3.26	2.16	2.07
23	c	2480	CLA	C4B-NB	3.26	1.38	1.34
23	B	518	CLA	C3D-CAD	-3.26	1.40	1.47
28	K	50	BCR	C26-C25	3.26	1.39	1.34
23	B	522	CLA	MG-NA	3.26	2.16	2.07
28	c	2489	BCR	C2-C1	3.26	1.62	1.54
23	c	2480	CLA	MG-NA	3.25	2.16	2.07
28	F	48	BCR	C29-C30	3.24	1.62	1.54
23	d	2354	CLA	CAA-C2A	3.24	1.59	1.54
28	C	488	BCR	C5-C6	3.24	1.39	1.34
23	c	2483	CLA	C1A-NA	3.24	1.39	1.32
24	a	2350	PHO	C4D-CHA	-3.24	1.41	1.45
28	C	489	BCR	C5-C6	3.24	1.39	1.34
23	B	525	CLA	C1A-NA	3.24	1.39	1.32
23	C	485	CLA	C1B-CHB	-3.23	1.30	1.39
25	E	84	HEM	CHB-C1B	3.23	1.40	1.35
23	c	2477	CLA	C4B-NB	3.23	1.38	1.34
23	c	2478	CLA	C4B-NB	3.22	1.38	1.34
25	V	138	HEM	CHC-C4B	3.22	1.46	1.39
28	B	529	BCR	C29-C30	3.22	1.62	1.54
23	B	524	CLA	C1B-CHB	-3.22	1.31	1.39
23	A	352	CLA	C4B-NB	3.22	1.38	1.34
25	v	2138	HEM	CMA-C3A	3.22	1.58	1.51
25	E	84	HEM	FE-NA	3.21	2.06	1.92
23	C	478	CLA	C1A-NA	3.21	1.39	1.32
23	c	2486	CLA	CAA-C2A	3.21	1.59	1.54
28	C	488	BCR	C26-C25	3.20	1.39	1.34
23	D	356	CLA	C4B-NB	3.20	1.38	1.34
23	C	484	CLA	C1A-NA	3.20	1.39	1.32
23	B	516	CLA	CAA-C2A	3.19	1.59	1.54
23	B	519	CLA	C1B-CHB	-3.19	1.31	1.39
28	C	489	BCR	C2-C1	3.19	1.62	1.54
23	b	2515	CLA	C1A-NA	3.18	1.39	1.32
26	D	357	PL9	C13-C14	3.18	1.39	1.32
23	C	478	CLA	MG-NA	3.17	2.16	2.07
23	b	2524	CLA	C1A-NA	3.17	1.39	1.32
23	c	2477	CLA	O2A-CGA	3.17	1.43	1.33
23	b	2526	CLA	C1B-NB	3.17	1.38	1.34
23	B	521	CLA	MG-NA	3.17	2.16	2.07
23	C	476	CLA	CAA-C2A	3.17	1.59	1.54
26	d	2358	PL9	C8-C9	3.17	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	522	CLA	C1B-C2B	3.17	1.44	1.40
23	d	2355	CLA	C3D-CAD	-3.17	1.40	1.47
23	C	482	CLA	C1A-NA	3.16	1.39	1.32
23	C	483	CLA	C4B-NB	3.16	1.38	1.34
23	C	486	CLA	C3B-CAB	-3.16	1.46	1.49
28	J	53	BCR	C2-C1	3.16	1.62	1.54
23	c	2478	CLA	C1B-C2B	3.16	1.44	1.40
23	c	2475	CLA	O2A-CGA	3.15	1.43	1.33
23	C	479	CLA	MG-NA	3.15	2.16	2.07
23	B	512	CLA	C4A-NA	-3.14	1.32	1.39
23	B	511	CLA	C3D-CAD	-3.14	1.40	1.47
23	C	484	CLA	CHB-C4A	3.14	1.43	1.36
23	B	527	CLA	MG-NC	3.14	2.16	2.07
28	K	50	BCR	C29-C30	3.13	1.62	1.54
23	b	2526	CLA	MG-NC	3.13	2.16	2.07
23	b	2521	CLA	C4-C3	3.13	1.58	1.50
23	b	2519	CLA	C1A-NA	3.13	1.39	1.32
23	b	2525	CLA	CAA-C2A	3.12	1.59	1.54
23	C	476	CLA	C4B-NB	3.12	1.38	1.34
23	B	523	CLA	C4B-NB	3.11	1.38	1.34
23	b	2511	CLA	C1C-NC	-3.11	1.35	1.38
24	d	2356	PHO	C3D-CAD	-3.11	1.41	1.47
23	C	486	CLA	C3D-CAD	-3.11	1.41	1.47
23	c	2486	CLA	C3D-CAD	-3.11	1.41	1.47
23	b	2515	CLA	MG-NA	3.11	2.16	2.07
26	D	357	PL9	C30-C29	3.11	1.58	1.50
23	c	2476	CLA	C1A-NA	3.11	1.39	1.32
26	D	357	PL9	C8-C9	3.11	1.39	1.32
23	c	2476	CLA	C4B-NB	3.11	1.38	1.34
25	v	2138	HEM	O2D-CGD	-3.10	1.19	1.30
23	B	520	CLA	C2-C3	3.09	1.39	1.32
23	D	354	CLA	CAA-C2A	3.09	1.59	1.54
23	b	2516	CLA	C4B-NB	3.09	1.38	1.34
23	c	2484	CLA	CAA-C2A	3.09	1.59	1.54
23	B	517	CLA	C1B-C2B	3.09	1.44	1.40
23	c	2478	CLA	MG-NA	3.09	2.16	2.07
23	B	515	CLA	C1B-CHB	-3.08	1.31	1.39
23	b	2516	CLA	C4A-NA	-3.08	1.32	1.39
23	B	512	CLA	CHB-C4A	3.08	1.43	1.36
23	A	352	CLA	CAA-C2A	3.08	1.59	1.54
27	d	2359	LMT	C3B-C2B	-3.08	1.44	1.52
27	d	2359	LMT	O1'-C1'	3.07	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2522	CLA	C1A-NA	3.07	1.39	1.32
23	B	516	CLA	CHB-C4A	3.07	1.43	1.36
23	B	525	CLA	MG-NA	3.07	2.16	2.07
23	B	513	CLA	CHB-C4A	3.07	1.43	1.36
23	C	487	CLA	MG-NC	3.06	2.16	2.07
23	C	475	CLA	MG-NA	3.06	2.16	2.07
23	C	475	CLA	C5-C3	3.06	1.58	1.51
23	c	2475	CLA	MG-NA	3.06	2.16	2.07
23	c	2482	CLA	C1A-NA	3.05	1.39	1.32
23	D	354	CLA	C1A-NA	3.04	1.39	1.32
23	c	2484	CLA	C1A-NA	3.04	1.38	1.32
23	d	2357	CLA	C4B-NB	3.04	1.38	1.34
25	E	84	HEM	C3B-C4B	3.03	1.48	1.44
23	B	511	CLA	CAA-CBA	-3.03	1.42	1.52
26	a	2352	PL9	C31-C29	3.03	1.58	1.51
23	b	2517	CLA	MG-NA	3.03	2.16	2.07
23	C	483	CLA	C1A-NA	3.03	1.38	1.32
23	b	2515	CLA	C1B-CHB	-3.02	1.31	1.39
23	c	2483	CLA	C4B-NB	3.02	1.38	1.34
25	V	138	HEM	CBC-CAC	3.02	1.46	1.28
23	c	2476	CLA	C4A-NA	-3.02	1.32	1.39
28	k	2050	BCR	C2-C1	3.02	1.61	1.54
23	C	484	CLA	CAA-C2A	3.02	1.59	1.54
23	C	477	CLA	O2A-CGA	3.01	1.42	1.33
23	b	2518	CLA	CAA-CBA	-3.00	1.42	1.52
23	A	349	CLA	C4B-NB	3.00	1.38	1.34
23	b	2524	CLA	C1B-CHB	-3.00	1.31	1.39
23	C	475	CLA	C4B-NB	2.99	1.38	1.34
23	c	2485	CLA	MG-NA	2.99	2.16	2.07
26	a	2352	PL9	C8-C9	2.99	1.39	1.32
23	b	2525	CLA	MG-NA	2.99	2.16	2.07
23	C	480	CLA	C1C-NC	-2.99	1.35	1.38
23	b	2519	CLA	C1B-CHB	-2.98	1.31	1.39
23	C	483	CLA	MG-NA	2.98	2.16	2.07
23	B	522	CLA	C1A-NA	2.98	1.38	1.32
23	c	2485	CLA	C1B-CHB	-2.98	1.31	1.39
25	e	2084	HEM	CMA-C3A	2.98	1.57	1.51
23	b	2523	CLA	C3D-CAD	-2.98	1.41	1.47
23	B	516	CLA	C1A-NA	2.98	1.38	1.32
23	B	520	CLA	C4B-NB	2.97	1.38	1.34
23	c	2476	CLA	C1C-NC	-2.97	1.35	1.38
23	c	2475	CLA	C5-C3	2.96	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2522	CLA	C3D-CAD	-2.96	1.41	1.47
23	b	2516	CLA	C5-C3	2.96	1.58	1.51
23	d	2357	CLA	MG-NC	2.96	2.16	2.07
23	b	2524	CLA	C1C-NC	-2.96	1.35	1.38
26	a	2352	PL9	C17-C18	-2.95	1.42	1.50
23	b	2511	CLA	C1B-CHB	-2.95	1.31	1.39
23	C	476	CLA	C1A-NA	2.95	1.38	1.32
23	B	519	CLA	C2-C3	2.94	1.38	1.32
23	C	477	CLA	C1B-NB	2.94	1.38	1.34
23	B	516	CLA	C5-C3	2.94	1.58	1.51
23	B	517	CLA	C1B-CHB	-2.94	1.31	1.39
23	C	481	CLA	C1A-NA	2.94	1.38	1.32
23	B	519	CLA	C1A-NA	2.94	1.38	1.32
23	C	482	CLA	CHB-C4A	2.94	1.43	1.36
23	b	2514	CLA	C1B-C2B	2.94	1.43	1.40
23	c	2475	CLA	C4-C3	2.94	1.58	1.50
23	c	2483	CLA	MG-NA	2.93	2.15	2.07
23	C	483	CLA	C5-C3	2.93	1.58	1.51
23	d	2354	CLA	C4A-NA	-2.93	1.32	1.39
26	D	357	PL9	C38-C39	2.93	1.40	1.34
23	C	481	CLA	C1B-NB	2.93	1.38	1.34
23	c	2483	CLA	C2-C3	2.92	1.38	1.32
23	C	479	CLA	CAA-CBA	-2.92	1.43	1.52
23	C	486	CLA	C1C-NC	-2.92	1.36	1.38
23	B	518	CLA	CAA-CBA	-2.92	1.43	1.52
23	C	475	CLA	O2A-CGA	2.92	1.42	1.33
24	A	351	PHO	C4D-CHA	-2.92	1.41	1.45
23	B	513	CLA	C4A-NA	-2.92	1.32	1.39
23	B	524	CLA	C1A-NA	2.92	1.38	1.32
28	C	489	BCR	C1-C6	2.92	1.58	1.53
25	v	2138	HEM	C1B-NB	2.92	1.46	1.39
23	c	2474	CLA	MG-NA	2.91	2.15	2.07
23	D	354	CLA	C4A-NA	-2.91	1.32	1.39
23	c	2481	CLA	C1B-NB	2.91	1.38	1.34
26	A	353	PL9	C31-C29	2.91	1.58	1.51
23	b	2515	CLA	CAA-CBA	-2.91	1.43	1.52
24	D	355	PHO	C3D-CAD	-2.91	1.41	1.47
23	A	348	CLA	C4A-NA	-2.91	1.32	1.39
23	A	348	CLA	C4B-NB	2.91	1.38	1.34
23	c	2476	CLA	CHB-C4A	2.91	1.43	1.36
23	b	2512	CLA	C3D-CAD	-2.91	1.41	1.47
25	e	2084	HEM	FE-NA	2.90	2.04	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2516	CLA	C1-C2	2.90	1.58	1.49
23	a	2348	CLA	C1B-CHB	-2.90	1.31	1.39
23	b	2519	CLA	CAA-CBA	-2.90	1.43	1.52
23	A	352	CLA	MG-NA	2.90	2.15	2.07
23	c	2480	CLA	C1C-NC	-2.89	1.36	1.38
23	c	2479	CLA	C4B-NB	2.89	1.38	1.34
23	b	2516	CLA	CHB-C4A	2.89	1.43	1.36
23	B	520	CLA	C4A-NA	-2.89	1.33	1.39
23	B	515	CLA	C3D-CAD	-2.89	1.41	1.47
26	A	353	PL9	C8-C9	2.89	1.38	1.32
23	b	2519	CLA	C2-C3	2.89	1.38	1.32
23	B	511	CLA	C4B-NB	2.88	1.38	1.34
25	v	2138	HEM	C4A-NA	2.88	1.42	1.36
23	b	2513	CLA	CHB-C4A	2.88	1.43	1.36
23	B	516	CLA	C1-C2	2.88	1.58	1.49
23	B	527	CLA	C1B-NB	2.88	1.38	1.34
28	k	2050	BCR	C30-C25	2.88	1.57	1.53
23	B	520	CLA	O2A-CGA	2.87	1.42	1.33
23	A	352	CLA	MG-NC	2.87	2.15	2.07
23	b	2512	CLA	CHB-C4A	2.87	1.43	1.36
23	a	2348	CLA	C1C-NC	-2.86	1.36	1.38
23	c	2482	CLA	CHB-C4A	2.86	1.43	1.36
23	B	517	CLA	C3D-CAD	-2.86	1.41	1.47
23	d	2357	CLA	CHB-C4A	2.86	1.43	1.36
23	B	521	CLA	C1B-NB	2.86	1.38	1.34
23	B	519	CLA	CAA-CBA	-2.86	1.43	1.52
26	d	2358	PL9	C38-C39	2.86	1.40	1.34
25	E	84	HEM	C4A-NA	2.86	1.42	1.36
23	b	2512	CLA	CAA-C2A	2.85	1.59	1.54
23	c	2483	CLA	CHB-C4A	2.85	1.43	1.36
25	V	138	HEM	O2A-CGA	-2.85	1.20	1.30
23	C	484	CLA	MG-NC	2.84	2.15	2.07
23	A	352	CLA	C1A-NA	2.84	1.38	1.32
23	D	356	CLA	C1C-NC	-2.84	1.36	1.38
23	B	521	CLA	C4-C3	2.84	1.57	1.50
23	C	476	CLA	C4A-NA	-2.84	1.33	1.39
23	b	2521	CLA	C4B-NB	2.83	1.38	1.34
23	b	2511	CLA	C4B-NB	2.83	1.38	1.34
28	d	2360	BCR	C14-C13	2.83	1.39	1.35
23	B	514	CLA	C1B-C2B	2.83	1.43	1.40
23	b	2524	CLA	C4A-NA	-2.82	1.33	1.39
23	B	515	CLA	CAA-CBA	-2.82	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2348	CLA	C1A-NA	2.82	1.38	1.32
25	e	2084	HEM	C1A-C2A	2.82	1.48	1.43
23	B	512	CLA	C4-C3	2.82	1.57	1.50
23	C	485	CLA	C1C-NC	-2.81	1.36	1.38
23	B	527	CLA	C2-C3	2.81	1.38	1.32
23	A	348	CLA	C1B-CHB	-2.81	1.32	1.39
23	c	2475	CLA	C1A-NA	2.81	1.38	1.32
23	B	512	CLA	C1A-NA	2.81	1.38	1.32
25	V	138	HEM	CBD-CGD	-2.80	1.43	1.50
23	B	515	CLA	C1A-NA	2.80	1.38	1.32
23	B	524	CLA	CAA-C2A	2.80	1.59	1.54
23	B	525	CLA	C3B-C4B	2.80	1.44	1.40
23	c	2484	CLA	C4-C3	2.79	1.57	1.50
23	C	487	CLA	OBD-CAD	2.79	1.26	1.22
23	B	516	CLA	C4A-NA	-2.79	1.33	1.39
23	a	2349	CLA	CAA-CBA	-2.79	1.43	1.52
23	C	477	CLA	C3D-CAD	-2.78	1.41	1.47
28	K	50	BCR	C12-C13	-2.78	1.39	1.45
23	c	2480	CLA	C1A-NA	2.78	1.38	1.32
28	b	2527	BCR	C1-C6	2.78	1.57	1.53
23	b	2525	CLA	OBD-CAD	2.78	1.26	1.22
23	c	2474	CLA	C4-C3	2.78	1.57	1.50
23	c	2478	CLA	C2-C3	2.77	1.38	1.32
23	D	356	CLA	MG-NC	2.77	2.15	2.07
23	B	525	CLA	CAA-C2A	2.77	1.59	1.54
23	C	480	CLA	CAA-CBA	-2.77	1.43	1.52
28	K	50	BCR	C1-C6	2.77	1.57	1.53
23	b	2521	CLA	C4A-NA	-2.77	1.33	1.39
23	b	2511	CLA	CAA-CBA	-2.77	1.43	1.52
23	b	2524	CLA	MG-NA	2.76	2.15	2.07
23	B	523	CLA	C1A-NA	2.76	1.38	1.32
23	C	476	CLA	MG-NC	2.76	2.15	2.07
23	C	484	CLA	C4-C3	2.76	1.57	1.50
26	A	353	PL9	C27-C28	-2.76	1.42	1.50
23	B	523	CLA	C3D-CAD	-2.76	1.41	1.47
23	B	523	CLA	C4A-NA	-2.75	1.33	1.39
23	c	2486	CLA	MG-NC	2.75	2.15	2.07
23	B	525	CLA	OBD-CAD	2.75	1.26	1.22
23	d	2357	CLA	C4-C3	2.75	1.57	1.50
28	b	2528	BCR	C24-C23	2.75	1.41	1.32
23	A	349	CLA	MG-NA	2.75	2.15	2.07
23	a	2349	CLA	C4B-NB	2.74	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	483	CLA	CHB-C4A	2.74	1.43	1.36
23	b	2523	CLA	CHB-C4A	2.74	1.43	1.36
23	C	480	CLA	C4A-NA	-2.74	1.33	1.39
23	c	2475	CLA	C4A-NA	-2.74	1.33	1.39
23	b	2525	CLA	CHB-C4A	2.74	1.42	1.36
23	a	2349	CLA	C1A-NA	2.74	1.38	1.32
28	K	50	BCR	C21-C22	-2.73	1.32	1.35
23	C	475	CLA	C4-C3	2.73	1.57	1.50
26	d	2358	PL9	C30-C29	2.73	1.57	1.50
23	b	2518	CLA	MG-NA	2.73	2.15	2.07
26	a	2352	PL9	C27-C28	-2.72	1.42	1.50
23	c	2481	CLA	CHB-C4A	2.72	1.42	1.36
25	e	2084	HEM	O1A-CGA	2.72	1.32	1.22
23	c	2481	CLA	CAA-CBA	-2.72	1.43	1.52
23	B	512	CLA	MG-NA	2.72	2.15	2.07
23	d	2355	CLA	C1B-CHB	-2.71	1.32	1.39
23	C	476	CLA	CHB-C4A	2.71	1.42	1.36
23	B	518	CLA	C1B-CHB	-2.71	1.32	1.39
23	c	2483	CLA	C5-C3	2.71	1.57	1.51
23	C	483	CLA	C4A-NA	-2.71	1.33	1.39
23	c	2478	CLA	CAA-C2A	2.71	1.59	1.54
23	c	2476	CLA	C3D-CAD	-2.71	1.41	1.47
23	b	2511	CLA	C1B-NB	2.71	1.38	1.34
28	K	50	BCR	C2-C1	2.71	1.61	1.54
23	B	513	CLA	MG-NC	2.70	2.15	2.07
23	B	524	CLA	O2A-CGA	2.70	1.41	1.33
23	B	511	CLA	C1B-CHB	-2.70	1.32	1.39
23	B	523	CLA	C1C-NC	-2.70	1.36	1.38
23	c	2484	CLA	CHB-C4A	2.69	1.42	1.36
23	C	476	CLA	MG-NA	2.69	2.15	2.07
23	c	2487	CLA	C3B-C4B	2.69	1.44	1.40
27	d	2359	LMT	C2-C1	2.69	1.63	1.50
23	c	2474	CLA	C1C-NC	-2.69	1.36	1.38
23	b	2515	CLA	C3A-C4A	-2.69	1.44	1.51
23	a	2351	CLA	C1A-NA	2.69	1.38	1.32
23	C	476	CLA	C1C-NC	-2.69	1.36	1.38
23	a	2351	CLA	MG-NA	2.68	2.15	2.07
23	B	513	CLA	C2-C3	2.68	1.38	1.32
26	D	357	PL9	C41-C39	2.68	1.55	1.40
23	C	485	CLA	MG-NA	2.68	2.15	2.07
23	C	478	CLA	C1B-CHB	-2.68	1.32	1.39
23	A	350	CLA	C4A-NA	-2.67	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	353	PL9	C17-C18	-2.67	1.42	1.50
25	V	138	HEM	C2C-C1C	2.68	1.51	1.43
23	d	2355	CLA	O2A-CGA	2.67	1.41	1.33
23	a	2351	CLA	CAA-C2A	2.67	1.58	1.54
23	b	2520	CLA	C4-C3	2.67	1.57	1.50
23	d	2357	CLA	MG-NA	2.66	2.15	2.07
27	B	526	LMT	C2-C1	2.66	1.63	1.50
23	C	474	CLA	C4A-NA	-2.66	1.33	1.39
23	b	2519	CLA	C1-C2	2.66	1.58	1.49
23	D	354	CLA	CHB-C4A	2.66	1.42	1.36
27	d	2359	LMT	C4'-C5'	2.66	1.60	1.52
23	c	2481	CLA	C1A-NA	2.66	1.38	1.32
23	A	349	CLA	C3D-CAD	-2.66	1.41	1.47
23	D	354	CLA	C4B-NB	2.66	1.37	1.34
26	D	357	PL9	C32-C33	-2.65	1.42	1.50
23	B	520	CLA	C1C-NC	-2.65	1.36	1.38
26	d	2358	PL9	C41-C39	2.65	1.54	1.40
23	C	482	CLA	C5-C3	2.65	1.57	1.51
23	c	2474	CLA	C4B-NB	2.65	1.37	1.34
23	c	2483	CLA	C4-C3	2.65	1.57	1.50
23	C	485	CLA	C1A-NA	2.65	1.38	1.32
23	c	2486	CLA	C1B-CHB	-2.64	1.32	1.39
23	c	2485	CLA	CAA-CBA	-2.64	1.43	1.52
23	d	2357	CLA	C3D-CAD	-2.64	1.42	1.47
23	c	2482	CLA	C4A-NA	-2.64	1.33	1.39
23	c	2483	CLA	CAA-CBA	-2.63	1.44	1.52
23	A	350	CLA	C4B-NB	2.64	1.37	1.34
23	D	356	CLA	CHB-C4A	2.63	1.42	1.36
23	C	475	CLA	MG-NC	2.63	2.15	2.07
23	b	2520	CLA	C4B-NB	2.63	1.37	1.34
25	e	2084	HEM	C4A-CHB	2.63	1.47	1.39
23	B	527	CLA	CHB-C4A	2.63	1.42	1.36
23	A	350	CLA	C1C-NC	-2.63	1.36	1.38
23	c	2478	CLA	C1B-CHB	-2.63	1.32	1.39
23	a	2351	CLA	MG-NC	2.63	2.15	2.07
23	A	350	CLA	CHB-C4A	2.62	1.42	1.36
23	a	2349	CLA	C1C-NC	-2.62	1.36	1.38
23	B	522	CLA	C3D-CAD	-2.62	1.42	1.47
23	B	515	CLA	C3A-C4A	-2.62	1.44	1.51
23	c	2477	CLA	C4A-NA	-2.62	1.33	1.39
23	B	517	CLA	MG-NA	2.62	2.15	2.07
23	C	476	CLA	C3D-CAD	-2.62	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2518	CLA	MG-NB	2.62	2.10	2.05
23	B	524	CLA	MG-NA	2.62	2.15	2.07
23	C	474	CLA	CAA-CBA	-2.62	1.44	1.52
23	C	477	CLA	C4A-NA	-2.61	1.33	1.39
23	B	523	CLA	MG-NA	2.62	2.15	2.07
23	b	2514	CLA	C5-C3	2.62	1.57	1.51
23	c	2487	CLA	C4-C3	2.61	1.57	1.50
23	b	2522	CLA	C4A-NA	-2.61	1.33	1.39
23	b	2517	CLA	C1B-CHB	-2.61	1.32	1.39
23	A	352	CLA	C4-C3	2.61	1.57	1.50
23	a	2348	CLA	CHC-C1C	2.61	1.44	1.35
23	C	478	CLA	CAA-C2A	2.61	1.58	1.54
23	b	2515	CLA	C3B-CAB	-2.61	1.46	1.49
23	B	520	CLA	C1-C2	2.61	1.57	1.49
23	C	475	CLA	C1B-CHB	-2.60	1.32	1.39
23	a	2349	CLA	CHB-C4A	2.60	1.42	1.36
23	b	2520	CLA	O2A-CGA	2.60	1.41	1.33
23	b	2513	CLA	MG-NA	2.60	2.14	2.07
23	B	512	CLA	CAA-C2A	2.60	1.58	1.54
23	B	517	CLA	C1A-NA	2.60	1.38	1.32
23	B	517	CLA	C3A-C4A	-2.60	1.44	1.51
23	B	511	CLA	MG-NC	2.60	2.14	2.07
23	b	2511	CLA	C3D-CAD	-2.60	1.42	1.47
23	b	2520	CLA	C1-C2	2.60	1.57	1.49
26	a	2352	PL9	C35-C34	2.59	1.57	1.50
28	K	50	BCR	C33-C5	2.59	1.55	1.51
23	B	514	CLA	MG-NA	2.59	2.14	2.07
25	E	84	HEM	O1A-CGA	2.59	1.31	1.22
23	C	483	CLA	CAA-CBA	-2.59	1.44	1.52
23	c	2475	CLA	C3B-CAB	-2.59	1.46	1.49
23	d	2355	CLA	C4B-NB	2.59	1.37	1.34
28	k	2050	BCR	C12-C13	-2.58	1.40	1.45
23	B	516	CLA	C6-C5	2.58	1.62	1.52
23	c	2476	CLA	CAA-C2A	2.58	1.58	1.54
25	e	2084	HEM	CMC-C2C	2.58	1.55	1.47
26	a	2352	PL9	C41-C39	2.58	1.54	1.40
23	c	2485	CLA	MG-NC	2.58	2.14	2.07
28	B	528	BCR	C33-C5	2.58	1.55	1.51
23	B	527	CLA	C4-C3	2.58	1.57	1.50
23	c	2480	CLA	CAA-CBA	-2.57	1.44	1.52
23	b	2526	CLA	C3B-CAB	2.57	1.51	1.49
26	d	2358	PL9	C35-C34	2.57	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2523	CLA	C4B-NB	2.57	1.37	1.34
23	B	519	CLA	C1-C2	2.57	1.57	1.49
23	b	2521	CLA	CAA-CBA	-2.57	1.44	1.52
23	B	511	CLA	C3A-C4A	-2.56	1.44	1.51
23	c	2482	CLA	C5-C3	2.56	1.57	1.51
23	B	517	CLA	C4A-NA	-2.56	1.33	1.39
23	C	478	CLA	C1B-C2B	2.56	1.43	1.40
23	b	2516	CLA	C1A-NA	2.56	1.37	1.32
23	B	514	CLA	C3A-C4A	-2.56	1.44	1.51
25	E	84	HEM	CHC-C1C	2.56	1.41	1.36
23	a	2349	CLA	C4A-NA	-2.55	1.33	1.39
23	b	2524	CLA	O2A-CGA	2.55	1.41	1.33
26	A	353	PL9	C30-C29	2.55	1.57	1.50
23	b	2511	CLA	MG-NA	2.55	2.14	2.07
23	C	482	CLA	C4A-NA	-2.55	1.33	1.39
23	B	516	CLA	CAA-CBA	-2.55	1.44	1.52
26	A	353	PL9	C18-C19	2.55	1.38	1.32
23	d	2355	CLA	C4A-NA	-2.55	1.33	1.39
23	c	2484	CLA	C3D-CAD	-2.55	1.42	1.47
23	c	2474	CLA	C1A-NA	2.55	1.37	1.32
23	C	482	CLA	C3D-CAD	-2.54	1.42	1.47
23	B	519	CLA	MG-ND	-2.54	1.99	2.05
23	B	511	CLA	C1B-NB	2.54	1.37	1.34
23	b	2511	CLA	O2A-CGA	2.54	1.41	1.33
23	c	2475	CLA	C1-C2	2.54	1.57	1.49
23	b	2514	CLA	MG-NA	2.54	2.14	2.07
23	c	2485	CLA	C1A-NA	2.54	1.37	1.32
23	c	2475	CLA	C1C-NC	-2.54	1.36	1.38
23	B	523	CLA	MG-NC	2.53	2.14	2.07
23	c	2479	CLA	MG-NA	2.53	2.14	2.07
23	C	487	CLA	C1B-CHB	-2.53	1.32	1.39
23	b	2518	CLA	CHB-C4A	2.53	1.42	1.36
23	C	475	CLA	C1-C2	2.53	1.57	1.49
23	b	2512	CLA	MG-NA	2.53	2.14	2.07
28	k	2050	BCR	C21-C22	-2.52	1.32	1.35
23	a	2348	CLA	C4B-NB	2.52	1.37	1.34
23	b	2525	CLA	C1C-NC	-2.52	1.36	1.38
23	B	516	CLA	C4-C3	2.52	1.57	1.50
23	c	2484	CLA	C4A-NA	-2.52	1.33	1.39
23	c	2480	CLA	C4A-NA	-2.52	1.33	1.39
23	C	483	CLA	C2-C3	2.52	1.38	1.32
23	a	2351	CLA	C4-C3	2.52	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	513	CLA	MG-NA	2.52	2.14	2.07
25	v	2138	HEM	C4A-C3A	2.52	1.43	1.40
23	C	475	CLA	C1C-NC	-2.51	1.36	1.38
28	b	2528	BCR	C38-C26	2.51	1.55	1.51
28	c	2489	BCR	C21-C22	2.51	1.39	1.35
23	c	2487	CLA	C1C-NC	-2.51	1.36	1.38
23	b	2522	CLA	C4-C3	2.51	1.57	1.50
25	v	2138	HEM	C3C-C2C	2.51	1.48	1.43
23	C	486	CLA	C1B-CHB	-2.50	1.32	1.39
23	b	2524	CLA	C4B-NB	2.50	1.37	1.34
25	e	2084	HEM	FE-NB	2.50	2.07	1.97
23	b	2517	CLA	CAA-CBA	-2.50	1.44	1.52
23	a	2351	CLA	C4C-C3C	2.50	1.49	1.45
23	A	348	CLA	CHC-C1C	2.50	1.43	1.35
23	c	2482	CLA	C3D-CAD	-2.50	1.42	1.47
26	a	2352	PL9	C30-C29	2.50	1.57	1.50
28	K	50	BCR	C20-C21	-2.50	1.36	1.43
23	B	527	CLA	MG-NB	2.49	2.10	2.05
23	D	356	CLA	C4-C3	2.49	1.57	1.50
26	A	353	PL9	C41-C39	2.49	1.54	1.40
23	b	2520	CLA	CHB-C4A	2.49	1.42	1.36
28	F	48	BCR	C14-C13	2.49	1.39	1.35
23	A	352	CLA	C3D-CAD	-2.49	1.42	1.47
23	c	2481	CLA	C1C-NC	-2.49	1.36	1.38
23	C	481	CLA	C4-C3	2.49	1.57	1.50
23	b	2511	CLA	C1A-NA	2.49	1.37	1.32
27	B	526	LMT	C4'-C5'	2.49	1.59	1.52
23	A	349	CLA	CAA-C2A	2.49	1.58	1.54
23	B	511	CLA	MG-NA	2.49	2.14	2.07
25	E	84	HEM	C3C-C2C	-2.48	1.39	1.43
26	d	2358	PL9	C32-C33	-2.48	1.43	1.50
23	b	2512	CLA	C4-C3	2.48	1.57	1.50
25	V	138	HEM	FE-ND	2.48	2.06	1.97
23	A	349	CLA	C1B-CHB	-2.48	1.33	1.39
24	d	2356	PHO	C4D-CHA	-2.48	1.42	1.45
23	b	2523	CLA	MG-NA	2.48	2.14	2.07
23	A	349	CLA	O2A-CGA	2.47	1.41	1.33
23	C	484	CLA	OBD-CAD	2.47	1.25	1.22
23	C	474	CLA	MG-NA	2.47	2.14	2.07
23	c	2474	CLA	CAA-CBA	-2.47	1.44	1.52
23	b	2519	CLA	MG-NA	2.47	2.14	2.07
28	k	2050	BCR	C20-C21	-2.47	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	351	PHO	C1D-ND	-2.47	1.34	1.38
23	c	2475	CLA	C4B-NB	2.47	1.37	1.34
23	b	2516	CLA	C1C-NC	-2.47	1.36	1.38
23	B	511	CLA	C1A-NA	2.47	1.37	1.32
23	b	2516	CLA	CAA-CBA	-2.47	1.44	1.52
23	D	356	CLA	MG-NA	2.47	2.14	2.07
23	d	2354	CLA	CHB-C4A	2.47	1.42	1.36
28	j	2053	BCR	C38-C26	2.47	1.55	1.51
23	c	2479	CLA	C3A-C4A	-2.46	1.45	1.51
23	b	2515	CLA	C4-C3	2.46	1.57	1.50
23	C	486	CLA	C1B-NB	2.46	1.37	1.34
23	b	2520	CLA	MG-NC	2.46	2.14	2.07
23	b	2513	CLA	MG-NC	2.46	2.14	2.07
23	B	519	CLA	C5-C3	2.46	1.57	1.51
26	A	353	PL9	C35-C34	2.46	1.57	1.50
23	B	521	CLA	CAA-CBA	-2.46	1.44	1.52
23	C	487	CLA	C3B-C4B	2.46	1.44	1.40
23	b	2518	CLA	C4-C3	2.45	1.57	1.50
23	B	518	CLA	MG-NC	2.45	2.14	2.07
25	E	84	HEM	C2A-C3A	2.45	1.44	1.37
23	b	2518	CLA	C1B-CHB	-2.45	1.33	1.39
23	c	2479	CLA	C1B-CHB	-2.45	1.33	1.39
23	b	2522	CLA	CAA-C2A	2.45	1.58	1.54
23	A	350	CLA	CAA-CBA	-2.44	1.44	1.52
23	B	525	CLA	CHB-C4A	2.44	1.42	1.36
23	b	2511	CLA	C4A-NA	-2.44	1.33	1.39
28	k	2050	BCR	C5-C6	2.44	1.38	1.34
23	C	480	CLA	CHB-C4A	2.44	1.42	1.36
23	A	349	CLA	C4A-NA	-2.44	1.33	1.39
23	b	2524	CLA	C3D-CAD	-2.44	1.42	1.47
23	c	2478	CLA	OBD-CAD	2.44	1.25	1.22
23	C	478	CLA	C2-C3	2.44	1.37	1.32
23	b	2520	CLA	C4A-NA	-2.44	1.33	1.39
28	k	2050	BCR	C16-C17	-2.44	1.36	1.43
24	d	2356	PHO	CHA-C1A	2.44	1.42	1.37
23	B	525	CLA	C3B-C2B	-2.43	1.37	1.41
23	C	474	CLA	MG-NC	2.43	2.14	2.07
23	b	2514	CLA	C3A-C4A	-2.43	1.45	1.51
23	d	2357	CLA	C5-C3	2.43	1.57	1.51
28	K	50	BCR	C16-C15	-2.43	1.29	1.35
23	b	2512	CLA	C1A-NA	2.43	1.37	1.32
23	b	2511	CLA	C1-C2	2.43	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	524	CLA	C3D-CAD	-2.43	1.42	1.47
28	k	2050	BCR	C33-C5	2.43	1.55	1.51
23	B	522	CLA	CHB-C4A	2.43	1.42	1.36
23	A	348	CLA	C1A-NA	2.43	1.37	1.32
23	c	2483	CLA	C1C-NC	-2.42	1.36	1.38
28	K	50	BCR	C16-C17	-2.42	1.36	1.43
23	b	2511	CLA	CHC-C1C	2.42	1.43	1.35
23	b	2517	CLA	C1A-NA	2.42	1.37	1.32
23	b	2517	CLA	C3A-C4A	-2.42	1.45	1.51
28	b	2528	BCR	C5-C6	2.42	1.38	1.34
28	c	2488	BCR	C19-C18	-2.42	1.40	1.45
23	a	2348	CLA	C3D-CAD	-2.42	1.42	1.47
26	D	357	PL9	C35-C34	2.42	1.56	1.50
23	C	486	CLA	C4B-NB	2.42	1.37	1.34
23	b	2523	CLA	C1A-NA	2.42	1.37	1.32
23	b	2523	CLA	C4A-NA	-2.42	1.33	1.39
23	b	2511	CLA	MG-NC	2.42	2.14	2.07
23	C	482	CLA	MG-NC	2.42	2.14	2.07
23	b	2517	CLA	C3D-CAD	-2.41	1.42	1.47
23	D	356	CLA	C1C-C2C	2.41	1.49	1.44
23	B	512	CLA	MG-NC	2.41	2.14	2.07
23	c	2481	CLA	C4-C3	2.41	1.56	1.50
23	C	485	CLA	C4-C3	2.41	1.56	1.50
23	b	2519	CLA	C4A-NA	-2.41	1.34	1.39
23	B	518	CLA	C4A-NA	-2.41	1.34	1.39
23	C	483	CLA	MG-NC	2.41	2.14	2.07
28	k	2050	BCR	C16-C15	-2.40	1.29	1.35
23	b	2517	CLA	C4A-NA	-2.40	1.34	1.39
23	C	478	CLA	OBD-CAD	2.40	1.25	1.22
23	C	479	CLA	C1B-CHB	-2.40	1.33	1.39
23	c	2475	CLA	C1B-CHB	-2.40	1.33	1.39
23	B	520	CLA	C3D-CAD	-2.39	1.42	1.47
23	B	511	CLA	O2A-CGA	2.39	1.40	1.33
23	c	2485	CLA	C4-C3	2.40	1.56	1.50
23	c	2484	CLA	MG-NC	2.39	2.14	2.07
24	a	2350	PHO	C1D-ND	-2.39	1.35	1.38
23	C	481	CLA	MG-NC	2.39	2.14	2.07
23	A	348	CLA	CAA-CBA	-2.39	1.44	1.52
23	c	2480	CLA	CHB-C4A	2.39	1.42	1.36
23	B	520	CLA	MG-NA	2.39	2.14	2.07
23	C	474	CLA	C1B-CHB	-2.39	1.33	1.39
23	b	2518	CLA	C3B-CAB	-2.39	1.47	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	487	CLA	C4-C3	2.39	1.56	1.50
23	B	523	CLA	CHB-C4A	2.39	1.42	1.36
23	C	474	CLA	C4B-NB	2.39	1.37	1.34
23	b	2525	CLA	C4-C3	2.38	1.56	1.50
23	B	517	CLA	CAA-CBA	-2.38	1.44	1.52
23	B	520	CLA	MG-NC	2.38	2.14	2.07
23	A	350	CLA	C1A-NA	2.38	1.37	1.32
26	d	2358	PL9	C37-C38	-2.38	1.43	1.50
23	C	478	CLA	O2A-CGA	2.38	1.40	1.33
23	b	2519	CLA	C4-C3	2.38	1.56	1.50
27	B	526	LMT	O1'-C1'	2.38	1.44	1.40
23	B	518	CLA	MG-NA	2.37	2.14	2.07
23	a	2351	CLA	C1B-CHB	-2.37	1.33	1.39
23	b	2513	CLA	C2-C3	2.37	1.37	1.32
23	B	521	CLA	C4A-NA	-2.37	1.34	1.39
23	b	2520	CLA	MG-NA	2.37	2.14	2.07
23	b	2524	CLA	CAA-C2A	2.36	1.58	1.54
23	B	511	CLA	CHC-C1C	2.36	1.43	1.35
28	c	2489	BCR	C33-C5	2.36	1.55	1.51
23	b	2514	CLA	C4-C3	2.36	1.56	1.50
25	v	2138	HEM	C2B-C1B	-2.36	1.44	1.44
26	d	2358	PL9	C2-C3	2.36	1.41	1.34
23	b	2526	CLA	CHB-C4A	2.35	1.42	1.36
23	c	2485	CLA	CBA-CGA	-2.35	1.43	1.50
26	a	2352	PL9	C40-C39	2.35	1.56	1.48
23	C	481	CLA	C4A-NA	-2.35	1.34	1.39
23	b	2515	CLA	C4A-NA	-2.35	1.34	1.39
23	b	2513	CLA	C4-C3	2.35	1.56	1.50
23	c	2482	CLA	MG-NC	2.35	2.14	2.07
23	B	519	CLA	C4B-NB	2.35	1.37	1.34
23	b	2514	CLA	C2-C3	2.35	1.37	1.32
23	b	2511	CLA	C1C-C2C	2.35	1.49	1.44
23	C	484	CLA	C3D-CAD	-2.35	1.42	1.47
23	b	2511	CLA	C3A-C4A	-2.35	1.45	1.51
23	B	512	CLA	C3D-CAD	-2.35	1.42	1.47
23	C	480	CLA	C1A-NA	2.34	1.37	1.32
23	A	348	CLA	C3D-CAD	-2.34	1.42	1.47
23	b	2526	CLA	C4-C3	2.34	1.56	1.50
23	b	2517	CLA	C1C-NC	-2.34	1.36	1.38
23	b	2524	CLA	C3B-CAB	-2.34	1.47	1.49
23	b	2523	CLA	CHC-C1C	2.33	1.43	1.35
23	d	2357	CLA	CAA-C2A	2.33	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2350	PHO	C4-C3	2.33	1.56	1.50
24	D	355	PHO	C1D-ND	-2.33	1.35	1.38
23	B	522	CLA	C1B-CHB	-2.33	1.33	1.39
23	c	2477	CLA	MG-NC	2.33	2.14	2.07
28	K	50	BCR	C15-C14	-2.33	1.36	1.43
23	c	2483	CLA	C3D-CAD	-2.33	1.42	1.47
23	B	514	CLA	C5-C3	2.33	1.56	1.51
23	A	352	CLA	C1B-CHB	-2.33	1.33	1.39
23	b	2520	CLA	CHC-C1C	2.33	1.43	1.35
23	B	523	CLA	C2A-C1A	-2.32	1.48	1.52
23	B	527	CLA	C4C-C3C	2.32	1.49	1.45
23	c	2481	CLA	C3D-CAD	-2.32	1.42	1.47
23	d	2355	CLA	MG-NA	2.32	2.14	2.07
23	c	2476	CLA	CHC-C1C	2.32	1.43	1.35
23	c	2478	CLA	MG-NC	2.32	2.14	2.07
23	c	2476	CLA	MG-NC	2.32	2.14	2.07
23	C	483	CLA	CAA-C2A	2.32	1.58	1.54
26	D	357	PL9	C2-C3	2.32	1.41	1.34
24	D	355	PHO	C4D-CHA	-2.31	1.42	1.45
23	c	2487	CLA	C4B-NB	2.31	1.37	1.34
23	B	511	CLA	C4A-NA	-2.31	1.34	1.39
23	c	2475	CLA	MG-NC	2.31	2.14	2.07
23	C	481	CLA	CHB-C4A	2.31	1.42	1.36
23	b	2526	CLA	CMB-C2B	2.31	1.56	1.51
28	j	2053	BCR	C33-C5	2.31	1.54	1.51
23	C	485	CLA	CAA-CBA	-2.31	1.45	1.52
23	b	2525	CLA	MG-NC	2.31	2.14	2.07
23	B	519	CLA	C3B-C2B	-2.30	1.37	1.41
28	B	529	BCR	C38-C26	2.30	1.54	1.51
23	B	521	CLA	MG-NB	2.30	2.10	2.05
23	b	2520	CLA	C5-C3	2.29	1.56	1.51
23	C	475	CLA	CAA-CBA	-2.30	1.45	1.52
23	B	520	CLA	C4-C3	2.29	1.56	1.50
26	D	357	PL9	C37-C38	-2.29	1.43	1.50
23	A	349	CLA	C1A-NA	2.29	1.37	1.32
23	b	2517	CLA	C4B-NB	2.29	1.37	1.34
23	c	2478	CLA	CHB-C4A	2.29	1.41	1.36
23	b	2523	CLA	C1C-C2C	2.29	1.49	1.44
23	B	511	CLA	C1-C2	2.29	1.56	1.49
23	B	514	CLA	C4-C3	2.29	1.56	1.50
23	c	2474	CLA	C1B-CHB	-2.29	1.33	1.39
23	b	2525	CLA	C3B-C2B	-2.29	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2475	CLA	CAA-CBA	-2.29	1.45	1.52
23	C	482	CLA	C1B-NB	2.28	1.37	1.34
23	b	2514	CLA	C4A-NA	-2.28	1.34	1.39
23	c	2478	CLA	C4A-NA	-2.28	1.34	1.39
23	b	2521	CLA	CHB-C4A	2.28	1.41	1.36
23	D	356	CLA	C1A-NA	2.28	1.37	1.32
23	B	515	CLA	C4-C3	2.28	1.56	1.50
23	C	475	CLA	C1A-NA	2.28	1.37	1.32
23	b	2516	CLA	C6-C5	2.28	1.61	1.52
23	C	486	CLA	MG-NC	2.27	2.13	2.07
23	B	514	CLA	C3D-CAD	-2.27	1.42	1.47
23	C	475	CLA	C4A-NA	-2.27	1.34	1.39
25	E	84	HEM	C4B-NB	2.27	1.43	1.37
23	b	2526	CLA	C4C-C3C	2.27	1.49	1.45
23	c	2474	CLA	C1B-NB	2.27	1.37	1.34
28	c	2488	BCR	C33-C5	2.27	1.54	1.51
23	B	521	CLA	CHB-C4A	2.26	1.41	1.36
23	C	480	CLA	C4B-NB	2.26	1.37	1.34
23	c	2486	CLA	C4-C3	2.26	1.56	1.50
23	C	484	CLA	CHC-C1C	2.26	1.43	1.35
23	b	2523	CLA	C1C-NC	-2.26	1.36	1.38
23	b	2521	CLA	C1B-NB	2.26	1.37	1.34
23	d	2355	CLA	CHC-C1C	2.26	1.43	1.35
23	C	479	CLA	C1B-NB	2.26	1.37	1.34
23	B	527	CLA	CMB-C2B	2.25	1.56	1.51
23	A	350	CLA	MG-NC	2.25	2.13	2.07
23	B	521	CLA	MG-NC	2.25	2.13	2.07
23	c	2486	CLA	C1B-NB	2.25	1.37	1.34
23	C	481	CLA	CAA-CBA	-2.25	1.45	1.52
23	C	477	CLA	CHB-C4A	2.25	1.41	1.36
24	d	2356	PHO	C1D-ND	-2.25	1.35	1.38
23	C	478	CLA	C3D-CAD	-2.25	1.42	1.47
23	b	2526	CLA	MG-NB	2.24	2.10	2.05
26	A	353	PL9	C40-C39	2.24	1.56	1.48
28	b	2528	BCR	C37-C22	2.24	1.54	1.51
23	B	525	CLA	C4-C3	2.24	1.56	1.50
28	K	50	BCR	C24-C25	-2.24	1.38	1.46
23	B	521	CLA	C1B-CHB	-2.24	1.33	1.39
23	C	479	CLA	CHB-C4A	2.24	1.41	1.36
23	b	2523	CLA	MG-NC	2.24	2.13	2.07
24	D	355	PHO	CHA-C1A	2.24	1.42	1.37
23	c	2480	CLA	C1B-CHB	-2.24	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	483	CLA	C4-C3	2.24	1.56	1.50
24	a	2350	PHO	CAA-CBA	-2.23	1.45	1.52
23	b	2523	CLA	C4-C3	2.23	1.56	1.50
23	B	514	CLA	C2-C3	2.23	1.37	1.32
28	d	2360	BCR	C24-C23	2.23	1.39	1.32
23	b	2521	CLA	C5-C3	2.23	1.56	1.51
23	B	520	CLA	CHC-C1C	2.23	1.43	1.35
23	B	519	CLA	C4-C3	2.23	1.56	1.50
23	C	479	CLA	C3A-C4A	-2.23	1.45	1.51
23	a	2348	CLA	C3B-C2B	-2.23	1.37	1.41
23	b	2516	CLA	C4-C3	2.23	1.56	1.50
23	C	478	CLA	C4A-NA	-2.23	1.34	1.39
23	B	527	CLA	C3B-CAB	2.23	1.51	1.49
23	B	514	CLA	C4A-NA	-2.22	1.34	1.39
23	B	522	CLA	C4A-NA	-2.22	1.34	1.39
28	k	2050	BCR	C11-C10	-2.22	1.37	1.43
25	v	2138	HEM	CAD-C3D	-2.22	1.43	1.51
23	b	2521	CLA	CMB-C2B	2.22	1.56	1.51
23	C	482	CLA	C4-C3	2.22	1.56	1.50
26	D	357	PL9	C7-C8	-2.22	1.47	1.50
23	C	479	CLA	C3D-CAD	-2.22	1.42	1.47
23	B	516	CLA	C4B-NB	2.22	1.37	1.34
23	b	2523	CLA	C5-C3	2.22	1.56	1.51
23	c	2475	CLA	OBD-CAD	2.21	1.25	1.22
23	d	2357	CLA	C1A-NA	2.21	1.37	1.32
23	A	349	CLA	CAA-CBA	-2.21	1.45	1.52
23	b	2516	CLA	O2A-CGA	2.21	1.40	1.33
23	c	2480	CLA	C4-C3	2.21	1.56	1.50
23	c	2479	CLA	C2-C3	2.21	1.37	1.32
25	v	2138	HEM	CBC-CAC	2.21	1.41	1.28
28	j	2053	BCR	C37-C22	2.21	1.54	1.51
23	C	485	CLA	MG-NC	2.20	2.13	2.07
23	b	2522	CLA	C1B-CHB	-2.20	1.33	1.39
25	V	138	HEM	FE-NB	2.20	2.05	1.97
23	C	481	CLA	C3D-CAD	-2.20	1.42	1.47
23	B	523	CLA	C1B-CHB	-2.20	1.33	1.39
24	A	351	PHO	C4-C3	2.20	1.56	1.50
23	C	478	CLA	C4B-NB	2.20	1.37	1.34
23	C	478	CLA	MG-NC	2.19	2.13	2.07
23	D	356	CLA	C3D-CAD	-2.19	1.42	1.47
25	v	2138	HEM	C4B-NB	2.19	1.43	1.37
23	b	2525	CLA	C1B-CHB	-2.19	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	488	BCR	C23-C22	-2.19	1.41	1.45
23	b	2516	CLA	MG-NC	2.19	2.13	2.07
23	a	2348	CLA	CAA-CBA	-2.18	1.45	1.52
23	c	2483	CLA	C4A-NA	-2.18	1.34	1.39
23	B	523	CLA	CHC-C1C	2.18	1.42	1.35
23	B	519	CLA	C4A-NA	-2.18	1.34	1.39
24	A	351	PHO	C3D-CAD	-2.19	1.42	1.47
28	k	2050	BCR	C15-C14	-2.18	1.37	1.43
28	c	2488	BCR	C11-C10	-2.18	1.37	1.43
24	a	2350	PHO	C4B-NB	2.18	1.38	1.36
23	B	521	CLA	C1A-NA	2.18	1.37	1.32
23	C	477	CLA	MG-NC	2.18	2.13	2.07
23	c	2487	CLA	C2A-C1A	2.18	1.56	1.52
23	C	484	CLA	C1B-NB	2.18	1.37	1.34
23	b	2518	CLA	C3B-C2B	-2.17	1.37	1.41
23	A	348	CLA	CBA-CGA	-2.17	1.43	1.50
23	c	2486	CLA	C4B-NB	2.17	1.37	1.34
23	B	520	CLA	C1B-CHB	-2.17	1.33	1.39
25	e	2084	HEM	C4B-NB	2.17	1.43	1.37
23	c	2482	CLA	C4-C3	2.17	1.56	1.50
23	b	2517	CLA	C4-C3	2.17	1.56	1.50
23	C	483	CLA	C3D-CAD	-2.17	1.42	1.47
23	b	2523	CLA	C2A-C1A	-2.16	1.48	1.52
28	C	488	BCR	C17-C18	-2.16	1.32	1.35
23	B	513	CLA	C1C-NC	-2.16	1.36	1.38
23	d	2354	CLA	C5-C3	2.16	1.56	1.51
23	b	2518	CLA	CHC-C1C	2.16	1.42	1.35
23	c	2478	CLA	C3A-C4A	-2.16	1.45	1.51
23	C	474	CLA	C4-C3	2.16	1.56	1.50
23	b	2518	CLA	C3A-C4A	-2.16	1.45	1.51
28	J	53	BCR	C38-C26	2.16	1.54	1.51
23	c	2476	CLA	C1C-C2C	2.15	1.49	1.44
23	C	486	CLA	C4-C3	2.15	1.56	1.50
23	c	2476	CLA	CMB-C2B	2.15	1.56	1.51
24	d	2356	PHO	C4-C3	2.15	1.56	1.50
23	B	523	CLA	C4-C3	2.15	1.56	1.50
24	a	2350	PHO	CHA-C1A	2.15	1.42	1.37
23	B	521	CLA	CHC-C1C	2.15	1.42	1.35
23	B	520	CLA	CHB-C4A	2.15	1.41	1.36
23	a	2351	CLA	CHB-C4A	2.15	1.41	1.36
23	B	513	CLA	C4-C3	2.15	1.56	1.50
23	C	480	CLA	C4-C3	2.15	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	529	BCR	C20-C21	-2.15	1.37	1.43
23	c	2474	CLA	C4A-NA	-2.14	1.34	1.39
23	c	2487	CLA	OBD-CAD	2.14	1.25	1.22
28	c	2488	BCR	C20-C21	-2.14	1.37	1.43
23	c	2482	CLA	C4C-C3C	2.14	1.49	1.45
26	d	2358	PL9	C22-C23	-2.14	1.44	1.50
28	F	48	BCR	C24-C23	2.14	1.39	1.32
23	a	2349	CLA	C1B-NB	2.14	1.37	1.34
23	d	2357	CLA	C2A-C1A	-2.14	1.48	1.52
28	c	2489	BCR	C37-C22	2.13	1.54	1.51
28	K	50	BCR	C5-C6	2.13	1.37	1.34
23	b	2522	CLA	C5-C3	2.13	1.56	1.51
23	B	515	CLA	C4A-NA	-2.13	1.34	1.39
23	c	2487	CLA	C1B-CHB	-2.13	1.34	1.39
23	c	2476	CLA	C4-C3	2.13	1.56	1.50
23	B	522	CLA	CAA-C2A	2.13	1.57	1.54
23	a	2351	CLA	C3D-CAD	-2.13	1.43	1.47
23	C	481	CLA	C1C-NC	-2.13	1.36	1.38
23	c	2479	CLA	C3D-CAD	-2.13	1.43	1.47
28	B	529	BCR	C5-C6	2.13	1.37	1.34
23	d	2354	CLA	MG-NC	2.13	2.13	2.07
23	B	511	CLA	C3B-CAB	-2.12	1.47	1.49
23	c	2479	CLA	C1C-NC	-2.12	1.36	1.38
23	c	2477	CLA	CMB-C2B	2.12	1.56	1.51
23	C	484	CLA	C4A-NA	-2.12	1.34	1.39
23	B	527	CLA	OBD-CAD	2.12	1.25	1.22
23	B	527	CLA	C1-C2	2.12	1.56	1.49
23	c	2486	CLA	CHB-C4A	2.12	1.41	1.36
23	d	2355	CLA	C1A-NA	2.12	1.36	1.32
23	B	519	CLA	C3A-C4A	-2.12	1.46	1.51
25	V	138	HEM	CHD-C1D	2.12	1.44	1.39
28	B	529	BCR	C37-C22	2.12	1.54	1.51
23	B	518	CLA	C3A-C4A	-2.11	1.46	1.51
23	D	356	CLA	CAA-CBA	-2.11	1.45	1.52
25	V	138	HEM	O1D-CGD	2.11	1.29	1.22
23	A	348	CLA	MG-NC	2.11	2.13	2.07
23	b	2519	CLA	C3D-CAD	-2.11	1.43	1.47
23	c	2479	CLA	MG-NC	2.11	2.13	2.07
23	D	356	CLA	CAA-C2A	2.10	1.57	1.54
23	B	518	CLA	CHB-C4A	2.10	1.41	1.36
23	C	487	CLA	C4A-NA	-2.10	1.34	1.39
23	C	479	CLA	C2-C3	2.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2478	CLA	O2A-CGA	2.10	1.39	1.33
23	c	2482	CLA	C1B-NB	2.10	1.37	1.34
28	c	2488	BCR	C23-C22	-2.10	1.41	1.45
28	b	2527	BCR	C38-C26	2.10	1.54	1.51
23	b	2523	CLA	C1B-NB	2.10	1.37	1.34
23	C	477	CLA	C1A-NA	2.10	1.36	1.32
28	C	488	BCR	C11-C10	-2.09	1.37	1.43
23	C	486	CLA	C5-C3	2.09	1.56	1.51
26	d	2358	PL9	C7-C8	-2.09	1.47	1.50
23	b	2520	CLA	C3D-CAD	-2.09	1.43	1.47
23	C	475	CLA	C3A-C4A	-2.09	1.46	1.51
23	C	475	CLA	C3D-CAD	-2.09	1.43	1.47
23	B	520	CLA	C1A-NA	2.09	1.36	1.32
23	c	2485	CLA	C3D-CAD	-2.09	1.43	1.47
23	b	2518	CLA	C2-C3	2.08	1.37	1.32
23	c	2483	CLA	CHC-C1C	2.08	1.42	1.35
23	a	2349	CLA	MG-NC	2.08	2.13	2.07
23	B	512	CLA	CHC-C1C	2.08	1.42	1.35
26	a	2352	PL9	C32-C33	-2.08	1.44	1.50
23	C	474	CLA	C1A-NA	2.08	1.36	1.32
23	B	522	CLA	C4-C3	2.08	1.56	1.50
23	c	2475	CLA	CHC-C1C	2.08	1.42	1.35
23	b	2520	CLA	C1B-NB	2.08	1.37	1.34
28	K	50	BCR	C14-C13	-2.08	1.33	1.35
23	B	518	CLA	C4B-NB	2.08	1.37	1.34
23	B	522	CLA	MG-NC	2.07	2.13	2.07
23	c	2480	CLA	MG-NC	2.07	2.13	2.07
23	c	2479	CLA	CHB-C4A	2.07	1.41	1.36
23	C	480	CLA	C3D-CAD	-2.07	1.43	1.47
23	c	2479	CLA	C4-C3	2.07	1.56	1.50
23	C	477	CLA	C1B-CHB	-2.06	1.34	1.39
23	c	2477	CLA	C1A-NA	2.06	1.36	1.32
23	D	356	CLA	C2A-C1A	-2.06	1.48	1.52
23	C	480	CLA	C1B-NB	2.06	1.37	1.34
23	c	2487	CLA	CMA-C3A	2.06	1.57	1.53
23	b	2518	CLA	O2A-CGA	2.06	1.39	1.33
23	c	2480	CLA	C1B-NB	2.06	1.37	1.34
23	A	352	CLA	C1C-NC	-2.06	1.36	1.38
23	B	519	CLA	C1C-NC	-2.06	1.36	1.38
23	c	2479	CLA	C4A-NA	-2.06	1.34	1.39
23	b	2512	CLA	MG-NC	2.05	2.13	2.07
23	B	511	CLA	C2-C3	2.05	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	489	BCR	C33-C5	2.05	1.54	1.51
28	k	2050	BCR	C14-C13	-2.05	1.33	1.35
23	c	2487	CLA	C5-C3	2.05	1.56	1.51
23	c	2477	CLA	CHB-C4A	2.05	1.41	1.36
23	C	485	CLA	C3A-C4A	-2.05	1.46	1.51
23	B	516	CLA	MG-NC	2.05	2.13	2.07
23	C	478	CLA	C3A-C4A	-2.05	1.46	1.51
23	B	517	CLA	C4-C3	2.05	1.55	1.50
23	c	2481	CLA	MG-NC	2.05	2.13	2.07
23	c	2474	CLA	MG-NC	2.04	2.13	2.07
23	B	518	CLA	CHC-C1C	2.04	1.42	1.35
23	B	517	CLA	C3B-C2B	-2.04	1.37	1.41
28	J	53	BCR	C37-C22	2.04	1.54	1.51
23	c	2480	CLA	C3D-CAD	-2.04	1.43	1.47
23	B	527	CLA	C1B-CHB	-2.04	1.34	1.39
23	B	517	CLA	MG-NC	2.04	2.13	2.07
28	C	488	BCR	C19-C18	-2.04	1.41	1.45
23	b	2523	CLA	CBA-CGA	-2.03	1.44	1.50
23	B	514	CLA	CHC-C1C	2.03	1.42	1.35
23	b	2526	CLA	C2-C3	2.03	1.37	1.32
25	e	2084	HEM	C2A-C3A	2.03	1.43	1.37
23	c	2485	CLA	C3A-C4A	-2.03	1.46	1.51
26	a	2352	PL9	C37-C38	-2.03	1.44	1.50
28	j	2053	BCR	C1-C6	2.03	1.56	1.53
23	d	2357	CLA	CAA-CBA	-2.03	1.46	1.52
26	A	353	PL9	C32-C33	-2.03	1.44	1.50
23	C	477	CLA	C1-C2	2.03	1.55	1.49
23	c	2486	CLA	MG-NB	2.03	2.09	2.05
23	B	525	CLA	C1B-CHB	-2.03	1.34	1.39
25	V	138	HEM	CBA-CGA	-2.03	1.45	1.50
23	C	482	CLA	C1-C2	2.02	1.55	1.49
23	C	477	CLA	C2-C3	2.02	1.37	1.32
23	c	2475	CLA	CHB-C4A	2.02	1.41	1.36
25	v	2138	HEM	CBA-CGA	-2.02	1.45	1.50
23	b	2513	CLA	C1B-CHB	-2.02	1.34	1.39
23	c	2481	CLA	C1C-C2C	2.02	1.48	1.44
23	c	2485	CLA	MG-NB	2.02	2.09	2.05
23	b	2516	CLA	MG-NB	2.02	2.09	2.05
23	C	474	CLA	CHB-C4A	2.02	1.41	1.36
25	v	2138	HEM	C3C-CAC	2.02	1.46	1.40
23	C	475	CLA	CHC-C1C	2.02	1.42	1.35
23	b	2523	CLA	C1B-CHB	-2.02	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	511	CLA	C1C-NC	-2.01	1.36	1.38
23	B	511	CLA	C4-C3	2.01	1.55	1.50
25	v	2138	HEM	FE-NA	2.01	2.01	1.92
23	B	515	CLA	CHC-C1C	2.01	1.42	1.35
23	d	2355	CLA	C1B-NB	2.01	1.37	1.34
23	C	475	CLA	CHB-C4A	2.01	1.41	1.36
23	B	522	CLA	C1B-NB	2.01	1.37	1.34
23	c	2481	CLA	C1B-CHB	-2.01	1.34	1.39
23	D	354	CLA	CHC-C1C	2.01	1.42	1.35
23	B	514	CLA	O2A-CGA	2.01	1.39	1.33
23	B	518	CLA	MG-NB	2.01	2.09	2.05
26	A	353	PL9	C2-C3	2.01	1.40	1.34
23	B	516	CLA	C3D-CAD	-2.01	1.43	1.47
23	c	2477	CLA	CHC-C1C	2.01	1.42	1.35
23	b	2519	CLA	C3A-C4A	-2.01	1.46	1.51
23	d	2354	CLA	C3D-CAD	-2.01	1.43	1.47
23	C	486	CLA	CHB-C4A	2.00	1.41	1.36
23	B	511	CLA	MG-NB	2.00	2.09	2.05
24	A	351	PHO	C1B-NB	-2.00	1.35	1.38
23	B	515	CLA	C3B-C2B	-2.00	1.37	1.41

All (2016) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	138	HEM	C3B-C4B-NB	-12.21	105.26	114.00
23	B	520	CLA	CBA-CAA-C2A	9.75	142.93	114.01
23	b	2520	CLA	CBA-CAA-C2A	9.73	142.88	114.01
23	B	520	CLA	CAA-C2A-C1A	-9.72	87.37	111.62
23	b	2520	CLA	CAA-C2A-C1A	-9.70	87.43	111.62
25	V	138	HEM	CBD-CAD-C3D	-8.27	96.33	114.37
23	c	2477	CLA	CAA-C2A-C1A	-8.00	91.66	111.62
23	C	477	CLA	CAA-C2A-C1A	-7.88	91.96	111.62
27	d	2359	LMT	O1'-C1-C2	7.85	140.53	109.87
23	C	477	CLA	CBA-CAA-C2A	7.85	137.30	114.01
27	B	526	LMT	O1'-C1-C2	7.84	140.49	109.87
23	c	2477	CLA	CBA-CAA-C2A	7.75	137.00	114.01
23	A	349	CLA	C1-C2-C3	7.55	139.61	126.19
23	B	519	CLA	CAA-C2A-C1A	-7.43	93.09	111.62
23	b	2519	CLA	CAA-C2A-C1A	-7.40	93.15	111.62
25	v	2138	HEM	C3A-C4A-NA	7.38	114.98	109.41
23	d	2355	CLA	C1-C2-C3	7.20	138.98	126.19
25	E	84	HEM	C3A-C4A-NA	7.17	114.83	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	519	CLA	C1-C2-C3	7.06	138.74	126.19
23	d	2354	CLA	C1-C2-C3	7.02	138.66	126.19
23	D	354	CLA	C1-C2-C3	6.98	138.59	126.19
23	b	2519	CLA	C1-C2-C3	6.94	138.52	126.19
23	C	481	CLA	CBA-CAA-C2A	6.90	134.49	114.01
26	a	2352	PL9	C22-C23-C24	6.80	142.47	127.80
23	c	2481	CLA	CBA-CAA-C2A	6.68	133.84	114.01
23	b	2516	CLA	O2A-C1-C2	6.64	122.93	108.55
28	b	2527	BCR	C33-C5-C6	6.62	132.01	124.51
28	B	528	BCR	C33-C5-C6	6.62	132.01	124.51
23	B	516	CLA	O2A-C1-C2	6.61	122.88	108.55
23	B	527	CLA	O2A-C1-C2	-6.44	94.60	108.55
26	D	357	PL9	C37-C36-C34	6.41	133.97	112.74
25	V	138	HEM	C4A-CHB-C1B	-6.39	119.06	127.47
26	d	2358	PL9	C37-C36-C34	6.38	133.88	112.74
23	b	2526	CLA	O2A-C1-C2	-6.38	94.73	108.55
23	b	2524	CLA	C1-C2-C3	6.38	137.53	126.19
23	b	2519	CLA	CBA-CAA-C2A	6.37	132.92	114.01
25	E	84	HEM	C3B-C4B-NB	-6.33	109.47	114.00
26	A	353	PL9	C21-C22-C23	-6.29	93.65	111.62
23	B	519	CLA	CBA-CAA-C2A	6.17	132.33	114.01
26	A	353	PL9	C22-C23-C24	6.16	141.08	127.80
23	B	524	CLA	C1-C2-C3	6.13	137.08	126.19
25	v	2138	HEM	CBD-CAD-C3D	-6.13	101.00	114.37
23	C	483	CLA	CBA-CAA-C2A	6.13	132.20	114.01
28	B	529	BCR	C38-C26-C25	6.08	131.40	124.51
24	D	355	PHO	C3D-C4D-CHA	6.07	115.90	109.18
26	a	2352	PL9	C21-C22-C23	-6.05	94.33	111.62
24	d	2356	PHO	C3D-C4D-CHA	6.02	115.84	109.18
24	a	2350	PHO	C3D-C4D-CHA	6.01	115.84	109.18
26	A	353	PL9	C37-C36-C34	5.99	132.56	112.74
23	c	2483	CLA	CAA-C2A-C1A	-5.98	96.70	111.62
28	d	2360	BCR	C33-C5-C6	5.95	131.26	124.51
24	A	351	PHO	C3D-C4D-CHA	5.92	115.74	109.18
23	c	2483	CLA	CBA-CAA-C2A	5.89	131.48	114.01
25	v	2138	HEM	CMD-C2D-C3D	5.88	138.92	125.60
26	a	2352	PL9	C37-C36-C34	5.88	132.20	112.74
25	V	138	HEM	C3A-C4A-NA	5.85	113.83	109.41
23	C	483	CLA	CAA-C2A-C1A	-5.81	97.11	111.62
28	B	529	BCR	C20-C21-C22	-5.80	118.94	127.29
26	A	353	PL9	C35-C34-C36	-5.76	106.63	115.39
23	b	2520	CLA	CAA-CBA-CGA	-5.73	94.80	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	48	BCR	C16-C17-C18	5.71	135.53	127.29
28	F	48	BCR	C33-C5-C6	5.70	130.97	124.51
23	B	520	CLA	CAA-CBA-CGA	-5.68	94.95	113.27
25	e	2084	HEM	C3B-C4B-NB	-5.67	109.94	114.00
28	j	2053	BCR	C33-C5-C6	5.66	130.92	124.51
28	b	2527	BCR	C38-C26-C25	5.66	130.92	124.51
25	V	138	HEM	CHC-C1C-NC	5.64	129.63	124.73
25	V	138	HEM	C4A-NA-C1A	-5.63	99.35	106.76
28	d	2360	BCR	C16-C17-C18	5.55	135.29	127.29
23	A	348	CLA	C2B-C3B-CAB	-5.54	115.98	127.33
28	B	528	BCR	C38-C26-C25	5.50	130.75	124.51
28	J	53	BCR	C33-C5-C6	5.48	130.72	124.51
26	a	2352	PL9	C35-C34-C36	-5.48	107.05	115.39
28	J	53	BCR	C38-C26-C25	5.48	130.72	124.51
28	b	2528	BCR	C38-C26-C25	5.46	130.70	124.51
28	c	2489	BCR	C33-C5-C6	5.40	130.63	124.51
28	b	2528	BCR	C20-C21-C22	-5.38	119.53	127.29
28	j	2053	BCR	C38-C26-C25	5.32	130.53	124.51
26	A	353	PL9	C36-C34-C33	5.31	131.30	121.08
28	C	489	BCR	C33-C5-C6	5.28	130.49	124.51
28	F	48	BCR	C38-C26-C25	5.26	130.47	124.51
23	C	475	CLA	O2A-CGA-CBA	5.23	128.40	111.94
23	c	2481	CLA	CAA-C2A-C1A	-5.22	98.59	111.62
23	c	2475	CLA	O2A-C1-C2	5.22	119.87	108.55
23	a	2348	CLA	C2B-C3B-CAB	-5.22	116.65	127.33
23	C	475	CLA	O2A-C1-C2	5.21	119.85	108.55
26	a	2352	PL9	C36-C34-C33	5.19	131.08	121.08
23	c	2475	CLA	O2A-CGA-CBA	5.19	128.27	111.94
26	a	2352	PL9	C26-C24-C23	-5.15	111.17	121.08
23	D	354	CLA	C2B-C3B-CAB	-5.14	116.82	127.33
28	K	50	BCR	C38-C26-C25	5.12	130.31	124.51
26	D	357	PL9	C35-C34-C36	-5.11	107.61	115.39
23	B	516	CLA	O2A-CGA-CBA	5.07	127.90	111.94
23	B	511	CLA	CAA-C2A-C1A	-5.06	99.00	111.62
25	V	138	HEM	CHB-C1B-NB	5.05	131.25	124.31
23	A	348	CLA	C4B-C3B-CAB	5.05	137.40	127.18
23	b	2516	CLA	O2A-CGA-CBA	5.03	127.76	111.94
23	b	2511	CLA	CAA-C2A-C1A	-5.01	99.12	111.62
23	b	2513	CLA	C4A-NA-C1A	5.00	113.41	106.52
23	D	354	CLA	C4B-C3B-CAB	4.98	137.26	127.18
25	v	2138	HEM	C1A-CHA-C4D	-4.97	120.93	127.47
23	B	513	CLA	C4A-NA-C1A	4.95	113.34	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2520	CLA	C2B-C3B-CAB	-4.95	117.21	127.33
26	d	2358	PL9	C35-C34-C36	-4.94	107.87	115.39
28	d	2360	BCR	C38-C26-C25	4.93	130.10	124.51
23	C	481	CLA	CAA-C2A-C1A	-4.93	99.33	111.62
23	B	518	CLA	CAA-C2A-C1A	-4.91	99.37	111.62
23	D	354	CLA	O2A-C1-C2	4.89	119.14	108.55
25	e	2084	HEM	CBA-CAA-C2A	-4.87	104.11	112.69
28	k	2050	BCR	C38-C26-C25	4.85	130.00	124.51
23	c	2479	CLA	C4A-NA-C1A	4.84	113.19	106.52
23	d	2354	CLA	C2B-C3B-CAB	-4.84	117.43	127.33
23	B	512	CLA	C1-C2-C3	4.82	134.75	126.19
23	B	511	CLA	C4A-NA-C1A	4.80	113.13	106.52
23	a	2348	CLA	C4B-C3B-CAB	4.78	136.87	127.18
28	C	488	BCR	C38-C26-C25	4.79	129.93	124.51
23	B	514	CLA	CAA-C2A-C1A	-4.77	99.71	111.62
25	E	84	HEM	CBA-CAA-C2A	-4.76	104.30	112.69
23	b	2518	CLA	CAA-C2A-C1A	-4.76	99.76	111.62
28	F	48	BCR	C11-C10-C9	4.75	134.14	127.29
23	B	519	CLA	C4A-NA-C1A	4.75	113.06	106.52
23	b	2511	CLA	C4A-NA-C1A	4.74	113.05	106.52
23	B	519	CLA	C2B-C3B-CAB	-4.73	117.65	127.33
23	C	479	CLA	CAA-C2A-C1A	-4.73	99.82	111.62
23	C	478	CLA	C2B-C3B-CAB	-4.73	117.65	127.33
23	B	523	CLA	CAA-C2A-C1A	-4.72	99.85	111.62
28	C	488	BCR	C33-C5-C6	4.71	129.85	124.51
23	d	2357	CLA	C4A-NA-C1A	4.70	113.00	106.52
28	F	48	BCR	C8-C9-C10	-4.70	111.76	118.97
23	D	356	CLA	C4A-NA-C1A	4.69	112.99	106.52
23	B	520	CLA	C2B-C3B-CAB	-4.69	117.73	127.33
23	C	479	CLA	C4A-NA-C1A	4.69	112.98	106.52
25	v	2138	HEM	C4A-NA-C1A	-4.68	100.60	106.76
23	C	481	CLA	CAA-CBA-CGA	-4.68	98.19	113.27
23	B	516	CLA	C2B-C3B-CAB	-4.68	117.76	127.33
23	c	2479	CLA	CAA-C2A-C1A	-4.67	99.97	111.62
23	b	2514	CLA	CAA-C2A-C1A	-4.67	99.98	111.62
23	b	2512	CLA	C4A-NA-C1A	4.67	112.95	106.52
23	C	478	CLA	C4B-C3B-CAB	4.66	136.62	127.18
23	c	2478	CLA	C2B-C3B-CAB	-4.66	117.79	127.33
23	b	2512	CLA	C1-C2-C3	4.65	134.46	126.19
26	A	353	PL9	C26-C24-C23	-4.64	112.15	121.08
23	b	2523	CLA	C4A-NA-C1A	4.64	112.92	106.52
23	b	2519	CLA	C2B-C3B-CAB	-4.63	117.85	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2523	CLA	CAA-C2A-C1A	-4.62	100.09	111.62
28	K	50	BCR	C33-C5-C6	4.62	129.75	124.51
28	c	2488	BCR	C38-C26-C25	4.62	129.75	124.51
23	c	2481	CLA	CAA-CBA-CGA	-4.62	98.38	113.27
23	B	518	CLA	CBA-CAA-C2A	4.61	127.70	114.01
23	A	350	CLA	C2B-C3B-CAB	-4.60	117.92	127.33
25	v	2138	HEM	C3B-C4B-NB	-4.60	110.71	114.00
28	c	2488	BCR	C33-C5-C6	4.60	129.72	124.51
28	d	2360	BCR	C11-C10-C9	4.60	133.92	127.29
23	B	523	CLA	C4A-NA-C1A	4.59	112.85	106.52
23	a	2349	CLA	C2B-C3B-CAB	-4.58	117.95	127.33
23	d	2354	CLA	O2A-C1-C2	4.58	118.48	108.55
23	c	2478	CLA	C1-C2-C3	4.58	134.32	126.19
28	b	2527	BCR	C33-C5-C4	-4.58	104.94	113.34
23	C	486	CLA	C2B-C3B-CAB	-4.57	117.97	127.33
23	d	2354	CLA	C4B-C3B-CAB	4.57	136.42	127.18
23	B	512	CLA	C4A-NA-C1A	4.55	112.80	106.52
24	d	2356	PHO	CBD-CHA-C1A	4.54	134.49	126.57
23	B	517	CLA	C4A-NA-C1A	4.53	112.77	106.52
23	C	483	CLA	C4A-NA-C1A	4.52	112.76	106.52
23	A	352	CLA	C4A-NA-C1A	4.52	112.75	106.52
23	b	2523	CLA	CBA-CAA-C2A	4.52	127.41	114.01
23	B	523	CLA	CBA-CAA-C2A	4.51	127.39	114.01
23	b	2518	CLA	CBA-CAA-C2A	4.50	127.38	114.01
23	b	2511	CLA	C2B-C3B-CAB	-4.50	118.11	127.33
23	A	349	CLA	C4A-NA-C1A	4.50	112.72	106.52
23	b	2525	CLA	C4A-NA-C1A	4.50	112.72	106.52
28	d	2360	BCR	C8-C9-C10	-4.49	112.07	118.97
23	b	2522	CLA	C4A-NA-C1A	4.48	112.70	106.52
28	k	2050	BCR	C33-C5-C6	4.48	129.59	124.51
23	B	524	CLA	C4A-NA-C1A	4.48	112.70	106.52
23	C	476	CLA	C4A-NA-C1A	4.48	112.69	106.52
25	V	138	HEM	CHD-C4C-NC	-4.48	120.84	124.73
23	c	2483	CLA	C4A-NA-C1A	4.47	112.69	106.52
23	b	2516	CLA	C2B-C3B-CAB	-4.47	118.18	127.33
23	c	2478	CLA	C4A-NA-C1A	4.46	112.67	106.52
23	c	2486	CLA	C2B-C3B-CAB	-4.46	118.19	127.33
23	B	522	CLA	C4A-NA-C1A	4.46	112.67	106.52
23	b	2523	CLA	C2B-C3B-CAB	-4.45	118.21	127.33
23	C	484	CLA	C2B-C3B-CAB	-4.45	118.22	127.33
23	b	2520	CLA	C4A-NA-C1A	4.44	112.64	106.52
23	a	2351	CLA	C4A-NA-C1A	4.44	112.64	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	474	CLA	C4A-NA-C1A	4.43	112.63	106.52
23	C	478	CLA	C4A-NA-C1A	4.42	112.61	106.52
23	B	523	CLA	C2B-C3B-CAB	-4.42	118.28	127.33
23	b	2520	CLA	C4B-C3B-CAB	4.42	136.12	127.18
23	C	482	CLA	C4A-NA-C1A	4.42	112.61	106.52
23	C	483	CLA	C2B-C3B-CAB	-4.42	118.29	127.33
23	c	2483	CLA	C2B-C3B-CAB	-4.41	118.30	127.33
23	b	2518	CLA	C4A-NA-C1A	4.41	112.59	106.52
24	D	355	PHO	CBD-CHA-C1A	4.41	134.26	126.57
23	B	518	CLA	C4A-NA-C1A	4.40	112.59	106.52
28	F	48	BCR	C7-C8-C9	4.39	132.79	126.22
23	b	2524	CLA	C4A-NA-C1A	4.39	112.57	106.52
23	B	525	CLA	C4A-NA-C1A	4.39	112.57	106.52
23	c	2484	CLA	C4A-NA-C1A	4.38	112.56	106.52
23	b	2514	CLA	CAA-C2A-C3A	-4.38	102.69	113.04
23	b	2519	CLA	O2A-C1-C2	4.37	118.03	108.55
23	c	2478	CLA	C4B-C3B-CAB	4.37	136.03	127.18
26	D	357	PL9	C30-C29-C31	4.37	122.03	115.39
23	B	511	CLA	CBA-CAA-C2A	4.37	126.98	114.01
23	C	481	CLA	C4A-NA-C1A	4.37	112.54	106.52
23	B	518	CLA	C2B-C3B-CAB	-4.37	118.39	127.33
23	b	2519	CLA	C4A-NA-C1A	4.36	112.53	106.52
23	b	2511	CLA	CBA-CAA-C2A	4.36	126.95	114.01
27	d	2359	LMT	C1B-O1B-C4'	-4.35	106.88	117.99
28	c	2489	BCR	C38-C26-C25	4.35	129.44	124.51
23	c	2481	CLA	C4A-NA-C1A	4.35	112.52	106.52
23	c	2477	CLA	O2A-C1-C2	4.35	117.97	108.55
23	c	2480	CLA	C4A-NA-C1A	4.35	112.51	106.52
23	b	2515	CLA	C2B-C3B-CAB	-4.33	118.46	127.33
28	C	489	BCR	C38-C26-C25	4.33	129.42	124.51
23	b	2518	CLA	C2B-C3B-CAB	-4.33	118.47	127.33
23	b	2517	CLA	C4A-NA-C1A	4.32	112.48	106.52
23	C	478	CLA	C1-C2-C3	4.32	133.87	126.19
23	C	474	CLA	C2B-C3B-CAB	-4.31	118.50	127.33
23	B	520	CLA	C4A-NA-C1A	4.31	112.46	106.52
23	B	511	CLA	C2B-C3B-CAB	-4.31	118.51	127.33
23	c	2486	CLA	C4A-NA-C1A	4.30	112.45	106.52
23	b	2515	CLA	CBD-CHA-C1A	4.30	134.39	128.77
23	B	516	CLA	C4B-C3B-CAB	4.30	135.89	127.18
23	C	477	CLA	O2A-C1-C2	4.30	117.86	108.55
23	B	519	CLA	C4B-C3B-CAB	4.30	135.88	127.18
23	B	515	CLA	C2B-C3B-CAB	-4.30	118.53	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2479	CLA	C2B-C3B-CAB	-4.29	118.54	127.33
23	C	480	CLA	C4A-NA-C1A	4.29	112.43	106.52
23	d	2355	CLA	C4A-NA-C1A	4.29	112.43	106.52
23	C	484	CLA	C4A-NA-C1A	4.29	112.43	106.52
23	B	516	CLA	C4A-NA-C1A	4.28	112.43	106.52
25	e	2084	HEM	C3A-C4A-NA	4.28	112.65	109.41
23	B	514	CLA	O2A-C1-C2	4.28	117.82	108.55
23	b	2516	CLA	C4A-NA-C1A	4.28	112.42	106.52
24	A	351	PHO	C2B-C3B-CAB	-4.28	118.58	127.33
23	C	479	CLA	C2B-C3B-CAB	-4.27	118.60	127.33
23	B	522	CLA	C2B-C3B-CAB	-4.27	118.60	127.33
23	c	2474	CLA	C4A-NA-C1A	4.26	112.40	106.52
23	B	514	CLA	CAA-C2A-C3A	-4.25	102.98	113.04
25	V	138	HEM	CHD-C1D-ND	-4.26	121.05	124.58
23	B	517	CLA	C2B-C3B-CAB	-4.25	118.63	127.33
23	c	2476	CLA	C4A-NA-C1A	4.25	112.38	106.52
23	c	2475	CLA	C2B-C3B-CAB	-4.25	118.62	127.33
23	b	2519	CLA	C4B-C3B-CAB	4.25	135.78	127.18
28	B	528	BCR	C33-C5-C4	-4.25	105.53	113.34
23	A	352	CLA	C2B-C3B-CAB	-4.25	118.64	127.33
23	C	486	CLA	CBD-CHA-C1A	4.23	134.30	128.77
23	c	2484	CLA	C2B-C3B-CAB	-4.23	118.67	127.33
23	B	515	CLA	CBD-CHA-C1A	4.23	134.30	128.77
23	C	475	CLA	C4A-NA-C1A	4.23	112.35	106.52
23	B	519	CLA	O2A-C1-C2	4.22	117.69	108.55
23	c	2482	CLA	C4A-NA-C1A	4.21	112.33	106.52
23	B	514	CLA	C4A-NA-C1A	4.21	112.32	106.52
26	D	357	PL9	C36-C34-C33	4.20	129.17	121.08
23	b	2514	CLA	C4A-NA-C1A	4.20	112.31	106.52
23	b	2514	CLA	O2A-C1-C2	4.20	117.64	108.55
23	C	486	CLA	C4A-NA-C1A	4.19	112.29	106.52
23	c	2477	CLA	C2B-C3B-CAB	-4.19	118.76	127.33
26	d	2358	PL9	C30-C29-C31	4.19	121.75	115.39
23	C	480	CLA	C2B-C3B-CAB	-4.18	118.77	127.33
23	A	349	CLA	C2B-C3B-CAB	-4.18	118.77	127.33
23	d	2357	CLA	C2B-C3B-CAB	-4.18	118.78	127.33
23	b	2517	CLA	C2B-C3B-CAB	-4.18	118.78	127.33
23	C	475	CLA	C2B-C3B-CAB	-4.17	118.79	127.33
23	b	2516	CLA	C4B-C3B-CAB	4.16	135.60	127.18
23	c	2477	CLA	C7-C6-C5	-4.15	100.77	113.01
26	d	2358	PL9	C36-C34-C33	4.15	129.07	121.08
23	c	2486	CLA	CBD-CHA-C1A	4.15	134.19	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2351	CLA	C2B-C3B-CAB	-4.15	118.84	127.33
23	B	525	CLA	C2B-C3B-CAB	-4.13	118.87	127.33
23	A	348	CLA	O2A-C1-C2	4.13	117.50	108.55
23	c	2481	CLA	C2B-C3B-CAB	-4.13	118.88	127.33
27	B	526	LMT	C1B-O1B-C4'	-4.13	107.46	117.99
28	d	2360	BCR	C7-C8-C9	4.13	132.39	126.22
23	c	2487	CLA	CMB-C2B-C1B	-4.12	122.28	128.62
23	c	2480	CLA	C2B-C3B-CAB	-4.12	118.89	127.33
23	b	2515	CLA	C4A-NA-C1A	4.12	112.20	106.52
23	B	520	CLA	C4B-C3B-CAB	4.12	135.51	127.18
23	C	477	CLA	CAA-CBA-CGA	-4.12	100.00	113.27
24	a	2350	PHO	C2B-C3B-CAB	-4.12	118.90	127.33
23	C	477	CLA	C2B-C3B-CAB	-4.11	118.92	127.33
28	B	529	BCR	C2-C1-C6	4.11	117.27	110.44
23	b	2525	CLA	C2B-C3B-CAB	-4.11	118.92	127.33
23	C	484	CLA	C4B-C3B-CAB	4.11	135.49	127.18
23	C	482	CLA	C2B-C3B-CAB	-4.10	118.93	127.33
26	a	2352	PL9	C7-C8-C9	4.10	133.68	126.76
23	C	477	CLA	C7-C6-C5	-4.10	100.93	113.01
23	b	2526	CLA	C4A-NA-C1A	4.09	112.16	106.52
23	b	2526	CLA	C6-C5-C3	4.09	122.50	112.78
24	a	2350	PHO	CBD-CHA-C1A	4.09	133.70	126.57
24	A	351	PHO	CBD-CHA-C1A	4.08	133.69	126.57
23	c	2485	CLA	C4A-NA-C1A	4.08	112.15	106.52
26	a	2352	PL9	C25-C24-C23	4.07	131.59	123.52
23	B	513	CLA	CBA-CAA-C2A	4.07	126.10	114.01
23	C	481	CLA	C2B-C3B-CAB	-4.07	118.99	127.33
23	C	478	CLA	C2A-C1A-NA	-4.07	106.74	111.24
23	b	2522	CLA	C2B-C3B-CAB	-4.07	119.00	127.33
23	c	2479	CLA	CAA-CBA-CGA	-4.07	100.16	113.27
23	A	350	CLA	C4B-C3B-CAB	4.06	135.40	127.18
23	B	527	CLA	C6-C5-C3	4.06	122.42	112.78
23	a	2349	CLA	C4B-C3B-CAB	4.03	135.35	127.18
23	A	348	CLA	C4A-NA-C1A	4.03	112.08	106.52
23	c	2479	CLA	CBD-CHA-C1A	4.02	134.03	128.77
23	c	2477	CLA	CAA-CBA-CGA	-4.02	100.31	113.27
23	c	2474	CLA	C2B-C3B-CAB	-4.02	119.10	127.33
26	A	353	PL9	C7-C8-C9	4.02	133.55	126.76
23	C	483	CLA	C4B-C3B-CAB	4.02	135.32	127.18
23	B	527	CLA	C4A-NA-C1A	4.02	112.06	106.52
23	B	523	CLA	C4B-C3B-CAB	4.01	135.30	127.18
23	b	2513	CLA	C2B-C3B-CAB	-4.01	119.11	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2521	CLA	C2B-C3B-CAB	-4.01	119.12	127.33
23	D	356	CLA	C2B-C3B-CAB	-4.00	119.14	127.33
23	B	515	CLA	C4A-NA-C1A	3.99	112.03	106.52
23	B	521	CLA	C2B-C3B-CAB	-3.99	119.17	127.33
28	C	488	BCR	C16-C17-C18	3.99	133.03	127.29
23	c	2475	CLA	C4A-NA-C1A	3.98	112.01	106.52
23	d	2355	CLA	C2B-C3B-CAB	-3.98	119.18	127.33
23	B	514	CLA	C2B-C3B-CAB	-3.97	119.20	127.33
23	b	2523	CLA	C4B-C3B-CAB	3.97	135.22	127.18
23	D	356	CLA	C1-C2-C3	3.97	133.24	126.19
23	c	2476	CLA	C2B-C3B-CAB	-3.97	119.20	127.33
23	C	474	CLA	C4B-C3B-CAB	3.96	135.19	127.18
23	c	2482	CLA	C2B-C3B-CAB	-3.96	119.23	127.33
23	B	515	CLA	CAA-C2A-C3A	-3.95	103.70	113.04
23	c	2484	CLA	C4B-C3B-CAB	3.95	135.17	127.18
28	d	2360	BCR	C33-C5-C4	-3.95	106.09	113.34
23	A	349	CLA	C4B-C3B-CAB	3.94	135.16	127.18
23	C	485	CLA	C4A-NA-C1A	3.94	111.95	106.52
25	v	2138	HEM	C4A-CHB-C1B	-3.94	122.29	127.47
23	c	2483	CLA	C4B-C3B-CAB	3.94	135.15	127.18
23	C	479	CLA	CBA-CAA-C2A	3.93	125.69	114.01
23	d	2354	CLA	C4A-NA-C1A	3.93	111.94	106.52
23	C	487	CLA	CMB-C2B-C1B	-3.93	122.58	128.62
23	d	2357	CLA	C1-C2-C3	3.92	133.16	126.19
23	c	2476	CLA	C1-C2-C3	3.92	133.16	126.19
23	a	2351	CLA	C1-C2-C3	3.92	133.16	126.19
23	D	354	CLA	C4A-NA-C1A	3.92	111.92	106.52
23	a	2348	CLA	C4A-NA-C1A	3.92	111.92	106.52
28	b	2528	BCR	C2-C1-C6	3.91	116.94	110.44
23	b	2518	CLA	O2A-CGA-CBA	3.90	124.22	111.94
28	b	2527	BCR	C38-C26-C27	-3.90	106.17	113.34
23	B	517	CLA	C4B-C3B-CAB	3.90	135.08	127.18
23	b	2511	CLA	C4B-C3B-CAB	3.90	135.07	127.18
23	b	2524	CLA	C5-C3-C2	-3.89	113.61	121.08
28	J	53	BCR	C33-C5-C4	-3.88	106.20	113.34
23	c	2478	CLA	C2A-C1A-NA	-3.88	106.95	111.24
23	c	2487	CLA	C2B-C3B-CAB	-3.88	119.38	127.33
25	v	2138	HEM	CMC-C2C-C3C	3.88	135.30	126.16
23	c	2479	CLA	CBA-CAA-C2A	3.88	125.53	114.01
23	c	2479	CLA	C4B-C3B-CAB	3.88	135.03	127.18
23	B	513	CLA	C2B-C3B-CAB	-3.88	119.39	127.33
23	b	2521	CLA	C4A-NA-C1A	3.86	111.85	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	518	CLA	C4B-C3B-CAB	3.86	134.99	127.18
23	B	518	CLA	O2A-CGA-CBA	3.86	124.08	111.94
23	b	2514	CLA	C2B-C3B-CAB	-3.86	119.44	127.33
23	B	522	CLA	C4B-C3B-CAB	3.86	134.98	127.18
23	b	2513	CLA	C4B-C3B-CAB	3.85	134.98	127.18
23	b	2513	CLA	CAA-CBA-CGA	3.85	125.68	113.27
23	A	350	CLA	C4A-NA-C1A	3.85	111.83	106.52
23	C	485	CLA	OBD-CAD-CBD	-3.85	120.13	125.94
23	c	2477	CLA	C4A-NA-C1A	3.85	111.83	106.52
23	C	476	CLA	C2B-C3B-CAB	-3.85	119.45	127.33
23	C	479	CLA	C4B-C3B-CAB	3.84	134.95	127.18
23	B	521	CLA	C4A-NA-C1A	3.84	111.81	106.52
23	B	515	CLA	C4B-C3B-CAB	3.83	134.93	127.18
23	b	2517	CLA	C4B-C3B-CAB	3.83	134.93	127.18
23	A	349	CLA	CAA-C2A-C1A	-3.82	102.09	111.62
23	b	2515	CLA	CAA-C2A-C3A	-3.82	104.00	113.04
23	B	525	CLA	C3B-CAB-CBB	-3.82	118.05	125.95
28	K	50	BCR	C2-C1-C6	3.81	116.77	110.44
28	F	48	BCR	C33-C5-C4	-3.81	106.35	113.34
25	v	2138	HEM	CHC-C1C-NC	3.80	128.04	124.73
23	C	477	CLA	C4A-NA-C1A	3.80	111.76	106.52
23	b	2515	CLA	C4B-C3B-CAB	3.80	134.88	127.18
23	a	2348	CLA	O2A-C1-C2	3.80	116.78	108.55
23	B	514	CLA	CBA-CAA-C2A	3.80	125.28	114.01
28	B	529	BCR	C21-C20-C19	3.79	136.04	123.24
23	c	2478	CLA	CBD-CHA-C1A	3.79	133.73	128.77
28	c	2488	BCR	C16-C17-C18	3.79	132.75	127.29
23	b	2513	CLA	CBA-CAA-C2A	3.79	125.25	114.01
23	C	479	CLA	CAA-CBA-CGA	-3.78	101.07	113.27
28	B	528	BCR	C2-C1-C6	3.78	116.73	110.44
25	V	138	HEM	CHA-C1A-NA	-3.78	118.27	124.58
23	C	487	CLA	C2B-C3B-CAB	-3.78	119.59	127.33
23	B	513	CLA	CAA-CBA-CGA	3.78	125.44	113.27
23	C	487	CLA	C4A-NA-C1A	3.77	111.72	106.52
28	j	2053	BCR	C33-C5-C4	-3.77	106.41	113.34
23	c	2481	CLA	C2D-C1D-ND	3.77	112.26	109.41
28	k	2050	BCR	C2-C1-C6	3.77	116.70	110.44
23	C	480	CLA	C4B-C3B-CAB	3.76	134.80	127.18
28	B	528	BCR	C38-C26-C27	-3.76	106.44	113.34
23	A	349	CLA	C2D-C1D-ND	3.75	112.25	109.41
23	d	2355	CLA	C4B-C3B-CAB	3.75	134.78	127.18
23	C	485	CLA	C2B-C3B-CAB	-3.75	119.65	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2482	CLA	C1-C2-C3	3.75	132.85	126.19
23	C	486	CLA	C4B-C3B-CAB	3.75	134.76	127.18
23	C	479	CLA	CBD-CHA-C1A	3.75	133.67	128.77
28	b	2528	BCR	C21-C20-C19	3.74	135.88	123.24
23	b	2518	CLA	C4B-C3B-CAB	3.74	134.76	127.18
23	C	478	CLA	C2A-C1A-CHA	3.74	130.32	123.83
23	d	2357	CLA	C4B-C3B-CAB	3.74	134.76	127.18
28	F	48	BCR	C38-C26-C27	-3.74	106.46	113.34
23	a	2349	CLA	C4A-NA-C1A	3.74	111.68	106.52
23	b	2522	CLA	C4B-C3B-CAB	3.74	134.75	127.18
23	b	2525	CLA	C3B-CAB-CBB	-3.74	118.21	125.95
23	A	349	CLA	CBA-CAA-C2A	3.73	125.09	114.01
23	B	514	CLA	O2A-CGA-CBA	3.73	123.67	111.94
23	b	2522	CLA	CBD-CHA-C1A	3.73	133.64	128.77
23	c	2486	CLA	C4B-C3B-CAB	3.72	134.71	127.18
23	B	524	CLA	C2B-C3B-CAB	-3.72	119.71	127.33
23	B	524	CLA	OBD-CAD-CBD	-3.72	120.33	125.94
23	d	2355	CLA	CBA-CAA-C2A	3.72	125.04	114.01
25	v	2138	HEM	CHA-C4D-ND	3.71	129.41	124.31
24	a	2350	PHO	OBD-CAD-CBD	-3.71	120.34	125.94
25	e	2084	HEM	C4A-NA-C1A	-3.71	101.88	106.76
23	C	482	CLA	C4B-C3B-CAB	3.71	134.69	127.18
23	c	2474	CLA	CAA-C2A-C1A	-3.71	102.37	111.62
23	B	527	CLA	C1-O2A-CGA	3.71	127.36	116.98
23	B	520	CLA	CBD-CHA-C1A	3.70	133.61	128.77
28	B	529	BCR	C30-C25-C26	-3.70	117.24	122.60
23	d	2355	CLA	CAA-C2A-C1A	-3.70	102.38	111.62
23	C	482	CLA	C1-C2-C3	3.70	132.77	126.19
23	B	524	CLA	C5-C3-C2	-3.70	113.97	121.08
23	b	2520	CLA	CBD-CHA-C1A	3.70	133.60	128.77
23	C	476	CLA	C1-C2-C3	3.69	132.75	126.19
23	b	2524	CLA	C2B-C3B-CAB	-3.69	119.78	127.33
23	A	352	CLA	C4B-C3B-CAB	3.69	134.64	127.18
26	a	2352	PL9	C32-C31-C29	3.68	124.94	112.74
23	c	2478	CLA	C2A-C1A-CHA	3.68	130.21	123.83
23	C	474	CLA	CBA-CAA-C2A	3.68	124.94	114.01
23	A	350	CLA	CBA-CAA-C2A	3.68	124.93	114.01
23	b	2524	CLA	C1-O2A-CGA	3.68	127.29	116.98
28	B	529	BCR	C38-C26-C27	-3.68	106.59	113.34
23	c	2474	CLA	C4B-C3B-CAB	3.67	134.61	127.18
23	b	2526	CLA	C1-O2A-CGA	3.67	127.26	116.98
28	b	2527	BCR	C24-C23-C22	3.67	131.70	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	353	PL9	C32-C31-C29	3.66	124.87	112.74
23	B	513	CLA	C4B-C3B-CAB	3.66	134.59	127.18
23	c	2485	CLA	C2B-C3B-CAB	-3.65	119.85	127.33
23	c	2481	CLA	C4B-C3B-CAB	3.65	134.57	127.18
23	c	2474	CLA	CBA-CAA-C2A	3.65	124.84	114.01
23	a	2351	CLA	CAA-C2A-C3A	-3.65	104.42	113.04
23	b	2514	CLA	CBA-CAA-C2A	3.65	124.83	114.01
23	c	2482	CLA	C4B-C3B-CAB	3.64	134.56	127.18
23	b	2521	CLA	C4B-C3B-CAB	3.65	134.56	127.18
23	B	514	CLA	C4B-C3B-CAB	3.64	134.55	127.18
23	B	521	CLA	C4B-C3B-CAB	3.64	134.55	127.18
28	C	488	BCR	C38-C26-C27	-3.64	106.66	113.34
23	c	2483	CLA	CBD-CHA-C1A	3.63	133.52	128.77
23	c	2479	CLA	C2A-C1A-NA	-3.63	107.22	111.24
23	c	2480	CLA	CBA-CAA-C2A	3.63	124.79	114.01
23	c	2480	CLA	C4B-C3B-CAB	3.63	134.53	127.18
23	a	2351	CLA	C4B-C3B-CAB	3.62	134.52	127.18
23	B	522	CLA	CBD-CHA-C1A	3.62	133.51	128.77
28	J	53	BCR	C24-C23-C22	3.62	131.64	126.22
23	c	2476	CLA	C4B-C3B-CAB	3.62	134.51	127.18
28	B	528	BCR	C24-C23-C22	3.61	131.62	126.22
23	A	349	CLA	O2A-CGA-CBA	3.61	123.29	111.94
23	B	518	CLA	CAA-C2A-C3A	-3.61	104.52	113.04
23	B	511	CLA	C2A-C1A-NA	-3.60	107.26	111.24
24	D	355	PHO	C2B-C3B-CAB	-3.60	119.96	127.33
28	C	489	BCR	C33-C5-C4	-3.60	106.72	113.34
24	a	2350	PHO	C1-C2-C3	3.60	132.59	126.19
23	C	487	CLA	CAC-C3C-C4C	3.60	130.24	124.85
23	B	524	CLA	C1-O2A-CGA	3.60	127.06	116.98
23	B	519	CLA	CAA-CBA-CGA	-3.60	101.67	113.27
23	b	2511	CLA	C2A-C1A-NA	-3.59	107.27	111.24
23	c	2485	CLA	OBD-CAD-CBD	-3.59	120.51	125.94
23	b	2519	CLA	CBD-CHA-C1A	3.59	133.47	128.77
23	b	2518	CLA	O2A-C1-C2	3.59	116.33	108.55
23	C	477	CLA	C4B-C3B-CAB	3.59	134.44	127.18
23	c	2475	CLA	C4B-C3B-CAB	3.59	134.44	127.18
28	b	2528	BCR	C30-C25-C26	-3.58	117.41	122.60
23	C	478	CLA	CBD-CHA-C1A	3.58	133.45	128.77
28	j	2053	BCR	C24-C23-C22	3.58	131.57	126.22
26	A	353	PL9	C27-C26-C24	-3.58	100.89	112.74
23	C	482	CLA	CBD-CHA-C1A	3.58	133.44	128.77
24	d	2356	PHO	C2B-C3B-CAB	-3.58	120.00	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2523	CLA	C2D-C1D-ND	3.57	112.11	109.41
23	C	479	CLA	C2A-C1A-NA	-3.57	107.29	111.24
23	b	2517	CLA	CAA-C2A-C3A	-3.57	104.59	113.04
23	c	2477	CLA	C4B-C3B-CAB	3.57	134.40	127.18
23	D	356	CLA	C4B-C3B-CAB	3.57	134.40	127.18
23	B	511	CLA	C4B-C3B-CAB	3.57	134.40	127.18
23	d	2355	CLA	C2D-C1D-ND	3.56	112.10	109.41
23	B	512	CLA	CBD-CHA-C1A	3.56	133.43	128.77
23	b	2514	CLA	O2A-CGA-CBA	3.56	123.14	111.94
23	B	515	CLA	CBA-CAA-C2A	3.56	124.58	114.01
23	C	478	CLA	C2D-C1D-ND	3.56	112.10	109.41
23	a	2349	CLA	CAA-C2A-C1A	-3.56	102.75	111.62
23	C	480	CLA	CBA-CAA-C2A	3.56	124.56	114.01
23	c	2475	CLA	CBD-CHA-C1A	3.56	133.42	128.77
23	b	2524	CLA	OBD-CAD-CBD	-3.55	120.58	125.94
23	B	517	CLA	C2A-C1A-NA	-3.55	107.31	111.24
23	b	2526	CLA	CBD-CHA-C1A	3.55	133.41	128.77
25	E	84	HEM	CHC-C1C-NC	3.55	127.82	124.73
23	a	2349	CLA	CBA-CAA-C2A	3.55	124.55	114.01
23	c	2487	CLA	C4A-NA-C1A	3.54	111.41	106.52
23	C	474	CLA	CAA-C2A-C1A	-3.54	102.78	111.62
23	b	2525	CLA	CED-O2D-CGD	3.54	124.45	116.02
28	b	2527	BCR	C2-C1-C6	3.54	116.33	110.44
28	d	2360	BCR	C38-C26-C27	-3.54	106.84	113.34
25	E	84	HEM	CMA-C3A-C4A	-3.53	123.19	128.62
24	d	2356	PHO	CAA-C2A-C3A	-3.53	104.69	113.04
28	d	2360	BCR	C23-C24-C25	3.53	137.74	127.32
24	D	355	PHO	CAA-C2A-C3A	-3.52	104.71	113.04
25	E	84	HEM	CMA-C3A-C2A	3.52	131.59	124.94
23	b	2526	CLA	C7-C6-C5	-3.52	102.64	113.01
28	b	2527	BCR	C29-C30-C25	3.52	116.28	110.44
23	b	2514	CLA	C4B-C3B-CAB	3.51	134.29	127.18
28	C	489	BCR	C2-C1-C6	3.51	116.27	110.44
23	B	518	CLA	O2A-C1-C2	3.51	116.15	108.55
28	c	2488	BCR	C29-C30-C25	3.51	116.27	110.44
28	J	53	BCR	C29-C30-C25	3.51	116.27	110.44
23	a	2348	CLA	CAA-C2A-C3A	-3.49	104.78	113.04
23	c	2477	CLA	C6-C5-C3	3.49	121.09	112.78
23	A	352	CLA	CAA-C2A-C3A	-3.49	104.78	113.04
23	b	2526	CLA	CAA-CBA-CGA	-3.49	102.03	113.27
26	a	2352	PL9	C27-C26-C24	-3.49	101.19	112.74
23	B	517	CLA	CAA-C2A-C3A	-3.49	104.80	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	356	CLA	C2D-C1D-ND	3.48	112.04	109.41
23	C	481	CLA	C4B-C3B-CAB	3.48	134.23	127.18
23	B	525	CLA	CED-O2D-CGD	3.48	124.30	116.02
23	B	527	CLA	C2B-C3B-CAB	-3.48	120.20	127.33
23	b	2513	CLA	C2A-C1A-NA	-3.48	107.39	111.24
23	B	517	CLA	CBD-CHA-C1A	3.48	133.31	128.77
23	d	2355	CLA	CBD-CHA-C1A	3.47	133.31	128.77
28	c	2488	BCR	C8-C9-C10	-3.47	113.63	118.97
23	c	2483	CLA	C2D-C1D-ND	3.47	112.03	109.41
23	B	527	CLA	C7-C6-C5	-3.47	102.78	113.01
23	b	2515	CLA	C2A-C1A-NA	-3.47	107.41	111.24
23	c	2487	CLA	C4B-C3B-CAB	3.46	134.19	127.18
26	D	357	PL9	C32-C31-C29	3.46	124.19	112.74
28	C	489	BCR	C29-C30-C25	3.46	116.19	110.44
23	b	2515	CLA	CBA-CAA-C2A	3.46	124.27	114.01
23	B	523	CLA	CBD-CHA-C1A	3.46	133.29	128.77
26	A	353	PL9	C25-C24-C23	3.46	130.37	123.52
23	C	475	CLA	C4B-C3B-CAB	3.46	134.18	127.18
23	d	2355	CLA	O2A-CGA-CBA	3.45	122.81	111.94
28	B	528	BCR	C29-C30-C25	3.45	116.18	110.44
23	c	2483	CLA	O2A-CGA-CBA	3.45	122.80	111.94
23	A	349	CLA	CBD-CHA-C1A	3.45	133.28	128.77
28	B	529	BCR	C1-C6-C5	-3.44	117.62	122.60
23	d	2354	CLA	C2D-C1D-ND	3.44	112.01	109.41
28	c	2488	BCR	C38-C26-C27	-3.44	107.02	113.34
23	C	481	CLA	C2D-C1D-ND	3.43	112.00	109.41
23	C	483	CLA	CBD-CHA-C1A	3.43	133.26	128.77
25	V	138	HEM	O1D-CGD-CBD	-3.43	111.22	123.03
23	C	476	CLA	C4B-C3B-CAB	3.43	134.12	127.18
23	C	484	CLA	C1D-CHD-C4C	3.43	127.91	122.60
28	j	2053	BCR	C7-C8-C9	3.42	131.34	126.22
28	b	2528	BCR	C1-C6-C5	-3.42	117.65	122.60
23	B	520	CLA	C1-C2-C3	3.42	132.27	126.19
26	d	2358	PL9	C32-C31-C29	3.42	124.06	112.74
23	b	2517	CLA	C2A-C1A-NA	-3.42	107.46	111.24
23	B	513	CLA	C2A-C1A-NA	-3.41	107.47	111.24
23	B	527	CLA	C2D-C1D-ND	3.41	111.99	109.41
23	C	479	CLA	OBD-CAD-CBD	-3.41	120.79	125.94
23	b	2512	CLA	CMB-C2B-C1B	-3.41	123.37	128.62
28	c	2489	BCR	C33-C5-C4	-3.41	107.08	113.34
23	b	2512	CLA	CBD-CHA-C1A	3.41	133.23	128.77
28	b	2528	BCR	C38-C26-C27	-3.41	107.08	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	477	CLA	CBD-CHA-C1A	3.41	133.22	128.77
23	B	527	CLA	CBD-CHA-C1A	3.41	133.22	128.77
23	C	477	CLA	C1D-CHD-C4C	3.41	127.88	122.60
28	j	2053	BCR	C8-C9-C10	-3.41	113.74	118.97
23	b	2518	CLA	CBD-CHA-C1A	3.40	133.22	128.77
23	B	511	CLA	CAA-CBA-CGA	-3.40	102.31	113.27
23	b	2517	CLA	OBD-CAD-CBD	-3.40	120.81	125.94
23	B	513	CLA	CAA-C2A-C3A	-3.40	105.01	113.04
23	b	2513	CLA	C2D-C1D-ND	3.40	111.98	109.41
23	c	2478	CLA	O2A-CGA-CBA	3.40	122.62	111.94
23	b	2526	CLA	CBA-CAA-C2A	3.39	124.08	114.01
23	B	513	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
23	C	474	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
23	b	2523	CLA	CED-O2D-CGD	3.39	124.08	116.02
23	c	2478	CLA	C2D-C1D-ND	3.39	111.97	109.41
28	F	48	BCR	C16-C15-C14	3.39	130.86	123.36
23	C	478	CLA	O2A-CGA-CBA	3.39	122.59	111.94
23	B	524	CLA	C4B-C3B-CAB	3.39	134.03	127.18
23	B	518	CLA	CBD-CHA-C1A	3.38	133.19	128.77
23	c	2477	CLA	CBD-CHA-C1A	3.38	133.19	128.77
23	C	487	CLA	C4B-C3B-CAB	3.38	134.02	127.18
23	b	2519	CLA	CAA-CBA-CGA	-3.37	102.39	113.27
28	F	48	BCR	C2-C1-C6	3.37	116.04	110.44
23	B	527	CLA	CAA-CBA-CGA	-3.37	102.40	113.27
23	c	2477	CLA	O2A-CGA-CBA	3.37	122.54	111.94
23	A	348	CLA	OBD-CAD-CBD	-3.37	120.86	125.94
23	B	515	CLA	CED-O2D-CGD	3.36	124.02	116.02
23	B	527	CLA	CBA-CAA-C2A	3.36	124.00	114.01
23	C	478	CLA	CMB-C2B-C1B	-3.36	123.45	128.62
28	C	488	BCR	C33-C5-C4	-3.36	107.17	113.34
23	c	2487	CLA	CAC-C3C-C4C	3.36	129.88	124.85
23	b	2519	CLA	C2D-C1D-ND	3.36	111.95	109.41
23	A	350	CLA	CAA-C2A-C1A	-3.36	103.25	111.62
23	B	513	CLA	C7-C6-C5	-3.36	103.12	113.01
23	c	2482	CLA	CBD-CHA-C1A	3.36	133.16	128.77
23	B	525	CLA	CBD-CHA-C1A	3.36	133.16	128.77
23	c	2476	CLA	C7-C6-C5	-3.36	103.12	113.01
23	C	477	CLA	O2A-CGA-CBA	3.35	122.49	111.94
23	A	352	CLA	C1-C2-C3	3.35	132.15	126.19
23	c	2475	CLA	CED-O2D-CGD	3.35	123.99	116.02
23	c	2484	CLA	CBD-CHA-C1A	3.35	133.15	128.77
28	j	2053	BCR	C23-C22-C21	-3.35	113.83	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2520	CLA	C1-C2-C3	3.34	132.13	126.19
23	C	478	CLA	C1D-CHD-C4C	3.34	127.78	122.60
28	c	2489	BCR	C2-C1-C6	3.34	115.99	110.44
28	C	488	BCR	C8-C9-C10	-3.34	113.84	118.97
23	c	2476	CLA	CBD-CHA-C1A	3.34	133.14	128.77
28	C	489	BCR	C23-C24-C25	3.34	137.19	127.32
28	J	53	BCR	C38-C26-C27	-3.34	107.20	113.34
23	C	483	CLA	O2A-CGA-CBA	3.34	122.45	111.94
23	b	2519	CLA	CAA-C2A-C3A	-3.34	105.15	113.04
23	b	2517	CLA	CBD-CHA-C1A	3.34	133.13	128.77
28	F	48	BCR	C23-C24-C25	3.33	137.17	127.32
23	C	482	CLA	C1D-CHD-C4C	3.33	127.76	122.60
23	C	482	CLA	C1-O2A-CGA	3.33	126.31	116.98
25	E	84	HEM	C4A-NA-C1A	-3.33	102.38	106.76
23	C	476	CLA	CBD-CHA-C1A	3.33	133.12	128.77
28	b	2528	BCR	C29-C30-C25	3.33	115.97	110.44
23	c	2479	CLA	OBD-CAD-CBD	-3.33	120.92	125.94
28	K	50	BCR	C29-C30-C25	3.33	115.97	110.44
23	B	519	CLA	CBD-CHA-C1A	3.32	133.11	128.77
23	C	487	CLA	C1D-CHD-C4C	3.32	127.75	122.60
23	c	2486	CLA	C2D-C1D-ND	3.32	111.92	109.41
23	B	515	CLA	C2A-C1A-NA	-3.32	107.57	111.24
28	d	2360	BCR	C29-C30-C25	3.32	115.95	110.44
23	b	2524	CLA	C4B-C3B-CAB	3.31	133.89	127.18
23	b	2518	CLA	CAA-C2A-C3A	-3.31	105.21	113.04
23	C	484	CLA	C1-C2-C3	3.31	132.07	126.19
23	A	352	CLA	CBD-CHA-C1A	3.31	133.10	128.77
23	c	2478	CLA	CMB-C2B-C1B	-3.31	123.53	128.62
28	j	2053	BCR	C38-C26-C27	-3.31	107.27	113.34
23	d	2354	CLA	O2A-CGA-CBA	3.31	122.34	111.94
23	C	486	CLA	C2D-C1D-ND	3.30	111.91	109.41
23	B	523	CLA	CED-O2D-CGD	3.30	123.88	116.02
24	A	351	PHO	OBD-CAD-CBD	-3.30	120.95	125.94
23	B	523	CLA	CAA-CBA-CGA	-3.30	102.63	113.27
23	b	2523	CLA	CBD-CHA-C1A	3.30	133.08	128.77
23	B	513	CLA	C1-C2-C3	3.30	132.05	126.19
27	B	526	LMT	C1-O1'-C1'	-3.30	108.02	113.96
28	d	2360	BCR	C2-C1-C6	3.30	115.92	110.44
23	B	521	CLA	CED-O2D-CGD	3.30	123.86	116.02
28	d	2360	BCR	C16-C15-C14	3.30	130.66	123.36
23	C	475	CLA	CBD-CHA-C1A	3.29	133.07	128.77
23	A	348	CLA	CAA-C2A-C3A	-3.29	105.27	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	CAA-C2A-C1A	-3.29	103.42	111.62
23	b	2523	CLA	CAA-CBA-CGA	-3.28	102.68	113.27
23	D	354	CLA	O2A-CGA-CBA	3.28	122.27	111.94
23	C	477	CLA	C6-C5-C3	3.28	120.58	112.78
23	a	2348	CLA	C1-O2A-CGA	3.28	126.17	116.98
23	b	2513	CLA	CAA-C2A-C3A	-3.28	105.28	113.04
25	V	138	HEM	CMD-C2D-C3D	3.28	133.03	125.60
23	c	2487	CLA	C1D-CHD-C4C	3.27	127.68	122.60
28	c	2489	BCR	C7-C8-C9	3.28	131.12	126.22
23	b	2513	CLA	CBD-CHA-C1A	3.28	133.05	128.77
23	b	2526	CLA	C2B-C3B-CAB	-3.27	120.64	127.33
24	D	355	PHO	C7-C6-C5	-3.27	103.37	113.01
23	B	527	CLA	C4B-C3B-CAB	3.27	133.80	127.18
23	c	2486	CLA	C6-C5-C3	3.27	120.55	112.78
23	A	349	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
23	C	480	CLA	CAA-C2A-C1A	-3.27	103.47	111.62
23	d	2354	CLA	C1D-CHD-C4C	3.27	127.66	122.60
23	B	519	CLA	CAA-C2A-C3A	-3.26	105.33	113.04
23	c	2486	CLA	C1-C2-C3	3.26	131.98	126.19
28	K	50	BCR	C7-C8-C9	3.25	131.08	126.22
23	b	2515	CLA	C1-C2-C3	3.25	131.96	126.19
23	C	477	CLA	CED-O2D-CGD	3.25	123.75	116.02
23	b	2519	CLA	C2A-C1A-NA	-3.25	107.65	111.24
27	B	526	LMT	O1B-C1B-C2B	3.25	115.91	108.12
23	B	519	CLA	C2A-C1A-NA	-3.24	107.66	111.24
23	b	2511	CLA	CAA-CBA-CGA	-3.24	102.81	113.27
23	c	2477	CLA	CED-O2D-CGD	3.24	123.73	116.02
23	C	474	CLA	C2D-C1D-ND	3.24	111.86	109.41
27	d	2359	LMT	O1B-C1B-C2B	3.24	115.89	108.12
28	c	2489	BCR	C29-C30-C25	3.24	115.82	110.44
23	c	2482	CLA	C1D-CHD-C4C	3.24	127.62	122.60
28	k	2050	BCR	C29-C30-C25	3.24	115.82	110.44
28	k	2050	BCR	C7-C8-C9	3.24	131.06	126.22
23	B	513	CLA	CBD-CHA-C1A	3.23	132.99	128.77
23	B	512	CLA	OBD-CAD-CBD	-3.23	121.06	125.94
23	B	522	CLA	CMB-C2B-C1B	-3.23	123.65	128.62
23	b	2513	CLA	C1-C2-C3	3.23	131.93	126.19
23	b	2511	CLA	CAA-C2A-C3A	-3.23	105.41	113.04
23	a	2349	CLA	CBD-CHA-C1A	3.23	132.99	128.77
23	b	2516	CLA	C1D-CHD-C4C	3.23	127.60	122.60
23	b	2511	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
23	B	523	CLA	C2D-C1D-ND	3.22	111.84	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	486	CLA	C6-C5-C3	3.22	120.42	112.78
23	b	2514	CLA	C2A-C1A-NA	-3.21	107.69	111.24
23	B	513	CLA	C2D-C1D-ND	3.22	111.84	109.41
23	C	476	CLA	C2D-C1D-ND	3.21	111.84	109.41
24	A	351	PHO	C1-C2-C3	3.22	131.90	126.19
23	C	485	CLA	CED-O2D-CGD	3.21	123.67	116.02
28	c	2489	BCR	C23-C24-C25	3.21	136.80	127.32
23	d	2357	CLA	C2D-C1D-ND	3.21	111.83	109.41
23	B	513	CLA	C2A-C1A-CHA	3.21	129.39	123.83
23	c	2482	CLA	C1-O2A-CGA	3.20	125.96	116.98
23	B	517	CLA	O2A-CGA-CBA	3.20	122.02	111.94
23	A	348	CLA	C1-O2A-CGA	3.21	125.96	116.98
23	b	2515	CLA	CED-O2D-CGD	3.20	123.64	116.02
23	b	2522	CLA	CMB-C2B-C1B	-3.20	123.70	128.62
23	c	2485	CLA	CAA-C2A-C3A	-3.20	105.47	113.04
28	F	48	BCR	C29-C30-C25	3.19	115.75	110.44
23	C	483	CLA	C1D-CHD-C4C	3.19	127.55	122.60
28	B	529	BCR	C33-C5-C6	3.19	128.12	124.51
23	B	513	CLA	CAA-C2A-C1A	-3.19	103.67	111.62
23	b	2513	CLA	C7-C6-C5	-3.19	103.62	113.01
23	B	513	CLA	C2A-C3A-C4A	3.19	106.30	101.40
28	b	2528	BCR	C33-C5-C6	3.18	128.12	124.51
23	c	2484	CLA	C1-C2-C3	3.18	131.84	126.19
23	A	350	CLA	CBD-CHA-C1A	3.18	132.93	128.77
23	b	2514	CLA	C2D-C1D-ND	3.18	111.81	109.41
23	c	2485	CLA	C1D-CHD-C4C	3.18	127.53	122.60
28	c	2489	BCR	C38-C26-C27	-3.18	107.50	113.34
23	b	2525	CLA	CBD-CHA-C1A	3.18	132.92	128.77
23	b	2512	CLA	C1-O2A-CGA	3.18	125.87	116.98
23	d	2355	CLA	C5-C3-C2	-3.18	114.97	121.08
23	b	2511	CLA	C2D-C1D-ND	3.18	111.81	109.41
23	c	2486	CLA	O2A-CGA-CBA	3.17	121.92	111.94
28	C	489	BCR	C38-C26-C27	-3.17	107.51	113.34
23	b	2513	CLA	C2A-C3A-C4A	3.17	106.28	101.40
23	b	2516	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
23	B	522	CLA	C1D-CHD-C4C	3.17	127.51	122.60
23	b	2513	CLA	O2A-CGA-CBA	3.17	121.90	111.94
23	c	2485	CLA	CED-O2D-CGD	3.17	123.56	116.02
23	b	2519	CLA	OBD-CAD-CBD	-3.17	121.16	125.94
28	J	53	BCR	C23-C22-C21	-3.17	114.11	118.97
25	e	2084	HEM	C2A-C1A-NA	3.16	114.13	109.73
23	b	2513	CLA	C6-C5-C3	3.16	120.30	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	517	CLA	C1D-CHD-C4C	3.16	127.50	122.60
23	B	517	CLA	OBD-CAD-CBD	-3.16	121.17	125.94
23	b	2512	CLA	CMB-C2B-C3B	3.16	129.94	124.97
23	C	475	CLA	CAA-C2A-C3A	-3.16	105.57	113.04
23	a	2348	CLA	C2D-C1D-ND	3.15	111.79	109.41
23	c	2475	CLA	C2D-C1D-ND	3.15	111.79	109.41
23	c	2479	CLA	C6-C7-C8	3.15	124.21	115.14
28	B	529	BCR	C29-C30-C25	3.15	115.67	110.44
23	b	2524	CLA	CBD-CHA-C1A	3.14	132.88	128.77
23	b	2521	CLA	CED-O2D-CGD	3.14	123.49	116.02
23	C	486	CLA	CAA-C2A-C3A	-3.14	105.62	113.04
28	C	488	BCR	C29-C30-C25	3.14	115.66	110.44
23	c	2479	CLA	CED-O2D-CGD	3.14	123.48	116.02
27	d	2359	LMT	C1-O1'-C1'	-3.14	108.31	113.96
23	C	479	CLA	C7-C6-C5	-3.14	103.77	113.01
23	a	2351	CLA	CBD-CHA-C1A	3.14	132.87	128.77
23	c	2487	CLA	CED-O2D-CGD	3.14	123.48	116.02
23	B	525	CLA	C1D-CHD-C4C	3.14	127.46	122.60
23	C	483	CLA	C1-C2-C3	3.14	131.76	126.19
28	C	488	BCR	C23-C24-C25	3.13	136.57	127.32
23	B	513	CLA	C6-C5-C3	3.13	120.23	112.78
28	B	529	BCR	C37-C22-C21	-3.13	118.47	122.92
23	A	352	CLA	C1D-CHD-C4C	3.13	127.46	122.60
23	c	2485	CLA	CBD-CHA-C1A	3.13	132.86	128.77
23	C	483	CLA	C2D-C1D-ND	3.13	111.77	109.41
23	C	485	CLA	CAA-C2A-C3A	-3.13	105.65	113.04
23	C	481	CLA	OBD-CAD-CBD	-3.13	121.22	125.94
23	C	482	CLA	C2A-C3A-C4A	3.13	106.21	101.40
23	D	356	CLA	C1D-CHD-C4C	3.12	127.44	122.60
23	b	2522	CLA	C1D-CHD-C4C	3.12	127.44	122.60
23	c	2480	CLA	CAA-C2A-C1A	-3.12	103.83	111.62
23	a	2349	CLA	C7-C6-C5	-3.12	103.81	113.01
23	B	519	CLA	O2A-CGA-CBA	3.12	121.75	111.94
23	d	2354	CLA	CBD-CHA-C1A	3.12	132.84	128.77
23	C	486	CLA	C1-C2-C3	3.11	131.72	126.19
23	B	512	CLA	CMB-C2B-C1B	-3.11	123.83	128.62
23	c	2483	CLA	C6-C5-C3	3.11	120.18	112.78
23	B	525	CLA	C4B-C3B-CAB	3.11	133.48	127.18
23	D	354	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
23	c	2482	CLA	C2A-C3A-C4A	3.11	106.18	101.40
23	C	485	CLA	CBD-CHA-C1A	3.11	132.83	128.77
23	b	2525	CLA	C7-C6-C5	-3.11	103.86	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	520	CLA	OBD-CAD-CBD	-3.10	121.25	125.94
23	B	514	CLA	C2A-C1A-NA	-3.10	107.81	111.24
23	b	2526	CLA	C1D-CHD-C4C	3.10	127.41	122.60
23	B	519	CLA	C1D-CHD-C4C	3.10	127.41	122.60
23	D	354	CLA	CBD-CHA-C1A	3.10	132.82	128.77
23	D	354	CLA	C2D-C1D-ND	3.10	111.75	109.41
23	C	480	CLA	O2A-CGA-CBA	3.10	121.69	111.94
23	c	2476	CLA	C2D-C1D-ND	3.09	111.75	109.41
23	b	2513	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
23	C	483	CLA	C2A-C3A-C4A	3.09	106.16	101.40
23	b	2526	CLA	C2A-C1A-CHA	3.09	129.19	123.83
23	B	516	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
23	C	475	CLA	CED-O2D-CGD	3.09	123.38	116.02
28	c	2488	BCR	C33-C5-C4	-3.09	107.66	113.34
23	c	2484	CLA	C1D-CHD-C4C	3.09	127.39	122.60
23	c	2483	CLA	C1D-CHD-C4C	3.09	127.39	122.60
23	b	2526	CLA	C4B-C3B-CAB	3.09	133.43	127.18
23	B	519	CLA	C2D-C1D-ND	3.09	111.74	109.41
23	c	2476	CLA	C1D-CHD-C4C	3.09	127.39	122.60
23	B	515	CLA	C1-C2-C3	3.09	131.68	126.19
23	b	2517	CLA	O2A-CGA-CBA	3.09	121.66	111.94
23	a	2348	CLA	C1D-CHD-C4C	3.09	127.39	122.60
23	c	2487	CLA	CMB-C2B-C3B	3.09	129.83	124.97
28	J	53	BCR	C8-C9-C10	-3.09	114.22	118.97
23	C	486	CLA	O2A-CGA-CBA	3.09	121.64	111.94
23	A	349	CLA	C5-C3-C2	-3.08	115.15	121.08
23	b	2519	CLA	CED-O2D-CGD	3.08	123.35	116.02
23	a	2349	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
23	A	350	CLA	C7-C6-C5	-3.08	103.94	113.01
23	B	519	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
28	k	2050	BCR	C38-C26-C27	-3.08	107.69	113.34
23	B	525	CLA	C1-C2-C3	3.07	131.65	126.19
23	c	2484	CLA	CED-O2D-CGD	3.07	123.33	116.02
23	c	2474	CLA	O2A-C1-C2	3.07	115.21	108.55
23	c	2478	CLA	C1D-CHD-C4C	3.07	127.36	122.60
23	B	511	CLA	CED-O2D-CGD	3.07	123.33	116.02
23	B	516	CLA	CBA-CAA-C2A	3.07	123.11	114.01
23	c	2478	CLA	CED-O2D-CGD	3.06	123.31	116.02
23	B	524	CLA	CBD-CHA-C1A	3.06	132.78	128.77
23	B	523	CLA	C1D-CHD-C4C	3.06	127.35	122.60
23	B	512	CLA	C1-O2A-CGA	3.06	125.56	116.98
28	J	53	BCR	C2-C1-C6	3.06	115.53	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	355	PHO	O2A-CGA-CBA	3.06	121.57	111.94
23	b	2511	CLA	CED-O2D-CGD	3.06	123.30	116.02
23	B	512	CLA	C1D-CHD-C4C	3.06	127.35	122.60
23	C	486	CLA	OBD-CAD-CBD	-3.06	121.32	125.94
23	b	2524	CLA	C2D-C1D-ND	3.06	111.72	109.41
24	d	2356	PHO	C6-C5-C3	3.06	120.05	112.78
24	a	2350	PHO	C7-C6-C5	-3.06	104.00	113.01
23	A	350	CLA	OBD-CAD-CBD	-3.05	121.33	125.94
23	c	2479	CLA	C7-C6-C5	-3.05	104.01	113.01
24	d	2356	PHO	C7-C6-C5	-3.05	104.02	113.01
23	b	2525	CLA	C1D-CHD-C4C	3.05	127.33	122.60
23	d	2357	CLA	C1D-CHD-C4C	3.05	127.33	122.60
23	b	2513	CLA	C2A-C1A-CHA	3.05	129.11	123.83
23	D	354	CLA	C1D-CHD-C4C	3.05	127.33	122.60
23	C	487	CLA	CMB-C2B-C3B	3.05	129.77	124.97
23	C	476	CLA	C1D-CHD-C4C	3.05	127.32	122.60
23	c	2474	CLA	O2A-CGA-CBA	3.05	121.52	111.94
28	C	489	BCR	C7-C8-C9	3.04	130.77	126.22
23	D	356	CLA	CBD-CHA-C1A	3.04	132.75	128.77
23	c	2480	CLA	O2A-CGA-CBA	3.04	121.51	111.94
23	b	2519	CLA	C1D-CHD-C4C	3.04	127.32	122.60
23	d	2355	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
24	d	2356	PHO	O2A-CGA-CBA	3.04	121.50	111.94
23	C	485	CLA	C1D-CHD-C4C	3.04	127.31	122.60
23	c	2480	CLA	CBD-CHA-C1A	3.04	132.74	128.77
23	C	479	CLA	C6-C7-C8	3.04	123.88	115.14
23	C	484	CLA	C2D-C1D-ND	3.04	111.70	109.41
28	K	50	BCR	C38-C26-C27	-3.03	107.77	113.34
23	b	2526	CLA	C2A-C1A-NA	-3.03	107.89	111.24
23	b	2521	CLA	OBD-CAD-CBD	-3.03	121.36	125.94
23	c	2475	CLA	CAA-C2A-C3A	-3.03	105.87	113.04
28	b	2528	BCR	C33-C5-C4	-3.03	107.77	113.34
23	b	2519	CLA	O2A-CGA-CBA	3.03	121.48	111.94
23	C	474	CLA	O2A-CGA-CBA	3.03	121.47	111.94
28	c	2488	BCR	C23-C24-C25	3.03	136.27	127.32
23	b	2525	CLA	C4B-C3B-CAB	3.03	133.31	127.18
23	B	524	CLA	C7-C6-C5	-3.03	104.09	113.01
23	c	2477	CLA	C6-C7-C8	3.03	123.85	115.14
23	B	513	CLA	O2A-CGA-CBA	3.02	121.45	111.94
28	F	48	BCR	C34-C9-C8	3.02	122.98	118.09
23	C	480	CLA	CBD-CHA-C1A	3.02	132.72	128.77
28	J	53	BCR	C7-C8-C9	3.02	130.74	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	CED-O2D-CGD	3.02	123.20	116.02
23	C	475	CLA	C2D-C1D-ND	3.02	111.69	109.41
23	C	486	CLA	C7-C6-C5	-3.01	104.13	113.01
23	b	2513	CLA	C1D-CHD-C4C	3.01	127.27	122.60
23	C	485	CLA	CBA-CAA-C2A	3.01	122.95	114.01
23	C	474	CLA	C1-C2-C3	3.01	131.54	126.19
23	B	517	CLA	CAA-C2A-C1A	-3.01	104.12	111.62
23	a	2348	CLA	CBD-CHA-C1A	3.01	132.70	128.77
28	c	2489	BCR	C8-C9-C10	-3.01	114.35	118.97
23	B	525	CLA	C2D-C1D-ND	3.01	111.68	109.41
23	b	2522	CLA	C2D-C1D-ND	3.01	111.68	109.41
23	c	2484	CLA	C2D-C1D-ND	3.01	111.68	109.41
23	b	2525	CLA	C2A-C3A-C4A	3.01	106.02	101.40
23	b	2512	CLA	C1D-CHD-C4C	3.00	127.26	122.60
26	A	353	PL9	C27-C28-C29	-3.00	121.32	127.80
23	C	474	CLA	O2A-C1-C2	3.00	115.06	108.55
28	b	2528	BCR	C37-C22-C21	-3.00	118.66	122.92
23	C	477	CLA	C6-C7-C8	3.00	123.77	115.14
23	B	513	CLA	CED-O2D-CGD	3.00	123.15	116.02
23	C	476	CLA	C7-C6-C5	-3.00	104.18	113.01
23	c	2481	CLA	C7-C6-C5	-2.99	104.19	113.01
28	d	2360	BCR	C30-C25-C26	-3.00	118.26	122.60
23	b	2512	CLA	C2D-C1D-ND	2.99	111.67	109.41
23	B	522	CLA	C2D-C1D-ND	2.99	111.67	109.41
23	d	2354	CLA	OBD-CAD-CBD	-2.99	121.42	125.94
23	B	527	CLA	C2A-C1A-CHA	2.99	129.01	123.83
26	a	2352	PL9	C32-C33-C34	-2.99	121.35	127.80
23	b	2522	CLA	CED-O2D-CGD	2.99	123.13	116.02
23	C	481	CLA	C1D-CHD-C4C	2.99	127.23	122.60
23	C	474	CLA	C1D-CHD-C4C	2.99	127.23	122.60
23	c	2479	CLA	C1D-CHD-C4C	2.98	127.23	122.60
23	B	523	CLA	C16-C15-C13	2.98	123.73	115.14
23	A	349	CLA	CAA-C2A-C3A	-2.98	105.99	113.04
23	c	2474	CLA	C2D-C1D-ND	2.98	111.66	109.41
23	B	522	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
24	D	355	PHO	CED-O2D-CGD	2.98	123.11	116.02
23	a	2348	CLA	C2A-C3A-C4A	2.98	105.98	101.40
23	B	521	CLA	C1D-CHD-C4C	2.98	127.22	122.60
23	C	479	CLA	CED-O2D-CGD	2.98	123.11	116.02
23	B	525	CLA	O2A-CGA-CBA	2.98	121.31	111.94
23	C	483	CLA	C6-C5-C3	2.98	119.86	112.78
23	b	2525	CLA	O2A-CGA-CBA	2.98	121.31	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2483	CLA	C1-C2-C3	2.97	131.47	126.19
23	b	2522	CLA	CMB-C2B-C3B	2.98	129.66	124.97
28	F	48	BCR	C30-C25-C26	-2.97	118.29	122.60
23	B	511	CLA	CBD-CHA-C1A	2.97	132.65	128.77
23	d	2355	CLA	CMB-C2B-C1B	-2.97	124.05	128.62
23	C	484	CLA	CBD-CHA-C1A	2.97	132.65	128.77
23	A	348	CLA	CBD-CHA-C1A	2.97	132.65	128.77
23	b	2516	CLA	CBA-CAA-C2A	2.97	122.83	114.01
23	b	2516	CLA	C2D-C1D-ND	2.97	111.65	109.41
23	C	487	CLA	CED-O2D-CGD	2.97	123.08	116.02
23	B	515	CLA	CAA-CBA-CGA	-2.97	103.70	113.27
23	b	2517	CLA	CED-O2D-CGD	2.97	123.08	116.02
28	C	488	BCR	C2-C1-C6	2.97	115.37	110.44
23	C	485	CLA	C2A-C3A-C4A	2.97	105.96	101.40
23	B	511	CLA	C1D-CHD-C4C	2.97	127.20	122.60
23	B	511	CLA	C2D-C1D-ND	2.97	111.65	109.41
23	b	2511	CLA	C1D-CHD-C4C	2.96	127.20	122.60
23	c	2477	CLA	C1D-CHD-C4C	2.96	127.19	122.60
23	b	2516	CLA	CAA-C2A-C1A	-2.96	104.23	111.62
23	b	2523	CLA	C1D-CHD-C4C	2.96	127.19	122.60
23	C	481	CLA	O2A-CGA-CBA	2.96	121.25	111.94
23	c	2475	CLA	C1D-CHD-C4C	2.96	127.19	122.60
23	C	478	CLA	CAA-C2A-C3A	-2.96	106.05	113.04
23	b	2514	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
23	b	2524	CLA	O2A-CGA-CBA	2.96	121.24	111.94
23	C	481	CLA	C2A-C3A-C4A	2.96	105.95	101.40
23	b	2523	CLA	C16-C15-C13	2.96	123.65	115.14
23	B	516	CLA	C1D-CHD-C4C	2.95	127.18	122.60
23	C	475	CLA	C1D-CHD-C4C	2.95	127.17	122.60
23	c	2485	CLA	C4B-C3B-CAB	2.95	133.15	127.18
28	j	2053	BCR	C2-C1-C6	2.95	115.33	110.44
23	c	2485	CLA	C2A-C3A-C4A	2.95	105.93	101.40
23	b	2525	CLA	C1-C2-C3	2.95	131.42	126.19
28	K	50	BCR	C33-C5-C4	-2.94	107.93	113.34
23	b	2514	CLA	C1D-CHD-C4C	2.94	127.16	122.60
23	C	482	CLA	CBA-CAA-C2A	2.94	122.75	114.01
23	C	479	CLA	C1D-CHD-C4C	2.94	127.16	122.60
23	b	2514	CLA	CBD-CHA-C1A	2.94	132.62	128.77
23	b	2515	CLA	CAA-C2A-C1A	-2.94	104.29	111.62
24	A	351	PHO	C7-C6-C5	-2.94	104.34	113.01
23	d	2357	CLA	CBD-CHA-C1A	2.94	132.61	128.77
23	B	513	CLA	C1D-CHD-C4C	2.94	127.16	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	K	50	BCR	C23-C22-C21	-2.94	114.45	118.97
23	b	2511	CLA	CBD-CHA-C1A	2.94	132.61	128.77
23	b	2523	CLA	CMB-C2B-C1B	-2.94	124.11	128.62
23	c	2486	CLA	OBD-CAD-CBD	-2.94	121.51	125.94
23	b	2512	CLA	C6-C5-C3	2.93	119.75	112.78
23	C	474	CLA	C1-O2A-CGA	2.93	125.19	116.98
23	B	521	CLA	OBD-CAD-CBD	-2.93	121.52	125.94
28	F	48	BCR	C30-C25-C24	2.93	123.81	115.69
23	b	2517	CLA	CMB-C2B-C1B	-2.93	124.12	128.62
23	C	485	CLA	C4B-C3B-CAB	2.93	133.10	127.18
23	B	511	CLA	CAA-C2A-C3A	-2.93	106.12	113.04
23	C	479	CLA	C2D-C1D-ND	2.93	111.62	109.41
23	B	527	CLA	C1D-CHD-C4C	2.93	127.14	122.60
23	c	2486	CLA	C7-C6-C5	-2.92	104.40	113.01
23	c	2474	CLA	C1D-CHD-C4C	2.92	127.13	122.60
23	C	480	CLA	C1D-CHD-C4C	2.92	127.13	122.60
28	d	2360	BCR	C34-C9-C8	2.92	122.81	118.09
23	C	486	CLA	C2A-C3A-C4A	2.92	105.89	101.40
24	a	2350	PHO	CED-O2D-CGD	2.92	122.96	116.02
23	B	522	CLA	CMB-C2B-C3B	2.92	129.57	124.97
23	C	484	CLA	CED-O2D-CGD	2.92	122.96	116.02
28	c	2488	BCR	C2-C1-C6	2.92	115.29	110.44
28	b	2527	BCR	C23-C24-C25	2.91	135.92	127.32
23	b	2516	CLA	C5-C3-C2	2.91	126.69	121.08
23	B	517	CLA	C2D-C1D-ND	2.91	111.61	109.41
23	b	2526	CLA	C2D-C1D-ND	2.91	111.61	109.41
23	c	2481	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
23	B	524	CLA	CMB-C2B-C1B	-2.91	124.14	128.62
23	c	2478	CLA	C2A-C3A-C4A	2.91	105.88	101.40
26	d	2358	PL9	C31-C29-C28	-2.91	115.48	121.08
24	d	2356	PHO	CMB-C2B-C3B	2.91	129.55	124.97
23	b	2516	CLA	C6-C7-C8	2.91	123.52	115.14
26	D	357	PL9	C31-C29-C28	-2.91	115.49	121.08
23	a	2349	CLA	O2A-CGA-CBA	2.90	121.08	111.94
28	j	2053	BCR	C29-C30-C25	2.90	115.27	110.44
23	B	512	CLA	C7-C6-C5	-2.91	104.45	113.01
23	C	481	CLA	C7-C6-C5	-2.90	104.46	113.01
23	C	479	CLA	C6-C5-C3	2.90	119.68	112.78
23	B	512	CLA	CMB-C2B-C3B	2.90	129.54	124.97
23	B	522	CLA	CED-O2D-CGD	2.90	122.92	116.02
23	a	2351	CLA	C1D-CHD-C4C	2.90	127.10	122.60
23	c	2481	CLA	O2A-CGA-CBA	2.90	121.05	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	516	CLA	C6-C7-C8	2.90	123.48	115.14
23	C	480	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
23	c	2486	CLA	C2A-C3A-C4A	2.89	105.84	101.40
23	B	523	CLA	O2A-CGA-CBA	2.89	121.03	111.94
23	C	481	CLA	CBD-CHA-C1A	2.89	132.55	128.77
23	B	516	CLA	C2A-C3A-C4A	2.89	105.85	101.40
23	b	2520	CLA	O2D-CGD-CBD	2.89	117.22	111.33
23	b	2518	CLA	CED-O2D-CGD	2.89	122.89	116.02
23	C	486	CLA	C2A-C1A-CHA	2.89	128.83	123.83
28	B	529	BCR	C33-C5-C4	-2.89	108.04	113.34
23	a	2351	CLA	C2D-C1D-ND	2.89	111.59	109.41
23	c	2482	CLA	CBA-CAA-C2A	2.89	122.58	114.01
23	B	518	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
23	B	514	CLA	C1D-CHD-C4C	2.88	127.07	122.60
23	b	2521	CLA	C2D-C1D-ND	2.88	111.59	109.41
23	B	512	CLA	C2B-C3B-CAB	-2.88	121.42	127.33
23	B	512	CLA	C6-C5-C3	2.88	119.63	112.78
23	B	514	CLA	CBD-CHA-C1A	2.88	132.53	128.77
23	c	2481	CLA	CED-O2D-CGD	2.88	122.87	116.02
23	c	2480	CLA	CED-O2D-CGD	2.88	122.86	116.02
23	c	2486	CLA	C1D-CHD-C4C	2.88	127.06	122.60
28	C	489	BCR	C30-C25-C24	2.88	123.66	115.69
23	c	2481	CLA	C1D-CHD-C4C	2.87	127.06	122.60
23	B	514	CLA	CMB-C2B-C1B	-2.87	124.20	128.62
28	k	2050	BCR	C23-C22-C21	-2.87	114.55	118.97
23	c	2474	CLA	C7-C6-C5	-2.87	104.54	113.01
23	B	524	CLA	O2A-CGA-CBA	2.87	120.97	111.94
23	B	522	CLA	C2A-C1A-NA	-2.87	108.06	111.24
24	d	2356	PHO	C4D-CHA-CBD	-2.87	103.17	107.53
23	b	2514	CLA	CED-O2D-CGD	2.87	122.85	116.02
24	A	351	PHO	CED-O2D-CGD	2.87	122.85	116.02
23	B	512	CLA	C2D-C1D-ND	2.87	111.58	109.41
23	C	478	CLA	CED-O2D-CGD	2.87	122.84	116.02
23	C	477	CLA	C2D-C1D-ND	2.86	111.57	109.41
23	A	350	CLA	O2A-CGA-CBA	2.86	120.93	111.94
23	b	2514	CLA	CMB-C2B-C3B	2.86	129.47	124.97
23	b	2517	CLA	C2D-C1D-ND	2.86	111.57	109.41
23	B	523	CLA	CMB-C2B-C1B	-2.85	124.23	128.62
23	c	2487	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
23	C	485	CLA	C7-C6-C5	-2.85	104.60	113.01
23	A	352	CLA	C2D-C1D-ND	2.85	111.56	109.41
23	C	486	CLA	C1D-CHD-C4C	2.85	127.02	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	514	CLA	C2D-C1D-ND	2.85	111.56	109.41
23	C	487	CLA	CBD-CHA-C1A	2.85	132.49	128.77
23	B	524	CLA	CMB-C2B-C3B	2.85	129.46	124.97
23	b	2514	CLA	CMB-C2B-C1B	-2.85	124.24	128.62
23	d	2354	CLA	CBA-CAA-C2A	2.85	122.46	114.01
26	d	2358	PL9	C20-C19-C21	-2.85	111.06	115.39
23	B	524	CLA	CED-O2D-CGD	2.85	122.79	116.02
26	a	2352	PL9	C27-C28-C29	-2.84	121.66	127.80
28	k	2050	BCR	C8-C9-C10	-2.84	114.60	118.97
28	B	528	BCR	C23-C24-C25	2.84	135.72	127.32
28	B	528	BCR	C30-C25-C26	-2.85	118.48	122.60
24	A	351	PHO	CAA-C2A-C3A	-2.84	106.31	113.04
23	c	2474	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
23	a	2349	CLA	C1D-CHD-C4C	2.84	127.01	122.60
23	b	2512	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
23	B	524	CLA	C1D-CHD-C4C	2.84	127.00	122.60
23	c	2486	CLA	CAA-C2A-C3A	-2.84	106.33	113.04
28	k	2050	BCR	C33-C5-C4	-2.84	108.13	113.34
23	c	2478	CLA	CAA-C2A-C3A	-2.83	106.34	113.04
23	B	514	CLA	OBD-CAD-CBD	-2.83	121.66	125.94
23	B	520	CLA	C2A-C3A-C4A	2.83	105.75	101.40
23	b	2512	CLA	C7-C6-C5	-2.83	104.67	113.01
23	b	2526	CLA	CED-O2D-CGD	2.83	122.75	116.02
23	c	2480	CLA	C1D-CHD-C4C	2.83	126.99	122.60
25	v	2138	HEM	CMA-C3A-C2A	2.83	130.28	124.94
23	b	2515	CLA	CAA-CBA-CGA	-2.83	104.14	113.27
28	b	2527	BCR	C30-C25-C26	-2.83	118.50	122.60
28	c	2489	BCR	C30-C25-C24	2.83	123.52	115.69
23	A	349	CLA	CMB-C2B-C1B	-2.83	124.27	128.62
23	B	512	CLA	C4B-C3B-CAB	2.83	132.90	127.18
23	C	477	CLA	C16-C15-C13	2.82	123.27	115.14
23	D	354	CLA	C2A-C3A-C4A	2.82	105.74	101.40
28	B	528	BCR	C8-C9-C10	-2.82	114.63	118.97
23	B	519	CLA	CED-O2D-CGD	2.82	122.73	116.02
23	B	516	CLA	CAA-C2A-C1A	-2.82	104.58	111.62
28	B	528	BCR	C1-C6-C5	-2.82	118.51	122.60
23	c	2485	CLA	CBA-CAA-C2A	2.82	122.39	114.01
26	a	2352	PL9	C15-C14-C16	-2.82	111.10	115.39
23	B	511	CLA	C1-C2-C3	2.82	131.20	126.19
28	b	2527	BCR	C1-C6-C5	-2.82	118.52	122.60
23	b	2523	CLA	O2A-CGA-CBA	2.82	120.81	111.94
23	B	525	CLA	C7-C6-C5	-2.82	104.70	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	475	CLA	O1A-CGA-CBA	-2.82	112.16	123.78
24	d	2356	PHO	CED-O2D-CGD	2.82	122.72	116.02
23	B	521	CLA	C2D-C1D-ND	2.82	111.54	109.41
23	b	2520	CLA	OBD-CAD-CBD	-2.82	121.69	125.94
23	B	515	CLA	C2D-C1D-ND	2.81	111.54	109.41
23	b	2522	CLA	C2A-C1A-NA	-2.81	108.13	111.24
23	b	2521	CLA	C1D-CHD-C4C	2.81	126.95	122.60
23	b	2515	CLA	C2A-C1A-CHA	2.81	128.70	123.83
23	c	2475	CLA	O1A-CGA-CBA	-2.81	112.19	123.78
23	B	520	CLA	CED-O2D-CGD	2.81	122.70	116.02
23	A	350	CLA	C2A-C3A-C4A	2.81	105.72	101.40
23	A	350	CLA	C1D-CHD-C4C	2.81	126.95	122.60
24	D	355	PHO	C6-C5-C3	2.81	119.45	112.78
23	C	482	CLA	C6-C5-C3	2.80	119.45	112.78
23	c	2474	CLA	C1-C2-C3	2.81	131.17	126.19
23	b	2524	CLA	C7-C6-C5	-2.80	104.75	113.01
23	b	2512	CLA	C2B-C3B-CAB	-2.80	121.60	127.33
23	b	2511	CLA	C1-C2-C3	2.80	131.16	126.19
23	d	2354	CLA	C2A-C3A-C4A	2.80	105.70	101.40
23	b	2517	CLA	CAA-C2A-C1A	-2.79	104.65	111.62
28	K	50	BCR	C8-C9-C10	-2.79	114.68	118.97
23	B	521	CLA	CMB-C2B-C1B	-2.79	124.33	128.62
23	B	516	CLA	C5-C3-C2	2.79	126.46	121.08
23	b	2515	CLA	C1-O2A-CGA	2.79	124.79	116.98
25	e	2084	HEM	C2D-C1D-ND	-2.79	109.64	112.93
23	b	2524	CLA	C1D-CHD-C4C	2.79	126.93	122.60
23	B	514	CLA	CMB-C2B-C3B	2.79	129.36	124.97
28	F	48	BCR	C1-C6-C5	-2.79	118.56	122.60
23	C	477	CLA	CMB-C2B-C1B	-2.79	124.33	128.62
23	B	527	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
24	D	355	PHO	C4A-NA-C1A	2.78	112.08	108.42
23	B	515	CLA	C2A-C1A-CHA	2.78	128.65	123.83
23	b	2524	CLA	CED-O2D-CGD	2.78	122.63	116.02
23	b	2520	CLA	C2D-C1D-ND	2.78	111.51	109.41
25	v	2138	HEM	CMA-C3A-C4A	-2.78	124.35	128.62
23	b	2524	CLA	CMB-C2B-C1B	-2.77	124.35	128.62
23	A	348	CLA	CED-O2D-CGD	2.77	122.62	116.02
23	B	527	CLA	CED-O2D-CGD	2.77	122.62	116.02
23	B	518	CLA	CED-O2D-CGD	2.77	122.62	116.02
23	c	2482	CLA	C2D-C1D-ND	2.77	111.50	109.41
23	B	517	CLA	CMB-C2B-C1B	-2.77	124.36	128.62
23	b	2526	CLA	C6-C7-C8	2.77	123.12	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	520	CLA	O2A-CGA-CBA	2.77	120.65	111.94
28	B	528	BCR	C8-C7-C6	2.77	135.50	127.32
23	b	2524	CLA	C2A-C3A-C4A	2.77	105.65	101.40
23	c	2482	CLA	CED-O2D-CGD	2.76	122.59	116.02
26	a	2352	PL9	C31-C32-C33	2.76	119.51	111.62
28	C	488	BCR	C19-C18-C17	-2.76	114.73	118.97
23	B	525	CLA	C2A-C3A-C4A	2.76	105.65	101.40
23	D	356	CLA	C2A-C3A-C4A	2.76	105.64	101.40
26	A	353	PL9	C30-C29-C31	2.76	119.58	115.39
23	c	2474	CLA	CBD-CHA-C1A	2.76	132.38	128.77
23	C	483	CLA	CED-O2D-CGD	2.76	122.58	116.02
23	B	516	CLA	CBD-CHA-C1A	2.76	132.37	128.77
25	V	138	HEM	CHA-C4D-ND	2.76	128.09	124.31
23	c	2481	CLA	C1D-C2D-C3D	-2.75	104.53	106.78
23	b	2518	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
23	c	2479	CLA	C2D-C1D-ND	2.75	111.49	109.41
28	d	2360	BCR	C30-C25-C24	2.75	123.31	115.69
23	b	2521	CLA	CBD-CHA-C1A	2.75	132.37	128.77
23	B	511	CLA	CMB-C2B-C3B	2.75	129.30	124.97
28	J	53	BCR	C8-C7-C6	2.75	135.44	127.32
24	d	2356	PHO	C4A-NA-C1A	2.75	112.03	108.42
23	a	2351	CLA	C2A-C3A-C4A	2.75	105.62	101.40
23	a	2351	CLA	CED-O2D-CGD	2.75	122.55	116.02
23	b	2525	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
23	c	2483	CLA	CED-O2D-CGD	2.74	122.54	116.02
24	D	355	PHO	C4D-CHA-CBD	-2.74	103.36	107.53
23	b	2518	CLA	C1D-CHD-C4C	2.74	126.85	122.60
28	F	48	BCR	C24-C23-C22	2.74	130.32	126.22
23	c	2484	CLA	O2A-CGA-CBA	2.74	120.55	111.94
23	B	515	CLA	CAA-C2A-C1A	-2.74	104.79	111.62
23	A	352	CLA	C2A-C3A-C4A	2.74	105.61	101.40
23	B	523	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
23	c	2482	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
28	B	529	BCR	C1-C6-C7	2.74	123.27	115.69
23	d	2355	CLA	CAA-C2A-C3A	-2.74	106.57	113.04
23	B	515	CLA	C7-C6-C5	-2.73	104.95	113.01
23	c	2483	CLA	C2A-C3A-C4A	2.73	105.60	101.40
23	c	2474	CLA	O2D-CGD-CBD	2.73	116.89	111.33
28	C	489	BCR	C8-C9-C10	-2.73	114.78	118.97
26	D	357	PL9	C20-C19-C21	-2.72	111.25	115.39
23	c	2479	CLA	C6-C5-C3	2.72	119.26	112.78
24	d	2356	PHO	C1-C2-C3	2.72	131.03	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2351	CLA	OBD-CAD-CBD	-2.73	121.83	125.94
23	b	2512	CLA	C4B-C3B-CAB	2.72	132.69	127.18
23	b	2522	CLA	C16-C15-C13	2.72	122.97	115.14
23	b	2517	CLA	C1D-CHD-C4C	2.72	126.82	122.60
23	b	2517	CLA	C2A-C1A-CHA	2.72	128.54	123.83
23	B	520	CLA	C1D-CHD-C4C	2.72	126.81	122.60
23	B	511	CLA	CMB-C2B-C1B	-2.72	124.44	128.62
23	b	2526	CLA	CMB-C2B-C1B	-2.71	124.45	128.62
23	A	349	CLA	C1D-CHD-C4C	2.71	126.80	122.60
23	C	482	CLA	C2D-C1D-ND	2.71	111.46	109.41
23	C	480	CLA	CED-O2D-CGD	2.71	122.46	116.02
24	d	2356	PHO	C12-C11-C10	-2.71	99.13	113.02
26	A	353	PL9	C31-C32-C33	2.71	119.34	111.62
23	b	2514	CLA	C1D-C2D-C3D	-2.70	104.57	106.78
23	B	521	CLA	CBD-CHA-C1A	2.71	132.31	128.77
23	B	524	CLA	C2D-C1D-ND	2.70	111.45	109.41
23	C	484	CLA	O2A-CGA-CBA	2.70	120.45	111.94
23	c	2485	CLA	C7-C6-C5	-2.71	105.04	113.01
23	d	2357	CLA	C2A-C3A-C4A	2.70	105.56	101.40
28	b	2527	BCR	C23-C22-C21	-2.70	114.82	118.97
23	c	2480	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
23	C	482	CLA	CED-O2D-CGD	2.70	122.44	116.02
25	E	84	HEM	CBD-CAD-C3D	-2.70	108.48	114.37
23	A	348	CLA	C7-C6-C5	-2.70	105.05	113.01
23	C	479	CLA	CAA-C2A-C3A	-2.70	106.66	113.04
23	c	2486	CLA	C2A-C1A-CHA	2.69	128.50	123.83
28	k	2050	BCR	C34-C9-C8	2.70	122.45	118.09
23	c	2474	CLA	C1-O2A-CGA	2.69	124.53	116.98
23	B	516	CLA	C2D-C1D-ND	2.69	111.44	109.41
23	B	518	CLA	C1D-CHD-C4C	2.69	126.77	122.60
23	B	517	CLA	C2A-C1A-CHA	2.69	128.49	123.83
23	b	2512	CLA	CED-O2D-CGD	2.69	122.41	116.02
23	A	350	CLA	C2D-C1D-ND	2.69	111.44	109.41
23	d	2357	CLA	C1D-C2D-C3D	-2.69	104.58	106.78
23	c	2477	CLA	C16-C15-C13	2.69	122.88	115.14
23	C	474	CLA	CED-O2D-CGD	2.69	122.41	116.02
23	B	515	CLA	C1-O2A-CGA	2.69	124.51	116.98
23	C	476	CLA	C2A-C3A-C4A	2.69	105.53	101.40
23	b	2515	CLA	C1D-CHD-C4C	2.69	126.77	122.60
23	B	523	CLA	C2A-C3A-C4A	2.69	105.53	101.40
23	A	348	CLA	C1D-CHD-C4C	2.69	126.77	122.60
23	c	2481	CLA	CBD-CHA-C1A	2.69	132.28	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	483	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
23	B	527	CLA	C6-C7-C8	2.68	122.87	115.14
23	b	2526	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
23	B	522	CLA	C1-C2-C3	2.68	130.95	126.19
23	B	527	CLA	C2A-C1A-NA	-2.68	108.28	111.24
26	A	353	PL9	C32-C33-C34	-2.68	122.02	127.80
23	C	474	CLA	CBD-CHA-C1A	2.68	132.27	128.77
23	C	484	CLA	C2A-C3A-C4A	2.68	105.52	101.40
23	c	2485	CLA	O2A-CGA-CBA	2.68	120.36	111.94
23	b	2520	CLA	O2A-CGA-CBA	2.68	120.36	111.94
23	C	476	CLA	O2A-CGA-CBA	2.68	120.36	111.94
25	e	2084	HEM	O1D-CGD-CBD	-2.68	113.82	123.03
23	A	352	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
23	a	2348	CLA	C16-C15-C13	2.67	122.83	115.14
23	b	2521	CLA	CMB-C2B-C1B	-2.67	124.52	128.62
23	C	486	CLA	C2A-C1A-NA	-2.67	108.29	111.24
23	b	2511	CLA	C2A-C1A-CHA	2.67	128.45	123.83
23	C	484	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
23	c	2484	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
23	b	2526	CLA	C2A-C3A-C4A	2.67	105.50	101.40
23	b	2515	CLA	C2A-C3A-C4A	2.67	105.50	101.40
23	c	2477	CLA	OBD-CAD-CBD	-2.66	121.92	125.94
23	c	2486	CLA	CED-O2D-CGD	2.66	122.36	116.02
28	K	50	BCR	C36-C18-C19	2.66	122.40	118.09
24	D	355	PHO	C12-C11-C10	-2.66	99.37	113.02
23	B	527	CLA	CMB-C2B-C1B	-2.66	124.53	128.62
27	d	2359	LMT	C3'-C4'-C5'	-2.66	104.89	110.85
23	a	2349	CLA	C2A-C3A-C4A	2.65	105.48	101.40
23	b	2515	CLA	CMB-C2B-C1B	-2.65	124.54	128.62
23	B	520	CLA	C2D-C1D-ND	2.65	111.41	109.41
23	A	349	CLA	C2A-C3A-C4A	2.65	105.47	101.40
23	B	515	CLA	C2A-C3A-C4A	2.65	105.47	101.40
27	B	526	LMT	C3'-C4'-C5'	-2.65	104.90	110.85
28	b	2527	BCR	C8-C7-C6	2.65	135.14	127.32
28	d	2360	BCR	C24-C23-C22	2.65	130.18	126.22
23	C	486	CLA	C4D-CHA-CBD	-2.64	103.14	109.37
23	B	527	CLA	C1-C2-C3	2.64	130.89	126.19
28	j	2053	BCR	C8-C7-C6	2.64	135.12	127.32
23	A	352	CLA	C7-C6-C5	-2.64	105.22	113.01
28	b	2528	BCR	C1-C6-C7	2.64	123.00	115.69
25	V	138	HEM	C4B-CHC-C1C	-2.64	119.62	126.57
23	C	474	CLA	C6-C7-C8	2.64	122.73	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	522	CLA	C2A-C1A-CHA	2.64	128.40	123.83
25	E	84	HEM	O1D-CGD-CBD	-2.63	113.97	123.03
23	c	2479	CLA	C2A-C3A-C4A	2.63	105.45	101.40
23	C	482	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
23	B	525	CLA	C6-C5-C3	2.63	119.02	112.78
23	A	348	CLA	C16-C15-C13	2.63	122.70	115.14
23	b	2516	CLA	C2A-C3A-C4A	2.63	105.44	101.40
23	B	514	CLA	CED-O2D-CGD	2.62	122.26	116.02
28	k	2050	BCR	C36-C18-C19	2.63	122.34	118.09
24	D	355	PHO	CMB-C2B-C3B	2.62	129.10	124.97
23	C	484	CLA	CAA-C2A-C3A	-2.62	106.84	113.04
23	a	2348	CLA	O2D-CGD-CBD	2.62	116.67	111.33
23	b	2520	CLA	CED-O2D-CGD	2.62	122.25	116.02
23	C	486	CLA	CED-O2D-CGD	2.62	122.24	116.02
23	c	2477	CLA	C2D-C1D-ND	2.62	111.39	109.41
26	d	2358	PL9	C22-C21-C19	-2.62	104.07	112.74
23	B	524	CLA	C2A-C3A-C4A	2.62	105.42	101.40
23	C	485	CLA	C2D-C1D-ND	2.61	111.38	109.41
23	B	517	CLA	CED-O2D-CGD	2.61	122.23	116.02
23	d	2357	CLA	OBD-CAD-CBD	-2.61	122.00	125.94
25	v	2138	HEM	C3A-C4A-CHB	-2.61	121.05	126.00
23	b	2520	CLA	C2A-C3A-C4A	2.61	105.41	101.40
28	B	528	BCR	C23-C22-C21	-2.61	114.96	118.97
23	c	2481	CLA	C2A-C3A-C4A	2.61	105.41	101.40
23	b	2515	CLA	C2D-C1D-ND	2.61	111.38	109.41
23	a	2348	CLA	OBD-CAD-CBD	-2.61	122.01	125.94
23	c	2485	CLA	O2D-CGD-CBD	2.60	116.63	111.33
23	B	511	CLA	C2A-C1A-CHA	2.60	128.34	123.83
23	c	2479	CLA	O2A-CGA-CBA	2.60	120.12	111.94
23	A	349	CLA	CED-O2D-CGD	2.60	122.20	116.02
23	b	2520	CLA	C1D-CHD-C4C	2.60	126.63	122.60
28	c	2488	BCR	C19-C18-C17	-2.60	114.98	118.97
23	b	2522	CLA	C1-C2-C3	2.60	130.80	126.19
23	d	2355	CLA	C1D-CHD-C4C	2.60	126.63	122.60
28	B	529	BCR	C35-C13-C12	2.59	122.28	118.09
23	c	2476	CLA	O2A-CGA-CBA	2.59	120.10	111.94
27	B	526	LMT	O1'-C1'-C2'	2.59	111.48	108.18
23	c	2487	CLA	C2A-C3A-C4A	2.59	105.38	101.40
23	b	2523	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
23	b	2522	CLA	O2A-CGA-CBA	2.58	120.07	111.94
23	d	2355	CLA	C2A-C3A-C4A	2.58	105.38	101.40
23	C	476	CLA	C6-C7-C8	2.59	122.58	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	522	CLA	C16-C15-C13	2.58	122.58	115.14
23	C	478	CLA	C2A-C3A-C4A	2.58	105.37	101.40
23	c	2486	CLA	C2A-C1A-NA	-2.58	108.39	111.24
23	d	2357	CLA	O2D-CGD-CBD	2.58	116.59	111.33
23	c	2487	CLA	CBD-CHA-C1A	2.58	132.14	128.77
23	B	515	CLA	OBD-CAD-CBD	-2.58	122.05	125.94
23	B	522	CLA	O2A-CGA-CBA	2.58	120.05	111.94
23	b	2525	CLA	C2D-C1D-ND	2.58	111.36	109.41
23	B	518	CLA	C2A-C1A-NA	-2.58	108.39	111.24
23	c	2486	CLA	O2D-CGD-CBD	2.57	116.58	111.33
23	B	525	CLA	CBA-CAA-C2A	2.57	121.65	114.01
23	b	2524	CLA	CMB-C2B-C3B	2.57	129.02	124.97
23	B	511	CLA	OBD-CAD-CBD	-2.57	122.06	125.94
23	C	487	CLA	O2A-CGA-CBA	2.57	120.02	111.94
23	C	475	CLA	C2A-C1A-NA	-2.57	108.40	111.24
23	A	349	CLA	C1D-C2D-C3D	-2.57	104.68	106.78
23	b	2514	CLA	C3A-C2A-C1A	2.56	104.71	101.08
23	C	487	CLA	C2A-C3A-C4A	2.57	105.35	101.40
23	C	482	CLA	CMB-C2B-C1B	-2.56	124.68	128.62
23	b	2515	CLA	CMB-C2B-C3B	2.56	129.01	124.97
23	b	2522	CLA	C2A-C1A-CHA	2.56	128.27	123.83
23	C	480	CLA	C2D-C1D-ND	2.56	111.35	109.41
23	C	475	CLA	CMB-C2B-C1B	-2.56	124.69	128.62
23	C	477	CLA	C2A-C3A-C4A	2.55	105.33	101.40
23	b	2523	CLA	C1D-C2D-C3D	-2.55	104.69	106.78
23	c	2485	CLA	C1-C2-C3	2.55	130.72	126.19
28	d	2360	BCR	C20-C21-C22	2.55	130.97	127.29
28	k	2050	BCR	C37-C22-C23	2.55	122.22	118.09
23	b	2525	CLA	CBA-CAA-C2A	2.55	121.58	114.01
23	c	2483	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
28	b	2527	BCR	C7-C8-C9	2.55	130.02	126.22
23	C	485	CLA	C1-C2-C3	2.54	130.71	126.19
23	C	481	CLA	CED-O2D-CGD	2.54	122.07	116.02
23	C	474	CLA	C1D-C2D-C3D	-2.54	104.70	106.78
25	E	84	HEM	C4A-C3A-C2A	-2.54	105.23	107.00
23	A	352	CLA	C2A-C1A-NA	-2.54	108.43	111.24
23	C	485	CLA	CMB-C2B-C3B	2.54	128.97	124.97
23	c	2476	CLA	C2A-C3A-C4A	2.54	105.31	101.40
23	d	2355	CLA	O2A-C1-C2	-2.54	103.05	108.55
23	b	2511	CLA	CMB-C2B-C3B	2.54	128.97	124.97
23	a	2351	CLA	C7-C6-C5	-2.54	105.53	113.01
23	b	2516	CLA	CBD-CHA-C1A	2.54	132.09	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	479	CLA	C2A-C3A-C4A	2.54	105.30	101.40
23	C	477	CLA	OBD-CAD-CBD	-2.53	122.11	125.94
23	c	2482	CLA	CMB-C2B-C1B	-2.53	124.72	128.62
26	a	2352	PL9	C30-C29-C31	2.53	119.24	115.39
23	B	527	CLA	C2A-C3A-C4A	2.53	105.30	101.40
23	A	350	CLA	CMB-C2B-C1B	-2.53	124.72	128.62
28	b	2527	BCR	C8-C9-C10	-2.53	115.08	118.97
23	b	2512	CLA	C2A-C3A-C4A	2.53	105.29	101.40
23	C	485	CLA	O2D-CGD-CBD	2.53	116.49	111.33
23	C	474	CLA	O2D-CGD-CBD	2.53	116.48	111.33
28	d	2360	BCR	C1-C6-C5	-2.53	118.94	122.60
23	d	2354	CLA	CED-O2D-CGD	2.53	122.03	116.02
23	c	2477	CLA	CMB-C2B-C1B	-2.53	124.74	128.62
23	C	482	CLA	O2D-CGD-CBD	2.53	116.48	111.33
23	A	348	CLA	C2D-C1D-ND	2.53	111.32	109.41
23	c	2486	CLA	C4D-CHA-CBD	-2.52	103.43	109.37
23	B	515	CLA	C1D-CHD-C4C	2.52	126.52	122.60
23	b	2511	CLA	C1D-C2D-C3D	-2.52	104.72	106.78
23	b	2525	CLA	C6-C5-C3	2.52	118.78	112.78
28	b	2528	BCR	C30-C25-C24	2.52	122.68	115.69
24	D	355	PHO	OBD-CAD-CBD	-2.52	122.13	125.94
23	C	487	CLA	C1-C2-C3	2.52	130.67	126.19
23	B	515	CLA	CMB-C2B-C1B	-2.52	124.74	128.62
23	c	2474	CLA	CMB-C2B-C1B	-2.52	124.75	128.62
23	c	2483	CLA	C6-C7-C8	2.52	122.39	115.14
24	a	2350	PHO	CAA-C2A-C3A	-2.52	107.09	113.04
25	V	138	HEM	C2A-C1A-NA	2.52	113.23	109.73
23	c	2480	CLA	C2A-C3A-C4A	2.52	105.27	101.40
23	B	514	CLA	C1D-C2D-C3D	-2.52	104.73	106.78
23	d	2355	CLA	CED-O2D-CGD	2.52	122.00	116.02
28	K	50	BCR	C37-C22-C23	2.51	122.16	118.09
23	B	524	CLA	C4-C3-C5	2.51	119.21	115.39
23	b	2523	CLA	CMB-C2B-C3B	2.51	128.93	124.97
23	D	356	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
23	D	356	CLA	CED-O2D-CGD	2.51	122.00	116.02
28	j	2053	BCR	C37-C22-C23	2.51	122.16	118.09
23	c	2474	CLA	C2A-C3A-C4A	2.51	105.26	101.40
24	d	2356	PHO	CBA-CAA-C2A	2.51	121.47	114.01
23	B	522	CLA	C2A-C3A-C4A	2.51	105.26	101.40
23	C	487	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
23	b	2511	CLA	CMB-C2B-C1B	-2.51	124.77	128.62
23	C	479	CLA	O2A-CGA-CBA	2.51	119.82	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	480	CLA	CMB-C2B-C1B	-2.51	124.77	128.62
23	C	483	CLA	C6-C7-C8	2.50	122.35	115.14
23	B	511	CLA	O2A-CGA-CBA	2.50	119.81	111.94
23	B	522	CLA	C6-C5-C3	2.50	118.73	112.78
23	B	520	CLA	O2D-CGD-CBD	2.50	116.42	111.33
28	b	2528	BCR	C35-C13-C12	2.50	122.13	118.09
23	c	2478	CLA	CMB-C2B-C3B	2.50	128.90	124.97
23	c	2474	CLA	CED-O2D-CGD	2.50	121.95	116.02
23	b	2526	CLA	C4D-CHA-CBD	-2.49	103.50	109.37
28	C	488	BCR	C36-C18-C19	2.49	122.12	118.09
23	B	521	CLA	C2A-C3A-C4A	2.49	105.23	101.40
23	c	2476	CLA	CED-O2D-CGD	2.49	121.95	116.02
23	b	2515	CLA	C7-C6-C5	-2.49	105.67	113.01
23	C	474	CLA	C2A-C3A-C4A	2.49	105.23	101.40
23	b	2521	CLA	CMB-C2B-C3B	2.49	128.89	124.97
23	C	482	CLA	C4D-CHA-CBD	-2.49	103.51	109.37
23	c	2487	CLA	O2A-CGA-CBA	2.49	119.76	111.94
24	D	355	PHO	C4B-C3B-C2B	-2.49	105.80	107.60
23	d	2355	CLA	CMB-C2B-C3B	2.49	128.89	124.97
23	c	2481	CLA	CMB-C2B-C1B	-2.48	124.80	128.62
23	b	2511	CLA	C1-O2A-CGA	2.48	123.94	116.98
23	C	479	CLA	C2A-C1A-CHA	2.48	128.13	123.83
23	c	2485	CLA	CMB-C2B-C1B	-2.48	124.81	128.62
23	B	517	CLA	O2D-CGD-CBD	2.48	116.38	111.33
23	B	518	CLA	C1D-C2D-C3D	-2.48	104.75	106.78
23	c	2480	CLA	C2D-C1D-ND	2.48	111.28	109.41
23	C	474	CLA	C7-C6-C5	-2.48	105.71	113.01
23	C	484	CLA	CBA-CAA-C2A	2.48	121.37	114.01
23	A	352	CLA	CED-O2D-CGD	2.48	121.91	116.02
23	b	2518	CLA	CMB-C2B-C1B	-2.48	124.81	128.62
28	c	2489	BCR	C1-C6-C5	-2.47	119.02	122.60
23	C	478	CLA	CAA-C2A-C1A	2.48	117.80	111.62
23	C	487	CLA	C2D-C1D-ND	2.47	111.28	109.41
23	c	2484	CLA	CMB-C2B-C1B	-2.47	124.82	128.62
24	D	355	PHO	C1-C2-C3	2.47	130.58	126.19
23	b	2517	CLA	O2D-CGD-CBD	2.47	116.37	111.33
28	J	53	BCR	C30-C25-C26	-2.47	119.02	122.60
23	b	2526	CLA	CMB-C2B-C3B	2.47	128.86	124.97
24	a	2350	PHO	CMB-C2B-C3B	2.47	128.86	124.97
24	d	2356	PHO	C1D-C2D-C3D	-2.47	104.77	106.89
23	A	348	CLA	C2A-C3A-C4A	2.47	105.20	101.40
26	d	2358	PL9	C8-C7-C3	2.47	119.67	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	488	BCR	C34-C9-C8	2.47	122.08	118.09
23	D	356	CLA	C1D-C2D-C3D	-2.47	104.77	106.78
28	C	489	BCR	C30-C25-C26	-2.47	119.03	122.60
23	c	2484	CLA	CBA-CAA-C2A	2.46	121.33	114.01
24	D	355	PHO	CBA-CAA-C2A	2.47	121.33	114.01
24	d	2356	PHO	OBD-CAD-CBD	-2.47	122.22	125.94
28	C	489	BCR	C1-C6-C5	-2.46	119.03	122.60
23	b	2522	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
23	B	527	CLA	C4D-CHA-CBD	-2.46	103.57	109.37
23	b	2521	CLA	O2A-CGA-CBA	2.46	119.66	111.94
23	C	481	CLA	CMB-C2B-C1B	-2.45	124.85	128.62
24	A	351	PHO	O2A-CGA-CBA	2.45	119.66	111.94
23	c	2477	CLA	C2A-C3A-C4A	2.45	105.17	101.40
23	B	512	CLA	C2A-C3A-C4A	2.45	105.17	101.40
23	c	2484	CLA	C2A-C3A-C4A	2.45	105.17	101.40
23	b	2512	CLA	C6-C7-C8	2.45	122.20	115.14
23	b	2515	CLA	C4D-CHA-CBD	-2.45	103.60	109.37
23	c	2481	CLA	O2A-C1-C2	2.45	113.86	108.55
23	C	481	CLA	O2A-C1-C2	2.45	113.86	108.55
23	b	2517	CLA	CBA-CAA-C2A	2.45	121.28	114.01
23	B	518	CLA	C2D-C1D-ND	2.45	111.26	109.41
23	D	354	CLA	CBA-CAA-C2A	2.45	121.28	114.01
23	B	523	CLA	C1D-C2D-C3D	-2.44	104.78	106.78
23	B	525	CLA	OBD-CAD-CBD	-2.44	122.25	125.94
24	a	2350	PHO	O2A-CGA-CBA	2.44	119.63	111.94
23	c	2479	CLA	C2A-C1A-CHA	2.44	128.06	123.83
23	C	480	CLA	C2A-C3A-C4A	2.44	105.16	101.40
23	b	2518	CLA	C1D-C2D-C3D	-2.44	104.79	106.78
23	b	2518	CLA	C2A-C1A-NA	-2.44	108.55	111.24
26	D	357	PL9	C22-C21-C19	-2.44	104.66	112.74
23	C	485	CLA	O2A-CGA-CBA	2.44	119.61	111.94
23	C	478	CLA	CMB-C2B-C3B	2.44	128.81	124.97
23	b	2514	CLA	CAA-CBA-CGA	-2.44	105.41	113.27
28	K	50	BCR	C23-C24-C25	2.43	134.51	127.32
23	a	2349	CLA	CAA-C2A-C3A	-2.43	107.28	113.04
23	A	348	CLA	O2D-CGD-CBD	2.43	116.29	111.33
23	c	2475	CLA	C6-C7-C8	2.43	122.14	115.14
23	c	2478	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
23	B	519	CLA	CHB-C4A-NA	2.43	127.46	124.58
23	d	2355	CLA	C4D-CHA-CBD	-2.43	103.65	109.37
23	B	520	CLA	O2A-C1-C2	2.43	113.81	108.55
26	D	357	PL9	C7-C8-C9	2.43	130.86	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2487	CLA	C1-C2-C3	2.43	130.50	126.19
23	c	2482	CLA	C16-C15-C13	2.43	122.14	115.14
23	d	2357	CLA	C6-C5-C3	2.43	118.56	112.78
24	D	355	PHO	C1D-C2D-C3D	-2.43	104.81	106.89
28	B	529	BCR	C24-C23-C22	2.43	129.84	126.22
23	A	350	CLA	CAA-C2A-C3A	-2.43	107.31	113.04
23	b	2522	CLA	C2A-C3A-C4A	2.42	105.13	101.40
28	c	2488	BCR	C11-C10-C9	2.43	130.79	127.29
23	c	2477	CLA	CMB-C2B-C3B	2.42	128.78	124.97
23	B	513	CLA	O2D-CGD-CBD	2.42	116.27	111.33
23	B	511	CLA	C1D-C2D-C3D	-2.42	104.80	106.78
23	C	474	CLA	CAA-C2A-C3A	-2.42	107.31	113.04
23	c	2479	CLA	CHB-C4A-NA	2.42	127.45	124.58
25	e	2084	HEM	C2A-C1A-CHA	-2.42	121.42	126.00
28	b	2528	BCR	C34-C9-C8	2.42	122.00	118.09
23	a	2348	CLA	C7-C6-C5	-2.42	105.89	113.01
23	B	512	CLA	C6-C7-C8	2.42	122.10	115.14
23	c	2482	CLA	C6-C5-C3	2.41	118.52	112.78
23	C	487	CLA	C1-O2A-CGA	2.42	123.74	116.98
23	b	2517	CLA	C3A-C2A-C1A	2.41	104.50	101.08
23	a	2349	CLA	C2D-C1D-ND	2.41	111.23	109.41
23	c	2478	CLA	CAA-C2A-C1A	2.41	117.65	111.62
23	c	2476	CLA	C6-C7-C8	2.41	122.08	115.14
23	C	480	CLA	C7-C6-C5	-2.41	105.90	113.01
23	b	2513	CLA	O2D-CGD-CBD	2.41	116.25	111.33
23	a	2351	CLA	C1-O2A-CGA	2.41	123.74	116.98
23	C	477	CLA	CMB-C2B-C3B	2.41	128.76	124.97
26	D	357	PL9	C25-C24-C26	-2.41	111.73	115.39
26	d	2358	PL9	C7-C8-C9	2.41	130.82	126.76
23	C	483	CLA	CAA-CBA-CGA	-2.41	105.50	113.27
23	c	2475	CLA	OBD-CAD-CBD	-2.41	122.31	125.94
23	B	511	CLA	CHB-C4A-NA	2.40	127.42	124.58
23	c	2480	CLA	C7-C6-C5	-2.40	105.93	113.01
23	B	514	CLA	C3A-C2A-C1A	2.40	104.47	101.08
23	B	517	CLA	CMB-C2B-C3B	2.40	128.75	124.97
26	A	353	PL9	C15-C14-C16	-2.40	111.74	115.39
26	d	2358	PL9	C25-C24-C26	-2.40	111.74	115.39
23	b	2522	CLA	C6-C5-C3	2.40	118.48	112.78
23	B	511	CLA	C16-C15-C13	2.40	122.04	115.14
24	D	355	PHO	O2D-CGD-CBD	2.39	116.20	111.33
23	a	2348	CLA	C1D-C2D-C3D	-2.39	104.83	106.78
23	c	2487	CLA	C6-C7-C8	2.39	122.01	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	2527	BCR	C37-C22-C23	2.39	121.95	118.09
23	b	2522	CLA	C4D-CHA-CBD	-2.38	103.75	109.37
23	d	2355	CLA	C1D-C2D-C3D	-2.39	104.83	106.78
25	V	138	HEM	O2D-CGD-O1D	2.38	129.36	123.30
23	C	479	CLA	C16-C15-C13	2.38	122.00	115.14
23	C	482	CLA	C16-C15-C13	2.38	122.00	115.14
23	C	476	CLA	C6-C5-C3	2.38	118.44	112.78
23	B	513	CLA	OBD-CAD-C3D	2.38	132.34	127.91
25	V	138	HEM	CHC-C4B-NB	2.38	126.56	124.58
23	b	2524	CLA	C4-C3-C5	2.38	119.01	115.39
28	j	2053	BCR	C16-C17-C18	2.38	130.72	127.29
23	B	527	CLA	CMB-C2B-C3B	2.38	128.71	124.97
23	C	487	CLA	C2A-C1A-CHA	2.37	127.94	123.83
28	k	2050	BCR	C23-C24-C25	2.37	134.33	127.32
28	F	48	BCR	C20-C21-C22	2.38	130.72	127.29
23	b	2513	CLA	CMB-C2B-C1B	-2.38	124.97	128.62
23	C	476	CLA	CED-O2D-CGD	2.37	121.67	116.02
23	c	2474	CLA	C6-C7-C8	2.37	121.97	115.14
23	c	2475	CLA	C2A-C1A-NA	-2.37	108.62	111.24
28	b	2528	BCR	C35-C13-C14	-2.37	119.55	122.92
23	c	2487	CLA	C1-O2A-CGA	2.37	123.62	116.98
23	B	522	CLA	CAA-C2A-C3A	-2.37	107.44	113.04
23	c	2485	CLA	C12-C11-C10	-2.37	100.86	113.02
28	c	2488	BCR	C15-C16-C17	-2.37	118.11	123.36
23	D	354	CLA	CMB-C2B-C1B	-2.37	124.98	128.62
23	B	521	CLA	O2A-CGA-CBA	2.37	119.39	111.94
28	b	2528	BCR	C3-C4-C5	2.37	117.33	113.74
23	B	515	CLA	CMB-C2B-C3B	2.37	128.70	124.97
23	C	481	CLA	C1D-C2D-C3D	-2.36	104.85	106.78
23	c	2479	CLA	CAA-C2A-C3A	-2.37	107.45	113.04
23	b	2519	CLA	C2A-C3A-C4A	2.36	105.04	101.40
23	c	2484	CLA	CAA-C2A-C3A	-2.36	107.45	113.04
23	b	2519	CLA	CMB-C2B-C1B	-2.36	124.99	128.62
28	B	528	BCR	C12-C13-C14	-2.36	115.34	118.97
23	C	486	CLA	CBA-CAA-C2A	2.36	121.02	114.01
28	c	2488	BCR	C34-C9-C8	2.36	121.91	118.09
23	B	513	CLA	CMB-C2B-C1B	-2.36	124.99	128.62
28	j	2053	BCR	C35-C13-C12	2.36	121.91	118.09
23	c	2487	CLA	C2A-C1A-CHA	2.36	127.91	123.83
23	C	481	CLA	C4D-CHA-CBD	-2.36	103.82	109.37
23	b	2523	CLA	C2A-C3A-C4A	2.35	105.02	101.40
23	c	2484	CLA	C16-C15-C13	2.35	121.92	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2486	CLA	CBA-CAA-C2A	2.35	121.00	114.01
23	A	350	CLA	O2D-CGD-CBD	2.35	116.13	111.33
23	c	2483	CLA	C7-C6-C5	-2.35	106.08	113.01
23	C	474	CLA	C11-C12-C13	2.35	121.92	115.14
23	c	2482	CLA	C4D-CHA-CBD	-2.35	103.83	109.37
23	a	2351	CLA	C2A-C1A-NA	-2.35	108.64	111.24
23	b	2516	CLA	CMB-C2B-C1B	-2.35	125.01	128.62
28	B	529	BCR	C35-C13-C14	-2.35	119.59	122.92
23	A	349	CLA	C4D-CHA-CBD	-2.34	103.86	109.37
23	c	2487	CLA	CAA-C2A-C3A	-2.34	107.51	113.04
23	B	515	CLA	C4D-CHA-CBD	-2.34	103.86	109.37
23	C	478	CLA	C4D-CHA-CBD	-2.34	103.86	109.37
23	C	475	CLA	C6-C7-C8	2.34	121.87	115.14
23	c	2483	CLA	CAA-CBA-CGA	-2.34	105.73	113.27
23	C	485	CLA	CMB-C2B-C1B	-2.33	125.03	128.62
23	c	2485	CLA	CMB-C2B-C3B	2.33	128.65	124.97
23	d	2354	CLA	O2D-CGD-CBD	2.33	116.08	111.33
23	B	519	CLA	O2D-CGD-CBD	2.33	116.08	111.33
25	v	2138	HEM	C4A-C3A-C2A	-2.33	105.38	107.00
23	c	2485	CLA	CAA-C2A-C1A	-2.33	105.81	111.62
23	C	485	CLA	C12-C11-C10	-2.33	101.07	113.02
23	c	2479	CLA	C16-C15-C13	2.33	121.85	115.14
23	C	474	CLA	CMB-C2B-C1B	-2.33	125.04	128.62
26	D	357	PL9	C8-C7-C3	2.33	119.20	111.47
28	B	529	BCR	C30-C25-C24	2.33	122.14	115.69
28	B	529	BCR	C34-C9-C8	2.32	121.85	118.09
23	b	2517	CLA	CMB-C2B-C3B	2.32	128.63	124.97
23	c	2485	CLA	C2D-C1D-ND	2.32	111.17	109.41
23	C	476	CLA	O2D-CGD-CBD	2.32	116.06	111.33
23	a	2348	CLA	CED-O2D-CGD	2.32	121.54	116.02
23	C	487	CLA	CHB-C1B-NB	2.32	128.45	124.58
23	c	2478	CLA	C4D-CHA-CBD	-2.32	103.91	109.37
23	D	356	CLA	O2D-CGD-CBD	2.32	116.06	111.33
23	d	2354	CLA	CMB-C2B-C1B	-2.32	125.06	128.62
26	d	2358	PL9	C15-C14-C16	-2.32	111.86	115.39
23	C	485	CLA	C1D-C2D-C3D	-2.32	104.89	106.78
23	B	518	CLA	C4D-CHA-CBD	-2.32	103.91	109.37
28	C	489	BCR	C28-C27-C26	2.32	117.25	113.74
23	B	517	CLA	C2A-C3A-C4A	2.31	104.96	101.40
23	b	2526	CLA	C1-C2-C3	2.31	130.30	126.19
28	B	529	BCR	C3-C4-C5	2.31	117.25	113.74
23	c	2474	CLA	C11-C12-C13	2.31	121.80	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	351	PHO	C4A-NA-C1A	2.31	111.46	108.42
23	c	2486	CLA	C1D-C2D-C3D	-2.31	104.89	106.78
23	b	2525	CLA	C6-C7-C8	2.31	121.80	115.14
23	c	2476	CLA	O2D-CGD-CBD	2.31	116.04	111.33
23	c	2487	CLA	CHB-C1B-NB	2.31	128.44	124.58
23	C	479	CLA	C3A-C2A-C1A	2.31	104.35	101.08
23	c	2475	CLA	C2A-C3A-C4A	2.31	104.95	101.40
23	b	2518	CLA	CMB-C2B-C3B	2.31	128.60	124.97
23	B	514	CLA	CAA-CBA-CGA	-2.31	105.83	113.27
23	D	354	CLA	CED-O2D-CGD	2.31	121.50	116.02
28	J	53	BCR	C28-C27-C26	2.30	117.23	113.74
25	v	2138	HEM	C4B-CHC-C1C	-2.30	120.50	126.57
28	C	488	BCR	C15-C16-C17	-2.30	118.27	123.36
23	b	2512	CLA	O2A-CGA-CBA	2.30	119.18	111.94
23	C	485	CLA	C6-C5-C3	2.30	118.25	112.78
23	c	2474	CLA	CAA-C2A-C3A	-2.30	107.60	113.04
23	b	2522	CLA	CAA-C2A-C3A	-2.30	107.60	113.04
23	c	2485	CLA	C11-C12-C13	2.30	121.76	115.14
23	b	2515	CLA	C16-C15-C13	2.30	121.76	115.14
28	j	2053	BCR	C30-C25-C26	-2.30	119.27	122.60
23	b	2518	CLA	C4D-CHA-CBD	-2.30	103.96	109.37
23	c	2487	CLA	C6-C5-C3	2.30	118.24	112.78
23	C	486	CLA	C1D-C2D-C3D	-2.30	104.91	106.78
23	C	476	CLA	CMB-C2B-C1B	-2.30	125.09	128.62
23	B	517	CLA	C3A-C2A-C1A	2.29	104.33	101.08
23	c	2485	CLA	C1D-C2D-C3D	-2.30	104.91	106.78
23	b	2512	CLA	C1D-C2D-C3D	-2.29	104.91	106.78
23	C	485	CLA	OBD-CAD-C3D	2.29	132.18	127.91
23	b	2511	CLA	O2A-CGA-CBA	2.29	119.15	111.94
28	b	2528	BCR	C20-C19-C18	-2.29	119.85	126.38
23	b	2511	CLA	C16-C15-C13	2.29	121.73	115.14
28	F	48	BCR	C8-C7-C6	2.29	134.08	127.32
23	B	518	CLA	CMB-C2B-C1B	-2.29	125.10	128.62
28	d	2360	BCR	C15-C16-C17	-2.29	118.29	123.36
27	d	2359	LMT	O1'-C1'-C2'	2.29	111.09	108.18
23	A	352	CLA	C1-O2A-CGA	2.29	123.39	116.98
28	b	2528	BCR	C7-C8-C9	2.29	129.63	126.22
23	B	513	CLA	C6-C7-C8	2.29	121.72	115.14
28	B	528	BCR	C16-C17-C18	2.29	130.59	127.29
23	C	478	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
23	b	2516	CLA	O1A-CGA-CBA	-2.28	114.36	123.78
23	c	2481	CLA	C4D-CHA-CBD	-2.28	104.00	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	352	CLA	C2A-C1A-CHA	2.28	127.78	123.83
23	C	475	CLA	CMB-C2B-C3B	2.28	128.56	124.97
23	C	474	CLA	OBD-CAD-C3D	2.28	132.15	127.91
28	j	2053	BCR	C30-C25-C24	2.28	122.00	115.69
23	C	487	CLA	C6-C7-C8	2.28	121.70	115.14
23	b	2520	CLA	C4D-CHA-CBD	-2.28	104.01	109.37
23	A	352	CLA	C11-C12-C13	2.28	121.70	115.14
28	c	2488	BCR	C28-C27-C26	2.28	117.19	113.74
28	c	2489	BCR	C30-C25-C26	-2.27	119.31	122.60
23	A	350	CLA	OBD-CAD-C3D	2.27	132.14	127.91
23	B	511	CLA	C1-O2A-CGA	2.27	123.35	116.98
25	e	2084	HEM	CHA-C4D-ND	2.27	127.43	124.31
23	C	486	CLA	C6-C7-C8	2.27	121.67	115.14
23	c	2484	CLA	C1-O2A-CGA	2.27	123.33	116.98
26	A	353	PL9	C7-C3-C4	2.27	119.35	117.10
23	D	354	CLA	C16-C15-C13	2.26	121.66	115.14
23	C	480	CLA	CMB-C2B-C3B	2.26	128.53	124.97
23	B	522	CLA	C4D-CHA-CBD	-2.26	104.04	109.37
23	B	515	CLA	CHB-C4A-NA	2.26	127.26	124.58
25	E	84	HEM	O1A-CGA-CBA	-2.26	115.24	123.03
23	b	2515	CLA	OBD-CAD-CBD	-2.26	122.52	125.94
23	C	475	CLA	C2A-C1A-CHA	2.26	127.75	123.83
23	c	2482	CLA	C1D-C2D-C3D	-2.26	104.94	106.78
28	B	528	BCR	C7-C8-C9	2.26	129.60	126.22
23	C	484	CLA	C16-C15-C13	2.26	121.65	115.14
23	b	2513	CLA	C6-C7-C8	2.26	121.65	115.14
28	J	53	BCR	C30-C25-C24	2.26	121.95	115.69
23	c	2476	CLA	CMB-C2B-C1B	-2.26	125.15	128.62
28	F	48	BCR	C36-C18-C19	2.26	121.74	118.09
23	B	516	CLA	O1A-CGA-CBA	-2.26	114.47	123.78
23	b	2511	CLA	CHB-C4A-NA	2.25	127.25	124.58
23	C	475	CLA	C1D-C2D-C3D	-2.25	104.94	106.78
23	A	348	CLA	C2A-C1A-NA	-2.25	108.75	111.24
28	c	2489	BCR	C21-C20-C19	2.25	130.84	123.24
23	B	519	CLA	C2A-C3A-C4A	2.25	104.86	101.40
28	j	2053	BCR	C1-C6-C5	-2.25	119.34	122.60
23	C	485	CLA	C11-C12-C13	2.25	121.62	115.14
24	D	355	PHO	C2A-C1A-NA	-2.25	108.46	111.93
28	c	2488	BCR	C32-C1-C6	2.25	114.06	110.33
23	B	517	CLA	CBA-CAA-C2A	2.25	120.69	114.01
25	V	138	HEM	C3A-C4A-CHB	-2.25	121.73	126.00
23	c	2475	CLA	C4D-CHA-CBD	-2.25	104.07	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2478	CLA	O2D-CGD-CBD	2.25	115.91	111.33
23	a	2348	CLA	CMB-C2B-C1B	-2.25	125.16	128.62
23	a	2351	CLA	C1D-C2D-C3D	-2.25	104.94	106.78
23	c	2474	CLA	C1D-C2D-C3D	-2.25	104.95	106.78
23	B	515	CLA	O2D-CGD-CBD	2.24	115.90	111.33
23	B	518	CLA	C2A-C3A-C4A	2.24	104.85	101.40
28	K	50	BCR	C34-C9-C8	2.24	121.72	118.09
28	c	2488	BCR	C36-C18-C19	2.24	121.72	118.09
23	b	2511	CLA	C2A-C3A-C4A	2.24	104.85	101.40
23	c	2484	CLA	C6-C5-C3	2.24	118.10	112.78
23	B	511	CLA	C3A-C2A-C1A	2.24	104.25	101.08
23	C	475	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
28	C	489	BCR	C34-C9-C8	2.24	121.71	118.09
23	c	2484	CLA	C4D-CHA-CBD	-2.24	104.10	109.37
26	A	353	PL9	C36-C37-C38	2.24	118.01	111.62
23	B	520	CLA	CGD-CBD-CHA	2.23	118.56	110.96
23	B	523	CLA	CMB-C2B-C3B	2.23	128.49	124.97
23	C	487	CLA	C6-C5-C3	2.24	118.10	112.78
23	B	519	CLA	C11-C12-C13	2.23	121.57	115.14
23	B	512	CLA	O2A-CGA-CBA	2.23	118.97	111.94
23	B	512	CLA	CED-O2D-CGD	2.23	121.33	116.02
28	c	2489	BCR	C28-C27-C26	2.23	117.12	113.74
28	b	2528	BCR	C23-C24-C25	2.23	133.91	127.32
23	B	523	CLA	C4D-CHA-CBD	-2.23	104.12	109.37
23	B	523	CLA	C7-C6-C5	-2.23	106.43	113.01
26	D	357	PL9	C15-C14-C16	-2.23	112.00	115.39
23	c	2479	CLA	C1-C2-C3	2.23	130.15	126.19
23	B	524	CLA	OBD-CAD-C3D	2.23	132.06	127.91
23	b	2525	CLA	OBD-CAD-C3D	2.23	132.06	127.91
23	b	2520	CLA	O2A-C1-C2	2.23	113.38	108.55
24	a	2350	PHO	O2D-CGD-CBD	2.23	115.86	111.33
23	C	476	CLA	CBA-CAA-C2A	2.23	120.62	114.01
23	B	527	CLA	C1D-C2D-C3D	-2.23	104.96	106.78
23	a	2351	CLA	C11-C12-C13	2.22	121.54	115.14
28	J	53	BCR	C37-C22-C23	2.22	121.69	118.09
28	b	2527	BCR	C16-C17-C18	2.22	130.49	127.29
23	b	2515	CLA	CHB-C4A-NA	2.22	127.20	124.58
28	J	53	BCR	C1-C6-C5	-2.22	119.39	122.60
23	c	2479	CLA	C4D-CHA-CBD	-2.22	104.15	109.37
23	b	2518	CLA	C2D-C1D-ND	2.22	111.08	109.41
23	B	520	CLA	C4D-CHA-CBD	-2.21	104.16	109.37
23	B	513	CLA	C4D-CHA-CBD	-2.21	104.16	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	48	BCR	C15-C16-C17	-2.21	118.46	123.36
28	d	2360	BCR	C8-C7-C6	2.21	133.86	127.32
23	c	2487	CLA	C7-C6-C5	-2.21	106.49	113.01
23	b	2523	CLA	C7-C6-C5	-2.21	106.49	113.01
23	B	517	CLA	C1D-C2D-C3D	-2.21	104.97	106.78
23	C	483	CLA	CMB-C2B-C1B	-2.21	125.22	128.62
23	b	2525	CLA	O2D-CGD-CBD	2.21	115.84	111.33
23	B	514	CLA	C2A-C1A-CHA	2.21	127.66	123.83
23	d	2355	CLA	C4-C3-C5	2.21	118.75	115.39
23	D	356	CLA	O2A-CGA-CBA	2.21	118.88	111.94
25	v	2138	HEM	O1D-CGD-CBD	-2.21	115.44	123.03
23	A	350	CLA	CMA-C3A-C2A	-2.21	104.66	114.14
23	c	2480	CLA	CMB-C2B-C1B	-2.20	125.23	128.62
23	b	2511	CLA	C3A-C2A-C1A	2.20	104.20	101.08
24	A	351	PHO	O2D-CGD-CBD	2.21	115.82	111.33
23	b	2513	CLA	OBD-CAD-C3D	2.20	132.01	127.91
23	A	348	CLA	C1D-C2D-C3D	-2.20	104.98	106.78
28	d	2360	BCR	C36-C18-C19	2.21	121.66	118.09
26	a	2352	PL9	C36-C37-C38	2.20	117.91	111.62
23	b	2522	CLA	CBA-CAA-C2A	2.20	120.55	114.01
28	C	488	BCR	C28-C27-C26	2.20	117.08	113.74
23	b	2512	CLA	C4D-CHA-CBD	-2.20	104.18	109.37
23	C	487	CLA	C1D-C2D-C3D	-2.20	104.98	106.78
23	b	2524	CLA	O2D-CGD-CBD	2.20	115.82	111.33
23	C	484	CLA	CMB-C2B-C1B	-2.20	125.24	128.62
24	A	351	PHO	C4D-CHA-CBD	-2.20	104.19	107.53
23	D	356	CLA	C6-C5-C3	2.20	118.00	112.78
23	d	2357	CLA	O2A-CGA-CBA	2.20	118.85	111.94
23	b	2521	CLA	C2A-C3A-C4A	2.20	104.78	101.40
23	C	482	CLA	C1D-C2D-C3D	-2.20	104.99	106.78
23	B	524	CLA	O2D-CGD-CBD	2.20	115.81	111.33
23	b	2517	CLA	C2A-C3A-C4A	2.20	104.78	101.40
28	C	489	BCR	C8-C7-C6	2.20	133.80	127.32
23	c	2475	CLA	C2A-C1A-CHA	2.20	127.64	123.83
28	c	2488	BCR	C23-C22-C21	-2.20	115.60	118.97
23	B	525	CLA	C6-C7-C8	2.19	121.46	115.14
23	C	476	CLA	C1D-C2D-C3D	-2.19	104.99	106.78
23	c	2475	CLA	CMB-C2B-C1B	-2.19	125.25	128.62
23	B	521	CLA	CMB-C2B-C3B	2.19	128.42	124.97
23	C	475	CLA	C2A-C3A-C4A	2.19	104.77	101.40
23	C	478	CLA	C1-O2A-CGA	2.19	123.12	116.98
23	D	356	CLA	CMB-C2B-C1B	-2.19	125.25	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	529	BCR	C7-C8-C9	2.19	129.49	126.22
28	c	2489	BCR	C11-C10-C9	2.19	130.45	127.29
23	b	2520	CLA	CMB-C2B-C1B	-2.19	125.25	128.62
24	a	2350	PHO	C4D-CHA-CBD	-2.19	104.20	107.53
23	a	2351	CLA	C2A-C1A-CHA	2.19	127.62	123.83
23	d	2357	CLA	CED-O2D-CGD	2.19	121.22	116.02
28	B	529	BCR	C20-C19-C18	-2.19	120.14	126.38
23	C	476	CLA	CMB-C2B-C3B	2.19	128.41	124.97
23	B	512	CLA	C4D-CHA-CBD	-2.19	104.22	109.37
23	C	484	CLA	C6-C5-C3	2.19	117.98	112.78
23	B	511	CLA	C2A-C3A-C4A	2.18	104.76	101.40
23	C	487	CLA	CAA-C2A-C3A	-2.18	107.88	113.04
23	B	515	CLA	C16-C15-C13	2.18	121.43	115.14
23	C	479	CLA	CMB-C2B-C1B	-2.18	125.26	128.62
23	a	2349	CLA	C11-C12-C13	2.18	121.43	115.14
23	C	477	CLA	O2D-CGD-CBD	2.18	115.78	111.33
28	b	2527	BCR	C34-C9-C8	2.18	121.62	118.09
23	B	517	CLA	C4D-CHA-CBD	-2.18	104.23	109.37
23	b	2523	CLA	C6-C5-C3	2.18	117.96	112.78
23	B	514	CLA	CHB-C4A-NA	2.18	127.16	124.58
23	c	2479	CLA	C3A-C2A-C1A	2.18	104.17	101.08
23	b	2514	CLA	C2A-C1A-CHA	2.18	127.61	123.83
23	A	349	CLA	OBD-CAD-C3D	2.18	131.97	127.91
23	C	483	CLA	CAA-C2A-C3A	-2.18	107.89	113.04
23	A	348	CLA	O2A-CGA-CBA	2.18	118.80	111.94
23	b	2513	CLA	C4D-CHA-CBD	-2.18	104.24	109.37
28	J	53	BCR	C16-C17-C18	2.18	130.43	127.29
28	b	2527	BCR	C35-C13-C12	2.18	121.61	118.09
28	j	2053	BCR	C15-C14-C13	2.18	130.43	127.29
23	c	2485	CLA	C4D-CHA-CBD	-2.18	104.24	109.37
23	C	485	CLA	CHB-C4A-NA	2.17	127.15	124.58
23	C	483	CLA	C1D-C2D-C3D	-2.17	105.00	106.78
28	c	2489	BCR	C34-C9-C8	2.17	121.61	118.09
23	b	2519	CLA	O2D-CGD-CBD	2.17	115.76	111.33
28	B	529	BCR	C23-C24-C25	2.17	133.73	127.32
23	d	2355	CLA	C16-C15-C13	2.17	121.39	115.14
23	b	2514	CLA	CHB-C4A-NA	2.17	127.14	124.58
23	C	483	CLA	C7-C6-C5	-2.17	106.62	113.01
28	c	2488	BCR	C30-C25-C26	-2.17	119.46	122.60
23	b	2516	CLA	CED-O2D-CGD	2.17	121.17	116.02
23	d	2354	CLA	C16-C15-C13	2.17	121.38	115.14
23	C	475	CLA	C4D-CHA-CBD	-2.17	104.27	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	489	BCR	C21-C20-C19	2.16	130.54	123.24
23	D	356	CLA	C4D-CHA-CBD	-2.16	104.28	109.37
26	A	353	PL9	C7-C3-C2	-2.16	121.68	123.77
23	b	2516	CLA	OBD-CAD-C3D	2.16	131.93	127.91
23	b	2524	CLA	C1D-C2D-C3D	-2.16	105.02	106.78
26	a	2352	PL9	C37-C38-C39	-2.16	123.39	128.63
23	c	2476	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
23	b	2517	CLA	C4D-CHA-CBD	-2.16	104.29	109.37
23	B	522	CLA	CBA-CAA-C2A	2.16	120.41	114.01
23	c	2478	CLA	C1D-C2D-C3D	-2.15	105.02	106.78
23	a	2348	CLA	O2A-CGA-CBA	2.16	118.72	111.94
23	C	483	CLA	O2D-CGD-CBD	2.16	115.72	111.33
23	c	2476	CLA	CMB-C2B-C3B	2.15	128.36	124.97
25	E	84	HEM	CHD-C4C-NC	-2.16	122.86	124.73
23	C	481	CLA	CMB-C2B-C3B	2.15	128.36	124.97
28	d	2360	BCR	C28-C27-C26	2.15	117.01	113.74
23	B	519	CLA	CMB-C2B-C1B	-2.15	125.31	128.62
23	A	352	CLA	C4D-CHA-CBD	-2.15	104.30	109.37
23	C	487	CLA	C4D-CHA-CBD	-2.15	104.30	109.37
23	B	516	CLA	CMB-C2B-C1B	-2.15	125.31	128.62
23	B	524	CLA	C4D-CHA-CBD	-2.15	104.31	109.37
23	C	476	CLA	C2A-C1A-NA	-2.15	108.87	111.24
23	B	518	CLA	CMB-C2B-C3B	2.15	128.35	124.97
23	B	520	CLA	C1D-C2D-C3D	-2.15	105.03	106.78
23	A	349	CLA	O2A-C1-C2	-2.15	103.90	108.55
23	b	2519	CLA	C11-C12-C13	2.15	121.32	115.14
28	k	2050	BCR	C3-C4-C5	2.15	116.99	113.74
23	b	2514	CLA	C6-C7-C8	2.14	121.31	115.14
23	B	514	CLA	C6-C7-C8	2.14	121.31	115.14
23	b	2511	CLA	C4D-CHA-CBD	-2.14	104.33	109.37
23	A	349	CLA	C16-C15-C13	2.14	121.31	115.14
28	B	528	BCR	C37-C22-C23	2.14	121.56	118.09
23	a	2349	CLA	CMA-C3A-C2A	-2.14	104.95	114.14
23	A	349	CLA	C2A-C1A-NA	-2.14	108.88	111.24
23	D	354	CLA	C4D-CHA-CBD	-2.14	104.34	109.37
23	c	2480	CLA	C4D-CHA-CBD	-2.14	104.34	109.37
23	b	2521	CLA	OBD-CAD-C3D	2.14	131.88	127.91
23	c	2486	CLA	C6-C7-C8	2.13	121.28	115.14
23	b	2513	CLA	CMB-C2B-C3B	2.13	128.33	124.97
23	b	2523	CLA	C4D-CHA-CBD	-2.13	104.36	109.37
26	a	2352	PL9	C7-C3-C4	2.13	119.21	117.10
23	C	485	CLA	C5-C3-C2	-2.13	116.99	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2487	CLA	C1D-C2D-C3D	-2.13	105.04	106.78
23	B	516	CLA	O2A-CGA-O1A	-2.13	117.63	123.43
27	d	2359	LMT	C3-C2-C1	-2.12	103.29	113.58
23	c	2477	CLA	O2D-CGD-CBD	2.12	115.66	111.33
23	b	2516	CLA	C1D-C2D-C3D	-2.12	105.05	106.78
23	C	478	CLA	C3A-C2A-C1A	2.12	104.08	101.08
23	c	2480	CLA	O2D-CGD-CBD	2.12	115.65	111.33
23	C	482	CLA	CMB-C2B-C3B	2.12	128.31	124.97
23	C	479	CLA	CHB-C4A-NA	2.12	127.09	124.58
23	C	481	CLA	OBD-CAD-C3D	2.12	131.85	127.91
24	d	2356	PHO	C2A-C1A-NA	-2.12	108.66	111.93
23	c	2487	CLA	CHD-C4C-C3C	2.12	128.22	124.98
23	b	2524	CLA	C4D-CHA-CBD	-2.12	104.39	109.37
23	A	348	CLA	CMB-C2B-C1B	-2.12	125.37	128.62
23	B	520	CLA	CMB-C2B-C1B	-2.11	125.37	128.62
23	b	2518	CLA	C2A-C3A-C4A	2.11	104.65	101.40
23	A	349	CLA	CMB-C2B-C3B	2.11	128.30	124.97
23	C	480	CLA	C4D-CHA-CBD	-2.11	104.39	109.37
23	b	2524	CLA	OBD-CAD-C3D	2.11	131.84	127.91
23	c	2475	CLA	CMB-C2B-C3B	2.11	128.30	124.97
23	C	478	CLA	C1D-C2D-C3D	-2.11	105.06	106.78
23	C	485	CLA	CAA-C2A-C1A	-2.11	106.36	111.62
24	a	2350	PHO	C4A-NA-C1A	2.10	111.19	108.42
23	b	2517	CLA	C1D-C2D-C3D	-2.10	105.06	106.78
23	C	484	CLA	C1-O2A-CGA	2.11	122.88	116.98
28	b	2527	BCR	C28-C27-C26	2.10	116.93	113.74
23	c	2485	CLA	OBD-CAD-C3D	2.10	131.82	127.91
23	c	2476	CLA	C6-C5-C3	2.10	117.78	112.78
26	d	2358	PL9	C7-C3-C2	-2.10	121.74	123.77
23	d	2357	CLA	CMB-C2B-C1B	-2.10	125.39	128.62
23	B	513	CLA	CMB-C2B-C3B	2.10	128.28	124.97
23	C	479	CLA	C4D-CHA-CBD	-2.10	104.42	109.37
23	A	348	CLA	C2A-C1A-CHA	2.10	127.47	123.83
28	J	53	BCR	C20-C21-C22	2.10	130.32	127.29
23	c	2481	CLA	CMB-C2B-C3B	2.10	128.27	124.97
28	b	2527	BCR	C12-C13-C14	-2.09	115.75	118.97
23	c	2483	CLA	O2D-CGD-CBD	2.09	115.60	111.33
28	C	488	BCR	C11-C10-C9	2.09	130.31	127.29
23	d	2357	CLA	C7-C6-C5	-2.09	106.84	113.01
23	C	487	CLA	CHD-C4C-C3C	2.09	128.18	124.98
23	c	2483	CLA	CMB-C2B-C1B	-2.09	125.40	128.62
23	B	521	CLA	C1D-C2D-C3D	-2.09	105.07	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	515	CLA	O2A-CGA-CBA	2.09	118.52	111.94
23	C	484	CLA	C4D-CHA-CBD	-2.09	104.45	109.37
23	c	2485	CLA	C5-C3-C2	-2.09	117.06	121.08
23	c	2476	CLA	C4D-CHA-CBD	-2.09	104.46	109.37
28	J	53	BCR	C35-C13-C12	2.09	121.47	118.09
23	c	2487	CLA	C4D-CHA-CBD	-2.09	104.46	109.37
23	a	2351	CLA	CMB-C2B-C3B	2.09	128.26	124.97
23	c	2485	CLA	CHB-C4A-NA	2.09	127.05	124.58
23	C	484	CLA	C7-C6-C5	-2.08	106.87	113.01
23	b	2525	CLA	CAA-C2A-C3A	-2.09	108.11	113.04
23	c	2483	CLA	C16-C15-C13	2.08	121.14	115.14
23	a	2348	CLA	C4D-CHA-CBD	-2.08	104.47	109.37
25	v	2138	HEM	CAA-C2A-C1A	-2.08	119.21	125.50
23	b	2520	CLA	C6-C7-C8	2.08	121.14	115.14
24	d	2356	PHO	C3D-C4D-ND	2.08	110.44	106.97
23	B	518	CLA	C2A-C1A-CHA	2.08	127.44	123.83
28	C	488	BCR	C30-C25-C26	-2.08	119.59	122.60
23	a	2351	CLA	O2A-CGA-CBA	2.08	118.49	111.94
23	B	517	CLA	C7-C6-C5	-2.08	106.88	113.01
23	c	2481	CLA	C11-C12-C13	2.08	121.13	115.14
23	c	2476	CLA	CBA-CAA-C2A	2.08	120.18	114.01
23	B	516	CLA	O2D-CGD-CBD	2.08	115.56	111.33
23	c	2487	CLA	C2D-C1D-ND	2.08	110.98	109.41
28	K	50	BCR	C19-C18-C17	-2.08	115.78	118.97
23	B	511	CLA	C4D-CHA-CBD	-2.08	104.48	109.37
28	B	528	BCR	C3-C4-C5	2.08	116.89	113.74
23	D	356	CLA	C7-C6-C5	-2.07	106.90	113.01
23	c	2483	CLA	C4D-CHA-CBD	-2.07	104.49	109.37
26	a	2352	PL9	C21-C19-C18	-2.07	117.09	121.08
24	a	2350	PHO	C2A-C1A-NA	-2.07	108.73	111.93
28	C	488	BCR	C37-C22-C23	2.07	121.44	118.09
25	v	2138	HEM	O2D-CGD-O1D	2.07	128.57	123.30
28	B	529	BCR	C16-C17-C18	2.07	130.28	127.29
23	c	2478	CLA	C1-O2A-CGA	2.07	122.77	116.98
23	C	477	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
28	C	488	BCR	C1-C6-C7	2.07	121.42	115.69
23	d	2354	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
23	C	479	CLA	CMB-C2B-C3B	2.07	128.23	124.97
23	D	356	CLA	CMB-C2B-C3B	2.07	128.22	124.97
28	j	2053	BCR	C36-C18-C19	2.07	121.43	118.09
23	A	352	CLA	O2D-CGD-CBD	2.06	115.54	111.33
23	B	513	CLA	C1D-C2D-C3D	-2.06	105.10	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	2488	BCR	C1-C6-C7	2.06	121.41	115.69
23	b	2519	CLA	C3A-C2A-C1A	2.06	104.00	101.08
23	B	519	CLA	C2A-C1A-CHA	2.06	127.40	123.83
25	e	2084	HEM	CHB-C4A-NA	-2.06	121.14	124.58
23	B	512	CLA	C1D-C2D-C3D	-2.06	105.10	106.78
23	A	352	CLA	CAA-CBA-CGA	2.06	119.91	113.27
26	A	353	PL9	C21-C19-C18	-2.06	117.12	121.08
23	C	479	CLA	C1-C2-C3	2.06	129.84	126.19
24	a	2350	PHO	OBD-CAD-C3D	2.06	131.88	127.96
23	c	2474	CLA	C6-C5-C3	2.06	117.67	112.78
24	d	2356	PHO	C2A-C3A-C4A	2.06	105.75	101.11
28	c	2489	BCR	C1-C6-C7	2.05	121.38	115.69
23	B	514	CLA	C2A-C3A-C4A	2.05	104.56	101.40
23	a	2351	CLA	O2D-CGD-CBD	2.05	115.52	111.33
27	B	526	LMT	C3-C2-C1	-2.05	103.63	113.58
23	d	2357	CLA	C4D-CHA-CBD	-2.05	104.54	109.37
23	C	475	CLA	C16-C15-C13	2.05	121.05	115.14
23	a	2349	CLA	CMB-C2B-C1B	-2.05	125.47	128.62
23	a	2349	CLA	OBD-CAD-C3D	2.05	131.73	127.91
28	J	53	BCR	C36-C18-C19	2.05	121.41	118.09
23	B	523	CLA	C6-C5-C3	2.05	117.65	112.78
23	C	476	CLA	C4D-CHA-CBD	-2.05	104.55	109.37
23	b	2524	CLA	C2A-C1A-CHA	2.05	127.38	123.83
25	E	84	HEM	C3A-C4A-CHB	-2.05	122.12	126.00
25	e	2084	HEM	O1A-CGA-CBA	-2.05	115.99	123.03
26	D	357	PL9	C7-C3-C2	-2.04	121.80	123.77
23	c	2484	CLA	C7-C6-C5	-2.04	106.99	113.01
23	A	349	CLA	O2D-CGD-CBD	2.04	115.50	111.33
23	C	483	CLA	C4D-CHA-CBD	-2.04	104.56	109.37
23	c	2479	CLA	CMB-C2B-C1B	-2.04	125.48	128.62
28	k	2050	BCR	C19-C18-C17	-2.04	115.83	118.97
23	A	348	CLA	C4D-CHA-CBD	-2.04	104.56	109.37
23	B	524	CLA	C1D-C2D-C3D	-2.04	105.11	106.78
28	K	50	BCR	C1-C6-C5	-2.04	119.65	122.60
23	C	487	CLA	C11-C12-C13	2.04	121.01	115.14
23	C	480	CLA	O2D-CGD-CBD	2.04	115.49	111.33
23	a	2351	CLA	CAA-C2A-C1A	2.04	116.71	111.62
23	a	2348	CLA	C1C-NC-C4C	2.04	108.95	106.36
23	c	2477	CLA	OBD-CAD-C3D	2.04	131.70	127.91
23	B	513	CLA	CHB-C4A-NA	2.04	126.99	124.58
27	d	2359	LMT	O6B-C6B-C5B	2.04	118.37	111.36
28	F	48	BCR	C40-C30-C25	2.04	113.70	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	j	2053	BCR	C34-C9-C8	2.04	121.38	118.09
23	c	2487	CLA	O2A-C1-C2	-2.03	104.14	108.55
23	B	525	CLA	CMB-C2B-C3B	2.03	128.17	124.97
28	k	2050	BCR	C1-C6-C7	2.03	121.33	115.69
23	b	2516	CLA	O2A-CGA-O1A	-2.03	117.88	123.43
23	B	525	CLA	O2D-CGD-CBD	2.03	115.47	111.33
23	B	521	CLA	CBA-CAA-C2A	2.03	120.05	114.01
28	J	53	BCR	C11-C10-C9	2.03	130.22	127.29
23	c	2478	CLA	C3A-C2A-C1A	2.03	103.95	101.08
26	A	353	PL9	C37-C38-C39	-2.03	123.71	128.63
28	c	2488	BCR	C37-C22-C23	2.03	121.38	118.09
23	c	2478	CLA	C7-C6-C5	-2.03	107.03	113.01
23	B	514	CLA	C4D-CHA-CBD	-2.03	104.59	109.37
28	K	50	BCR	C1-C6-C7	2.03	121.31	115.69
23	c	2486	CLA	O1D-CGD-CBD	-2.03	120.27	124.42
23	B	511	CLA	C11-C12-C13	2.03	120.98	115.14
23	b	2519	CLA	CHB-C4A-NA	2.03	126.98	124.58
23	C	482	CLA	CAA-CBA-CGA	2.03	119.80	113.27
23	C	480	CLA	C6-C5-C3	2.03	117.60	112.78
23	b	2518	CLA	CHB-C4A-NA	2.03	126.98	124.58
25	E	84	HEM	CMD-C2D-C3D	2.03	130.19	125.60
24	A	351	PHO	CMB-C2B-C3B	2.03	128.16	124.97
23	b	2522	CLA	C7-C6-C5	-2.02	107.05	113.01
23	C	474	CLA	C4D-CHA-CBD	-2.02	104.60	109.37
23	b	2521	CLA	CAA-CBA-CGA	-2.02	106.75	113.27
23	B	516	CLA	C1C-NC-C4C	2.02	108.93	106.36
23	A	350	CLA	C1-O2A-CGA	2.02	122.64	116.98
23	c	2480	CLA	CMB-C2B-C3B	2.02	128.15	124.97
23	b	2511	CLA	O2D-CGD-CBD	2.02	115.45	111.33
28	C	489	BCR	C11-C10-C9	2.02	130.21	127.29
23	C	486	CLA	CMB-C2B-C1B	-2.02	125.51	128.62
23	c	2480	CLA	CAA-C2A-C3A	-2.02	108.26	113.04
23	c	2475	CLA	C1D-C2D-C3D	-2.02	105.13	106.78
23	C	475	CLA	C6-C5-C3	2.02	117.58	112.78
23	C	484	CLA	C1D-C2D-C3D	-2.02	105.13	106.78
23	c	2483	CLA	CAA-C2A-C3A	-2.02	108.27	113.04
23	A	350	CLA	C11-C12-C13	2.02	120.95	115.14
28	k	2050	BCR	C16-C17-C18	2.02	130.20	127.29
23	a	2349	CLA	O2D-CGD-CBD	2.02	115.44	111.33
23	B	522	CLA	C7-C6-C5	-2.02	107.07	113.01
23	a	2348	CLA	C2A-C1A-NA	-2.01	109.02	111.24
23	B	523	CLA	C6-C7-C8	2.01	120.94	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2477	CLA	C4D-CHA-CBD	-2.01	104.63	109.37
24	D	355	PHO	C2A-C3A-C4A	2.01	105.65	101.11
23	b	2521	CLA	C4D-CHA-CBD	-2.01	104.63	109.37
27	B	526	LMT	C1'-O5'-C5'	2.01	117.64	113.73
23	c	2479	CLA	OBD-CAD-C3D	2.01	131.65	127.91
23	B	521	CLA	OBD-CAD-C3D	2.01	131.65	127.91
24	A	351	PHO	C4B-C3B-C2B	-2.01	106.14	107.60
23	b	2519	CLA	CMB-C2B-C3B	2.01	128.13	124.97
28	B	528	BCR	C34-C9-C8	2.01	121.34	118.09
23	b	2514	CLA	O2D-CGD-CBD	2.01	115.42	111.33
23	B	522	CLA	C1-O2A-CGA	2.01	122.61	116.98
23	b	2513	CLA	C1-O2A-CGA	2.01	122.61	116.98
23	c	2485	CLA	C2A-C1A-NA	-2.01	109.02	111.24
28	b	2528	BCR	C16-C17-C18	2.01	130.19	127.29
23	c	2482	CLA	O2D-CGD-CBD	2.01	115.42	111.33
23	c	2482	CLA	CAA-CBA-CGA	2.00	119.73	113.27
24	a	2350	PHO	C3D-C4D-ND	2.01	110.31	106.97
23	c	2485	CLA	C6-C5-C3	2.01	117.55	112.78
28	C	488	BCR	C23-C22-C21	-2.00	115.89	118.97
23	C	485	CLA	C4D-CHA-CBD	-2.00	104.66	109.37
25	V	138	HEM	C1B-NB-C4B	2.00	107.21	105.16
23	b	2515	CLA	O2D-CGD-CBD	2.00	115.41	111.33
23	C	479	CLA	OBD-CAD-C3D	2.00	131.63	127.91
23	b	2524	CLA	C2A-C1A-NA	-2.00	109.03	111.24

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	a	2350	PHO	C2A
24	a	2350	PHO	C13
24	a	2350	PHO	C8
24	D	355	PHO	C2A
24	D	355	PHO	C13
24	D	355	PHO	C8
24	d	2356	PHO	C2A
24	d	2356	PHO	C13
24	d	2356	PHO	C8
24	A	351	PHO	C2A
24	A	351	PHO	C13
24	A	351	PHO	C8

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/344 (96%)	0.16	6 (1%) 65 33	33, 60, 91, 104	0
1	a	333/344 (96%)	0.08	2 (0%) 86 59	39, 63, 92, 105	0
2	B	476/510 (93%)	0.02	7 (1%) 70 36	39, 65, 89, 105	0
2	b	476/510 (93%)	0.13	11 (2%) 57 27	39, 65, 89, 106	0
3	C	421/473 (89%)	-0.00	5 (1%) 75 42	34, 69, 89, 103	0
3	c	421/473 (89%)	-0.03	2 (0%) 88 64	36, 71, 90, 107	0
4	D	339/352 (96%)	0.07	4 (1%) 75 42	22, 60, 92, 106	0
4	d	339/352 (96%)	0.05	6 (1%) 65 33	31, 62, 92, 106	0
5	E	76/84 (90%)	-0.07	2 (2%) 53 24	55, 76, 94, 107	0
5	e	76/84 (90%)	-0.12	1 (1%) 74 40	60, 79, 96, 107	0
6	F	33/45 (73%)	-0.18	0 100 100	49, 68, 92, 107	0
6	f	33/45 (73%)	0.06	2 (6%) 21 9	49, 70, 92, 101	0
7	H	53/66 (80%)	-0.08	1 (1%) 64 32	46, 73, 104, 106	0
7	h	53/66 (80%)	-0.16	1 (1%) 64 32	56, 74, 106, 109	0
8	I	38/38 (100%)	-0.04	2 (5%) 25 10	60, 76, 100, 102	0
8	i	38/38 (100%)	-0.28	0 100 100	59, 76, 100, 104	0
9	J	38/40 (95%)	-0.00	0 100 100	60, 79, 99, 103	0
9	j	38/40 (95%)	0.25	1 (2%) 53 24	61, 82, 98, 107	0
10	K	37/37 (100%)	-0.23	0 100 100	61, 71, 95, 95	0
10	k	37/37 (100%)	-0.01	0 100 100	65, 73, 96, 97	0
11	L	37/37 (100%)	0.13	1 (2%) 52 24	39, 58, 101, 104	0
11	l	37/37 (100%)	0.28	1 (2%) 52 24	34, 61, 99, 101	0
12	M	30/36 (83%)	0.05	0 100 100	45, 56, 79, 88	0
12	m	30/36 (83%)	0.07	0 100 100	44, 56, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	246/246 (100%)	0.12	3 (1%) 75 42	41, 75, 100, 110	0
13	o	246/246 (100%)	0.19	1 (0%) 90 71	46, 75, 99, 107	0
14	T	31/32 (96%)	0.16	0 100 100	27, 54, 86, 89	0
14	t	31/32 (96%)	-0.06	0 100 100	32, 53, 90, 93	0
15	U	105/134 (78%)	0.18	2 (1%) 64 32	41, 67, 91, 104	0
15	u	105/134 (78%)	-0.04	2 (1%) 64 32	46, 68, 92, 103	0
16	V	137/137 (100%)	-0.12	0 100 100	42, 66, 80, 88	0
16	v	137/137 (100%)	0.17	3 (2%) 59 28	46, 70, 85, 90	0
17	X	40/50 (80%)	0.09	3 (7%) 14 7	67, 74, 102, 109	0
17	x	40/50 (80%)	0.10	0 100 100	67, 77, 104, 108	0
18	N	0/37	-	-	-	-
18	n	0/37	-	-	-	-
19	Z	58/62 (93%)	-0.33	0 100 100	62, 80, 93, 102	0
19	z	58/62 (93%)	0.20	2 (3%) 43 19	70, 81, 94, 106	0
All	All	5056/5520 (91%)	0.05	71 (1%) 72 38	22, 68, 95, 110	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	X	47	GLN	5.9
6	f	2012	TYR	5.8
16	v	2100	ILE	4.1
13	O	62	GLU	4.1
4	D	242	GLU	4.0
4	d	2222	LEU	3.7
6	f	2013	PRO	3.7
5	E	8	PRO	3.6
2	b	2006	TYR	3.5
2	B	266	GLU	3.5
1	A	263	ALA	3.5
1	a	2026	ASN	3.4
4	d	2219	GLU	3.3
1	A	243	GLU	3.3
11	L	11	GLU	3.2
1	A	262	TYR	3.1
17	X	48	ARG	3.1
4	D	241	GLU	2.9
2	b	2086	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	b	2343	HIS	2.9
1	A	242	GLU	2.8
1	A	241	GLN	2.8
5	E	9	PHE	2.7
4	d	2255	GLN	2.7
7	H	62	LYS	2.7
8	I	28	PRO	2.7
15	U	35	THR	2.7
2	B	78	TRP	2.7
4	d	2223	PHE	2.7
19	z	2037	LYS	2.6
2	b	2138	MET	2.6
3	C	456	GLU	2.6
2	B	6	TYR	2.6
3	C	203	THR	2.5
2	B	235	GLU	2.5
17	X	46	VAL	2.5
2	b	2091	TRP	2.5
2	b	2124	ARG	2.4
16	v	2105	ARG	2.4
7	h	2013	LEU	2.4
11	l	2001	MET	2.4
13	O	229	GLU	2.4
16	v	2095	LEU	2.4
15	u	2053	GLU	2.4
19	z	2003	ILE	2.3
4	D	239	GLN	2.3
3	C	47	GLY	2.3
2	b	2298	LEU	2.3
4	d	2224	GLN	2.3
15	U	38	GLU	2.2
3	c	2110	PRO	2.2
9	j	2040	LEU	2.2
1	A	264	SER	2.2
3	c	2456	GLU	2.2
4	D	240	ALA	2.2
13	O	63	ALA	2.2
3	C	391	ARG	2.2
2	b	2341	LYS	2.2
2	B	233	ASN	2.2
3	C	366	LEU	2.2
13	o	2214	THR	2.1

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Mol	Chain	Res	Type	RSRZ
5	e	2009	PHE	2.1
2	b	2344	ALA	2.1
1	a	2190	HIS	2.1
2	B	471	ALA	2.0
2	B	72	THR	2.0
15	u	2052	GLY	2.0
8	I	25	SER	2.0
4	d	2264	LYS	2.0
2	b	2471	ALA	2.0
2	b	2128	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CLA	C	487	65/65	0.78	9.89	87,101,114,118	0
28	BCR	J	53	40/40	0.45	7.24	70,88,100,100	0
28	BCR	C	488	40/40	0.58	6.34	75,83,92,95	0
28	BCR	c	2488	40/40	0.94	6.26	76,84,93,96	0
28	BCR	b	2527	40/40	0.51	5.73	64,78,84,86	0
28	BCR	B	528	40/40	0.44	5.63	63,79,85,87	0
28	BCR	K	50	40/40	0.62	5.59	79,85,96,101	0
28	BCR	C	489	40/40	0.52	5.47	85,90,100,100	0
23	CLA	b	2516	65/65	0.32	4.90	42,54,93,94	0
26	PL9	D	357	45/55	0.44	4.73	71,80,86,88	0
28	BCR	k	2050	40/40	0.71	4.59	80,85,97,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	BCR	d	2360	40/40	0.34	3.79	67,79,91,93	0
28	BCR	B	529	40/40	0.69	3.73	76,93,105,106	0
23	CLA	c	2487	65/65	0.58	3.59	88,101,114,118	0
23	CLA	b	2517	65/65	0.49	3.56	64,71,80,89	0
23	CLA	A	352	65/65	0.41	3.51	48,65,101,102	0
23	CLA	C	480	65/65	0.47	3.23	64,79,82,87	0
23	CLA	C	481	65/65	0.38	3.09	54,60,84,88	0
28	BCR	F	48	40/40	0.30	2.91	66,80,91,92	0
27	LMT	d	2359	35/35	0.38	2.90	73,82,91,92	0
26	PL9	d	2358	45/55	0.58	2.53	70,80,87,89	0
23	CLA	c	2478	65/65	0.52	2.31	55,66,87,92	0
23	CLA	C	482	65/65	0.43	2.26	71,80,97,98	0
23	CLA	B	527	65/65	0.44	2.24	84,89,106,109	0
23	CLA	C	485	65/65	0.35	2.24	64,75,91,95	0
23	CLA	b	2521	65/65	0.37	2.17	67,71,80,82	0
28	BCR	b	2528	40/40	0.50	2.15	77,92,105,106	0
23	CLA	c	2486	65/65	0.47	2.14	79,84,92,94	0
23	CLA	B	516	65/65	0.38	2.14	44,55,92,93	0
23	CLA	c	2483	65/65	0.30	2.11	68,74,100,106	0
23	CLA	b	2526	65/65	0.39	2.04	82,89,106,110	0
23	CLA	B	511	65/65	0.34	2.01	58,81,92,97	0
23	CLA	C	486	65/65	0.32	1.93	78,84,91,95	0
23	CLA	B	518	65/65	0.43	1.91	51,61,86,89	0
25	HEM	e	2084	43/43	0.34	1.90	75,79,100,108	0
24	PHO	D	355	64/64	0.33	1.86	62,69,103,111	0
23	CLA	c	2485	65/65	0.40	1.72	61,75,90,94	0
23	CLA	c	2477	65/65	0.41	1.70	73,79,98,101	0
23	CLA	a	2349	65/65	0.32	1.66	36,54,93,95	0
26	PL9	a	2352	45/55	0.44	1.63	77,85,90,91	0
23	CLA	d	2357	65/65	0.34	1.60	68,77,91,95	0
23	CLA	C	484	65/65	0.37	1.59	76,87,101,102	0
23	CLA	b	2513	65/65	0.32	1.55	45,57,102,106	0
23	CLA	b	2522	65/65	0.60	1.55	69,75,87,88	0
23	CLA	B	519	65/65	0.46	1.55	58,67,90,91	0
23	CLA	B	524	65/65	0.41	1.49	56,68,75,88	0
23	CLA	c	2479	65/65	0.43	1.49	57,76,80,84	0
23	CLA	b	2519	65/65	0.38	1.48	60,66,90,91	0
28	BCR	c	2489	40/40	0.59	1.48	85,90,100,100	0
25	HEM	V	138	43/43	0.26	1.47	44,49,56,57	0
23	CLA	D	356	65/65	0.28	1.37	69,77,90,95	0
23	CLA	c	2475	65/65	0.36	1.34	66,80,97,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	d	2355	65/65	0.31	1.33	19,32,75,86	0
23	CLA	C	476	65/65	0.27	1.33	49,62,75,78	0
23	CLA	b	2518	65/65	0.38	1.31	53,60,86,88	0
23	CLA	b	2511	65/65	0.42	1.30	58,81,92,97	0
23	CLA	d	2354	65/65	0.28	1.23	40,47,75,80	0
23	CLA	c	2481	65/65	0.32	1.17	55,60,85,89	0
23	CLA	b	2524	65/65	0.51	1.15	56,68,76,89	0
23	CLA	C	475	65/65	0.34	1.10	66,80,97,103	0
23	CLA	c	2480	65/65	0.32	1.03	65,80,82,87	0
24	PHO	d	2356	64/64	0.29	1.03	62,70,103,111	0
26	PL9	A	353	45/55	0.62	1.03	77,86,91,92	0
23	CLA	B	513	65/65	0.34	0.97	46,57,102,106	0
27	LMT	B	526	35/35	0.36	0.97	72,82,90,91	0
23	CLA	C	478	65/65	0.38	0.94	55,65,87,91	0
23	CLA	c	2476	65/65	0.26	0.93	50,64,75,78	0
23	CLA	C	477	65/65	0.29	0.89	71,79,97,100	0
23	CLA	c	2482	65/65	0.44	0.80	72,81,97,98	0
24	PHO	a	2350	64/64	0.34	0.80	56,66,81,82	0
23	CLA	B	517	65/65	0.36	0.78	65,71,79,89	0
28	BCR	j	2053	40/40	0.43	0.76	71,87,100,101	0
23	CLA	b	2514	65/65	0.33	0.70	59,67,79,82	0
23	CLA	c	2474	65/65	0.26	0.67	70,76,88,89	0
23	CLA	a	2348	65/65	0.28	0.61	44,50,65,69	0
23	CLA	B	512	65/65	0.24	0.51	37,50,63,67	0
23	CLA	b	2525	65/65	0.35	0.48	73,80,89,91	0
23	CLA	C	479	65/65	0.31	0.44	57,76,80,83	0
25	HEM	E	84	43/43	0.26	0.42	64,79,100,108	0
23	CLA	a	2351	65/65	0.23	0.38	50,66,101,102	0
23	CLA	C	483	65/65	0.26	0.35	67,73,101,106	0
23	CLA	B	514	65/65	0.29	0.32	60,67,79,82	0
23	CLA	C	474	65/65	0.20	0.31	69,76,87,89	0
23	CLA	b	2512	65/65	0.24	0.30	34,50,63,66	0
23	CLA	c	2484	65/65	0.29	0.27	77,87,101,102	0
23	CLA	B	521	65/65	0.28	0.22	67,72,80,81	0
23	CLA	D	354	65/65	0.28	0.20	42,46,76,81	0
23	CLA	A	349	65/65	0.32	0.12	19,31,76,86	0
23	CLA	B	522	65/65	0.21	0.11	71,75,87,88	0
23	CLA	A	348	65/65	0.32	0.10	44,50,65,70	0
23	CLA	A	350	65/65	0.39	0.08	36,52,92,95	0
23	CLA	B	523	65/65	0.29	0.05	60,64,94,109	0
23	CLA	B	520	65/65	0.28	0.05	63,68,79,79	0
23	CLA	b	2520	65/65	0.30	0.04	61,68,78,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	HEM	v	2138	43/43	0.22	0.04	40,50,55,57	0
21	BCT	D	353	4/4	0.21	0.03	66,66,69,69	0
24	PHO	A	351	64/64	0.26	-0.04	55,65,80,82	0
23	CLA	b	2523	65/65	0.24	-0.08	59,64,94,108	0
21	BCT	a	2346	4/4	0.33	-0.11	71,72,73,76	0
23	CLA	B	525	65/65	0.21	-0.19	72,80,89,92	0
23	CLA	B	515	65/65	0.22	-0.19	45,66,84,87	0
23	CLA	b	2515	65/65	0.22	-0.43	43,66,84,87	0
21	BCT	A	346	4/4	0.22	-0.77	70,70,71,74	0
21	BCT	d	2353	4/4	0.14	-1.39	66,68,69,69	0
22	OEC	a	2347	9/9	0.21	-1.51	68,70,74,75	0
20	FE	A	345	1/1	0.10	-1.60	58,58,58,58	0
22	OEC	A	347	9/9	0.19	-1.74	66,69,73,74	0
20	FE	a	2345	1/1	0.06	-3.06	67,67,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.