



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:37 AM GMT

PDB ID : 2AXT
Title : Crystal Structure of Photosystem II from Thermosynechococcus elongatus
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.
Deposited on : 2005-09-06
Resolution : 3.00 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>

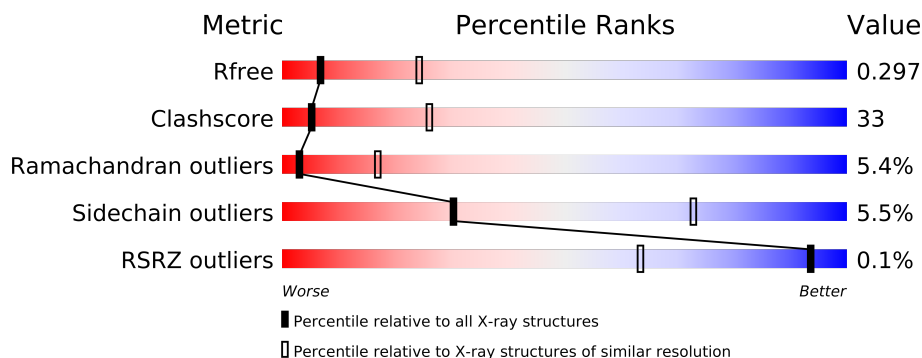
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	

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Mol	Chain	Length	Quality of chain
8	I	38	
8	i	38	
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	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	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
19	CA	K	56	-	X
21	BCT	D	353	-	X
22	UNK	C	474	-	X
22	UNK	C	478	-	X
22	UNK	C	479	-	X
22	UNK	C	481	-	X
22	UNK	C	483	-	X
22	UNK	C	486	-	X
22	UNK	C	489	-	X
22	UNK	c	5474	-	X
22	UNK	c	5475	-	X
22	UNK	c	5477	-	X
22	UNK	c	5478	-	X
22	UNK	c	5479	-	X
22	UNK	c	5484	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
22	UNK	c	5485	-	X
22	UNK	c	5486	-	X
22	UNK	c	5488	-	X
22	UNK	c	5489	-	X
22	UNK	c	5490	-	X
23	CLA	B	511	-	X
23	CLA	C	495	-	X
23	CLA	a	5560	-	X
23	CLA	a	5563	-	X
23	CLA	b	5511	-	X
23	CLA	b	5516	-	X
23	CLA	c	5503	-	X
26	PQ9	A	564	-	X
26	PQ9	a	5564	-	X
28	BCR	A	566	-	X
28	BCR	C	505	-	X
28	BCR	D	357	-	X
28	BCR	H	107	-	X
28	BCR	X	130	-	X
28	BCR	b	5529	-	X
28	BCR	c	5504	-	X
28	BCR	c	5505	-	X
28	BCR	d	5357	-	X
28	BCR	h	5107	-	X
28	BCR	x	5130	-	X
29	MGE	D	359	-	X
29	MGE	d	5359	-	X
33	LMT	A	569	-	X
33	LMT	T	217	-	X
33	LMT	a	5568	-	X
33	LMT	t	5217	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 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	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	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
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	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	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

- 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 Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	110	3	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	110	3	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

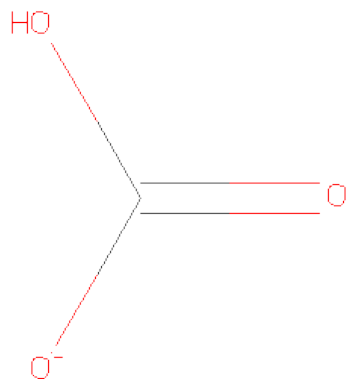
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	1	Total	Ca	0	0
			1	1		
19	k	1	Total	Ca	0	0
			1	1		

- Molecule 20 is FE (II) ION (three-letter code: FE2) (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: CHO₃).

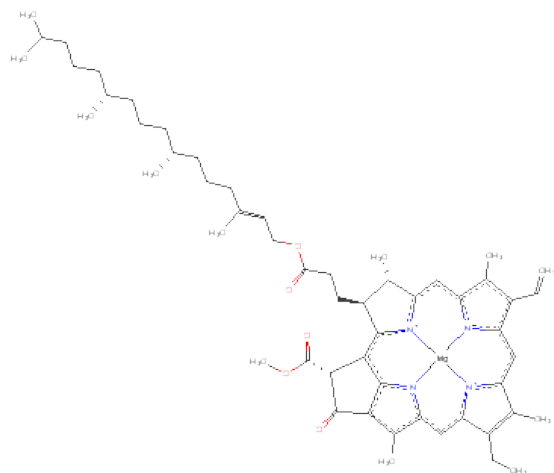


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is UNKNOWN (three-letter code: UNK) (formula: $C_4H_9NO_2$).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	C	17	Total	C	0	0
			152	152		
22	c	17	Total	C	0	0
			152	152		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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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	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			56	46	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	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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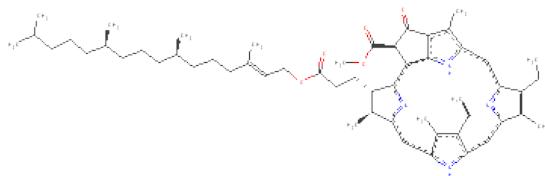
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
23	d	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
23	b	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 56	C 46	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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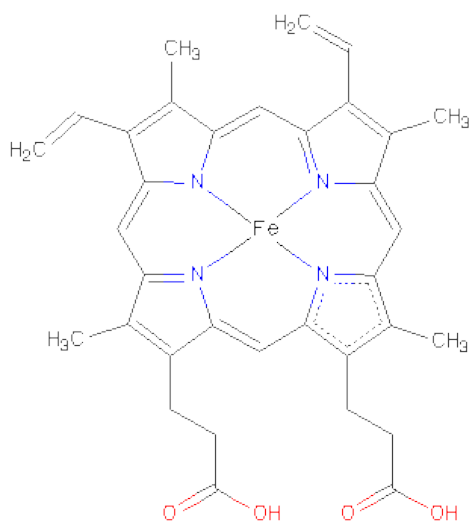
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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



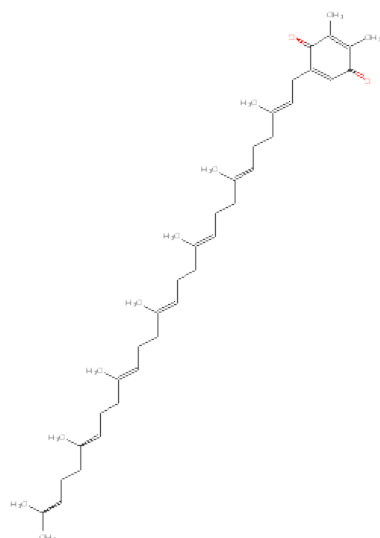
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



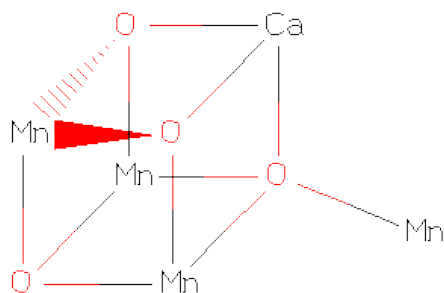
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



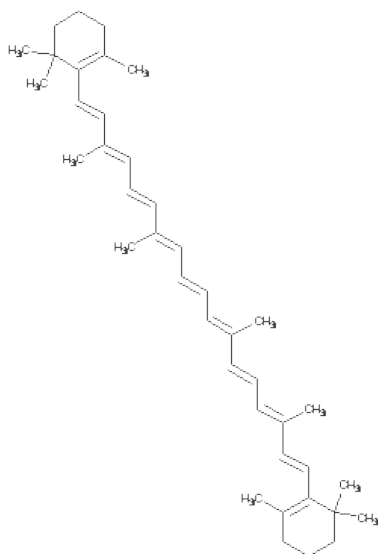
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O		
			30	28	2		
26	A	1	Total	C	O		
			30	28	2		
26	d	1	Total	C	O		
			30	28	2		
26	a	1	Total	C	O		
			30	28	2		

- Molecule 27 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn₄O₄).



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

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



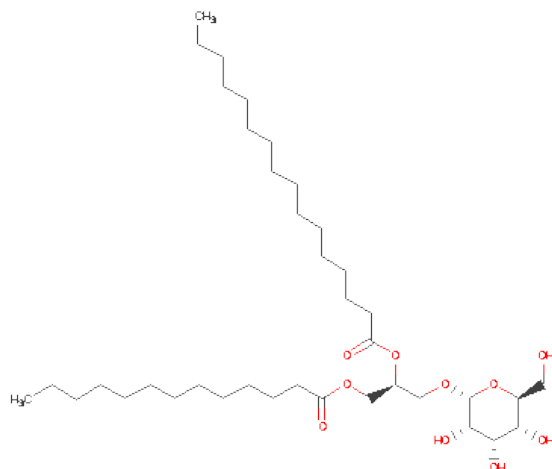
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		

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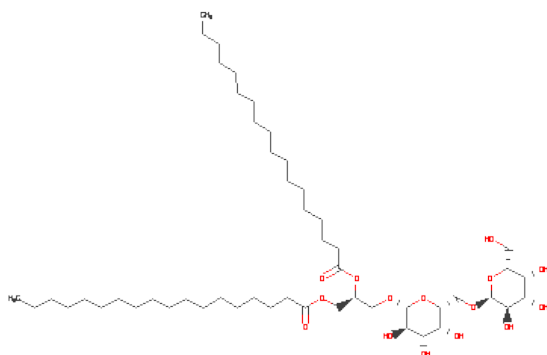
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	t	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	H	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	X	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	a	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	T	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	h	1	Total C 40 40	0	0
28	d	1	Total C 40 40	0	0
28	x	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0

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



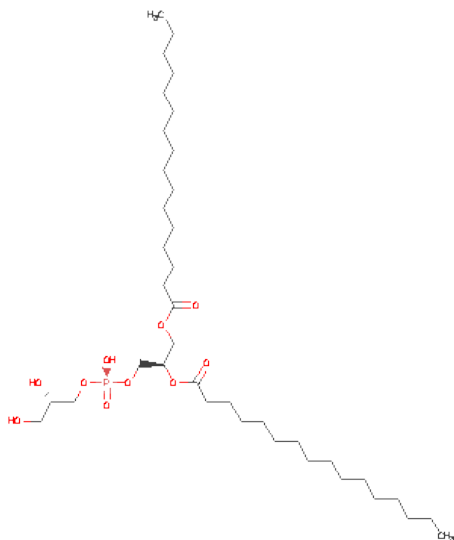
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	I	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			47	37	10		
29	D	1	Total	C	O	0	0
			41	31	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			48	38	10		
29	i	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			47	37	10		
29	d	1	Total	C	O	0	0
			41	31	10		
29	l	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



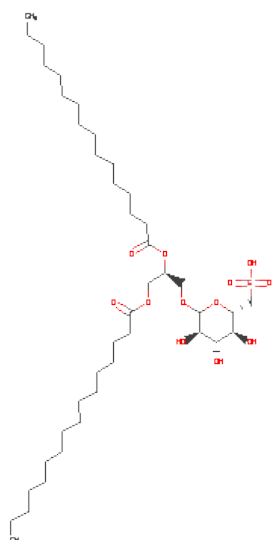
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total	C	O	0	0
			54	39	15		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			39	28	10	1		
31	a	1	Total	C	O	P	0	0
			39	28	10	1		

- Molecule 32 is 1,2-di-O-acyl-3-O-[6-deoxy-6-sulfo-alpha-D-glucopyranosyl]-sn-glycerol (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



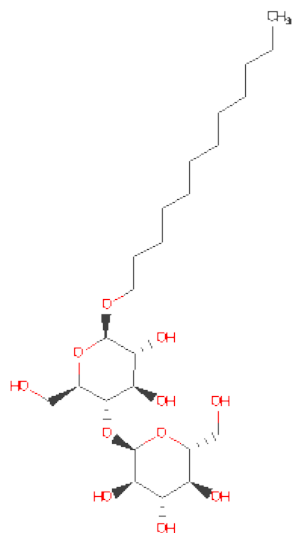
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			54	41	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	a	1	Total	C	O	S	0	0
			26	13	12	1		
32	t	1	Total	C	O	S	0	0
			47	34	12	1		
32	d	1	Total	C	O	S	0	0
			54	41	12	1		
32	A	1	Total	C	O	S	0	0
			26	13	12	1		
32	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



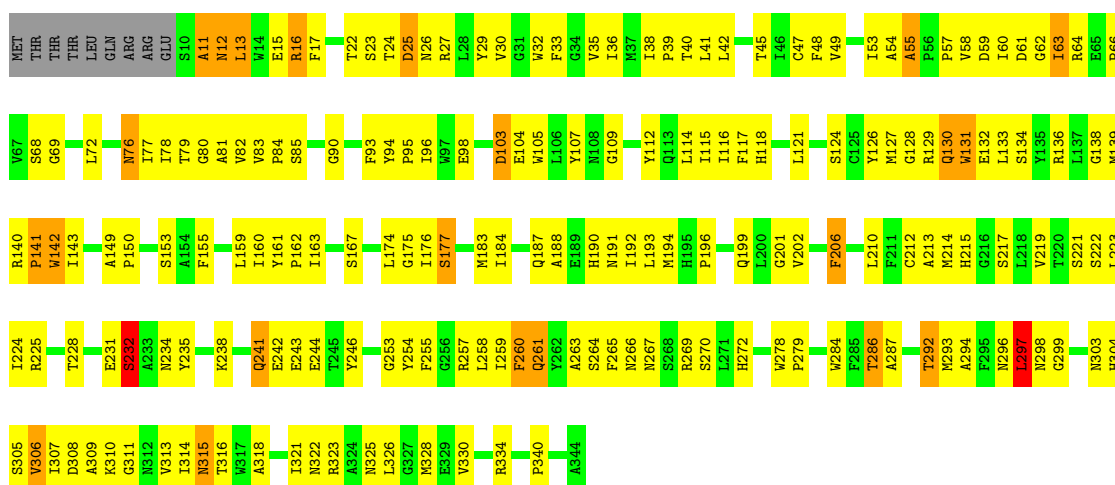
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O		0	0
			35	24	11			
33	m	1	Total	C	O		0	0
			35	24	11			
33	T	1	Total	C	O		0	0
			35	24	11			
33	a	1	Total	C	O		0	0
			35	24	11			
33	M	1	Total	C	O		0	0
			35	24	11			
33	t	1	Total	C	O		0	0
			35	24	11			

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.

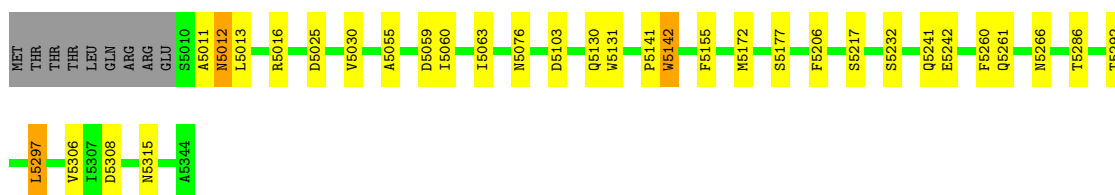
- Molecule 1: Photosystem Q(B) protein

Chain A:



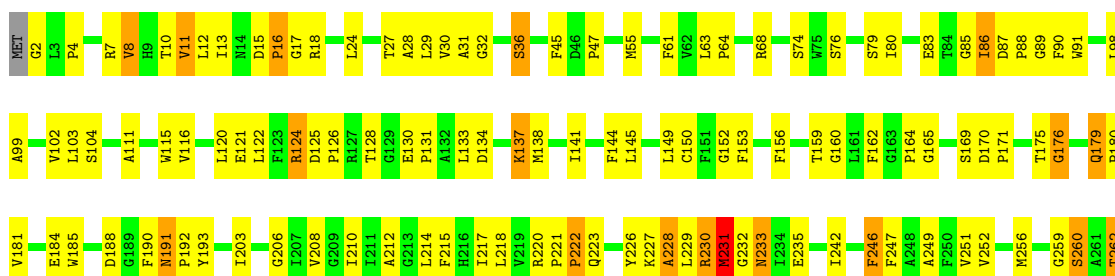
- Molecule 1: Photosystem Q(B) protein

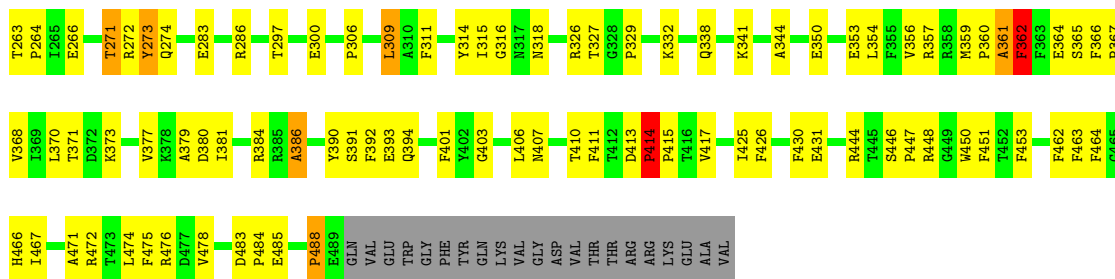
Chain a:



- Molecule 2: CP47 protein

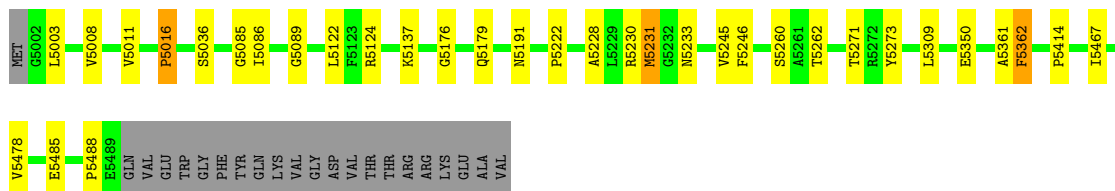
Chain B:





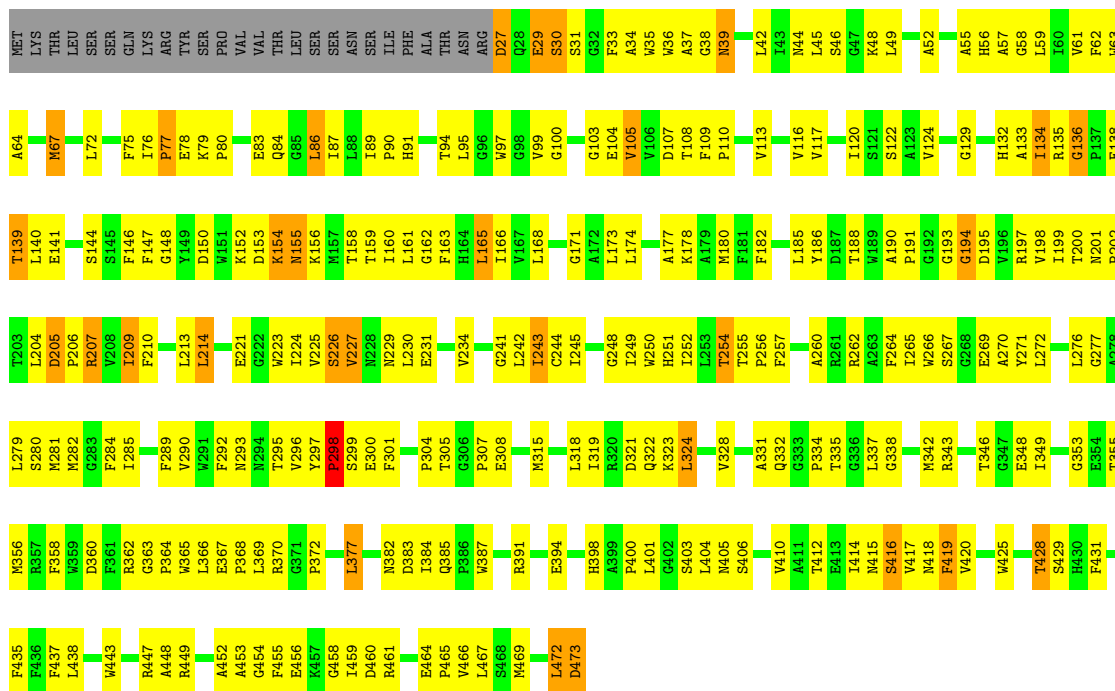
- Molecule 2: CP47 protein

Chain b:



- Molecule 3: photosystem II CP43 protein

Chain C:



- Molecule 3: photosystem II CP43 protein

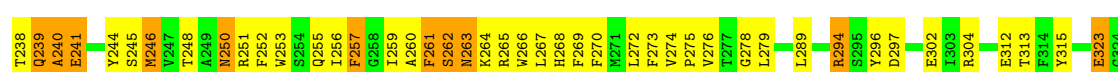
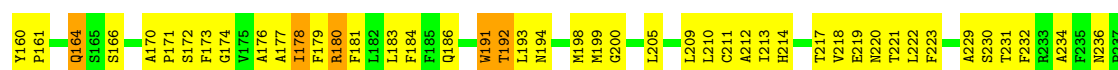
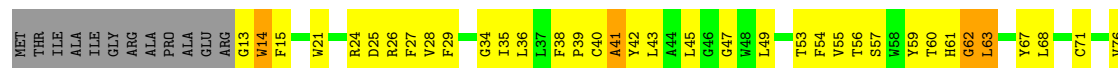
Chain c:





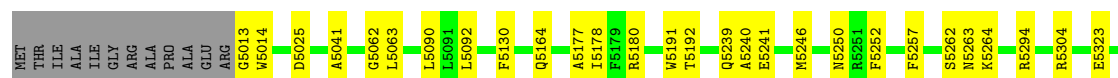
- Molecule 4: photosystem II reaction center D2 protein

Chain D:



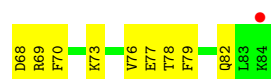
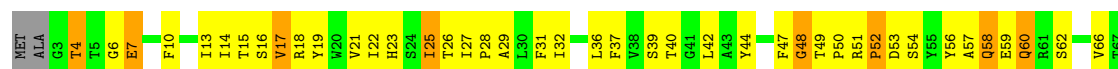
- Molecule 4: photosystem II reaction center D2 protein

Chain d:



- Molecule 5: Cytochrome b559 alpha subunit

Chain E:



- Molecule 5: Cytochrome b559 alpha subunit

Chain e:



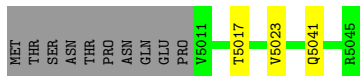
- Molecule 6: Cytochrome b559 beta subunit

Chain F:



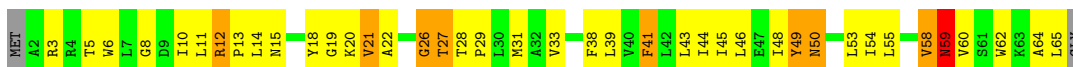
- Molecule 6: Cytochrome b559 beta subunit

Chain f:



- Molecule 7: Photosystem II reaction center H protein

Chain H:



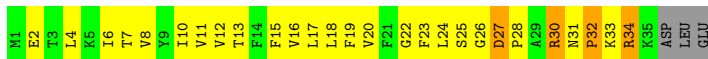
- Molecule 7: Photosystem II reaction center H protein

Chain h:



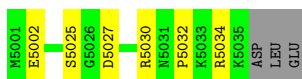
- Molecule 8: Photosystem II reaction center I protein

Chain I:



- Molecule 8: Photosystem II reaction center I protein

Chain i:



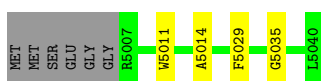
- Molecule 9: Photosystem II reaction center J protein

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:



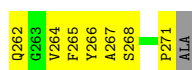
- Molecule 12: Photosystem II reaction center M protein

Chain m:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



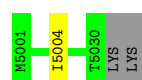
- Molecule 14: Photosystem II reaction center T protein

Chain T:



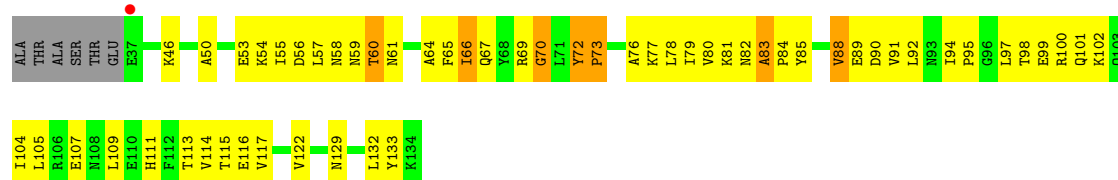
- Molecule 14: Photosystem II reaction center T protein

Chain t:



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



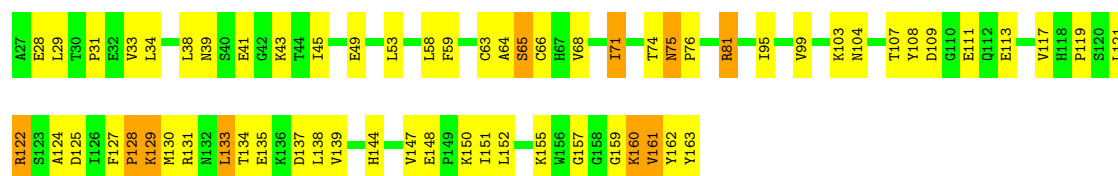
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



- Molecule 16: Cytochrome c-550

Chain V:



- Molecule 16: Cytochrome c-550

Chain v:



- Molecule 17: Unassigned subunits

Chain X: 



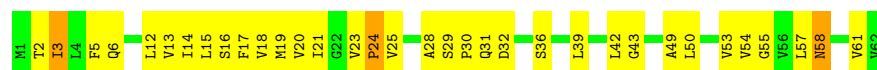
- Molecule 17: Unassigned subunits

Chain x: 



- Molecule 18: Photosystem II reaction center Z protein

Chain Z: 



- Molecule 18: 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	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.250 , 0.297	Depositor DCC
R_{free} test set	1781 reflections (1.25%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 155340 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: LHG, PHO, MGE, DGD, CA, LMT, CLA, BCT, FE2, PQ9, OEC, HEM, BCR, SQD

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	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00
13	o	5223	ILE	CB-CA-C	-5.19	101.21	111.60
2	b	5003	LEU	N-CA-C	-5.06	97.34	111.00
13	o	5271	PRO	N-CA-C	-5.03	99.02	112.10
13	O	223	ILE	CB-CA-C	-5.03	101.55	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	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	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	63	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	z	442	0	457	0	0
19	K	1	0	0	0	0
19	k	1	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	D	4	0	0	0	0
21	d	4	0	0	0	0
22	C	152	0	17	2	0
22	c	152	0	17	0	0
23	A	250	0	265	15	0
23	B	1007	0	1088	74	0
23	C	774	0	783	51	0
23	D	115	0	111	8	0
23	a	250	0	265	0	0
23	b	1007	0	1088	0	0
23	c	774	0	783	0	0
23	d	115	0	111	0	0
24	A	128	0	148	12	0
24	a	128	0	148	0	0
25	F	43	0	30	3	0
25	V	43	0	30	2	0
25	f	43	0	30	0	0
25	v	43	0	30	0	0
26	A	30	0	37	2	0
26	D	30	0	37	7	0
26	a	30	0	37	0	0
26	d	30	0	37	0	0
27	A	5	0	0	0	0
27	a	5	0	0	0	0
28	A	40	0	56	1	0
28	B	120	0	168	6	0
28	C	120	0	168	20	0
28	D	40	0	56	4	0
28	H	40	0	56	3	0
28	T	40	0	56	5	0
28	X	40	0	56	9	0
28	a	40	0	56	0	0
28	b	120	0	168	0	0
28	c	120	0	168	0	0
28	d	40	0	56	0	0
28	h	40	0	56	0	0
28	t	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	x	40	0	56	0	0
29	B	48	0	72	1	0
29	D	136	0	194	10	0
29	I	48	0	72	1	0
29	L	48	0	72	2	0
29	b	48	0	72	0	0
29	d	136	0	194	0	0
29	i	48	0	72	0	0
29	l	48	0	72	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	A	39	0	51	4	0
31	a	39	0	51	0	0
32	A	80	0	92	0	0
32	L	47	0	60	0	0
32	a	26	0	15	0	0
32	d	54	0	77	0	0
32	t	47	0	60	0	0
33	A	35	0	46	0	0
33	M	35	0	46	0	0
33	T	35	0	46	3	0
33	a	35	0	46	0	0
33	m	35	0	46	0	0
33	t	35	0	46	0	0
All	All	48254	0	47107	1544	0

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 33.

All (1544) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:X:126:UNK:NE	17:X:126:UNK:CD	1.46	1.53
17:X:126:UNK:CZ	17:X:126:UNK:NE	1.33	1.43
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:NE2	17:X:26:UNK:CD	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07
3:C:473:ASP:HB3	14:T:26:PRO:HB3	1.33	1.05
1:A:322:ASN:HD21	3:C:412:THR:HA	1.24	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.40	1.01
13:O:98:THR:HG22	13:O:99:ARG:H	1.21	1.01
2:B:329:PRO:HB3	23:B:517:CLA:HED1	1.43	1.00
16:V:38:LEU:HB2	16:V:45:ILE:HG13	1.45	0.99
2:B:68:ARG:HH22	23:B:514:CLA:HED1	1.28	0.98
2:B:263:THR:HG21	2:B:448:ARG:HH12	1.28	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.45	0.98
1:A:310:LYS:HB2	16:V:28:GLU:HB3	1.45	0.98
1:A:190:HIS:HA	1:A:298:ASN:HD22	1.26	0.97
3:C:204:LEU:HD23	3:C:204:LEU:H	1.28	0.96
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.44	0.96
2:B:149:LEU:HG	23:B:513:CLA:HBC1	1.46	0.96
13:O:45:CYS:HB2	13:O:46:PRO:HD2	1.47	0.96
13:O:179:THR:HG22	13:O:181:ASN:H	1.30	0.95
23:C:493:CLA:H191	23:C:493:CLA:HMD2	1.49	0.95
15:U:113:THR:HG22	15:U:114:VAL:N	1.84	0.93
3:C:269:GLU:HG2	3:C:448:ALA:HB2	1.50	0.93
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.49	0.92
8:I:34:ARG:NE	8:I:34:ARG:H	1.67	0.92
17:X:126:UNK:CZ	17:X:126:UNK:CD	2.47	0.92
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.52	0.92
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.52	0.91
8:I:33:LYS:HA	8:I:34:ARG:HH21	1.34	0.91
10:K:39:TRP:HE1	17:X:31:UNK:HG3	1.33	0.91
23:B:515:CLA:H141	23:B:520:CLA:HMA2	1.54	0.90
28:D:357:BCR:H403	9:J:25:VAL:HG21	1.52	0.89
17:X:86:UNK:O	17:X:87:UNK:HB2	1.73	0.89
4:D:186:GLN:HB2	23:D:354:CLA:HBC1	1.52	0.89
18:Z:36:SER:HA	18:Z:39:LEU:HD12	1.53	0.89
1:A:225:ARG:HH12	2:B:483:ASP:HA	1.35	0.89
15:U:50:ALA:CB	15:U:113:THR:HG21	2.04	0.89
8:I:34:ARG:HE	8:I:34:ARG:H	0.92	0.89
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.54	0.88
17:X:12:UNK:HG3	18:Z:17:PHE:CE1	2.10	0.87
3:C:254:THR:HG22	3:C:255:THR:H	1.40	0.87
3:C:473:ASP:HB3	14:T:26:PRO:CB	2.04	0.87
17:X:6:UNK:NE2	17:X:6:UNK:CG	2.43	0.87
23:B:518:CLA:HAB	4:D:123:ILE:HG23	1.55	0.86
10:K:28:ILE:HA	10:K:31:LEU:HD12	1.57	0.86
29:D:360:MGE:H6D2	11:L:15:THR:HG21	1.57	0.86
2:B:271:THR:H	2:B:274:GLN:HE21	1.17	0.86
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.04	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:327:THR:HG22	23:B:517:CLA:H12	1.58	0.86
13:O:145:LEU:HD23	13:O:175:PRO:HG2	1.57	0.86
16:V:159:GLY:O	16:V:161:VAL:N	2.08	0.86
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.05	0.86
13:O:145:LEU:CD2	13:O:175:PRO:HG2	2.06	0.86
17:X:26:UNK:NE2	17:X:26:UNK:CG	2.44	0.86
10:K:45:PHE:O	10:K:46:ARG:OXT	1.95	0.85
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.42	0.85
16:V:38:LEU:HD13	16:V:45:ILE:HD11	1.57	0.84
1:A:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
1:A:306:VAL:O	1:A:306:VAL:HG23	1.77	0.84
14:T:29:ILE:HD12	14:T:29:ILE:H	1.43	0.84
23:C:493:CLA:HBA1	23:C:493:CLA:HBD	1.59	0.83
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.60	0.83
18:Z:5:PHE:HA	18:Z:57:LEU:HD13	1.59	0.83
7:H:38:PHE:HB2	28:H:107:BCR:H10C	1.61	0.83
1:A:279:PRO:HB2	24:A:561:PHO:HBC1	1.58	0.83
3:C:209:ILE:HG23	28:C:506:BCR:H382	1.61	0.83
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.58	0.83
8:I:34:ARG:HE	8:I:34:ARG:N	1.76	0.83
23:B:518:CLA:H42	4:D:127:LEU:HD11	1.60	0.83
2:B:263:THR:HG22	2:B:448:ARG:HH22	1.44	0.83
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.60	0.82
3:C:293:ASN:ND2	3:C:296:VAL:HG22	1.94	0.82
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.62	0.82
17:X:126:UNK:NE	17:X:126:UNK:CG	2.47	0.82
13:O:151:LEU:HD13	13:O:223:ILE:HD11	1.59	0.82
13:O:45:CYS:H	13:O:72:GLN:NE2	1.77	0.82
3:C:406:SER:O	3:C:418:ASN:HB2	1.78	0.81
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
4:D:192:THR:HG23	23:D:354:CLA:HBC2	1.60	0.81
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.62	0.81
5:E:18:ARG:HG2	5:E:22:ILE:HD11	1.62	0.81
28:C:504:BCR:H353	28:X:130:BCR:H321	1.62	0.81
3:C:116:VAL:HG11	28:C:505:BCR:H323	1.62	0.80
6:F:21:VAL:O	6:F:25:THR:HG23	1.80	0.80
4:D:351:ALA:O	4:D:352:LEU:OXT	1.99	0.80
3:C:464:GLU:HB2	3:C:467:LEU:HD12	1.61	0.80
23:C:491:CLA:HMB3	28:C:506:BCR:H403	1.62	0.80
13:O:73:PRO:HG3	13:O:102:THR:HB	1.63	0.80
1:A:201:GLY:HA3	1:A:286:THR:HG23	1.62	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:27:PHE:HD2	4:D:28:VAL:HG23	1.45	0.80
18:Z:49:ALA:O	18:Z:53:VAL:HG23	1.82	0.79
1:A:60:ILE:HG23	1:A:61:ASP:H	1.45	0.79
1:A:41:LEU:O	1:A:45:THR:HG22	1.82	0.79
1:A:225:ARG:NH1	2:B:483:ASP:HA	1.96	0.79
4:D:161:PRO:HG2	4:D:170:ALA:HB2	1.63	0.79
3:C:27:ASP:HB2	23:C:501:CLA:HED2	1.64	0.79
13:O:56:TYR:O	13:O:161:SER:HA	1.82	0.79
3:C:365:TRP:HB3	3:C:391:ARG:HD3	1.65	0.78
15:U:58:ASN:ND2	15:U:114:VAL:HG13	1.98	0.78
1:A:190:HIS:HA	1:A:298:ASN:ND2	1.98	0.78
13:O:98:THR:HG22	13:O:99:ARG:N	1.99	0.78
15:U:94:ILE:HB	15:U:97:LEU:HD11	1.66	0.78
3:C:42:LEU:HD21	23:C:501:CLA:H2A	1.66	0.78
3:C:405:ASN:HD22	30:C:509:DGD:HD5	1.48	0.78
17:X:126:UNK:NE	17:X:126:UNK:NH2	2.31	0.78
3:C:346:THR:O	13:O:40:GLY:HA2	1.84	0.78
14:T:4:ILE:HG13	28:T:5104:BCR:H383	1.65	0.78
8:I:16:VAL:O	8:I:20:VAL:HG23	1.82	0.77
4:D:266:TRP:HD1	29:D:360:MGE:H3D	1.48	0.77
17:X:126:UNK:NH1	17:X:126:UNK:NE	2.30	0.77
17:X:12:UNK:HG3	18:Z:17:PHE:HE1	1.49	0.77
5:E:18:ARG:O	5:E:22:ILE:HG13	1.85	0.77
3:C:39:ASN:HB2	23:C:498:CLA:HBA1	1.66	0.77
3:C:186:TYR:O	3:C:230:LEU:HD11	1.84	0.77
3:C:282:MET:HA	3:C:285:ILE:HD12	1.67	0.77
2:B:116:VAL:HG21	28:B:529:BCR:H271	1.67	0.77
13:O:155:THR:HG22	13:O:167:ASP:O	1.86	0.77
1:A:142:TRP:HZ2	3:C:447:ARG:HD2	1.50	0.76
17:X:126:UNK:O	17:X:127:UNK:HB2	1.86	0.76
15:U:88:VAL:O	15:U:91:VAL:HG23	1.85	0.76
2:B:68:ARG:NH2	23:B:514:CLA:HED1	2.00	0.76
16:V:64:ALA:O	16:V:68:VAL:HG13	1.86	0.76
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.68	0.76
1:A:257:ARG:HH11	1:A:257:ARG:HG3	1.51	0.76
15:U:113:THR:CG2	15:U:114:VAL:H	1.94	0.76
2:B:263:THR:HG21	2:B:448:ARG:NH1	1.99	0.76
6:F:19:ARG:O	6:F:23:VAL:HG23	1.85	0.76
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.21	0.75
3:C:298:PRO:O	3:C:299:SER:HB3	1.85	0.75
3:C:276:LEU:HD21	23:C:498:CLA:HBB1	1.69	0.75
6:F:34:LEU:HD22	9:J:24:ILE:HD13	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:266:TRP:CD1	29:D:360:MGE:H3D	2.22	0.75
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.69	0.75
4:D:337:GLU:HG2	4:D:339:PHE:CZ	2.22	0.75
1:A:202:VAL:O	1:A:206:PHE:HB2	1.87	0.74
13:O:52:ALA:HB1	13:O:230:VAL:H	1.52	0.74
3:C:103:GLY:HA3	3:C:301:PHE:HE1	1.51	0.74
3:C:419:PHE:HA	30:C:508:DGD:HE5	1.70	0.74
2:B:150:CYS:HB2	23:B:513:CLA:HMC3	1.69	0.74
23:A:558:CLA:HBB1	23:D:354:CLA:NB	2.02	0.74
3:C:204:LEU:O	3:C:205:ASP:HB3	1.85	0.74
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	0.73
3:C:449:ARG:HH22	8:I:27:ASP:HB3	1.51	0.73
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.70	0.73
15:U:50:ALA:HB3	15:U:113:THR:HG21	1.70	0.73
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.53	0.73
1:A:309:ALA:HB3	16:V:28:GLU:HG3	1.68	0.73
2:B:27:THR:O	23:B:515:CLA:HBC1	1.89	0.73
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.19	0.72
13:O:144:LEU:HD23	13:O:144:LEU:H	1.54	0.72
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.71	0.72
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.71	0.72
3:C:204:LEU:CD2	3:C:204:LEU:H	2.02	0.72
24:A:562:PHO:HBC1	4:D:275:PRO:HB2	1.71	0.72
5:E:17:VAL:O	5:E:21:VAL:HG23	1.89	0.72
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	0.72
23:B:518:CLA:HMD1	23:B:520:CLA:HAB	1.70	0.72
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.54	0.72
3:C:337:LEU:HD23	13:O:131:PRO:HG3	1.71	0.72
3:C:464:GLU:CB	3:C:467:LEU:HD12	2.20	0.72
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.20	0.72
3:C:29:GLU:HB3	10:K:46:ARG:O	1.89	0.72
28:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	0.72
3:C:334:PRO:HA	13:O:179:THR:HB	1.72	0.71
3:C:293:ASN:ND2	3:C:296:VAL:H	1.87	0.71
15:U:66:ILE:HG12	15:U:72:TYR:CG	2.25	0.71
2:B:271:THR:HG23	2:B:273:TYR:H	1.56	0.71
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.25	0.71
1:A:224:ILE:HG22	2:B:484:PRO:HG3	1.71	0.71
10:K:17:ILE:HD11	18:Z:6:GLN:HE21	1.56	0.71
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.26	0.71
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.55	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.25	0.71
4:D:36:LEU:O	4:D:39:PRO:HD2	1.89	0.70
2:B:263:THR:CG2	2:B:448:ARG:HH12	2.02	0.70
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.19	0.70
1:A:306:VAL:HG21	1:A:316:THR:HG23	1.74	0.70
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.26	0.70
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.56	0.69
12:M:25:LEU:O	12:M:28:GLN:HG3	1.92	0.69
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.07	0.69
24:A:562:PHO:H42	4:D:41:ALA:HB1	1.74	0.69
2:B:271:THR:CG2	2:B:273:TYR:H	2.04	0.69
2:B:371:THR:HG22	2:B:377:VAL:HA	1.73	0.69
3:C:42:LEU:HD13	23:C:501:CLA:HMA3	1.74	0.69
10:K:17:ILE:CD1	18:Z:6:GLN:HE21	2.05	0.69
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.74	0.69
18:Z:21:ILE:O	18:Z:25:VAL:HG23	1.91	0.69
3:C:241:GLY:C	3:C:243:ILE:H	1.96	0.69
13:O:73:PRO:CG	13:O:102:THR:HB	2.22	0.69
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.75	0.69
23:C:495:CLA:HBD	23:C:495:CLA:HBA1	1.75	0.69
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
7:H:11:LEU:C	7:H:13:PRO:HD2	2.14	0.69
11:L:14:ARG:HG2	12:M:26:TYR:HE1	1.58	0.69
3:C:214:LEU:H	3:C:214:LEU:HD23	1.58	0.69
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.68
18:Z:15:LEU:HD23	18:Z:50:LEU:HD12	1.75	0.68
23:A:559:CLA:HED2	4:D:198:MET:SD	2.33	0.68
2:B:126:PRO:HG3	7:H:12:ARG:NH2	2.09	0.68
3:C:84:GLN:HB2	3:C:86:LEU:HD22	1.75	0.68
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	0.68
1:A:22:THR:HG23	1:A:136:ARG:HH11	1.59	0.68
3:C:363:GLY:O	3:C:367:GLU:HG2	1.93	0.68
5:E:58:GLN:HE22	16:V:28:GLU:HA	1.58	0.68
2:B:344:ALA:HB2	2:B:401:PHE:CE1	2.29	0.68
4:D:84:SER:HB2	5:E:68:ASP:HA	1.74	0.68
28:C:505:BCR:H312	18:Z:55:GLY:HA2	1.75	0.68
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.11	0.68
1:A:270:SER:HA	4:D:232:PHE:CE2	2.29	0.68
13:O:36:ILE:HG23	13:O:41:LEU:HB2	1.76	0.68
1:A:47:CYS:SG	1:A:114:LEU:HD23	2.34	0.67
5:E:4:THR:HG23	17:X:90:UNK:CD2	2.24	0.67
2:B:231:MET:HG3	23:B:520:CLA:HAC2	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:B:515:CLA:HMB3	23:B:516:CLA:H11	1.76	0.67
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	0.67
2:B:222:PRO:HG3	7:H:27:THR:H	1.60	0.67
3:C:124:VAL:HB	28:C:505:BCR:H362	1.77	0.67
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.24	0.67
4:D:261:PHE:O	4:D:262:SER:HB3	1.94	0.67
2:B:191:ASN:HD22	2:B:192:PRO:CD	2.07	0.67
4:D:89:LEU:HG	7:H:50:ASN:OD1	1.95	0.67
13:O:234:THR:OG1	13:O:236:GLU:HG2	1.95	0.67
13:O:163:THR:H	13:O:166:THR:HG23	1.60	0.67
3:C:150:ASP:O	3:C:153:ASP:HB3	1.96	0.67
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.75	0.67
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	0.67
17:X:54:UNK:HB1	17:X:57:UNK:CG2	2.25	0.67
5:E:40:THR:HG21	17:X:102:UNK:CB	2.25	0.67
3:C:153:ASP:O	3:C:155:ASN:N	2.28	0.66
3:C:210:PHE:O	3:C:213:LEU:HB2	1.95	0.66
2:B:353:GLU:HB3	2:B:373:LYS:NZ	2.10	0.66
1:A:60:ILE:HG23	1:A:61:ASP:N	2.09	0.66
10:K:35:LEU:HD22	17:X:17:UNK:CB	2.26	0.66
13:O:32:THR:H	13:O:35:ASP:HB2	1.61	0.66
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.78	0.66
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.78	0.66
14:T:4:ILE:HD13	14:T:4:ILE:C	2.16	0.66
3:C:56:HIS:C	3:C:58:GLY:H	1.99	0.66
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.11	0.66
2:B:463:PHE:HZ	23:B:518:CLA:HBB1	1.61	0.65
28:X:130:BCR:H331	28:X:130:BCR:HC8	1.78	0.65
4:D:267:LEU:HD23	4:D:267:LEU:C	2.17	0.65
2:B:297:THR:CB	2:B:300:GLU:HG3	2.26	0.65
13:O:77:LEU:N	13:O:77:LEU:HD12	2.10	0.65
5:E:10:PHE:O	5:E:13:ILE:HG22	1.95	0.65
10:K:23:ASP:OD2	17:X:6:UNK:NE2	2.34	0.65
5:E:22:ILE:HG23	17:X:116:UNK:HA	1.78	0.65
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.25	0.65
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.25	0.65
1:A:270:SER:HA	4:D:232:PHE:HE2	1.61	0.65
10:K:28:ILE:O	10:K:31:LEU:HB2	1.97	0.65
3:C:466:VAL:HA	3:C:469:MET:HE3	1.79	0.65
1:A:76:ASN:ND2	1:A:79:THR:H	1.95	0.65
17:X:51:UNK:O	17:X:52:UNK:C	2.44	0.65
2:B:176:GLY:HA3	2:B:266:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:A:558:CLA:H143	24:A:561:PHO:H62	1.78	0.65
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.62	0.65
2:B:392:PHE:O	2:B:393:GLU:HB2	1.96	0.65
5:E:78:THR:O	5:E:82:GLN:HG2	1.97	0.65
1:A:94:TYR:OH	1:A:104:GLU:HG2	1.97	0.65
23:C:501:CLA:H151	18:Z:20:VAL:HG13	1.78	0.64
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.80	0.64
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.80	0.64
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.33	0.64
3:C:265:ILE:HD13	23:C:495:CLA:HED1	1.78	0.64
3:C:449:ARG:NH2	8:I:27:ASP:HB3	2.12	0.64
1:A:305:SER:O	1:A:306:VAL:C	2.35	0.64
2:B:223:GLN:HE22	2:B:227:LYS:HD3	1.62	0.64
3:C:279:LEU:HA	3:C:282:MET:HE3	1.80	0.64
4:D:210:LEU:HD21	26:D:356:PQ9:H17	1.80	0.64
6:F:37:ILE:HG22	9:J:28:PHE:CE1	2.33	0.64
23:C:495:CLA:CMD	23:C:497:CLA:HAB	2.27	0.64
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.33	0.64
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.80	0.64
2:B:223:GLN:HE22	2:B:227:LYS:CD	2.10	0.64
1:A:134:SER:HB2	1:A:139:MET:HG3	1.79	0.63
16:V:95:ILE:O	16:V:99:VAL:HG23	1.97	0.63
1:A:187:GLN:HG3	1:A:325:ASN:OD1	1.98	0.63
28:C:504:BCR:H311	28:C:504:BCR:H343	1.81	0.63
28:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
7:H:12:ARG:N	7:H:13:PRO:HD2	2.13	0.63
13:O:184:ASP:HB2	13:O:185:PRO:HD2	1.80	0.63
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	0.63
23:B:519:CLA:HMC2	28:H:107:BCR:H343	1.81	0.63
16:V:49:GLU:O	16:V:53:LEU:HG	1.98	0.63
2:B:120:LEU:HD13	23:B:526:CLA:HMD2	1.79	0.63
4:D:229:ALA:O	4:D:231:THR:HG23	1.97	0.63
1:A:243:GLU:HA	4:D:241:GLU:HA	1.80	0.63
4:D:36:LEU:C	4:D:39:PRO:HD2	2.19	0.63
3:C:248:GLY:O	3:C:252:ILE:HG13	1.97	0.63
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	0.63
3:C:343:ARG:HB2	13:O:101:THR:HG23	1.80	0.63
16:V:38:LEU:HD13	16:V:45:ILE:CD1	2.29	0.63
4:D:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:43:LEU:HD23	17:X:60:UNK:CZ	2.29	0.63
2:B:208:VAL:HG21	23:B:512:CLA:HMC1	1.81	0.63
3:C:52:ALA:HA	23:C:501:CLA:HMB3	1.80	0.63
3:C:417:VAL:O	3:C:417:VAL:HG22	1.99	0.63
1:A:16:ARG:HD3	1:A:17:PHE:N	2.14	0.63
13:O:45:CYS:HB2	13:O:46:PRO:CD	2.27	0.63
15:U:82:ASN:HB2	15:U:85:TYR:OH	1.99	0.63
7:H:6:TRP:O	7:H:10:ILE:HG13	1.99	0.63
3:C:158:THR:HG22	3:C:251:HIS:O	1.99	0.63
5:E:23:HIS:C	5:E:25:ILE:H	2.02	0.62
15:U:89:GLU:CD	15:U:89:GLU:H	2.02	0.62
2:B:246:PHE:C	2:B:246:PHE:CD1	2.72	0.62
5:E:57:ALA:O	5:E:59:GLU:N	2.32	0.62
16:V:135:GLU:O	16:V:139:VAL:HG23	1.98	0.62
13:O:110:GLU:O	13:O:110:GLU:HG3	1.99	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.81	0.62
1:A:40:THR:HG21	1:A:121:LEU:HB3	1.81	0.62
13:O:45:CYS:H	13:O:72:GLN:HE22	1.48	0.62
23:C:501:CLA:H171	18:Z:20:VAL:HA	1.79	0.62
1:A:72:LEU:HD23	14:T:3:THR:HG21	1.82	0.62
13:O:183:LEU:HD22	13:O:187:GLY:O	1.99	0.62
2:B:2:GLY:HA3	11:L:11:GLU:OE1	2.00	0.62
4:D:103:ARG:NH1	5:E:77:GLU:HG3	2.15	0.62
13:O:46:PRO:HB2	13:O:266:TYR:CG	2.35	0.62
3:C:55:ALA:HB1	28:C:504:BCR:H373	1.82	0.62
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.30	0.62
4:D:90:LEU:HD23	4:D:109:GLY:HA2	1.81	0.62
1:A:253:GLY:O	1:A:257:ARG:HD2	2.00	0.61
2:B:357:ARG:NH2	4:D:337:GLU:HG3	2.14	0.61
17:X:28:UNK:CG2	18:Z:29:SER:HA	2.30	0.61
1:A:49:VAL:O	1:A:53:ILE:HG13	2.00	0.61
6:F:41:GLN:HE21	6:F:41:GLN:HA	1.64	0.61
17:X:26:UNK:HG2	17:X:26:UNK:NE2	2.20	0.61
2:B:329:PRO:CB	23:B:517:CLA:HED1	2.26	0.61
3:C:35:TRP:NE1	3:C:36:TRP:HD1	1.99	0.61
1:A:25:ASP:HB3	4:D:251:ARG:HH22	1.65	0.61
6:F:41:GLN:NE2	6:F:41:GLN:HA	2.15	0.61
3:C:90:PRO:O	3:C:94:THR:HG23	2.01	0.61
6:F:31:ILE:HG13	25:F:51:HEM:HMC2	1.82	0.61
16:V:39:ASN:HD21	16:V:41:GLU:HB2	1.64	0.61
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.01	0.61
7:H:21:VAL:HG22	7:H:22:ALA:O	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
3:C:298:PRO:O	3:C:299:SER:CB	2.48	0.61
5:E:10:PHE:HA	5:E:13:ILE:HG22	1.83	0.61
2:B:247:PHE:O	2:B:251:VAL:HG23	2.00	0.61
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.82	0.61
2:B:31:ALA:HB2	23:B:515:CLA:HBC3	1.83	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	0.61
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
22:C:474:UNK:C15	26:D:356:PQ9:H293	2.31	0.61
1:A:64:ARG:C	1:A:66:PRO:HD3	2.21	0.61
2:B:185:TRP:HH2	2:B:203:ILE:HG21	1.66	0.61
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.31	0.60
13:O:128:ASP:OD2	13:O:149:LYS:HG2	2.01	0.60
2:B:271:THR:HG22	2:B:274:GLN:H	1.64	0.60
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.16	0.60
5:E:56:TYR:HB3	5:E:60:GLN:HG3	1.83	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	0.60
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.83	0.60
15:U:66:ILE:HG22	15:U:66:ILE:O	2.01	0.60
5:E:36:LEU:HA	5:E:39:SER:HB3	1.82	0.60
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.15	0.60
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.16	0.60
2:B:137:LYS:O	2:B:141:ILE:HG13	2.02	0.60
14:T:21:ILE:HD12	28:T:5104:BCR:H332	1.83	0.60
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	0.60
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
9:J:8:ILE:H	9:J:8:ILE:HD12	1.66	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	0.60
7:H:49:TYR:CD2	30:H:208:DGD:HB22	2.37	0.60
2:B:10:THR:O	2:B:13:ILE:HG13	2.02	0.60
1:A:315:ASN:O	4:D:63:LEU:HB3	2.02	0.60
15:U:117:VAL:HG13	15:U:122:VAL:HG21	1.82	0.60
2:B:229:LEU:O	2:B:231:MET:N	2.35	0.60
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
3:C:230:LEU:O	3:C:234:VAL:HG23	2.01	0.59
4:D:337:GLU:HG2	4:D:339:PHE:CE2	2.36	0.59
5:E:60:GLN:HG3	5:E:60:GLN:O	2.01	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59
13:O:55:ALA:O	13:O:57:PRO:HD3	2.02	0.59
13:O:179:THR:CG2	13:O:180:ALA:N	2.65	0.59
3:C:458:GLY:HA2	4:D:222:LEU:O	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:428:THR:HG22	3:C:429:SER:N	2.17	0.59
13:O:112:LYS:HE2	13:O:114:ASN:HB3	1.84	0.59
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.32	0.59
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.84	0.59
16:V:147:VAL:O	16:V:150:LYS:HB2	2.02	0.59
4:D:60:THR:HG23	4:D:61:HIS:N	2.18	0.59
18:Z:14:ILE:O	18:Z:18:VAL:HG23	2.02	0.59
1:A:326:LEU:CD2	3:C:412:THR:HB	2.33	0.59
18:Z:16:SER:O	18:Z:20:VAL:HG23	2.03	0.59
7:H:62:TRP:CD1	30:H:208:DGD:HE5	2.37	0.59
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.84	0.59
13:O:230:VAL:HG12	13:O:231:ASP:N	2.17	0.59
2:B:384:ARG:NH1	15:U:132:LEU:HD22	2.18	0.59
7:H:29:PRO:O	7:H:33:VAL:HG23	2.02	0.59
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.38	0.59
4:D:279:LEU:HD22	23:D:354:CLA:HBA2	1.85	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
1:A:307:ILE:HD11	1:A:311:GLY:O	2.00	0.58
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.84	0.58
4:D:39:PRO:O	4:D:43:LEU:HB2	2.03	0.58
13:O:204:LYS:HB3	13:O:206:GLU:HG2	1.85	0.58
3:C:265:ILE:HG22	3:C:270:ALA:CB	2.33	0.58
3:C:465:PRO:C	3:C:469:MET:HE2	2.23	0.58
3:C:315:MET:O	3:C:319:ILE:HG13	2.04	0.58
1:A:131:TRP:CE3	1:A:132:GLU:N	2.72	0.58
13:O:76:PHE:C	13:O:77:LEU:HD12	2.23	0.58
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.85	0.58
3:C:456:GLU:N	3:C:456:GLU:OE1	2.35	0.58
18:Z:5:PHE:CA	18:Z:57:LEU:HD13	2.32	0.58
4:D:102:THR:O	4:D:105:CYS:HB2	2.04	0.58
4:D:120:PHE:HA	4:D:123:ILE:HD12	1.85	0.58
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.39	0.58
17:X:7:UNK:O	17:X:11:UNK:HG2	2.04	0.58
2:B:471:ALA:O	2:B:475:PHE:HB2	2.04	0.58
24:A:562:PHO:CMC	4:D:279:LEU:HD11	2.34	0.58
2:B:24:LEU:HD21	23:B:526:CLA:HAB	1.86	0.58
13:O:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58
2:B:149:LEU:HG	23:B:513:CLA:CBC	2.28	0.58
4:D:103:ARG:HD3	4:D:106:GLN:OE1	2.04	0.58
4:D:110:LEU:O	4:D:114:ILE:HG13	2.04	0.58
13:O:152:VAL:HG13	13:O:152:VAL:O	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:ALA:O	1:A:55:ALA:HB2	2.03	0.57
3:C:452:ALA:C	3:C:454:GLY:N	2.56	0.57
13:O:65:ARG:HA	13:O:111:LEU:H	1.68	0.57
1:A:62:GLY:HA3	3:C:356:MET:SD	2.44	0.57
3:C:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	0.57
5:E:60:GLN:C	5:E:62:SER:H	2.07	0.57
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.69	0.57
6:F:34:LEU:HD22	9:J:24:ILE:CD1	2.32	0.57
4:D:343:GLU:HG2	16:V:161:VAL:HG11	1.86	0.57
1:A:217:SER:HA	4:D:272:LEU:HD12	1.86	0.57
13:O:142:ILE:HD12	13:O:142:ILE:N	2.19	0.57
8:I:27:ASP:N	8:I:28:PRO:CD	2.67	0.57
9:J:14:ALA:HB1	28:X:130:BCR:H393	1.85	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	1.85	0.57
2:B:150:CYS:HA	23:B:513:CLA:HBC2	1.87	0.57
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.57
18:Z:39:LEU:O	18:Z:42:LEU:HB3	2.05	0.57
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.04	0.57
3:C:428:THR:CG2	30:C:508:DGD:HA91	2.35	0.57
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	0.57
4:D:261:PHE:HB2	26:D:356:PQ9:H92	1.84	0.57
4:D:239:GLN:O	4:D:240:ALA:HB3	2.05	0.57
4:D:273:PHE:CZ	29:L:210:MGE:H3B2	2.40	0.57
3:C:44:ASN:O	3:C:45:LEU:HG	2.04	0.57
10:K:18:PHE:O	10:K:19:ASP:C	2.43	0.57
14:T:4:ILE:O	14:T:4:ILE:HD13	2.04	0.57
5:E:15:THR:HG23	9:J:8:ILE:O	2.04	0.57
4:D:239:GLN:O	4:D:240:ALA:CB	2.53	0.57
13:O:168:PHE:CD1	13:O:168:PHE:N	2.71	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	0.57
13:O:172:PHE:CE2	13:O:223:ILE:HG12	2.39	0.57
23:B:518:CLA:HMA1	4:D:130:PHE:CE1	2.40	0.57
4:D:14:TRP:HD1	4:D:15:PHE:N	2.03	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57
9:J:15:THR:HG22	10:K:38:VAL:HG22	1.85	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
6:F:40:MET:HA	6:F:43:ILE:HG13	1.84	0.57
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
4:D:348:ARG:NH2	4:D:352:LEU:OXT	2.37	0.57
13:O:73:PRO:HG2	13:O:102:THR:OG1	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.35	0.57
13:O:145:LEU:O	13:O:147:THR:HG22	2.05	0.56
2:B:391:SER:OG	2:B:394:GLN:HB2	2.05	0.56
2:B:138:MET:SD	23:B:525:CLA:HAC1	2.45	0.56
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	0.56
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.26	0.56
4:D:221:THR:HG22	4:D:245:SER:H	1.69	0.56
13:O:163:THR:H	13:O:166:THR:CG2	2.18	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
16:V:39:ASN:ND2	16:V:41:GLU:HB2	2.20	0.56
1:A:213:ALA:O	1:A:217:SER:HB2	2.06	0.56
8:I:19:PHE:CE1	8:I:23:PHE:HE2	2.24	0.56
3:C:27:ASP:O	10:K:46:ARG:HD3	2.06	0.56
3:C:72:LEU:HD11	3:C:108:THR:OG1	2.05	0.56
3:C:198:VAL:HG12	3:C:200:THR:HG23	1.87	0.56
3:C:56:HIS:C	3:C:58:GLY:N	2.59	0.56
16:V:81:ARG:HH11	16:V:81:ARG:HG3	1.71	0.56
3:C:315:MET:CE	3:C:319:ILE:HD11	2.35	0.56
1:A:29:TYR:HD1	1:A:133:LEU:HB2	1.69	0.56
15:U:77:LYS:O	15:U:81:LYS:HB2	2.06	0.56
8:I:11:VAL:O	8:I:15:PHE:HD1	1.89	0.56
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.41	0.56
2:B:55:MET:HE3	2:B:80:ILE:HG12	1.87	0.56
2:B:353:GLU:HB3	2:B:373:LYS:HZ3	1.71	0.56
4:D:103:ARG:HH12	5:E:77:GLU:HG3	1.70	0.56
9:J:33:TYR:O	9:J:34:ALA:HB3	2.04	0.56
4:D:178:ILE:HG22	4:D:179:PHE:N	2.21	0.56
3:C:293:ASN:HD21	3:C:296:VAL:H	1.51	0.56
1:A:13:LEU:N	1:A:13:LEU:HD23	2.21	0.56
2:B:467:ILE:HD13	4:D:126:MET:SD	2.46	0.56
1:A:221:SER:HA	4:D:139:ARG:HB2	1.86	0.56
2:B:63:LEU:N	2:B:64:PRO:HD2	2.21	0.56
16:V:107:THR:HG22	16:V:108:TYR:H	1.69	0.55
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.41	0.55
3:C:194:GLY:O	3:C:195:ASP:HB2	2.06	0.55
3:C:332:GLN:HA	3:C:338:GLY:HA2	1.88	0.55
10:K:39:TRP:O	10:K:43:VAL:HG23	2.05	0.55
3:C:348:GLU:OE2	13:O:37:VAL:HA	2.06	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.89	0.55
16:V:103:LYS:O	16:V:122:ARG:HG3	2.07	0.55
3:C:400:PRO:C	3:C:401:LEU:HD23	2.26	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:260:ALA:O	3:C:264:PHE:HD2	1.89	0.55
3:C:284:PHE:HB3	30:C:507:DGD:HA51	1.87	0.55
13:O:163:THR:HG23	13:O:165:SER:H	1.71	0.55
16:V:124:ALA:HB1	16:V:131:ARG:HG3	1.87	0.55
4:D:176:ALA:C	4:D:178:ILE:H	2.10	0.55
15:U:72:TYR:CB	15:U:73:PRO:CD	2.84	0.55
1:A:38:ILE:O	1:A:42:LEU:HG	2.07	0.55
6:F:18:VAL:HG13	6:F:19:ARG:N	2.22	0.55
5:E:13:ILE:HD13	25:F:51:HEM:O1D	2.07	0.55
2:B:283:GLU:OE1	2:B:286:ARG:HD2	2.07	0.55
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.34	0.55
1:A:224:ILE:CG2	2:B:484:PRO:HG3	2.35	0.55
2:B:233:ASN:HD22	2:B:233:ASN:C	2.10	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
2:B:229:LEU:O	2:B:230:ARG:C	2.44	0.55
3:C:42:LEU:CD1	23:C:501:CLA:HMA3	2.36	0.55
3:C:209:ILE:CG2	28:C:506:BCR:H382	2.35	0.55
1:A:264:SER:OG	1:A:265:PHE:N	2.40	0.55
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.89	0.55
23:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
10:K:39:TRP:NE1	17:X:31:UNK:HG3	2.12	0.55
18:Z:23:VAL:HB	18:Z:24:PRO:HD3	1.89	0.55
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.55
16:V:159:GLY:O	16:V:160:LYS:C	2.45	0.55
2:B:18:ARG:HG3	2:B:18:ARG:HH11	1.70	0.55
13:O:47:THR:HG22	13:O:48:LEU:N	2.22	0.55
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.70	0.55
3:C:37:ALA:HA	23:C:498:CLA:O1A	2.06	0.55
13:O:145:LEU:HD23	13:O:175:PRO:CG	2.34	0.55
3:C:466:VAL:HA	3:C:469:MET:CE	2.36	0.55
9:J:14:ALA:CB	28:X:130:BCR:H393	2.38	0.54
3:C:416:SER:O	3:C:417:VAL:CG1	2.55	0.54
2:B:10:THR:C	2:B:12:LEU:H	2.10	0.54
4:D:346:LEU:O	4:D:348:ARG:HG3	2.07	0.54
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.82	0.54
13:O:75:THR:HG22	13:O:77:LEU:HD11	1.88	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.71	0.54
30:C:509:DGD:HD2	9:J:32:ALA:O	2.06	0.54
3:C:91:HIS:HB3	23:C:493:CLA:HBA2	1.88	0.54
10:K:43:VAL:HG12	10:K:46:ARG:HG3	1.90	0.54
28:B:527:BCR:H322	29:B:530:MGE:H2G	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.37	0.54
3:C:405:ASN:HD22	30:C:509:DGD:C5D	2.19	0.54
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.89	0.54
3:C:55:ALA:HB1	28:C:504:BCR:C37	2.37	0.54
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.35	0.54
5:E:25:ILE:O	5:E:29:ALA:HB2	2.08	0.54
4:D:325:ILE:O	4:D:329:MET:HB3	2.08	0.54
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	0.54
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	0.54
3:C:418:ASN:HB3	30:C:509:DGD:HE2	1.89	0.54
3:C:52:ALA:HB1	23:C:499:CLA:HAB	1.89	0.54
2:B:221:PRO:O	7:H:21:VAL:HG23	2.08	0.54
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.43	0.54
3:C:75:PHE:CE2	3:C:77:PRO:HA	2.43	0.54
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.33	0.54
2:B:392:PHE:O	2:B:393:GLU:CB	2.54	0.54
15:U:57:LEU:HD22	15:U:79:ILE:CG2	2.37	0.54
10:K:45:PHE:O	10:K:46:ARG:C	2.46	0.54
1:A:174:LEU:HD22	24:A:561:PHO:H152	1.89	0.54
5:E:76:VAL:O	5:E:79:PHE:HB2	2.07	0.54
4:D:100:ASP:OD1	4:D:102:THR:HG22	2.07	0.54
3:C:201:ASN:N	3:C:202:PRO:HD3	2.22	0.54
3:C:276:LEU:CD2	23:C:498:CLA:HBB1	2.37	0.54
4:D:67:TYR:CD2	4:D:76:VAL:HG11	2.43	0.54
12:M:26:TYR:O	12:M:29:THR:HB	2.08	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	0.54
4:D:45:LEU:HD13	4:D:49:LEU:HD12	1.90	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.89	0.53
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.89	0.53
3:C:99:VAL:HG23	3:C:100:GLY:H	1.72	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.53
1:A:159:LEU:O	1:A:163:ILE:HG13	2.08	0.53
1:A:76:ASN:HD22	1:A:76:ASN:C	2.11	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	0.53
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.44	0.53
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
17:X:72:UNK:O	17:X:73:UNK:C	2.57	0.53
2:B:124:ARG:O	7:H:12:ARG:NH2	2.42	0.53
14:T:29:ILE:CD1	14:T:29:ILE:H	2.18	0.53
11:L:11:GLU:HG2	11:L:12:LEU:N	2.24	0.53
11:L:14:ARG:HG3	11:L:14:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:84:GLN:HB2	3:C:86:LEU:CD2	2.37	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.90	0.53
3:C:158:THR:O	3:C:251:HIS:HB3	2.07	0.53
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.37	0.53
10:K:14:ALA:HB2	18:Z:61:VAL:HG11	1.90	0.53
4:D:14:TRP:HD1	4:D:15:PHE:H	1.55	0.53
5:E:51:ARG:O	5:E:53:ASP:N	2.41	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.28	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
2:B:12:LEU:HB2	23:B:522:CLA:HMC2	1.90	0.53
3:C:48:LYS:HE2	3:C:133:ALA:HA	1.90	0.53
1:A:286:THR:HB	23:A:558:CLA:O1D	2.09	0.53
13:O:162:ILE:HA	13:O:166:THR:HG21	1.90	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CD2	2.44	0.53
17:X:122:UNK:C	17:X:124:UNK:N	2.70	0.53
1:A:314:ILE:CG2	1:A:314:ILE:O	2.55	0.53
1:A:40:THR:HG22	1:A:118:HIS:O	2.09	0.53
3:C:193:GLY:O	3:C:194:GLY:C	2.47	0.53
4:D:172:SER:O	4:D:173:PHE:HB2	2.08	0.53
16:V:74:THR:O	16:V:75:ASN:HB2	2.07	0.53
3:C:29:GLU:HG3	3:C:30:SER:N	2.22	0.53
15:U:72:TYR:O	15:U:73:PRO:C	2.46	0.53
4:D:221:THR:O	4:D:221:THR:HG22	2.08	0.53
1:A:238:LYS:O	1:A:241:GLN:HB3	2.09	0.53
1:A:124:SER:O	1:A:127:MET:HB3	2.09	0.53
1:A:183:MET:HA	23:A:558:CLA:HMD2	1.90	0.53
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.44	0.53
3:C:377:LEU:HB2	13:O:106:GLN:HG2	1.91	0.53
1:A:176:ILE:HD13	23:A:559:CLA:HED3	1.91	0.53
24:A:561:PHO:NC	4:D:209:LEU:HD12	2.24	0.53
1:A:141:PRO:O	1:A:143:ILE:N	2.38	0.53
2:B:102:VAL:HA	28:B:528:BCR:C40	2.39	0.52
2:B:152:GLY:C	23:B:516:CLA:HMC3	2.30	0.52
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
23:C:492:CLA:H111	23:C:493:CLA:HMB2	1.90	0.52
29:D:360:MGE:H241	14:T:13:ILE:HG21	1.90	0.52
10:K:31:LEU:HB3	28:X:130:BCR:C15	2.39	0.52
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.52
13:O:33:TYR:C	13:O:35:ASP:H	2.12	0.52
5:E:32:ILE:O	5:E:36:LEU:HG	2.10	0.52
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.75	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.71	0.52
2:B:476:ARG:HG3	2:B:476:ARG:HH11	1.74	0.52
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
3:C:318:LEU:HD23	3:C:318:LEU:O	2.10	0.52
3:C:63:TRP:O	3:C:64:ALA:C	2.47	0.52
2:B:263:THR:O	2:B:263:THR:HG22	2.08	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	0.52
3:C:103:GLY:HA3	3:C:301:PHE:CE1	2.37	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
2:B:391:SER:OG	2:B:394:GLN:NE2	2.43	0.52
3:C:56:HIS:O	3:C:58:GLY:N	2.42	0.52
17:X:12:UNK:CG	18:Z:17:PHE:CE1	2.90	0.52
5:E:69:ARG:O	5:E:70:PHE:HB2	2.09	0.52
4:D:93:TRP:HZ2	23:D:355:CLA:O1A	1.93	0.52
1:A:103:ASP:OD1	1:A:103:ASP:N	2.40	0.52
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.45	0.52
4:D:348:ARG:HH21	4:D:352:LEU:C	2.12	0.52
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.24	0.52
14:T:1:MET:C	14:T:4:ILE:HG22	2.30	0.52
3:C:29:GLU:C	3:C:31:SER:H	2.13	0.52
2:B:220:ARG:HD2	7:H:20:LYS:O	2.10	0.52
13:O:206:GLU:CD	13:O:206:GLU:H	2.13	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	0.52
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.52
2:B:214:LEU:O	2:B:218:LEU:HG	2.09	0.52
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.44	0.52
16:V:134:THR:HG23	16:V:137:ASP:OD2	2.10	0.52
8:I:13:THR:O	8:I:17:LEU:HG	2.09	0.52
2:B:262:THR:C	2:B:264:PRO:HD3	2.30	0.52
2:B:362:PHE:HE2	4:D:164:GLN:NE2	2.08	0.52
1:A:63:ILE:CG2	3:C:335:THR:HG21	2.40	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.45	0.52
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.91	0.52
3:C:116:VAL:HG21	28:C:505:BCR:C32	2.40	0.52
23:C:503:CLA:HMC2	28:C:505:BCR:H372	1.91	0.52
1:A:64:ARG:O	1:A:66:PRO:HD3	2.10	0.52
2:B:137:LYS:HD2	7:H:14:LEU:O	2.10	0.52
1:A:27:ARG:NH1	1:A:27:ARG:O	2.43	0.52
13:O:118:SER:HB3	13:O:157:PRO:HA	1.90	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:L:2:GLU:HB3	11:L:3:PRO:HD2	1.92	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
16:V:33:VAL:HG12	16:V:33:VAL:O	2.10	0.52
9:J:24:ILE:HG23	9:J:25:VAL:N	2.24	0.51
18:Z:57:LEU:O	18:Z:61:VAL:HG23	2.10	0.51
1:A:257:ARG:HH12	1:A:261:GLN:CD	2.13	0.51
13:O:110:GLU:OE2	13:O:112:LYS:HB2	2.10	0.51
4:D:14:TRP:CD1	4:D:15:PHE:N	2.78	0.51
2:B:413:ASP:OD1	2:B:415:PRO:HD2	2.09	0.51
4:D:223:PHE:CZ	4:D:245:SER:HB3	2.44	0.51
13:O:144:LEU:N	13:O:144:LEU:HD23	2.23	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
13:O:172:PHE:HE2	13:O:223:ILE:HG12	1.75	0.51
2:B:463:PHE:CZ	23:B:518:CLA:HBB1	2.43	0.51
16:V:59:PHE:HA	16:V:63:CYS:SG	2.50	0.51
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
2:B:212:ALA:HB2	23:B:519:CLA:HMC3	1.91	0.51
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.91	0.51
1:A:192:ILE:HG23	1:A:193:LEU:N	2.25	0.51
23:C:493:CLA:HBA1	23:C:493:CLA:CBF	2.37	0.51
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
17:X:76:UNK:O	17:X:77:UNK:C	2.57	0.51
14:T:4:ILE:HB	33:T:217:LMT:O6'	2.11	0.51
1:A:326:LEU:HD21	3:C:412:THR:HB	1.93	0.51
2:B:229:LEU:HD11	23:B:519:CLA:O1A	2.11	0.51
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	0.51
15:U:69:ARG:O	15:U:70:GLY:C	2.47	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
2:B:380:ASP:OD2	2:B:380:ASP:C	2.47	0.51
14:T:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
2:B:233:ASN:ND2	2:B:235:GLU:H	2.08	0.51
10:K:39:TRP:HE1	17:X:31:UNK:CG	2.14	0.51
14:T:29:ILE:HD12	14:T:29:ILE:N	2.18	0.51
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.92	0.51
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.45	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
3:C:438:LEU:HD11	23:C:495:CLA:HBB1	1.92	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.51
23:C:495:CLA:HMD3	23:C:497:CLA:HAB	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
2:B:31:ALA:O	2:B:32:GLY:C	2.49	0.51
3:C:226:SER:HA	30:C:507:DGD:HE62	1.93	0.51
3:C:438:LEU:CD2	30:C:507:DGD:HAH2	2.41	0.51
3:C:449:ARG:HG3	3:C:449:ARG:O	2.10	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.93	0.51
6:F:11:VAL:HG12	6:F:12:SER:N	2.26	0.51
3:C:48:LYS:HE2	3:C:132:HIS:O	2.11	0.51
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.51
2:B:175:THR:HG22	2:B:175:THR:O	2.11	0.51
8:I:4:LEU:O	8:I:8:VAL:HG23	2.11	0.51
23:B:517:CLA:H202	11:L:27:LEU:HD11	1.93	0.50
2:B:233:ASN:C	2:B:233:ASN:ND2	2.64	0.50
17:X:85:UNK:C	17:X:86:UNK:OD1	2.59	0.50
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.09	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HH11	1.75	0.50
4:D:63:LEU:N	4:D:63:LEU:HD12	2.26	0.50
3:C:372:PRO:O	13:O:36:ILE:HD12	2.11	0.50
23:B:525:CLA:H162	23:B:525:CLA:H112	1.93	0.50
3:C:146:PHE:HD2	3:C:147:PHE:CE1	2.29	0.50
3:C:140:LEU:HB2	3:C:148:GLY:HA2	1.93	0.50
6:F:45:ARG:HG2	6:F:45:ARG:OXT	2.11	0.50
3:C:150:ASP:HB3	3:C:153:ASP:CB	2.32	0.50
23:A:560:CLA:HAB	23:D:354:CLA:H72	1.93	0.50
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
3:C:241:GLY:C	3:C:243:ILE:N	2.64	0.50
15:U:64:ALA:O	15:U:67:GLN:HG2	2.10	0.50
14:T:15:ALA:HB2	28:T:5104:BCR:H14C	1.92	0.50
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.32	0.50
13:O:145:LEU:CD2	13:O:175:PRO:CG	2.86	0.50
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.36	0.50
22:C:484:UNK:HG1	22:C:485:UNK:C	2.40	0.50
10:K:19:ASP:N	10:K:20:PRO:HD2	2.26	0.50
1:A:22:THR:HG23	1:A:136:ARG:NH1	2.26	0.50
10:K:37:PHE:HB3	28:X:130:BCR:C40	2.42	0.50
2:B:368:VAL:HG11	2:B:381:ILE:CD1	2.37	0.50
3:C:245:ILE:O	3:C:249:ILE:HD13	2.12	0.50
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.93	0.50
1:A:62:GLY:O	1:A:63:ILE:O	2.29	0.50
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.93	0.50
2:B:231:MET:C	2:B:233:ASN:H	2.15	0.50
10:K:43:VAL:HG21	17:X:31:UNK:HG3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:Z:36:SER:CA	18:Z:39:LEU:HD12	2.35	0.50
12:M:15:VAL:O	12:M:19:SER:HB2	2.12	0.50
1:A:72:LEU:HD22	33:T:217:LMT:O3'	2.12	0.50
13:O:147:THR:HG21	13:O:175:PRO:HD2	1.93	0.50
4:D:60:THR:HG23	4:D:61:HIS:H	1.77	0.50
2:B:341:LYS:O	2:B:406:LEU:HB2	2.11	0.50
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.50
2:B:15:ASP:O	2:B:17:GLY:N	2.45	0.50
3:C:178:LYS:HD2	3:C:182:PHE:O	2.11	0.50
2:B:463:PHE:CZ	2:B:467:ILE:HD12	2.46	0.50
1:A:299:GLY:O	3:C:403:SER:HB2	2.11	0.50
16:V:128:PRO:O	16:V:130:MET:N	2.45	0.50
13:O:216:PHE:C	13:O:216:PHE:CD2	2.85	0.50
2:B:31:ALA:HB2	23:B:515:CLA:CBC	2.42	0.49
4:D:176:ALA:C	4:D:178:ILE:N	2.66	0.49
4:D:35:ILE:O	4:D:35:ILE:HG22	2.12	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.11	0.49
7:H:59:ASN:OD1	7:H:59:ASN:O	2.29	0.49
13:O:73:PRO:CG	13:O:102:THR:CB	2.90	0.49
3:C:416:SER:O	3:C:417:VAL:HG12	2.11	0.49
2:B:246:PHE:C	2:B:246:PHE:HD1	2.15	0.49
2:B:286:ARG:HD3	2:B:286:ARG:C	2.33	0.49
16:V:144:HIS:CE1	16:V:148:GLU:OE2	2.65	0.49
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.46	0.49
2:B:474:LEU:HD11	23:B:518:CLA:HAA1	1.94	0.49
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	0.49
5:E:47:PHE:O	5:E:49:THR:N	2.45	0.49
3:C:67:MET:HE1	23:C:494:CLA:NC	2.26	0.49
16:V:104:ASN:HD21	16:V:113:GLU:CD	2.14	0.49
4:D:55:VAL:HG12	4:D:56:THR:N	2.26	0.49
3:C:46:SER:HA	3:C:49:LEU:HB3	1.93	0.49
9:J:12:ILE:O	9:J:16:VAL:HG23	2.12	0.49
3:C:277:GLY:C	23:C:495:CLA:HBC2	2.33	0.49
13:O:51:THR:O	13:O:52:ALA:O	2.30	0.49
3:C:188:THR:HG23	3:C:300:GLU:OE2	2.13	0.49
4:D:102:THR:CG2	4:D:103:ARG:N	2.74	0.49
13:O:216:PHE:C	13:O:216:PHE:HD2	2.15	0.49
2:B:13:ILE:HG22	2:B:13:ILE:O	2.11	0.49
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.28	0.49
2:B:124:ARG:HD3	2:B:131:PRO:N	2.28	0.49
2:B:222:PRO:HG3	7:H:27:THR:N	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
2:B:145:LEU:CD1	23:B:525:CLA:HMB2	2.43	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.92	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	0.49
2:B:165:GLY:HA3	2:B:179:GLN:O	2.11	0.49
3:C:199:ILE:N	3:C:199:ILE:HD12	2.27	0.49
2:B:271:THR:HB	2:B:274:GLN:HG3	1.95	0.49
13:O:65:ARG:HG2	13:O:66:ILE:N	2.27	0.49
1:A:78:ILE:O	1:A:177:SER:HB2	2.12	0.49
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.95	0.49
3:C:78:GLU:OE2	3:C:78:GLU:HA	2.12	0.49
10:K:43:VAL:HG12	10:K:43:VAL:O	2.13	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
13:O:101:THR:O	13:O:101:THR:HG22	2.13	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
3:C:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
1:A:232:SER:OG	1:A:235:TYR:CD1	2.65	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.32	0.49
3:C:281:MET:HG3	29:I:201:MGE:H231	1.94	0.49
3:C:250:TRP:HE1	23:C:496:CLA:HED1	1.78	0.49
18:Z:28:ALA:O	18:Z:30:PRO:HD3	2.12	0.49
8:I:24:LEU:C	8:I:26:GLY:H	2.16	0.49
28:T:5104:BCR:H23C	28:T:5104:BCR:H403	1.95	0.49
15:U:73:PRO:HD2	16:V:109:ASP:HB3	1.94	0.49
6:F:40:MET:O	6:F:42:PHE:N	2.46	0.49
2:B:28:ALA:O	2:B:104:SER:HB2	2.13	0.49
2:B:153:PHE:N	23:B:516:CLA:HMC3	2.27	0.49
3:C:269:GLU:CG	3:C:448:ALA:HB2	2.34	0.49
3:C:162:GLY:O	3:C:166:ILE:HG13	2.12	0.49
1:A:58:VAL:O	1:A:60:ILE:N	2.46	0.49
16:V:128:PRO:O	16:V:129:LYS:C	2.51	0.49
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
1:A:153:SER:CB	23:A:558:CLA:H43	2.43	0.48
4:D:57:SER:O	4:D:63:LEU:O	2.31	0.48
13:O:259:VAL:HG12	13:O:260:LYS:N	2.28	0.48
13:O:33:TYR:O	13:O:37:VAL:HG23	2.13	0.48
13:O:75:THR:HG22	13:O:77:LEU:CD1	2.43	0.48
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.48
13:O:154:SER:O	13:O:168:PHE:HA	2.13	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.30	0.48
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:342:MET:HE3	3:C:353:GLY:H	1.78	0.48
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.48
3:C:369:LEU:HD21	3:C:384:ILE:HG12	1.95	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
15:U:72:TYR:CG	15:U:73:PRO:N	2.79	0.48
1:A:140:ARG:NH2	31:A:567:LHG:O5	2.46	0.48
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.94	0.48
12:M:33:GLN:C	12:M:35:SER:H	2.16	0.48
11:L:14:ARG:HG2	12:M:26:TYR:CE1	2.44	0.48
23:B:520:CLA:OBD	23:B:520:CLA:H151	2.13	0.48
2:B:18:ARG:NH1	2:B:18:ARG:HG3	2.28	0.48
10:K:15:TYR:C	10:K:17:ILE:H	2.17	0.48
1:A:228:THR:OG1	1:A:231:GLU:HG2	2.13	0.48
13:O:264:VAL:HG12	13:O:265:PHE:N	2.29	0.48
13:O:83:LYS:O	13:O:84:ASN:CB	2.60	0.48
23:B:513:CLA:H2	23:B:515:CLA:H91	1.95	0.48
3:C:48:LYS:HB3	23:C:501:CLA:HMA2	1.95	0.48
4:D:312:GLU:HB2	13:O:185:PRO:HB3	1.96	0.48
18:Z:15:LEU:O	18:Z:19:MET:HG2	2.13	0.48
16:V:39:ASN:OD1	16:V:43:LYS:N	2.46	0.48
4:D:246:MET:HE3	4:D:263:ASN:H	1.78	0.48
2:B:124:ARG:HD3	2:B:130:GLU:C	2.33	0.48
29:L:210:MGE:H5A2	12:M:22:LEU:HD21	1.94	0.48
4:D:180:ARG:HD3	4:D:180:ARG:C	2.33	0.48
4:D:67:TYR:CE2	4:D:76:VAL:HG11	2.48	0.48
10:K:17:ILE:HG22	10:K:17:ILE:O	2.14	0.48
2:B:353:GLU:HB3	2:B:373:LYS:HZ1	1.78	0.48
2:B:86:ILE:C	2:B:86:ILE:HD12	2.33	0.48
4:D:126:MET:HE1	4:D:147:SER:HA	1.95	0.48
29:D:358:MGE:O3D	9:J:37:GLY:HA3	2.14	0.48
17:X:86:UNK:N	17:X:86:UNK:OD1	2.45	0.48
16:V:160:LYS:O	16:V:161:VAL:C	2.52	0.48
3:C:116:VAL:HG13	3:C:117:VAL:N	2.29	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.49	0.48
3:C:435:PHE:O	3:C:438:LEU:N	2.47	0.48
1:A:153:SER:HB3	23:A:558:CLA:H43	1.96	0.48
3:C:254:THR:HG22	3:C:255:THR:N	2.19	0.48
13:O:33:TYR:C	13:O:35:ASP:N	2.66	0.48
3:C:229:ASN:HD22	3:C:231:GLU:HG2	1.79	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:61:PHE:CZ	23:B:517:CLA:HBB1	2.49	0.48
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.14	0.48
18:Z:20:VAL:O	18:Z:24:PRO:HG2	2.14	0.48
18:Z:5:PHE:HE1	18:Z:54:VAL:HG13	1.79	0.48
15:U:73:PRO:HG2	16:V:109:ASP:N	2.29	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
7:H:45:ILE:O	7:H:46:LEU:C	2.51	0.48
1:A:191:ASN:ND2	1:A:194:MET:HB2	2.28	0.48
1:A:77:ILE:HD13	11:L:29:LEU:HG	1.96	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
17:X:3:UNK:C	17:X:5:UNK:N	2.76	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.47
13:O:67:ALA:HB3	13:O:268:SER:OG	2.14	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.47	0.47
3:C:59:LEU:HD13	23:C:500:CLA:HMD2	1.96	0.47
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	0.47
13:O:73:PRO:HG2	13:O:102:THR:CB	2.45	0.47
11:L:14:ARG:HH11	11:L:14:ARG:HG3	1.78	0.47
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.48	0.47
9:J:18:GLY:O	9:J:22:ILE:HG12	2.14	0.47
2:B:12:LEU:HD12	23:B:522:CLA:HBB1	1.96	0.47
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47
31:A:567:LHG:HC61	3:C:443:TRP:HH2	1.77	0.47
1:A:303:ASN:O	3:C:415:ASN:OD1	2.32	0.47
1:A:78:ILE:HD13	11:L:33:SER:HB2	1.96	0.47
2:B:262:THR:O	2:B:262:THR:CG2	2.61	0.47
3:C:449:ARG:HD3	23:C:495:CLA:HED1	1.95	0.47
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.36	0.47
3:C:62:PHE:CE2	10:K:28:ILE:HB	2.50	0.47
3:C:293:ASN:HD21	3:C:295:THR:HB	1.79	0.47
3:C:459:ILE:HD12	4:D:245:SER:OG	2.13	0.47
2:B:191:ASN:HD22	2:B:192:PRO:N	2.12	0.47
4:D:213:ILE:HG23	4:D:214:HIS:N	2.28	0.47
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.28	0.47
11:L:12:LEU:HD12	12:M:25:LEU:HD12	1.95	0.47
6:F:11:VAL:HG12	6:F:12:SER:H	1.79	0.47
3:C:152:LYS:O	3:C:154:LYS:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:T:4:ILE:HB	33:T:217:LMT:C6'	2.44	0.47
2:B:228:ALA:O	2:B:230:ARG:NH1	2.47	0.47
4:D:49:LEU:HD13	28:D:357:BCR:C15	2.45	0.47
13:O:147:THR:OG1	13:O:148:VAL:N	2.47	0.47
7:H:12:ARG:HG3	7:H:12:ARG:NH1	2.30	0.47
1:A:314:ILE:HG22	1:A:314:ILE:O	2.14	0.47
11:L:14:ARG:HD3	12:M:26:TYR:OH	2.15	0.47
1:A:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
1:A:213:ALA:O	1:A:217:SER:CB	2.63	0.47
13:O:169:LYS:HG2	13:O:224:SER:HB2	1.96	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
16:V:134:THR:N	16:V:137:ASP:OD2	2.45	0.47
16:V:144:HIS:HE1	16:V:148:GLU:OE2	1.97	0.47
15:U:105:LEU:O	15:U:109:LEU:HG	2.15	0.47
23:B:518:CLA:HMB1	4:D:126:MET:HB3	1.97	0.47
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.95	0.47
2:B:179:GLN:HE21	2:B:179:GLN:HA	1.78	0.47
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.91	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:7:ARG:NH2	29:D:359:MGE:O3D	2.47	0.47
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.47
23:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47
23:A:558:CLA:H201	29:D:360:MGE:H232	1.96	0.47
7:H:12:ARG:HG3	7:H:12:ARG:HH11	1.80	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HE3	1.96	0.47
4:D:251:ARG:HE	4:D:255:GLN:NE2	2.12	0.47
9:J:33:TYR:CD2	9:J:33:TYR:N	2.83	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	0.47
1:A:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
17:X:111:UNK:C	17:X:113:UNK:N	2.76	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47
13:O:79:LYS:HA	13:O:90:GLU:O	2.15	0.47
17:X:75:UNK:O	17:X:79:UNK:HG2	2.15	0.47
4:D:102:THR:HG23	4:D:103:ARG:N	2.29	0.47
6:F:41:GLN:HE21	6:F:41:GLN:CA	2.26	0.47
2:B:145:LEU:HD11	23:B:525:CLA:HMB2	1.96	0.47
1:A:29:TYR:CD1	1:A:133:LEU:HB2	2.49	0.47
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.30	0.47
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.15	0.47
16:V:162:TYR:O	16:V:163:TYR:OXT	2.33	0.47
4:D:40:CYS:O	4:D:41:ALA:C	2.53	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:55:ALA:C	28:C:504:BCR:H373	2.35	0.47
1:A:306:VAL:O	1:A:306:VAL:CG2	2.49	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	0.47
1:A:140:ARG:HH22	31:A:567:LHG:P	2.38	0.47
2:B:29:LEU:HD12	23:B:524:CLA:HBB2	1.95	0.47
4:D:68:LEU:HD21	5:E:44:TYR:CD1	2.50	0.47
14:T:1:MET:O	14:T:1:MET:HG2	2.14	0.47
15:U:73:PRO:HG2	16:V:109:ASP:H	1.80	0.47
4:D:214:HIS:HA	26:D:356:PQ9:O4	2.15	0.47
1:A:296:ASN:HB2	3:C:400:PRO:O	2.15	0.47
3:C:201:ASN:OD1	3:C:201:ASN:O	2.33	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
17:X:114:UNK:O	17:X:117:UNK:HB1	2.15	0.47
16:V:133:LEU:H	16:V:133:LEU:HD23	1.80	0.47
3:C:255:THR:HG23	3:C:256:PRO:CD	2.41	0.46
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.46
2:B:169:SER:HA	2:B:176:GLY:HA2	1.97	0.46
13:O:225:LEU:HD12	13:O:225:LEU:N	2.29	0.46
8:I:6:ILE:O	8:I:10:ILE:HG12	2.15	0.46
23:B:513:CLA:H162	7:H:38:PHE:HE2	1.80	0.46
13:O:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
3:C:453:ALA:CB	8:I:31:ASN:ND2	2.76	0.46
3:C:415:ASN:O	3:C:416:SER:CB	2.64	0.46
3:C:180:MET:CE	3:C:202:PRO:HG2	2.45	0.46
3:C:460:ASP:O	3:C:461:ARG:C	2.52	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
2:B:390:TYR:CD1	2:B:390:TYR:N	2.83	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.50	0.46
8:I:32:PRO:O	8:I:33:LYS:HG3	2.14	0.46
9:J:21:VAL:HA	9:J:24:ILE:HG22	1.97	0.46
4:D:222:LEU:HA	4:D:244:TYR:HA	1.97	0.46
3:C:290:VAL:HG23	3:C:297:TYR:CE1	2.50	0.46
3:C:89:ILE:N	3:C:90:PRO:CD	2.79	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	1.97	0.46
17:X:126:UNK:N	17:X:126:UNK:CD	2.77	0.46
6:F:25:THR:O	6:F:29:PRO:HG2	2.15	0.46
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.51	0.46
1:A:60:ILE:CG2	1:A:61:ASP:H	2.23	0.46
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
13:O:47:THR:HG22	13:O:48:LEU:H	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:80:GLU:O	13:O:81:GLU:C	2.53	0.46
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	0.46
15:U:98:THR:C	15:U:100:ARG:H	2.16	0.46
15:U:113:THR:O	15:U:114:VAL:HG23	2.16	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
1:A:183:MET:HB3	23:A:558:CLA:HBC2	1.98	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
18:Z:5:PHE:HA	18:Z:57:LEU:CD1	2.40	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
14:T:11:ALA:HB3	28:T:5104:BCR:H363	1.96	0.46
2:B:263:THR:CG2	2:B:448:ARG:NH1	2.70	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
3:C:39:ASN:OD1	23:C:499:CLA:HBB2	2.16	0.46
12:M:9:ILE:N	12:M:9:ILE:HD12	2.30	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
6:F:45:ARG:CG	6:F:45:ARG:OXT	2.64	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.46
23:C:497:CLA:H142	28:C:506:BCR:H362	1.96	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
5:E:23:HIS:C	5:E:25:ILE:N	2.69	0.46
5:E:59:GLU:O	5:E:60:GLN:C	2.53	0.46
4:D:106:GLN:NE2	5:E:48:GLY:HA3	2.31	0.46
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.46
17:X:112:UNK:C	17:X:114:UNK:N	2.79	0.46
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	0.46
15:U:59:ASN:O	15:U:60:THR:C	2.54	0.46
2:B:10:THR:O	2:B:12:LEU:N	2.49	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
1:A:210:LEU:O	1:A:210:LEU:HD12	2.16	0.46
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
1:A:63:ILE:HG21	3:C:335:THR:HG21	1.97	0.46
1:A:57:PRO:HA	1:A:68:SER:HA	1.97	0.46
17:X:117:UNK:HB1	17:X:117:UNK:NZ	2.31	0.46
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.46	0.46
2:B:462:PHE:CE1	23:B:523:CLA:HMB3	2.50	0.46
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:149:LEU:HB2	23:B:514:CLA:H203	1.97	0.46
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.46
2:B:249:ALA:O	2:B:252:VAL:HG22	2.16	0.46
23:B:518:CLA:H51	23:B:519:CLA:H101	1.97	0.46
1:A:60:ILE:CG2	1:A:61:ASP:N	2.79	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.46
4:D:229:ALA:O	4:D:231:THR:N	2.49	0.46
1:A:26:ASN:O	1:A:27:ARG:C	2.54	0.46
13:O:116:ASP:O	13:O:158:ASN:N	2.35	0.46
13:O:151:LEU:HD12	13:O:171:GLU:O	2.17	0.45
3:C:410:VAL:HG12	3:C:412:THR:H	1.80	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
1:A:126:TYR:O	1:A:130:GLN:HG3	2.16	0.45
1:A:163:ILE:HD13	30:C:507:DGD:HB22	1.97	0.45
2:B:356:VAL:HA	2:B:370:LEU:HD23	1.96	0.45
13:O:114:ASN:O	13:O:115:SER:O	2.33	0.45
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.45
3:C:400:PRO:O	3:C:401:LEU:HD23	2.15	0.45
23:D:355:CLA:H3A	23:D:355:CLA:HBA2	1.53	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
7:H:44:ILE:O	7:H:48:ILE:HG13	2.16	0.45
2:B:329:PRO:HD3	23:B:517:CLA:HED2	1.98	0.45
13:O:98:THR:CG2	13:O:99:ARG:H	2.04	0.45
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.97	0.45
6:F:30:THR:HG22	6:F:34:LEU:HD12	1.98	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45
13:O:70:CYS:SG	13:O:71:LEU:N	2.89	0.45
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
2:B:156:PHE:HB2	23:B:516:CLA:HAC1	1.99	0.45
23:B:511:CLA:CAA	28:H:107:BCR:H19C	2.47	0.45
3:C:453:ALA:HB1	8:I:31:ASN:HD22	1.81	0.45
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.45
1:A:306:VAL:HG21	1:A:316:THR:CG2	2.42	0.45
11:L:14:ARG:HH11	11:L:14:ARG:CG	2.29	0.45
3:C:331:ALA:O	3:C:338:GLY:HA2	2.17	0.45
15:U:115:THR:HG22	15:U:116:GLU:N	2.32	0.45
26:A:564:PQ9:H91	26:A:564:PQ9:H61	1.69	0.45
2:B:215:PHE:C	2:B:215:PHE:CD2	2.89	0.45
2:B:235:GLU:O	2:B:235:GLU:HG2	2.16	0.45
3:C:334:PRO:HG2	4:D:350:ASN:ND2	2.32	0.45
1:A:22:THR:O	1:A:22:THR:HG22	2.16	0.45
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.45
13:O:265:PHE:C	13:O:265:PHE:CD1	2.90	0.45
1:A:131:TRP:CZ2	23:C:495:CLA:HAA1	2.51	0.45
3:C:299:SER:OG	3:C:304:PRO:HA	2.17	0.45
9:J:8:ILE:N	9:J:8:ILE:HD12	2.30	0.45
4:D:213:ILE:CG2	4:D:214:HIS:N	2.79	0.45
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.45
2:B:193:TYR:CE1	2:B:260:SER:N	2.84	0.45
3:C:139:THR:HG23	3:C:139:THR:O	2.16	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	0.45
4:D:179:PHE:O	4:D:183:LEU:HG	2.17	0.45
1:A:210:LEU:HD13	24:A:562:PHO:ND	2.31	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	0.45
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.97	0.45
3:C:250:TRP:HE1	23:C:496:CLA:CED	2.30	0.45
13:O:70:CYS:O	13:O:265:PHE:HB2	2.16	0.45
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.45
15:U:50:ALA:O	15:U:53:GLU:HB2	2.17	0.45
10:K:46:ARG:HH22	17:X:31:UNK:CG2	2.30	0.45
2:B:271:THR:HG22	2:B:274:GLN:N	2.31	0.45
4:D:96:GLU:H	4:D:96:GLU:CD	2.20	0.45
15:U:92:LEU:HD11	15:U:109:LEU:HD11	1.98	0.45
18:Z:2:THR:O	18:Z:3:ILE:C	2.55	0.45
2:B:124:ARG:HE	2:B:131:PRO:HG3	1.82	0.45
2:B:124:ARG:NH1	2:B:124:ARG:CG	2.77	0.45
13:O:160:THR:O	13:O:161:SER:O	2.34	0.45
13:O:166:THR:O	13:O:167:ASP:HB3	2.16	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	0.45
2:B:98:LEU:O	2:B:99:ALA:C	2.55	0.45
3:C:264:PHE:CD2	3:C:264:PHE:N	2.85	0.45
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.78	0.45
7:H:55:LEU:HB2	7:H:58:VAL:HG21	1.98	0.45
3:C:349:ILE:HD13	13:O:127:ILE:CD1	2.47	0.45
13:O:139:GLY:O	13:O:140:GLU:O	2.34	0.45
23:B:514:CLA:O1A	23:B:515:CLA:HBA1	2.16	0.45
3:C:305:THR:CG2	3:C:307:PRO:HD2	2.31	0.45
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.99	0.45
23:A:559:CLA:H61	24:A:561:PHO:HMB3	1.99	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	0.45
1:A:40:THR:CG2	1:A:118:HIS:O	2.65	0.45
4:D:68:LEU:HB2	6:F:40:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:U:56:ASP:HB3	15:U:60:THR:H	1.82	0.45
13:O:59:ASP:C	13:O:61:SER:H	2.21	0.45
2:B:10:THR:HG23	2:B:13:ILE:HD11	1.99	0.45
23:B:519:CLA:HBA2	7:H:31:MET:SD	2.57	0.45
2:B:7:ARG:O	2:B:8:VAL:C	2.55	0.45
4:D:130:PHE:HE2	4:D:140:PRO:HB2	1.81	0.45
4:D:244:TYR:OH	4:D:264:LYS:HD3	2.17	0.45
6:F:18:VAL:CG1	6:F:19:ARG:N	2.80	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.45
2:B:297:THR:H	2:B:300:GLU:CD	2.20	0.45
2:B:171:PRO:HD3	7:H:65:LEU:C	2.37	0.45
23:B:517:CLA:H3A	23:B:517:CLA:HBA2	1.71	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
25:F:51:HEM:HAD2	25:F:51:HEM:HHA	1.67	0.44
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.52	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
4:D:100:ASP:C	4:D:100:ASP:OD1	2.55	0.44
8:I:17:LEU:O	8:I:18:LEU:C	2.55	0.44
12:M:31:SER:C	12:M:33:GLN:H	2.21	0.44
4:D:302:GLU:OE1	13:O:186:LYS:CE	2.65	0.44
12:M:33:GLN:O	12:M:35:SER:N	2.50	0.44
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.51	0.44
3:C:265:ILE:HB	23:C:495:CLA:HED3	1.98	0.44
28:C:504:BCR:H11C	28:X:130:BCR:H322	1.99	0.44
2:B:124:ARG:HA	2:B:131:PRO:HA	1.99	0.44
5:E:60:GLN:C	5:E:62:SER:N	2.71	0.44
15:U:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.52	0.44
13:O:81:GLU:O	13:O:82:PRO:C	2.56	0.44
1:A:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	0.44
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.64	0.44
17:X:126:UNK:HB2	17:X:127:UNK:H	1.41	0.44
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.19	0.44
3:C:116:VAL:O	3:C:117:VAL:C	2.56	0.44
16:V:63:CYS:SG	25:V:552:HEM:HAB	2.57	0.44
16:V:64:ALA:O	16:V:66:CYS:N	2.51	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
5:E:28:PRO:O	5:E:32:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.00	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.82	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
4:D:85:MET:HE3	4:D:107:LEU:HB3	1.99	0.44
3:C:257:PHE:CD1	3:C:257:PHE:N	2.85	0.44
17:X:128:UNK:O	17:X:129:UNK:C	2.66	0.44
3:C:42:LEU:HD11	23:C:501:CLA:C1A	2.48	0.44
3:C:292:PHE:HB3	30:C:507:DGD:HD62	1.99	0.44
23:A:558:CLA:HBD	23:A:559:CLA:HAC2	1.99	0.44
10:K:21:LEU:HD11	28:X:130:BCR:HC42	1.99	0.44
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.00	0.44
10:K:17:ILE:CD1	18:Z:6:GLN:NE2	2.78	0.44
4:D:60:THR:CG2	4:D:61:HIS:H	2.31	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:452:ALA:C	3:C:454:GLY:H	2.21	0.44
24:A:561:PHO:HED2	4:D:257:PHE:CE2	2.52	0.44
5:E:17:VAL:HA	9:J:8:ILE:HD11	2.00	0.44
5:E:26:THR:O	5:E:29:ALA:HB3	2.18	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.33	0.44
10:K:13:GLU:O	10:K:16:ALA:HB3	2.18	0.44
13:O:241:PHE:CD1	13:O:241:PHE:C	2.90	0.44
2:B:450:TRP:O	2:B:451:PHE:C	2.55	0.44
5:E:51:ARG:O	5:E:54:SER:N	2.48	0.44
2:B:476:ARG:HG3	2:B:476:ARG:NH1	2.33	0.44
15:U:98:THR:C	15:U:100:ARG:N	2.71	0.44
3:C:135:ARG:O	3:C:136:GLY:O	2.35	0.44
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.44	0.44
3:C:405:ASN:HB2	30:C:509:DGD:HG32	2.00	0.44
23:C:501:CLA:HMD2	10:K:40:GLN:CD	2.37	0.44
13:O:52:ALA:HA	13:O:230:VAL:O	2.18	0.44
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.99	0.44
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.48	0.44
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	0.43
2:B:450:TRP:O	2:B:453:PHE:N	2.51	0.43
10:K:15:TYR:OH	18:Z:58:ASN:HB2	2.17	0.43
11:L:7:ARG:HD2	11:L:7:ARG:HA	1.69	0.43
2:B:341:LYS:HB3	2:B:406:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:21:TRP:CE2	4:D:26:ARG:NH2	2.78	0.43
3:C:321:ASP:OD2	15:U:129:ASN:HB2	2.18	0.43
3:C:225:VAL:HG12	3:C:225:VAL:O	2.18	0.43
2:B:36:SER:OG	28:B:528:BCR:H362	2.18	0.43
23:C:498:CLA:H122	23:C:500:CLA:HED1	2.00	0.43
3:C:134:ILE:HD11	23:C:501:CLA:H92	2.00	0.43
4:D:256:ILE:O	4:D:256:ILE:HG12	2.19	0.43
4:D:263:ASN:HB3	29:D:360:MGE:O3D	2.19	0.43
7:H:19:GLY:O	7:H:21:VAL:HG12	2.17	0.43
2:B:193:TYR:HE1	2:B:260:SER:N	2.17	0.43
4:D:93:TRP:CZ2	23:D:355:CLA:O1A	2.71	0.43
2:B:217:ILE:HG22	2:B:218:LEU:HD23	1.99	0.43
1:A:48:PHE:HA	1:A:115:ILE:CD1	2.48	0.43
16:V:117:VAL:O	16:V:117:VAL:HG12	2.17	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.91	0.43
2:B:31:ALA:N	23:B:515:CLA:HBC3	2.33	0.43
3:C:305:THR:HB	3:C:308:GLU:HB2	1.99	0.43
28:D:357:BCR:H383	29:D:358:MGE:H6B1	2.00	0.43
15:U:78:LEU:HD13	15:U:97:LEU:HD21	2.01	0.43
13:O:231:ASP:O	13:O:232:GLY:C	2.56	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.54	0.43
18:Z:12:LEU:HA	18:Z:50:LEU:HD13	1.99	0.43
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43
23:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43
1:A:76:ASN:HD21	1:A:79:THR:H	1.66	0.43
23:B:520:CLA:H122	23:B:522:CLA:H43	2.00	0.43
4:D:120:PHE:CD1	4:D:123:ILE:HD12	2.53	0.43
4:D:157:PHE:CE2	4:D:171:PRO:HB2	2.53	0.43
23:C:491:CLA:H42	23:C:492:CLA:HMD1	2.00	0.43
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.43
26:D:356:PQ9:H61	26:D:356:PQ9:H91	1.75	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
2:B:332:LYS:HG3	2:B:444:ARG:HH21	1.84	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
2:B:318:ASN:ND2	2:B:361:ALA:HB2	2.34	0.43
28:X:130:BCR:HC31	18:Z:13:VAL:HG13	2.00	0.43
17:X:102:UNK:O	17:X:103:UNK:C	2.66	0.43
3:C:33:PHE:HE1	4:D:229:ALA:HB2	1.82	0.43
13:O:153:ALA:HB1	13:O:168:PHE:HB3	2.00	0.43
5:E:6:GLY:O	5:E:7:GLU:HG2	2.18	0.43
1:A:32:TRP:CE2	8:I:22:GLY:HA3	2.53	0.43
23:C:498:CLA:H191	30:C:509:DGD:HA91	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:148:ALA:CB	4:D:149:PRO:HD3	2.35	0.43
4:D:246:MET:HE3	4:D:263:ASN:N	2.34	0.43
1:A:225:ARG:NH1	2:B:484:PRO:HD3	2.34	0.43
2:B:271:THR:HG22	2:B:273:TYR:N	2.34	0.43
2:B:188:ASP:C	2:B:190:PHE:H	2.22	0.43
2:B:191:ASN:HD22	2:B:191:ASN:C	2.20	0.43
1:A:25:ASP:HA	4:D:251:ARG:NH2	2.32	0.43
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.54	0.43
6:F:22:ALA:O	6:F:24:HIS:N	2.52	0.43
1:A:284:TRP:O	1:A:287:ALA:HB3	2.18	0.43
17:X:127:UNK:CG	17:X:128:UNK:N	2.81	0.43
3:C:206:PRO:O	3:C:207:ARG:C	2.57	0.43
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.43
4:D:53:THR:HG22	4:D:67:TYR:CE1	2.53	0.43
2:B:208:VAL:HG21	23:B:512:CLA:CMC	2.48	0.43
2:B:403:GLY:O	2:B:407:ASN:HB2	2.18	0.43
1:A:35:VAL:HG22	28:A:566:BCR:HC42	2.00	0.43
14:T:4:ILE:CD1	14:T:4:ILE:C	2.85	0.43
4:D:178:ILE:CG2	4:D:179:PHE:N	2.81	0.43
3:C:205:ASP:C	3:C:205:ASP:OD2	2.57	0.43
23:C:491:CLA:CAD	23:C:493:CLA:H12	2.49	0.43
2:B:368:VAL:O	2:B:368:VAL:HG13	2.19	0.43
13:O:231:ASP:OD1	13:O:231:ASP:O	2.37	0.43
3:C:214:LEU:N	3:C:214:LEU:HD23	2.31	0.43
2:B:360:PRO:O	2:B:362:PHE:N	2.51	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	0.43
3:C:168:LEU:HD13	23:C:497:CLA:H2	2.01	0.43
28:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	0.43
3:C:180:MET:SD	3:C:202:PRO:HG2	2.57	0.43
4:D:134:ARG:HA	4:D:134:ARG:NE	2.34	0.43
3:C:385:GLN:HB2	3:C:387:TRP:CD1	2.54	0.43
23:B:515:CLA:CHA	23:B:515:CLA:HBA1	2.48	0.43
3:C:404:LEU:C	3:C:406:SER:H	2.23	0.43
4:D:35:ILE:O	4:D:39:PRO:HG2	2.18	0.43
15:U:66:ILE:HD11	15:U:72:TYR:CZ	2.54	0.43
2:B:221:PRO:O	2:B:222:PRO:C	2.56	0.43
13:O:32:THR:H	13:O:35:ASP:CB	2.28	0.43
2:B:464:PHE:HD2	23:B:521:CLA:HAC2	1.83	0.43
3:C:394:GLU:O	3:C:398:HIS:HD2	2.02	0.43
3:C:323:LYS:O	3:C:324:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:T:22:PHE:O	14:T:23:PHE:CD2	2.71	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.00	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
3:C:87:ILE:C	3:C:90:PRO:HD2	2.39	0.42
3:C:417:VAL:O	3:C:417:VAL:HG13	2.18	0.42
3:C:201:ASN:O	3:C:202:PRO:C	2.58	0.42
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.54	0.42
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.79	0.42
2:B:31:ALA:CA	23:B:515:CLA:HBC3	2.49	0.42
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.01	0.42
3:C:29:GLU:O	3:C:31:SER:N	2.52	0.42
3:C:452:ALA:O	3:C:454:GLY:N	2.52	0.42
1:A:206:PHE:CD1	24:A:562:PHO:HBB2	2.54	0.42
2:B:271:THR:CG2	2:B:273:TYR:N	2.79	0.42
2:B:271:THR:HG22	2:B:273:TYR:H	1.82	0.42
13:O:120:THR:OG1	13:O:154:SER:HB3	2.19	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.42
3:C:104:GLU:O	3:C:105:VAL:C	2.57	0.42
17:X:118:UNK:C	17:X:120:UNK:N	2.80	0.42
4:D:313:THR:C	4:D:315:TYR:N	2.72	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
23:B:518:CLA:HBA1	23:B:518:CLA:HBD	2.00	0.42
4:D:246:MET:CE	4:D:264:LYS:HG3	2.49	0.42
4:D:40:CYS:O	4:D:43:LEU:N	2.52	0.42
11:L:12:LEU:CD1	12:M:25:LEU:HD12	2.49	0.42
2:B:90:PHE:CZ	2:B:98:LEU:HD23	2.55	0.42
3:C:201:ASN:N	3:C:202:PRO:CD	2.82	0.42
2:B:314:TYR:CZ	2:B:316:GLY:HA3	2.55	0.42
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.85	0.42
13:O:30:THR:HG22	13:O:31:LEU:N	2.33	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
1:A:225:ARG:HH12	2:B:483:ASP:CA	2.19	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
1:A:261:GLN:O	1:A:264:SER:HB3	2.19	0.42
4:D:103:ARG:HA	4:D:103:ARG:HD3	1.81	0.42
23:B:524:CLA:H102	28:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:N	3:C:147:PHE:CD1	2.85	0.42
1:A:69:GLY:O	1:A:80:GLY:HA2	2.19	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	0.42
4:D:47:GLY:HA2	28:D:357:BCR:H332	2.01	0.42
2:B:271:THR:HG22	2:B:274:GLN:HG3	2.02	0.42
2:B:214:LEU:O	2:B:217:ILE:HB	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:125:ASP:O	2:B:128:THR:O	2.38	0.42
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.79	0.42
23:B:516:CLA:H72	28:B:529:BCR:H311	2.02	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.25	0.42
3:C:113:VAL:O	3:C:117:VAL:HG23	2.20	0.42
16:V:64:ALA:O	16:V:65:SER:C	2.57	0.42
17:X:23:UNK:CG2	18:Z:25:VAL:HG11	2.50	0.42
17:X:54:UNK:O	17:X:55:UNK:C	2.66	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	0.42
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.42
3:C:171:GLY:HA3	23:C:502:CLA:H41	2.01	0.42
3:C:472:LEU:HD12	3:C:472:LEU:H	1.84	0.42
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.42
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.42
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.49	0.42
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	0.42
1:A:33:PHE:CE1	1:A:128:GLY:HA3	2.55	0.42
14:T:2:GLU:O	14:T:3:THR:C	2.57	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:103:LEU:HD21	23:B:515:CLA:HMC3	2.01	0.42
3:C:168:LEU:CD1	23:C:497:CLA:H2	2.49	0.42
1:A:184:ILE:HA	23:A:558:CLA:HBC1	2.02	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
25:V:552:HEM:HAD2	25:V:552:HEM:HHA	1.56	0.42
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
12:M:15:VAL:O	12:M:19:SER:CB	2.68	0.42
7:H:54:ILE:O	7:H:55:LEU:HD23	2.20	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
23:B:515:CLA:H152	23:B:520:CLA:HED1	2.02	0.42
7:H:12:ARG:N	7:H:13:PRO:CD	2.82	0.42
1:A:257:ARG:HH12	1:A:261:GLN:NE2	2.18	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.83	0.42
11:L:12:LEU:HD13	12:M:25:LEU:HB2	2.02	0.42
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.82	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:B:30:VAL:O	2:B:30:VAL:HG12	2.19	0.42
16:V:29:LEU:HG	16:V:29:LEU:O	2.18	0.42
13:O:98:THR:CG2	13:O:99:ARG:N	2.70	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:44:LYS:HA	13:O:72:GLN:CD	2.40	0.42
3:C:405:ASN:ND2	30:C:509:DGD:HD5	2.26	0.42
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	0.42
4:D:274:VAL:HG13	26:D:356:PQ9:H251	2.02	0.42
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	0.42
3:C:138:GLU:O	3:C:139:THR:HB	2.20	0.42
5:E:37:PHE:CD1	5:E:42:LEU:HD23	2.55	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.20	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
13:O:266:TYR:CG	13:O:267:ALA:N	2.88	0.41
13:O:45:CYS:CB	13:O:46:PRO:HD2	2.31	0.41
23:C:493:CLA:H171	23:C:500:CLA:HBB2	2.01	0.41
23:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	0.41
1:A:314:ILE:O	1:A:315:ASN:O	2.38	0.41
4:D:270:PHE:HZ	26:D:356:PQ9:H243	1.85	0.41
2:B:462:PHE:CZ	23:B:523:CLA:HMB3	2.55	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
3:C:61:VAL:O	3:C:62:PHE:C	2.57	0.41
31:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
4:D:267:LEU:C	4:D:267:LEU:CD2	2.88	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	0.41
3:C:322:GLN:O	3:C:324:LEU:N	2.49	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
2:B:10:THR:C	2:B:12:LEU:N	2.73	0.41
8:I:33:LYS:HA	8:I:34:ARG:NH2	2.16	0.41
6:F:40:MET:C	6:F:42:PHE:N	2.74	0.41
16:V:75:ASN:N	16:V:76:PRO:HD3	2.35	0.41
13:O:106:GLN:N	13:O:106:GLN:HE21	2.18	0.41
15:U:69:ARG:HG3	15:U:70:GLY:N	2.33	0.41
3:C:120:ILE:C	3:C:122:SER:H	2.23	0.41
3:C:120:ILE:C	3:C:122:SER:N	2.73	0.41
1:A:76:ASN:ND2	1:A:76:ASN:C	2.73	0.41
3:C:334:PRO:O	13:O:182:PHE:HB2	2.19	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.55	0.41
17:X:52:UNK:O	17:X:54:UNK:N	2.54	0.41
23:B:513:CLA:CGA	23:B:513:CLA:H3A	2.50	0.41
4:D:178:ILE:O	4:D:181:PHE:N	2.54	0.41
8:I:27:ASP:O	8:I:28:PRO:C	2.58	0.41
3:C:166:ILE:HG23	3:C:245:ILE:CG2	2.42	0.41
3:C:419:PHE:CD1	3:C:419:PHE:C	2.93	0.41
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.41
2:B:208:VAL:HG12	2:B:208:VAL:O	2.20	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.20	0.41
3:C:190:ALA:HB3	3:C:193:GLY:C	2.41	0.41
17:X:120:UNK:C	17:X:122:UNK:N	2.82	0.41
1:A:292:THR:C	1:A:294:ALA:H	2.23	0.41
4:D:259:ILE:HG22	4:D:260:ALA:N	2.34	0.41
1:A:54:ALA:O	1:A:55:ALA:CB	2.69	0.41
28:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
13:O:77:LEU:N	13:O:77:LEU:CD1	2.81	0.41
23:B:521:CLA:C4	23:B:524:CLA:HBC3	2.50	0.41
3:C:75:PHE:CE2	3:C:105:VAL:HG11	2.56	0.41
3:C:95:LEU:O	3:C:185:LEU:HD23	2.21	0.41
2:B:359:MET:HB2	2:B:425:ILE:HG23	2.02	0.41
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.01	0.41
16:V:59:PHE:CD1	16:V:63:CYS:HB2	2.56	0.41
16:V:64:ALA:HB1	16:V:68:VAL:HG12	2.03	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.21	0.41
7:H:46:LEU:HD11	30:H:208:DGD:HA22	2.02	0.41
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.41
2:B:61:PHE:HZ	23:B:517:CLA:HBB1	1.85	0.41
4:D:159:ILE:O	4:D:160:TYR:C	2.58	0.41
3:C:418:ASN:HB3	30:C:509:DGD:C2E	2.51	0.41
3:C:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
17:X:4:UNK:O	17:X:5:UNK:C	2.69	0.41
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.20	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	0.41
1:A:321:ILE:HG22	1:A:322:ASN:N	2.35	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
3:C:56:HIS:O	3:C:59:LEU:N	2.53	0.41
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	0.41
3:C:42:LEU:HG	23:C:501:CLA:O1D	2.20	0.41
10:K:43:VAL:HG21	17:X:31:UNK:CG	2.51	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:17:ILE:HD11	18:Z:6:GLN:NE2	2.31	0.41
2:B:272:ARG:HH12	4:D:164:GLN:HG3	1.86	0.41
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
3:C:416:SER:C	3:C:417:VAL:HG12	2.41	0.41
3:C:229:ASN:HD22	3:C:231:GLU:CG	2.34	0.41
23:C:502:CLA:HBA2	23:C:502:CLA:O2D	2.20	0.41
10:K:18:PHE:CD1	10:K:18:PHE:N	2.89	0.41
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.28	0.41
3:C:438:LEU:HD21	30:C:507:DGD:HAH2	2.02	0.41
3:C:109:PHE:O	3:C:110:PRO:C	2.59	0.41
1:A:13:LEU:H	1:A:13:LEU:CD2	2.33	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
3:C:146:PHE:CD2	3:C:147:PHE:CE1	3.09	0.41
1:A:78:ILE:HD12	1:A:78:ILE:N	2.36	0.41
2:B:410:THR:HG22	2:B:411:PHE:N	2.36	0.41
5:E:16:SER:OG	5:E:19:TYR:HB2	2.21	0.41
2:B:68:ARG:HH12	23:B:514:CLA:CED	2.33	0.40
23:B:518:CLA:HBA1	23:B:518:CLA:CHA	2.51	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	0.40
4:D:38:PHE:HZ	4:D:128:ARG:NH2	2.18	0.40
1:A:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
23:C:494:CLA:HBA1	23:C:494:CLA:CHA	2.52	0.40
2:B:87:ASP:O	2:B:88:PRO:C	2.58	0.40
12:M:17:VAL:HG12	12:M:18:PRO:N	2.35	0.40
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.40
3:C:173:LEU:HD23	3:C:173:LEU:HA	1.86	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
2:B:12:LEU:CD1	23:B:522:CLA:HBB1	2.51	0.40
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.89	0.40
10:K:45:PHE:C	10:K:46:ARG:OXT	2.58	0.40
8:I:31:ASN:HB2	8:I:32:PRO:HD2	2.03	0.40
24:A:561:PHO:HND	4:D:209:LEU:HD12	1.87	0.40
13:O:142:ILE:N	13:O:142:ILE:CD1	2.84	0.40
2:B:74:SER:C	2:B:76:SER:N	2.74	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
15:U:69:ARG:HB2	15:U:69:ARG:HE	1.69	0.40
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.40
8:I:30:ARG:H	8:I:30:ARG:HG2	1.60	0.40
2:B:450:TRP:HB3	23:B:517:CLA:HMB2	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:164:PRO:HD3	23:B:516:CLA:O1D	2.22	0.40
2:B:230:ARG:NH1	2:B:474:LEU:HD22	2.36	0.40
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.79	0.40
23:C:491:CLA:HMA1	28:C:506:BCR:H401	2.02	0.40
17:X:85:UNK:N	17:X:85:UNK:OD1	2.54	0.40
1:A:206:PHE:HA	1:A:206:PHE:HD2	1.75	0.40
29:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.40
4:D:103:ARG:O	4:D:106:GLN:N	2.55	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40
17:X:62:UNK:O	17:X:66:UNK:N	2.55	0.40
14:T:22:PHE:O	14:T:23:PHE:CG	2.75	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
1:A:131:TRP:CD2	1:A:132:GLU:N	2.89	0.40
4:D:34:GLY:C	4:D:36:LEU:H	2.25	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
3:C:252:ILE:HG22	3:C:252:ILE:O	2.21	0.40
8:I:24:LEU:O	8:I:26:GLY:N	2.48	0.40
1:A:255:PHE:CE2	26:A:564:PQ9:H151	2.57	0.40
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.40
15:U:54:LYS:HB3	15:U:111:HIS:O	2.21	0.40

There are no symmetry-related clashes.

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	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	4	22
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	3	18
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	5	26
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	3	16
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	3	15
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	4	21
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	4	24
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	2	8
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	2	8
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	14
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	14
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	1	4
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	1	4
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	7	34
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	7	34
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	1	5
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	1	5
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	16
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	5
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	3	16
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	5
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	2	14
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	2	14
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	2	9
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	2	9
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	2	8
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	2	8
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	3	18
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	3	18
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	2	10
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	2	10
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	3	17

All (269) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN
2	B	230	ARG
2	B	260	SER
2	B	362	PHE
2	B	488	PRO
3	C	154	LYS
3	C	324	LEU
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	257	PHE
4	D	262	SER
5	E	7	GLU
5	E	58	GLN
5	E	60	GLN
7	H	18	TYR
7	H	64	ALA
13	O	46	PRO
13	O	52	ALA
13	O	86	ARG
13	O	115	SER
13	O	140	GLU
13	O	175	PRO
15	U	72	TYR
15	U	73	PRO
15	U	83	ALA
16	V	133	LEU
16	V	160	LYS
1	a	5011	ALA
1	a	5012	ASN
1	a	5063	ILE
1	a	5141	PRO
1	a	5142	TRP
1	a	5315	ASN
2	b	5230	ARG
2	b	5260	SER
2	b	5362	PHE
2	b	5488	PRO

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Mol	Chain	Res	Type
3	c	5154	LYS
3	c	5226	SER
3	c	5324	LEU
3	c	5416	SER
4	d	5239	GLN
4	d	5240	ALA
4	d	5262	SER
5	e	5007	GLU
5	e	5058	GLN
5	e	5060	GLN
7	h	5018	TYR
7	h	5064	ALA
13	o	5046	PRO
13	o	5052	ALA
13	o	5086	ARG
13	o	5115	SER
13	o	5140	GLU
13	o	5175	PRO
15	u	5072	TYR
15	u	5073	PRO
15	u	5083	ALA
16	v	5133	LEU
16	v	5160	LYS
1	A	12	ASN
1	A	130	GLN
1	A	261	GLN
1	A	266	ASN
2	B	11	VAL
2	B	85	GLY
2	B	176	GLY
2	B	231	MET
3	C	57	ALA
3	C	136	GLY
3	C	139	THR
3	C	141	GLU
3	C	144	SER
3	C	207	ARG
3	C	209	ILE
3	C	226	SER
3	C	242	LEU
4	D	92	LEU
4	D	263	ASN

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Mol	Chain	Res	Type
5	E	48	GLY
7	H	26	GLY
8	I	25	SER
9	J	35	GLY
10	K	13	GLU
10	K	16	ALA
12	M	34	LYS
13	O	50	ASP
13	O	84	ASN
13	O	88	GLU
13	O	138	GLY
13	O	161	SER
15	U	70	GLY
18	Z	31	GLN
18	Z	32	ASP
1	a	5055	ALA
1	a	5130	GLN
1	a	5242	GLU
1	a	5266	ASN
2	b	5011	VAL
2	b	5085	GLY
3	c	5136	GLY
3	c	5141	GLU
3	c	5144	SER
3	c	5207	ARG
3	c	5209	ILE
4	d	5092	LEU
4	d	5192	THR
4	d	5252	PHE
4	d	5257	PHE
4	d	5263	ASN
5	e	5048	GLY
6	f	5041	GLN
7	h	5026	GLY
8	i	5025	SER
9	j	5035	GLY
10	k	5013	GLU
10	k	5016	ALA
12	m	5034	LYS
13	o	5050	ASP
13	o	5084	ASN
13	o	5088	GLU

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Mol	Chain	Res	Type
13	o	5138	GLY
13	o	5161	SER
13	o	5233	ARG
15	u	5070	GLY
18	z	5031	GLN
18	z	5032	ASP
1	A	55	ALA
1	A	59	ASP
1	A	242	GLU
1	A	306	VAL
2	B	228	ALA
3	C	39	ASN
3	C	194	GLY
3	C	221	GLU
4	D	25	ASP
4	D	192	THR
4	D	252	PHE
4	D	351	ALA
5	E	52	PRO
6	F	41	GLN
7	H	3	ARG
7	H	59	ASN
9	J	14	ALA
11	L	5	PRO
11	L	7	ARG
13	O	233	ARG
15	U	88	VAL
16	V	75	ASN
1	a	5059	ASP
1	a	5261	GLN
1	a	5306	VAL
2	b	5176	GLY
2	b	5228	ALA
3	c	5039	ASN
3	c	5057	ALA
3	c	5139	THR
3	c	5221	GLU
3	c	5242	LEU
4	d	5025	ASP
4	d	5041	ALA
4	d	5351	ALA
5	e	5052	PRO

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Mol	Chain	Res	Type
7	h	5059	ASN
9	j	5011	TRP
11	l	5005	PRO
11	l	5007	ARG
13	o	5167	ASP
13	o	5232	GLY
15	u	5088	VAL
16	v	5064	ALA
1	A	232	SER
1	A	260	PHE
2	B	91	TRP
2	B	485	GLU
3	C	30	SER
3	C	38	GLY
3	C	77	PRO
3	C	205	ASP
3	C	298	PRO
4	D	41	ALA
4	D	177	ALA
4	D	261	PHE
9	J	11	TRP
13	O	167	ASP
13	O	232	GLY
15	U	60	THR
16	V	65	SER
1	a	5260	PHE
2	b	5231	MET
2	b	5485	GLU
3	c	5194	GLY
3	c	5205	ASP
4	d	5062	GLY
7	h	5003	ARG
9	j	5014	ALA
16	v	5129	LYS
2	B	16	PRO
2	B	89	GLY
2	B	386	ALA
3	C	227	VAL
3	C	382	ASN
4	D	29	PHE
4	D	62	GLY
12	M	17	VAL

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Mol	Chain	Res	Type
13	O	139	GLY
16	V	129	LYS
1	a	5172	MET
1	a	5217	SER
2	b	5089	GLY
2	b	5122	LEU
2	b	5361	ALA
3	c	5030	SER
3	c	5077	PRO
3	c	5153	ASP
3	c	5227	VAL
3	c	5298	PRO
3	c	5382	ASN
4	d	5177	ALA
16	v	5075	ASN
2	B	361	ALA
3	C	243	ILE
13	O	185	PRO
3	c	5038	GLY
3	c	5134	ILE
4	d	5264	LYS
12	m	5017	VAL
13	o	5139	GLY
16	v	5065	SER
2	B	8	VAL
6	F	23	VAL
18	Z	24	PRO
2	b	5016	PRO
3	c	5243	ILE
13	o	5185	PRO
15	u	5066	ILE
2	B	414	PRO
3	C	105	VAL
3	C	134	ILE
13	O	117	GLY
2	b	5008	VAL
2	b	5414	PRO
18	z	5003	ILE
4	D	80	THR
18	Z	3	ILE
1	a	5060	ILE
3	c	5105	VAL

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Mol	Chain	Res	Type
6	f	5023	VAL
7	h	5058	VAL
18	z	5024	PRO
2	B	86	ILE
2	B	232	GLY
7	H	58	VAL
15	U	66	ILE
16	V	71	ILE
16	V	161	VAL
2	b	5086	ILE
10	k	5012	PRO
13	o	5117	GLY
5	E	25	ILE
5	e	5025	ILE
11	l	5003	PRO
15	u	5062	ILE
16	v	5071	ILE

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	269/280 (96%)	251 (93%)	18 (7%)	23	64
1	a	269/280 (96%)	252 (94%)	17 (6%)	25	66
2	B	378/407 (93%)	361 (96%)	17 (4%)	38	81
2	b	378/407 (93%)	360 (95%)	18 (5%)	35	79
3	C	341/374 (91%)	320 (94%)	21 (6%)	26	67
3	c	341/374 (91%)	320 (94%)	21 (6%)	26	67
4	D	273/283 (96%)	259 (95%)	14 (5%)	33	76
4	d	273/283 (96%)	258 (94%)	15 (6%)	30	73
5	E	68/73 (93%)	65 (96%)	3 (4%)	39	82
5	e	68/73 (93%)	66 (97%)	2 (3%)	55	90
6	F	27/39 (69%)	26 (96%)	1 (4%)	45	86
6	f	27/39 (69%)	26 (96%)	1 (4%)	45	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	50/55 (91%)	42 (84%)	8 (16%)	3	17
7	h	50/55 (91%)	43 (86%)	7 (14%)	5	23
8	I	32/35 (91%)	27 (84%)	5 (16%)	4	18
8	i	32/35 (91%)	27 (84%)	5 (16%)	4	18
9	J	22/28 (79%)	21 (96%)	1 (4%)	38	81
9	j	22/28 (79%)	21 (96%)	1 (4%)	38	81
10	K	29/30 (97%)	28 (97%)	1 (3%)	49	88
10	k	29/30 (97%)	28 (97%)	1 (3%)	49	88
11	L	34/35 (97%)	31 (91%)	3 (9%)	14	48
11	l	34/35 (97%)	31 (91%)	3 (9%)	14	48
12	M	32/33 (97%)	32 (100%)	0	100	100
12	m	32/33 (97%)	32 (100%)	0	100	100
13	O	181/208 (87%)	171 (94%)	10 (6%)	30	73
13	o	181/208 (87%)	172 (95%)	9 (5%)	34	77
14	T	26/29 (90%)	25 (96%)	1 (4%)	44	85
14	t	26/29 (90%)	25 (96%)	1 (4%)	44	85
15	U	83/89 (93%)	80 (96%)	3 (4%)	47	86
15	u	83/89 (93%)	80 (96%)	3 (4%)	47	86
16	V	117/117 (100%)	113 (97%)	4 (3%)	49	88
16	v	117/117 (100%)	111 (95%)	6 (5%)	33	76
18	Z	43/52 (83%)	42 (98%)	1 (2%)	63	93
18	z	43/52 (83%)	42 (98%)	1 (2%)	63	93
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	30	73

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	16	ARG
1	A	24	THR
1	A	25	ASP
1	A	30	VAL
1	A	76	ASN

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Mol	Chain	Res	Type
1	A	103	ASP
1	A	131	TRP
1	A	155	PHE
1	A	177	SER
1	A	206	PHE
1	A	232	SER
1	A	241	GLN
1	A	286	THR
1	A	292	THR
1	A	297	LEU
1	A	308	ASP
2	B	36	SER
2	B	124	ARG
2	B	137	LYS
2	B	179	GLN
2	B	191	ASN
2	B	222	PRO
2	B	231	MET
2	B	233	ASN
2	B	246	PHE
2	B	262	THR
2	B	271	THR
2	B	309	LEU
2	B	350	GLU
2	B	354	LEU
2	B	362	PHE
2	B	414	PRO
2	B	478	VAL
3	C	27	ASP
3	C	29	GLU
3	C	67	MET
3	C	86	LEU
3	C	97	TRP
3	C	155	ASN
3	C	165	LEU
3	C	191	PRO
3	C	214	LEU
3	C	244	CYS
3	C	254	THR
3	C	262	ARG
3	C	289	PHE
3	C	298	PRO

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Mol	Chain	Res	Type
3	C	355	THR
3	C	377	LEU
3	C	383	ASP
3	C	419	PHE
3	C	428	THR
3	C	472	LEU
3	C	473	ASP
4	D	14	TRP
4	D	63	LEU
4	D	130	PHE
4	D	164	GLN
4	D	178	ILE
4	D	180	ARG
4	D	191	TRP
4	D	241	GLU
4	D	246	MET
4	D	250	ASN
4	D	294	ARG
4	D	304	ARG
4	D	323	GLU
4	D	346	LEU
5	E	4	THR
5	E	17	VAL
5	E	52	PRO
6	F	17	THR
7	H	12	ARG
7	H	21	VAL
7	H	27	THR
7	H	41	PHE
7	H	49	TYR
7	H	50	ASN
7	H	53	LEU
7	H	59	ASN
8	I	2	GLU
8	I	27	ASP
8	I	30	ARG
8	I	32	PRO
8	I	34	ARG
9	J	29	PHE
10	K	11	LEU
11	L	3	PRO
11	L	14	ARG

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Mol	Chain	Res	Type
11	L	16	SER
13	O	46	PRO
13	O	50	ASP
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	120	THR
13	O	168	PHE
13	O	206	GLU
13	O	216	PHE
13	O	223	ILE
14	T	4	ILE
15	U	46	LYS
15	U	61	ASN
15	U	90	ASP
16	V	81	ARG
16	V	111	GLU
16	V	122	ARG
16	V	128	PRO
18	Z	58	ASN
1	a	5012	ASN
1	a	5013	LEU
1	a	5016	ARG
1	a	5025	ASP
1	a	5030	VAL
1	a	5076	ASN
1	a	5103	ASP
1	a	5131	TRP
1	a	5155	PHE
1	a	5177	SER
1	a	5206	PHE
1	a	5232	SER
1	a	5241	GLN
1	a	5286	THR
1	a	5292	THR
1	a	5297	LEU
1	a	5308	ASP
2	b	5016	PRO
2	b	5036	SER
2	b	5124	ARG
2	b	5137	LYS
2	b	5179	GLN

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Mol	Chain	Res	Type
2	b	5191	ASN
2	b	5222	PRO
2	b	5231	MET
2	b	5233	ASN
2	b	5245	VAL
2	b	5246	PHE
2	b	5262	THR
2	b	5271	THR
2	b	5309	LEU
2	b	5350	GLU
2	b	5362	PHE
2	b	5467	ILE
2	b	5478	VAL
3	c	5027	ASP
3	c	5029	GLU
3	c	5067	MET
3	c	5086	LEU
3	c	5097	TRP
3	c	5155	ASN
3	c	5165	LEU
3	c	5191	PRO
3	c	5214	LEU
3	c	5244	CYS
3	c	5254	THR
3	c	5262	ARG
3	c	5289	PHE
3	c	5298	PRO
3	c	5355	THR
3	c	5377	LEU
3	c	5383	ASP
3	c	5419	PHE
3	c	5428	THR
3	c	5472	LEU
3	c	5473	ASP
4	d	5014	TRP
4	d	5063	LEU
4	d	5090	LEU
4	d	5130	PHE
4	d	5164	GLN
4	d	5178	ILE
4	d	5180	ARG
4	d	5191	TRP

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Mol	Chain	Res	Type
4	d	5241	GLU
4	d	5246	MET
4	d	5250	ASN
4	d	5294	ARG
4	d	5304	ARG
4	d	5323	GLU
4	d	5346	LEU
5	e	5017	VAL
5	e	5052	PRO
6	f	5017	THR
7	h	5012	ARG
7	h	5021	VAL
7	h	5027	THR
7	h	5041	PHE
7	h	5049	TYR
7	h	5050	ASN
7	h	5059	ASN
8	i	5002	GLU
8	i	5027	ASP
8	i	5030	ARG
8	i	5032	PRO
8	i	5034	ARG
9	j	5029	PHE
10	k	5011	LEU
11	l	5010	VAL
11	l	5014	ARG
11	l	5016	SER
13	o	5046	PRO
13	o	5050	ASP
13	o	5097	VAL
13	o	5106	GLN
13	o	5114	ASN
13	o	5120	THR
13	o	5168	PHE
13	o	5216	PHE
13	o	5223	ILE
14	t	5004	ILE
15	u	5046	LYS
15	u	5061	ASN
15	u	5090	ASP
16	v	5035	THR
16	v	5037	PRO

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Mol	Chain	Res	Type
16	v	5081	ARG
16	v	5111	GLU
16	v	5122	ARG
16	v	5128	PRO
18	z	5058	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	75	ASN
1	A	76	ASN
1	A	118	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	234	ASN
1	A	241	GLN
1	A	272	HIS
1	A	296	ASN
1	A	298	ASN
1	A	304	HIS
1	A	322	ASN
2	B	157	HIS
2	B	179	GLN
2	B	191	ASN
2	B	223	GLN
2	B	233	ASN
2	B	274	GLN
2	B	394	GLN
2	B	438	ASN
3	C	155	ASN
3	C	201	ASN
3	C	229	ASN
3	C	293	ASN
3	C	322	GLN
3	C	332	GLN
3	C	398	HIS
3	C	415	ASN
4	D	61	HIS
4	D	98	GLN

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Mol	Chain	Res	Type
4	D	224	GLN
4	D	250	ASN
4	D	255	GLN
5	E	58	GLN
6	F	41	GLN
7	H	15	ASN
12	M	5	GLN
13	O	72	GLN
13	O	106	GLN
13	O	114	ASN
13	O	130	GLN
13	O	262	GLN
15	U	108	ASN
16	V	104	ASN
16	V	144	HIS
18	Z	6	GLN
1	a	5012	ASN
1	a	5019	ASN
1	a	5075	ASN
1	a	5076	ASN
1	a	5118	HIS
1	a	5165	GLN
1	a	5241	GLN
1	a	5272	HIS
1	a	5296	ASN
1	a	5298	ASN
1	a	5304	HIS
1	a	5322	ASN
2	b	5157	HIS
2	b	5179	GLN
2	b	5191	ASN
2	b	5223	GLN
2	b	5233	ASN
2	b	5274	GLN
2	b	5289	GLN
2	b	5394	GLN
2	b	5438	ASN
3	c	5155	ASN
3	c	5201	ASN
3	c	5229	ASN
3	c	5293	ASN
3	c	5332	GLN

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Mol	Chain	Res	Type
3	c	5398	HIS
3	c	5415	ASN
4	d	5061	HIS
4	d	5098	GLN
4	d	5164	GLN
4	d	5224	GLN
4	d	5250	ASN
4	d	5255	GLN
5	e	5058	GLN
6	f	5041	GLN
7	h	5015	ASN
7	h	5059	ASN
12	m	5005	GLN
13	o	5072	GLN
13	o	5106	GLN
13	o	5114	ASN
13	o	5130	GLN
13	o	5262	GLN
15	u	5108	ASN
16	v	5104	ASN
16	v	5144	HIS
18	z	5006	GLN

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 180 ligands modelled in this entry, 34 are unknown and 4 are monoatomic - leaving 142 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$
32	SQD	A	5212	-	24,26,54	3.70	13 (54%)	33,37,65	3.01	10 (30%)
23	CLA	A	558	1	73,73,73	1.44	10 (13%)	95,113,113	1.56	19 (20%)
23	CLA	A	559	-	73,73,73	1.32	9 (12%)	95,113,113	1.45	17 (17%)
23	CLA	A	560	-	73,73,73	1.40	10 (13%)	95,113,113	1.53	19 (20%)
24	PHO	A	561	-	69,69,69	1.75	9 (13%)	91,99,99	1.55	18 (19%)
24	PHO	A	562	-	69,69,69	2.09	7 (10%)	91,99,99	1.59	17 (18%)
23	CLA	A	563	-	62,63,73	1.59	13 (20%)	81,101,113	1.58	18 (22%)
26	PQ9	A	564	-	30,30,45	0.96	2 (6%)	37,39,57	1.60	8 (21%)
27	OEC	A	565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	A	566	-	41,41,41	1.55	7 (17%)	56,56,56	2.06	21 (37%)
31	LHG	A	567	-	38,38,48	1.81	5 (13%)	44,44,54	1.42	4 (9%)
32	SQD	A	568	-	54,54,54	2.81	28 (51%)	65,65,65	2.79	18 (27%)
33	LMT	A	569	-	36,36,36	1.47	6 (16%)	47,47,47	1.08	1 (2%)
23	CLA	B	511	-	48,49,73	2.09	13 (27%)	64,84,113	1.56	12 (18%)
23	CLA	B	512	2	73,73,73	1.47	9 (12%)	95,113,113	1.50	18 (18%)
23	CLA	B	513	2	73,73,73	1.55	13 (17%)	95,113,113	1.58	18 (18%)
23	CLA	B	514	2	73,73,73	1.57	11 (15%)	95,113,113	1.50	18 (18%)
23	CLA	B	515	-	73,73,73	1.49	12 (16%)	95,113,113	1.65	21 (22%)
23	CLA	B	516	-	73,73,73	1.54	10 (13%)	95,113,113	1.52	19 (20%)
23	CLA	B	517	-	73,73,73	1.55	12 (16%)	95,113,113	1.66	23 (24%)
23	CLA	B	518	2	73,73,73	1.56	14 (19%)	95,113,113	1.56	20 (21%)
23	CLA	B	519	-	73,73,73	1.64	12 (16%)	95,113,113	1.49	19 (20%)
23	CLA	B	520	-	73,73,73	1.51	13 (17%)	95,113,113	1.48	19 (20%)
23	CLA	B	521	2	73,73,73	1.52	13 (17%)	95,113,113	1.55	19 (20%)
23	CLA	B	522	-	73,73,73	1.57	13 (17%)	95,113,113	1.52	16 (16%)
23	CLA	B	523	-	73,73,73	1.53	12 (16%)	95,113,113	1.49	19 (20%)
23	CLA	B	524	2	64,64,73	2.20	13 (20%)	83,102,113	1.60	19 (22%)
23	CLA	B	525	-	73,73,73	1.59	12 (16%)	95,113,113	1.53	16 (16%)
23	CLA	B	526	-	73,73,73	1.66	16 (21%)	95,113,113	1.51	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	B	527	-	41,41,41	1.70	8 (19%)	56,56,56	2.00	16 (28%)
28	BCR	B	528	-	41,41,41	1.82	7 (17%)	56,56,56	1.93	16 (28%)
28	BCR	B	529	-	41,41,41	1.79	8 (19%)	56,56,56	2.14	20 (35%)
29	MGE	B	530	-	48,48,48	1.16	6 (12%)	56,56,56	1.22	6 (10%)
23	CLA	C	491	3	73,73,73	1.45	10 (13%)	95,113,113	1.43	17 (17%)
23	CLA	C	492	3	67,68,73	1.59	13 (19%)	87,107,113	1.58	18 (20%)
23	CLA	C	493	3	73,73,73	1.57	11 (15%)	95,113,113	1.57	20 (21%)
23	CLA	C	494	-	53,54,73	1.69	11 (20%)	71,90,113	1.82	18 (25%)
23	CLA	C	495	-	73,73,73	1.60	13 (17%)	95,113,113	1.63	20 (21%)
23	CLA	C	496	3	73,73,73	1.61	14 (19%)	95,113,113	1.53	19 (20%)
23	CLA	C	497	-	73,73,73	1.47	12 (16%)	95,113,113	1.53	21 (22%)
23	CLA	C	498	3	73,73,73	1.54	13 (17%)	95,113,113	1.54	18 (18%)
23	CLA	C	499	-	54,55,73	1.69	9 (16%)	72,91,113	1.79	20 (27%)
23	CLA	C	500	-	73,73,73	1.48	11 (15%)	95,113,113	1.45	19 (20%)
23	CLA	C	501	3	73,73,73	1.67	11 (15%)	95,113,113	1.51	19 (20%)
23	CLA	C	502	-	59,59,73	2.07	17 (28%)	77,96,113	1.70	19 (24%)
23	CLA	C	503	3	58,58,73	1.90	14 (24%)	75,95,113	1.58	15 (20%)
28	BCR	C	504	-	41,41,41	1.80	7 (17%)	56,56,56	2.14	23 (41%)
28	BCR	C	505	-	41,41,41	1.90	9 (21%)	56,56,56	2.05	18 (32%)
28	BCR	C	506	-	41,41,41	1.72	9 (21%)	56,56,56	2.14	21 (37%)
30	DGD	C	507	-	54,54,67	1.71	10 (18%)	68,68,81	1.52	7 (10%)
30	DGD	C	508	-	48,48,67	2.02	11 (22%)	62,62,81	1.75	11 (17%)
30	DGD	C	509	-	58,58,67	1.67	8 (13%)	72,72,81	1.43	7 (9%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	73,73,73	1.46	15 (20%)	95,113,113	1.62	17 (17%)
23	CLA	D	355	-	58,58,73	1.84	13 (22%)	75,95,113	1.61	17 (22%)
26	PQ9	D	356	-	30,30,45	0.93	1 (3%)	37,39,57	1.79	10 (27%)
28	BCR	D	357	-	41,41,41	1.91	9 (21%)	56,56,56	2.19	20 (35%)
29	MGE	D	358	-	47,47,48	1.26	6 (12%)	55,55,56	0.98	3 (5%)
29	MGE	D	359	-	41,41,48	2.09	6 (14%)	49,49,56	1.09	5 (10%)
29	MGE	D	360	-	48,48,48	0.90	3 (6%)	56,56,56	1.13	4 (7%)
25	HEM	F	51	5,6	49,50,50	3.39	28 (57%)	46,82,82	2.40	13 (28%)
28	BCR	H	107	-	41,41,41	2.03	7 (17%)	56,56,56	2.21	24 (42%)
30	DGD	H	208	-	55,55,67	1.72	11 (20%)	69,69,81	1.58	8 (11%)
29	MGE	I	201	-	48,48,48	1.07	6 (12%)	56,56,56	1.10	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MGE	L	210	-	48,48,48	0.94	3 (6%)	56,56,56	1.18	4 (7%)
32	SQD	L	5213	-	47,47,54	3.35	25 (53%)	58,58,65	2.90	14 (24%)
33	LMT	M	5216	-	36,36,36	1.40	7 (19%)	47,47,47	0.91	1 (2%)
33	LMT	T	217	-	36,36,36	1.36	4 (11%)	47,47,47	1.02	4 (8%)
28	BCR	T	5104	-	41,41,41	1.52	9 (21%)	56,56,56	2.23	23 (41%)
25	HEM	V	552	16	49,50,50	3.72	25 (51%)	46,82,82	2.31	14 (30%)
28	BCR	X	130	-	41,41,41	1.88	10 (24%)	56,56,56	2.47	23 (41%)
32	SQD	a	212	-	24,26,54	4.07	14 (58%)	33,37,65	3.11	10 (30%)
23	CLA	a	5558	1	73,73,73	1.46	15 (20%)	95,113,113	1.49	19 (20%)
23	CLA	a	5559	-	73,73,73	1.45	11 (15%)	95,113,113	1.47	16 (16%)
23	CLA	a	5560	-	73,73,73	1.51	13 (17%)	95,113,113	1.50	18 (18%)
24	PHO	a	5561	-	69,69,69	1.89	10 (14%)	91,99,99	1.51	14 (15%)
24	PHO	a	5562	-	69,69,69	2.02	8 (11%)	91,99,99	1.56	16 (17%)
23	CLA	a	5563	-	62,63,73	1.71	14 (22%)	81,101,113	1.54	15 (18%)
26	PQ9	a	5564	-	30,30,45	1.01	1 (3%)	37,39,57	1.57	8 (21%)
27	OEC	a	5565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	a	5566	-	41,41,41	1.62	7 (17%)	56,56,56	2.06	22 (39%)
31	LHG	a	5567	-	38,38,48	1.83	5 (13%)	44,44,54	1.38	4 (9%)
33	LMT	a	5568	-	36,36,36	1.40	6 (16%)	47,47,47	1.10	1 (2%)
23	CLA	b	5511	-	48,49,73	2.06	13 (27%)	64,84,113	1.57	14 (21%)
23	CLA	b	5512	2	73,73,73	1.39	10 (13%)	95,113,113	1.49	18 (18%)
23	CLA	b	5513	2	73,73,73	1.49	12 (16%)	95,113,113	1.58	23 (24%)
23	CLA	b	5514	2	73,73,73	1.52	12 (16%)	95,113,113	1.53	20 (21%)
23	CLA	b	5515	-	73,73,73	1.43	12 (16%)	95,113,113	1.60	22 (23%)
23	CLA	b	5516	-	73,73,73	1.56	12 (16%)	95,113,113	1.54	21 (22%)
23	CLA	b	5517	-	73,73,73	1.58	10 (13%)	95,113,113	1.59	20 (21%)
23	CLA	b	5518	2	73,73,73	1.61	11 (15%)	95,113,113	1.56	20 (21%)
23	CLA	b	5519	-	73,73,73	1.54	15 (20%)	95,113,113	1.51	21 (22%)
23	CLA	b	5520	-	73,73,73	1.52	14 (19%)	95,113,113	1.48	18 (18%)
23	CLA	b	5521	2	73,73,73	1.45	7 (9%)	95,113,113	1.56	20 (21%)
23	CLA	b	5522	-	73,73,73	1.57	14 (19%)	95,113,113	1.50	14 (14%)
23	CLA	b	5523	-	73,73,73	1.48	10 (13%)	95,113,113	1.55	21 (22%)
23	CLA	b	5524	2	64,64,73	2.34	13 (20%)	83,102,113	1.56	17 (20%)
23	CLA	b	5525	-	73,73,73	1.48	13 (17%)	95,113,113	1.50	18 (18%)
23	CLA	b	5526	-	73,73,73	1.71	18 (24%)	95,113,113	1.56	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	b	5527	-	41,41,41	1.50	8 (19%)	56,56,56	1.92	14 (25%)
28	BCR	b	5528	-	41,41,41	1.66	8 (19%)	56,56,56	1.96	17 (30%)
28	BCR	b	5529	-	41,41,41	1.65	9 (21%)	56,56,56	2.06	19 (33%)
29	MGE	b	5530	-	48,48,48	1.15	8 (16%)	56,56,56	1.15	6 (10%)
23	CLA	c	5491	3	73,73,73	1.65	12 (16%)	95,113,113	1.49	17 (17%)
23	CLA	c	5492	3	67,68,73	1.56	11 (16%)	87,107,113	1.60	19 (21%)
23	CLA	c	5493	3	73,73,73	1.65	13 (17%)	95,113,113	1.56	19 (20%)
23	CLA	c	5494	-	53,54,73	1.63	11 (20%)	71,90,113	1.76	18 (25%)
23	CLA	c	5495	-	73,73,73	1.73	13 (17%)	95,113,113	1.62	23 (24%)
23	CLA	c	5496	-	73,73,73	1.58	16 (21%)	95,113,113	1.50	18 (18%)
23	CLA	c	5497	-	73,73,73	1.49	13 (17%)	95,113,113	1.49	20 (21%)
23	CLA	c	5498	3	73,73,73	1.72	15 (20%)	95,113,113	1.57	18 (18%)
23	CLA	c	5499	-	54,55,73	1.78	11 (20%)	72,91,113	1.76	19 (26%)
23	CLA	c	5500	-	73,73,73	1.48	13 (17%)	95,113,113	1.49	19 (20%)
23	CLA	c	5501	3	73,73,73	1.76	14 (19%)	95,113,113	1.50	19 (20%)
23	CLA	c	5502	-	59,59,73	2.12	18 (30%)	77,96,113	1.69	18 (23%)
23	CLA	c	5503	3	58,58,73	1.95	15 (25%)	75,95,113	1.60	16 (21%)
28	BCR	c	5504	-	41,41,41	2.04	7 (17%)	56,56,56	2.11	23 (41%)
28	BCR	c	5505	-	41,41,41	1.92	9 (21%)	56,56,56	2.06	18 (32%)
28	BCR	c	5506	-	41,41,41	1.92	9 (21%)	56,56,56	2.07	20 (35%)
30	DGD	c	5507	-	54,54,67	1.52	11 (20%)	68,68,81	1.51	6 (8%)
30	DGD	c	5508	-	48,48,67	1.72	10 (20%)	62,62,81	1.80	12 (19%)
30	DGD	c	5509	-	58,58,67	1.55	6 (10%)	72,72,81	1.41	5 (6%)
21	BCT	d	5353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	5354	4	73,73,73	1.47	11 (15%)	95,113,113	1.61	20 (21%)
23	CLA	d	5355	-	58,58,73	1.83	15 (25%)	75,95,113	1.59	14 (18%)
26	PQ9	d	5356	-	30,30,45	0.85	1 (3%)	37,39,57	1.77	9 (24%)
28	BCR	d	5357	-	41,41,41	1.94	9 (21%)	56,56,56	2.25	21 (37%)
32	SQD	d	5358	-	54,54,54	2.96	26 (48%)	65,65,65	2.73	20 (30%)
29	MGE	d	5359	-	47,47,48	1.33	6 (12%)	55,55,56	0.98	3 (5%)
29	MGE	d	5360	-	41,41,48	2.00	6 (14%)	49,49,56	1.11	6 (12%)
29	MGE	d	5361	-	48,48,48	1.01	4 (8%)	56,56,56	1.07	3 (5%)
25	HEM	f	5051	5,6	49,50,50	3.40	27 (55%)	46,82,82	2.52	15 (32%)
28	BCR	h	5107	-	41,41,41	1.93	7 (17%)	56,56,56	2.21	25 (44%)
30	DGD	h	5208	-	55,55,67	1.93	9 (16%)	69,69,81	1.60	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MGE	i	5201	-	48,48,48	1.21	8 (16%)	56,56,56	1.11	5 (8%)
29	MGE	l	5210	-	48,48,48	0.87	3 (6%)	56,56,56	1.15	4 (7%)
33	LMT	m	216	-	36,36,36	1.42	7 (19%)	47,47,47	0.97	1 (2%)
28	BCR	t	104	-	41,41,41	1.63	9 (21%)	56,56,56	2.20	23 (41%)
32	SQD	t	213	-	47,47,54	3.33	24 (51%)	58,58,65	2.98	15 (25%)
33	LMT	t	5217	-	36,36,36	1.42	5 (13%)	47,47,47	1.00	3 (6%)
25	HEM	v	5552	16	49,50,50	4.00	26 (53%)	46,82,82	2.31	13 (28%)
28	BCR	x	5130	-	41,41,41	1.93	9 (21%)	56,56,56	2.45	24 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	A	5212	-	-	0/19/39/69	0/1/1/1
23	CLA	A	558	1	-	0/37/135/135	0/0/9/9
23	CLA	A	559	-	-	0/37/135/135	0/0/9/9
23	CLA	A	560	-	-	0/37/135/135	0/0/9/9
24	PHO	A	561	-	3/3/17/22	0/48/103/103	0/0/6/6
24	PHO	A	562	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	A	563	-	-	0/25/123/135	0/0/9/9
26	PQ9	A	564	-	-	0/23/43/61	0/1/1/1
27	OEC	A	565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	A	566	-	-	0/29/63/63	0/2/2/2
31	LHG	A	567	-	-	0/43/43/53	0/0/0/0
32	SQD	A	568	-	-	0/49/69/69	0/1/1/1
33	LMT	A	569	-	-	0/21/61/61	0/2/2/2
23	CLA	B	511	-	-	0/8/106/135	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	2	-	0/37/135/135	0/0/9/9
23	CLA	B	515	-	-	0/37/135/135	0/0/9/9
23	CLA	B	516	-	-	0/37/135/135	0/0/9/9
23	CLA	B	517	-	-	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	-	-	0/37/135/135	0/0/9/9
23	CLA	B	520	-	-	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	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	523	-	-	0/37/135/135	0/0/9/9
23	CLA	B	524	2	-	0/27/125/135	0/0/9/9
23	CLA	B	525	-	-	0/37/135/135	0/0/9/9
23	CLA	B	526	-	-	0/37/135/135	0/0/9/9
28	BCR	B	527	-	-	0/29/63/63	0/2/2/2
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
29	MGE	B	530	-	-	0/43/63/63	0/1/1/1
23	CLA	C	491	3	-	0/37/135/135	0/0/9/9
23	CLA	C	492	3	-	0/31/129/135	0/0/9/9
23	CLA	C	493	3	-	0/37/135/135	0/0/9/9
23	CLA	C	494	-	-	0/15/113/135	0/0/9/9
23	CLA	C	495	-	-	0/37/135/135	0/0/9/9
23	CLA	C	496	3	-	0/37/135/135	0/0/9/9
23	CLA	C	497	-	-	0/37/135/135	0/0/9/9
23	CLA	C	498	3	-	0/37/135/135	0/0/9/9
23	CLA	C	499	-	-	0/16/114/135	0/0/9/9
23	CLA	C	500	-	-	0/37/135/135	0/0/9/9
23	CLA	C	501	3	-	0/37/135/135	0/0/9/9
23	CLA	C	502	-	-	0/21/119/135	0/0/9/9
23	CLA	C	503	3	-	1/19/117/135	0/0/9/9
28	BCR	C	504	-	-	0/29/63/63	0/2/2/2
28	BCR	C	505	-	-	0/29/63/63	0/2/2/2
28	BCR	C	506	-	-	0/29/63/63	0/2/2/2
30	DGD	C	507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	C	509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	-	1/37/135/135	0/0/9/9
23	CLA	D	355	-	-	0/19/117/135	0/0/9/9
26	PQ9	D	356	-	-	0/23/43/61	0/1/1/1
28	BCR	D	357	-	-	0/29/63/63	0/2/2/2
29	MGE	D	358	-	-	0/42/62/63	0/1/1/1
29	MGE	D	359	-	-	0/36/56/63	0/1/1/1
29	MGE	D	360	-	-	0/43/63/63	0/1/1/1
25	HEM	F	51	5,6	-	0/14/114/114	0/0/8/8
28	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	I	201	-	-	0/43/63/63	0/1/1/1
29	MGE	L	210	-	-	0/43/63/63	0/1/1/1
32	SQD	L	5213	-	-	0/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	M	5216	-	-	0/21/61/61	0/2/2/2
33	LMT	T	217	-	-	0/21/61/61	0/2/2/2
28	BCR	T	5104	-	-	0/29/63/63	0/2/2/2
25	HEM	V	552	16	-	0/14/114/114	0/0/8/8
28	BCR	X	130	-	-	0/29/63/63	0/2/2/2
32	SQD	a	212	-	-	0/19/39/69	0/1/1/1
23	CLA	a	5558	1	-	0/37/135/135	0/0/9/9
23	CLA	a	5559	-	-	0/37/135/135	0/0/9/9
23	CLA	a	5560	-	-	0/37/135/135	0/0/9/9
24	PHO	a	5561	-	3/3/17/22	0/48/103/103	0/0/6/6
24	PHO	a	5562	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	a	5563	-	-	0/25/123/135	0/0/9/9
26	PQ9	a	5564	-	-	0/23/43/61	0/1/1/1
27	OEC	a	5565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	a	5566	-	-	0/29/63/63	0/2/2/2
31	LHG	a	5567	-	-	0/43/43/53	0/0/0/0
33	LMT	a	5568	-	-	0/21/61/61	0/2/2/2
23	CLA	b	5511	-	-	0/8/106/135	0/0/9/9
23	CLA	b	5512	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5513	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5514	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5515	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5516	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5517	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5518	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5519	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5520	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5521	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5522	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5523	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5524	2	-	0/27/125/135	0/0/9/9
23	CLA	b	5525	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5526	-	-	0/37/135/135	0/0/9/9
28	BCR	b	5527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5528	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5529	-	-	0/29/63/63	0/2/2/2
29	MGE	b	5530	-	-	0/43/63/63	0/1/1/1
23	CLA	c	5491	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5492	3	-	0/31/129/135	0/0/9/9
23	CLA	c	5493	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5494	-	-	0/15/113/135	0/0/9/9
23	CLA	c	5495	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	5496	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5497	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5498	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5499	-	-	0/16/114/135	0/0/9/9
23	CLA	c	5500	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5501	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5502	-	-	0/21/119/135	0/0/9/9
23	CLA	c	5503	3	-	1/19/117/135	0/0/9/9
28	BCR	c	5504	-	-	0/29/63/63	0/2/2/2
28	BCR	c	5505	-	-	0/29/63/63	0/2/2/2
28	BCR	c	5506	-	-	0/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	c	5509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	d	5353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	5354	4	-	1/37/135/135	0/0/9/9
23	CLA	d	5355	-	-	0/19/117/135	0/0/9/9
26	PQ9	d	5356	-	-	0/23/43/61	0/1/1/1
28	BCR	d	5357	-	-	0/29/63/63	0/2/2/2
32	SQD	d	5358	-	-	0/49/69/69	0/1/1/1
29	MGE	d	5359	-	-	0/42/62/63	0/1/1/1
29	MGE	d	5360	-	-	0/36/56/63	0/1/1/1
29	MGE	d	5361	-	-	0/43/63/63	0/1/1/1
25	HEM	f	5051	5,6	-	0/14/114/114	0/0/8/8
28	BCR	h	5107	-	-	0/29/63/63	0/2/2/2
30	DGD	h	5208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	i	5201	-	-	0/43/63/63	0/1/1/1
29	MGE	l	5210	-	-	0/43/63/63	0/1/1/1
33	LMT	m	216	-	-	0/21/61/61	0/2/2/2
28	BCR	t	104	-	-	0/29/63/63	0/2/2/2
32	SQD	t	213	-	-	0/42/62/69	0/1/1/1
33	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
25	HEM	v	5552	16	-	0/14/114/114	0/0/8/8
28	BCR	x	5130	-	-	0/29/63/63	0/2/2/2

All (1519) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	552	HEM	C2D-C1D	-17.32	1.40	1.44
25	v	5552	HEM	C2D-C1D	-16.89	1.40	1.44
25	F	51	HEM	C2D-C1D	-14.18	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	5358	SQD	C6-C5	-13.55	1.38	1.52
25	v	5552	HEM	C2B-C1B	13.48	1.47	1.44
23	b	5524	CLA	C11-C10	-13.48	1.49	1.55
25	f	5051	HEM	C2D-C1D	-13.26	1.41	1.44
24	A	562	PHO	CHC-C1C	12.90	1.44	1.35
23	B	524	CLA	C11-C10	-12.33	1.50	1.55
24	a	5562	PHO	CHC-C1C	12.26	1.43	1.35
32	A	5212	SQD	C6-C5	-10.99	1.41	1.52
29	D	359	MGE	C6A-C5A	-10.96	1.50	1.55
32	a	212	SQD	C6-C5	-10.80	1.41	1.52
32	A	568	SQD	C6-C5	-10.76	1.41	1.52
24	a	5561	PHO	CHC-C1C	10.58	1.42	1.35
29	d	5360	MGE	C6A-C5A	-10.41	1.51	1.55
30	h	5208	DGD	CFA-CEA	-10.37	1.51	1.55
32	t	213	SQD	C31-C30	10.09	1.59	1.55
32	L	5213	SQD	C6-S	9.72	1.88	1.77
30	C	508	DGD	CCA-CBA	-9.66	1.51	1.55
32	L	5213	SQD	C31-C30	8.73	1.58	1.55
24	A	561	PHO	CHC-C1C	8.56	1.41	1.35
25	V	552	HEM	C2B-C1B	8.40	1.46	1.44
25	V	552	HEM	C3D-C4D	8.35	1.46	1.44
25	v	5552	HEM	C3D-C4D	8.13	1.46	1.44
32	t	213	SQD	C6-C5	-8.11	1.43	1.52
32	A	568	SQD	C4-C3	7.80	1.73	1.52
32	t	213	SQD	C4-C3	7.77	1.73	1.52
32	a	212	SQD	C4-C3	7.74	1.73	1.52
25	F	51	HEM	C3D-C4D	7.58	1.46	1.44
25	f	5051	HEM	C3D-C4D	7.54	1.46	1.44
32	d	5358	SQD	C4-C3	7.48	1.72	1.52
32	L	5213	SQD	C4-C3	7.42	1.72	1.52
24	A	561	PHO	C1D-CHD	7.36	1.43	1.35
31	A	567	LHG	P-O5	7.34	1.79	1.51
30	C	509	DGD	CBA-CAA	-7.31	1.52	1.55
28	c	5504	BCR	C1-C6	7.30	1.64	1.53
31	a	5567	LHG	P-O5	7.25	1.79	1.51
30	H	208	DGD	CFA-CEA	-7.22	1.52	1.55
32	L	5213	SQD	C6-C5	-7.13	1.44	1.52
24	a	5561	PHO	C1D-CHD	6.96	1.43	1.35
32	A	5212	SQD	C4-C3	6.92	1.70	1.52
32	a	212	SQD	C6-S	6.87	1.85	1.77
23	c	5502	CLA	C1B-C2B	6.82	1.48	1.40
24	A	562	PHO	C1D-CHD	6.63	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5498	CLA	C3B-C4B	6.48	1.50	1.40
32	t	213	SQD	C6-S	6.48	1.84	1.77
23	c	5502	CLA	C3B-C4B	6.47	1.50	1.40
30	c	5509	DGD	CGB-CFB	-6.46	1.52	1.55
30	C	509	DGD	CGB-CFB	-6.42	1.52	1.55
23	c	5495	CLA	MG-NA	6.40	2.26	2.07
23	c	5493	CLA	C1B-C2B	6.40	1.48	1.40
28	c	5504	BCR	C30-C25	6.37	1.62	1.53
25	F	51	HEM	C2B-C1B	6.36	1.46	1.44
28	h	5107	BCR	C30-C25	6.36	1.62	1.53
28	H	107	BCR	C30-C25	6.30	1.62	1.53
23	B	511	CLA	C1B-C2B	6.28	1.48	1.40
23	c	5491	CLA	C1B-C2B	6.24	1.48	1.40
23	C	502	CLA	C1B-C2B	6.23	1.48	1.40
23	B	525	CLA	C1B-C2B	6.21	1.47	1.40
23	B	517	CLA	MG-NA	6.21	2.25	2.07
23	c	5501	CLA	C1B-C2B	6.14	1.47	1.40
24	a	5562	PHO	C1D-CHD	6.13	1.42	1.35
23	B	511	CLA	C4B-NB	6.09	1.42	1.34
32	a	212	SQD	O47-C7	6.07	1.47	1.34
23	b	5511	CLA	C1B-C2B	6.06	1.47	1.40
23	C	503	CLA	MG-NA	6.00	2.25	2.07
23	c	5503	CLA	MG-NA	6.00	2.25	2.07
28	B	528	BCR	C30-C25	5.97	1.62	1.53
23	c	5503	CLA	C1B-C2B	5.96	1.47	1.40
23	c	5499	CLA	C1B-C2B	5.93	1.47	1.40
30	C	507	DGD	CEA-CDA	-5.92	1.52	1.55
28	d	5357	BCR	C1-C6	5.88	1.62	1.53
23	B	525	CLA	C3B-C4B	5.88	1.49	1.40
23	C	498	CLA	C3B-C4B	5.83	1.49	1.40
23	C	503	CLA	C1B-C2B	5.80	1.47	1.40
32	t	213	SQD	O8-S	5.73	1.60	1.46
28	C	505	BCR	C30-C25	5.73	1.62	1.53
32	L	5213	SQD	O8-S	5.72	1.60	1.46
23	C	493	CLA	C1B-C2B	5.71	1.47	1.40
23	d	5355	CLA	C3B-C4B	5.72	1.49	1.40
23	b	5516	CLA	MG-NA	5.71	2.24	2.07
32	a	212	SQD	O8-S	5.71	1.60	1.46
23	d	5354	CLA	C3B-C4B	5.71	1.49	1.40
28	c	5505	BCR	C30-C25	5.67	1.61	1.53
23	C	495	CLA	MG-NA	5.67	2.24	2.07
23	C	501	CLA	MG-NA	5.62	2.23	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	513	CLA	C3B-C4B	5.61	1.49	1.40
30	C	507	DGD	C9B-C8B	-5.61	1.52	1.55
32	A	5212	SQD	O8-S	5.61	1.60	1.46
28	C	504	BCR	C1-C6	5.61	1.61	1.53
23	C	501	CLA	C1B-C2B	5.60	1.47	1.40
23	B	522	CLA	C1B-C2B	5.59	1.47	1.40
23	B	522	CLA	C3B-C4B	5.57	1.49	1.40
23	C	502	CLA	C3B-C4B	5.57	1.49	1.40
23	B	523	CLA	C1B-C2B	5.57	1.47	1.40
23	c	5501	CLA	C3B-C4B	5.56	1.49	1.40
24	a	5562	PHO	C3B-C4B	5.55	1.49	1.40
23	c	5498	CLA	MG-NA	5.54	2.23	2.07
23	C	492	CLA	C1B-C2B	5.54	1.47	1.40
23	b	5522	CLA	C3B-C4B	5.53	1.49	1.40
32	L	5213	SQD	O7-S	5.50	1.63	1.45
24	A	562	PHO	C3B-C4B	5.47	1.49	1.40
23	c	5495	CLA	C1B-C2B	5.47	1.47	1.40
25	V	552	HEM	CHA-C4D	5.47	1.43	1.35
23	C	496	CLA	C1B-C2B	5.44	1.47	1.40
23	b	5518	CLA	C3B-C4B	5.43	1.49	1.40
23	D	355	CLA	MG-NA	5.43	2.23	2.07
23	B	516	CLA	MG-NA	5.42	2.23	2.07
28	b	5528	BCR	C30-C25	5.40	1.61	1.53
23	c	5491	CLA	MG-NA	5.39	2.23	2.07
23	c	5500	CLA	C1B-C2B	5.35	1.46	1.40
28	B	528	BCR	C1-C6	5.34	1.61	1.53
25	f	5051	HEM	C4A-C3A	5.33	1.46	1.40
23	B	524	CLA	MG-NA	5.31	2.23	2.07
23	B	519	CLA	C1B-C2B	5.31	1.46	1.40
28	A	566	BCR	C1-C6	5.29	1.61	1.53
28	X	130	BCR	C5-C6	5.28	1.42	1.34
23	a	5563	CLA	C3B-C4B	5.27	1.48	1.40
30	H	208	DGD	O3G-C1D	5.24	1.49	1.40
23	C	503	CLA	C3B-C4B	5.23	1.48	1.40
23	b	5514	CLA	MG-NA	5.23	2.22	2.07
23	c	5492	CLA	C1C-NC	-5.23	1.34	1.38
23	C	491	CLA	C1B-C2B	5.23	1.46	1.40
23	B	512	CLA	C3B-C4B	5.22	1.48	1.40
23	b	5518	CLA	C1B-C2B	5.22	1.46	1.40
23	b	5526	CLA	C1B-C2B	5.21	1.46	1.40
25	v	5552	HEM	CHA-C4D	5.21	1.43	1.35
32	t	213	SQD	O7-S	5.20	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	5517	CLA	C1B-C2B	5.19	1.46	1.40
23	c	5493	CLA	C3B-C4B	5.18	1.48	1.40
23	b	5511	CLA	C4B-NB	5.16	1.40	1.34
28	H	107	BCR	C1-C6	5.17	1.61	1.53
23	B	515	CLA	C3B-C4B	5.16	1.48	1.40
23	c	5496	CLA	C1B-C2B	5.16	1.46	1.40
23	C	493	CLA	C3B-C4B	5.16	1.48	1.40
28	x	5130	BCR	C5-C6	5.14	1.42	1.34
32	A	5212	SQD	O47-C7	5.14	1.45	1.34
32	d	5358	SQD	O7-S	5.13	1.62	1.45
30	c	5508	DGD	CCA-CBA	-5.12	1.53	1.55
23	b	5513	CLA	C3B-C4B	5.11	1.48	1.40
29	d	5359	MGE	CCA-CBA	-5.11	1.53	1.55
23	D	355	CLA	C1B-C2B	5.10	1.46	1.40
23	D	355	CLA	C3B-C4B	5.10	1.48	1.40
23	B	516	CLA	C1B-C2B	5.10	1.46	1.40
23	B	521	CLA	C1B-C2B	5.09	1.46	1.40
28	B	527	BCR	C30-C25	5.08	1.61	1.53
23	b	5518	CLA	MG-NA	5.07	2.22	2.07
23	c	5495	CLA	C3B-C4B	5.06	1.48	1.40
23	c	5498	CLA	C1B-C2B	5.04	1.46	1.40
23	B	520	CLA	C1B-C2B	5.04	1.46	1.40
23	b	5522	CLA	C1B-C2B	5.04	1.46	1.40
23	C	495	CLA	C3B-C4B	5.03	1.48	1.40
23	B	519	CLA	C3B-C4B	5.02	1.48	1.40
23	b	5520	CLA	C1B-C2B	5.02	1.46	1.40
28	D	357	BCR	C26-C25	5.02	1.42	1.34
23	c	5501	CLA	MG-NA	5.02	2.22	2.07
23	a	5559	CLA	C1B-C2B	5.01	1.46	1.40
23	B	519	CLA	MG-NA	5.01	2.22	2.07
23	c	5503	CLA	C3B-C4B	5.01	1.48	1.40
23	B	518	CLA	MG-NA	5.00	2.22	2.07
28	D	357	BCR	C30-C25	4.96	1.60	1.53
28	B	527	BCR	C26-C25	4.94	1.42	1.34
23	C	502	CLA	C4B-NB	4.93	1.40	1.34
23	c	5502	CLA	MG-NA	4.93	2.21	2.07
28	h	5107	BCR	C1-C6	4.92	1.60	1.53
23	b	5515	CLA	C1B-C2B	4.92	1.46	1.40
23	B	526	CLA	C1B-C2B	4.91	1.46	1.40
23	b	5521	CLA	C1B-C2B	4.90	1.46	1.40
23	C	499	CLA	C1B-C2B	4.89	1.46	1.40
23	B	514	CLA	MG-NA	4.89	2.21	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	497	CLA	C1B-C2B	4.89	1.46	1.40
23	A	558	CLA	C3B-C4B	4.89	1.48	1.40
23	b	5523	CLA	C1B-C2B	4.88	1.46	1.40
23	B	515	CLA	C1B-C2B	4.87	1.46	1.40
23	C	499	CLA	MG-NA	4.86	2.21	2.07
32	t	213	SQD	C1-C2	4.86	1.67	1.52
25	f	5051	HEM	C2B-C1B	4.86	1.45	1.44
23	c	5496	CLA	C3B-C4B	4.85	1.48	1.40
23	a	5559	CLA	C3B-C4B	4.85	1.48	1.40
23	b	5517	CLA	MG-NA	4.85	2.21	2.07
23	b	5520	CLA	C3B-C4B	4.85	1.48	1.40
28	c	5505	BCR	C26-C25	4.83	1.42	1.34
23	D	354	CLA	C3B-C4B	4.82	1.48	1.40
23	b	5525	CLA	C3B-C4B	4.79	1.47	1.40
28	C	505	BCR	C26-C25	4.78	1.42	1.34
28	c	5506	BCR	C30-C25	4.77	1.60	1.53
23	d	5355	CLA	C1B-C2B	4.77	1.46	1.40
28	a	5566	BCR	C1-C6	4.77	1.60	1.53
23	b	5512	CLA	C3B-C4B	4.77	1.47	1.40
23	B	514	CLA	C1B-C2B	4.75	1.46	1.40
28	C	504	BCR	C30-C25	4.75	1.60	1.53
23	c	5492	CLA	C1B-C2B	4.74	1.46	1.40
28	B	529	BCR	C26-C25	4.74	1.41	1.34
23	B	518	CLA	C3B-C4B	4.73	1.47	1.40
23	d	5355	CLA	MG-NA	4.72	2.21	2.07
23	b	5519	CLA	C3B-C4B	4.72	1.47	1.40
28	d	5357	BCR	C5-C6	4.71	1.41	1.34
28	B	529	BCR	C30-C25	4.70	1.60	1.53
23	c	5502	CLA	C4B-NB	4.69	1.40	1.34
23	B	521	CLA	C3B-C4B	4.68	1.47	1.40
32	A	5212	SQD	O7-S	4.68	1.60	1.45
28	x	5130	BCR	C1-C6	4.67	1.60	1.53
28	x	5130	BCR	C30-C25	4.66	1.60	1.53
23	C	496	CLA	C3B-C4B	4.66	1.47	1.40
28	X	130	BCR	C1-C6	4.66	1.60	1.53
28	H	107	BCR	C26-C25	4.65	1.41	1.34
28	h	5107	BCR	C26-C25	4.65	1.41	1.34
23	C	494	CLA	C1B-C2B	4.64	1.46	1.40
23	B	518	CLA	C1B-C2B	4.63	1.46	1.40
30	h	5208	DGD	O3G-C1D	4.63	1.48	1.40
23	b	5525	CLA	C1B-C2B	4.62	1.45	1.40
23	C	502	CLA	MG-NA	4.61	2.20	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	5506	BCR	C5-C6	4.60	1.41	1.34
23	b	5514	CLA	C1B-C2B	4.60	1.45	1.40
23	c	5499	CLA	C3B-C4B	4.59	1.47	1.40
28	b	5527	BCR	C30-C25	4.58	1.60	1.53
25	v	5552	HEM	CBC-CAC	4.58	1.55	1.28
23	B	517	CLA	C1B-C2B	4.58	1.45	1.40
23	C	500	CLA	C1B-C2B	4.57	1.45	1.40
23	b	5512	CLA	C1B-C2B	4.57	1.45	1.40
23	B	512	CLA	C1B-C2B	4.56	1.45	1.40
23	b	5526	CLA	C3B-C4B	4.56	1.47	1.40
28	H	107	BCR	C29-C30	4.55	1.65	1.54
28	D	357	BCR	C5-C6	4.54	1.41	1.34
28	c	5505	BCR	C1-C6	4.54	1.60	1.53
23	C	502	CLA	C6-C5	4.54	1.57	1.55
28	X	130	BCR	C30-C25	4.54	1.60	1.53
23	B	511	CLA	C3B-C4B	4.54	1.47	1.40
28	b	5529	BCR	C30-C25	4.53	1.60	1.53
25	f	5051	HEM	CHA-C4D	4.53	1.42	1.35
32	A	568	SQD	C6-S	4.52	1.82	1.77
28	d	5357	BCR	C26-C25	4.52	1.41	1.34
23	C	494	CLA	C3B-C4B	4.51	1.47	1.40
23	c	5494	CLA	C3B-C4B	4.51	1.47	1.40
32	A	568	SQD	O8-S	4.51	1.57	1.46
23	b	5521	CLA	C3B-C4B	4.50	1.47	1.40
28	c	5506	BCR	C26-C25	4.50	1.41	1.34
23	a	5558	CLA	C1B-C2B	4.49	1.45	1.40
25	V	552	HEM	CBC-CAC	4.49	1.55	1.28
23	C	501	CLA	C3B-C4B	4.48	1.47	1.40
23	b	5521	CLA	C1A-NA	4.47	1.42	1.32
23	c	5491	CLA	C3B-C4B	4.46	1.47	1.40
23	c	5497	CLA	C1B-C2B	4.46	1.45	1.40
32	d	5358	SQD	O8-S	4.46	1.57	1.46
23	b	5524	CLA	C1B-C2B	4.44	1.45	1.40
23	b	5523	CLA	C1C-NC	-4.43	1.34	1.38
25	f	5051	HEM	CBC-CAC	4.43	1.54	1.28
23	C	491	CLA	C3B-C4B	4.42	1.47	1.40
23	B	520	CLA	C3B-C4B	4.40	1.47	1.40
23	b	5517	CLA	C3B-C4B	4.39	1.47	1.40
30	c	5508	DGD	C5B-C4B	-4.39	1.53	1.55
25	F	51	HEM	CBC-CAC	4.38	1.54	1.28
28	c	5506	BCR	C1-C6	4.38	1.60	1.53
25	f	5051	HEM	CAD-CBD	4.36	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	t	213	SQD	O5-C5	4.36	1.55	1.44
23	C	492	CLA	C3B-C4B	4.34	1.47	1.40
23	B	526	CLA	C3B-C4B	4.34	1.47	1.40
23	b	5519	CLA	C1B-C2B	4.33	1.45	1.40
23	B	523	CLA	C3B-C4B	4.33	1.47	1.40
23	b	5513	CLA	C1B-C2B	4.33	1.45	1.40
23	C	496	CLA	MG-NA	4.32	2.20	2.07
25	f	5051	HEM	C3C-CAC	4.32	1.54	1.40
23	a	5559	CLA	C1C-NC	-4.31	1.35	1.38
23	B	524	CLA	C1B-C2B	4.31	1.45	1.40
23	B	513	CLA	C1B-C2B	4.31	1.45	1.40
23	a	5563	CLA	C1B-C2B	4.31	1.45	1.40
32	a	212	SQD	O7-S	4.30	1.59	1.45
23	A	563	CLA	C3B-C4B	4.30	1.47	1.40
33	A	569	LMT	O1'-C1'	4.30	1.48	1.40
23	b	5524	CLA	C3B-C4B	4.30	1.47	1.40
23	c	5492	CLA	C3B-C4B	4.25	1.47	1.40
23	a	5560	CLA	C1B-C2B	4.23	1.45	1.40
23	a	5558	CLA	C3B-C4B	4.22	1.47	1.40
30	c	5508	DGD	O6D-C1D	4.22	1.52	1.41
23	B	514	CLA	C1C-NC	-4.22	1.35	1.38
32	L	5213	SQD	O48-C23	4.21	1.46	1.33
23	c	5493	CLA	C4B-NB	4.21	1.39	1.34
23	C	495	CLA	C1B-C2B	4.20	1.45	1.40
23	b	5516	CLA	C1B-C2B	4.20	1.45	1.40
31	a	5567	LHG	P-O3	4.19	1.78	1.59
32	a	212	SQD	C1-C2	4.17	1.64	1.52
23	C	498	CLA	MG-NA	4.17	2.19	2.07
23	A	560	CLA	CAA-C2A	4.14	1.61	1.54
24	A	561	PHO	C3B-C4B	4.14	1.46	1.40
28	T	5104	BCR	C5-C6	4.13	1.40	1.34
28	a	5566	BCR	C30-C25	4.13	1.59	1.53
23	b	5519	CLA	MG-NA	4.12	2.19	2.07
23	A	559	CLA	C1B-C2B	4.11	1.45	1.40
23	B	514	CLA	C3B-C4B	4.11	1.46	1.40
25	F	51	HEM	C3C-CAC	4.10	1.53	1.40
23	a	5560	CLA	C3B-C4B	4.09	1.46	1.40
23	c	5494	CLA	CAA-C2A	4.07	1.61	1.54
32	A	568	SQD	O7-S	4.06	1.58	1.45
28	C	506	BCR	C30-C25	4.05	1.59	1.53
23	b	5522	CLA	MG-NA	4.04	2.19	2.07
23	b	5524	CLA	MG-NA	4.04	2.19	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	5511	CLA	C3B-C4B	4.02	1.46	1.40
25	F	51	HEM	C4A-C3A	4.02	1.45	1.40
30	c	5509	DGD	O3G-C1D	4.02	1.47	1.40
23	b	5524	CLA	C1C-NC	-4.02	1.35	1.38
23	b	5511	CLA	MG-NA	4.02	2.19	2.07
23	B	517	CLA	C3B-C4B	4.01	1.46	1.40
23	c	5494	CLA	C1B-C2B	4.01	1.45	1.40
28	B	529	BCR	C1-C6	4.00	1.59	1.53
23	C	500	CLA	C3B-C4B	3.98	1.46	1.40
23	c	5502	CLA	C6-C5	3.98	1.56	1.55
23	c	5501	CLA	C1A-NA	3.98	1.41	1.32
25	v	5552	HEM	C1A-NA	3.98	1.44	1.36
23	a	5560	CLA	MG-NA	3.98	2.19	2.07
23	c	5500	CLA	C3B-C4B	3.97	1.46	1.40
23	B	519	CLA	C4B-NB	3.96	1.39	1.34
23	D	355	CLA	CAA-C2A	3.94	1.61	1.54
32	d	5358	SQD	C1-C2	3.94	1.64	1.52
32	L	5213	SQD	O5-C5	3.93	1.54	1.44
28	C	506	BCR	C5-C6	3.93	1.40	1.34
23	B	516	CLA	C3B-C4B	3.93	1.46	1.40
23	b	5523	CLA	C3B-C4B	3.93	1.46	1.40
23	c	5494	CLA	C1A-NA	3.93	1.40	1.32
23	b	5526	CLA	C3B-CAB	-3.91	1.45	1.49
23	B	524	CLA	C3B-C4B	3.91	1.46	1.40
25	V	552	HEM	C3C-CAC	3.91	1.52	1.40
28	A	566	BCR	C5-C6	3.90	1.40	1.34
28	b	5528	BCR	C1-C6	3.90	1.59	1.53
23	c	5499	CLA	MG-NA	3.89	2.18	2.07
23	C	494	CLA	CAA-C2A	3.89	1.61	1.54
25	V	552	HEM	C3B-CAB	3.89	1.52	1.40
29	B	530	MGE	O3G-C1D	3.89	1.47	1.40
25	f	5051	HEM	C1A-NA	3.89	1.44	1.36
28	C	504	BCR	C26-C25	3.88	1.40	1.34
23	B	525	CLA	C4B-NB	3.88	1.39	1.34
32	A	568	SQD	C1-C2	3.87	1.64	1.52
33	a	5568	LMT	O1'-C1'	3.87	1.47	1.40
33	M	5216	LMT	O1'-C1'	3.86	1.47	1.40
23	A	558	CLA	C1B-C2B	3.85	1.45	1.40
23	A	559	CLA	C3B-C4B	3.85	1.46	1.40
32	L	5213	SQD	C1-C2	3.85	1.64	1.52
23	A	563	CLA	C1C-NC	-3.84	1.35	1.38
23	b	5515	CLA	C3B-C4B	3.84	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	t	104	BCR	C5-C6	3.84	1.40	1.34
23	C	498	CLA	C1B-C2B	3.83	1.45	1.40
28	C	505	BCR	C1-C6	3.83	1.59	1.53
23	B	519	CLA	CAA-C2A	3.83	1.61	1.54
23	B	526	CLA	C1C-NC	-3.82	1.35	1.38
23	c	5501	CLA	CAA-C2A	3.82	1.61	1.54
23	B	526	CLA	MG-NA	3.81	2.18	2.07
23	C	493	CLA	MG-NA	3.81	2.18	2.07
28	t	104	BCR	C30-C25	3.80	1.59	1.53
25	f	5051	HEM	CHB-C1B	-3.80	1.30	1.35
28	C	506	BCR	C26-C25	3.80	1.40	1.34
25	f	5051	HEM	FE-NA	3.80	2.08	1.92
28	C	506	BCR	C2-C1	3.79	1.63	1.54
23	c	5498	CLA	C4B-NB	3.78	1.39	1.34
28	B	528	BCR	C26-C25	3.77	1.40	1.34
25	f	5051	HEM	CAA-C2A	3.77	1.58	1.52
23	C	499	CLA	C1A-NA	3.77	1.40	1.32
30	c	5507	DGD	C4D-C3D	3.76	1.62	1.52
23	C	497	CLA	C3B-CAB	-3.75	1.45	1.49
25	F	51	HEM	FE-NA	3.75	2.08	1.92
23	c	5497	CLA	C3B-CAB	-3.74	1.45	1.49
32	A	568	SQD	O48-C23	3.74	1.45	1.33
23	C	503	CLA	CAA-C2A	3.74	1.60	1.54
32	d	5358	SQD	O48-C23	3.74	1.45	1.33
23	A	558	CLA	C1C-NC	-3.74	1.35	1.38
30	c	5507	DGD	O5D-C1E	3.74	1.47	1.40
23	B	522	CLA	C4B-NB	3.74	1.39	1.34
23	C	499	CLA	C3B-C4B	3.73	1.46	1.40
32	d	5358	SQD	O47-C7	3.72	1.45	1.34
23	C	500	CLA	C1A-NA	3.72	1.40	1.32
23	A	563	CLA	C1B-C2B	3.71	1.44	1.40
25	F	51	HEM	CHA-C4D	3.71	1.41	1.35
28	c	5505	BCR	C5-C6	3.70	1.40	1.34
23	B	516	CLA	CAA-C2A	3.70	1.60	1.54
24	a	5561	PHO	C3B-C4B	3.70	1.46	1.40
23	c	5501	CLA	C1B-NB	3.69	1.39	1.34
28	c	5504	BCR	C29-C30	3.69	1.63	1.54
25	F	51	HEM	CAA-C2A	3.69	1.58	1.52
23	D	354	CLA	C1A-NA	3.69	1.40	1.32
29	D	359	MGE	O3G-C1D	3.69	1.46	1.40
32	a	212	SQD	O5-C5	3.68	1.53	1.44
29	d	5361	MGE	O6D-C1D	3.68	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	552	HEM	C1A-NA	3.67	1.43	1.36
29	L	210	MGE	O6D-C1D	3.67	1.51	1.41
23	B	513	CLA	CAA-C2A	3.66	1.60	1.54
32	t	213	SQD	O48-C23	3.66	1.44	1.33
25	v	5552	HEM	C3C-CAC	3.66	1.51	1.40
23	c	5499	CLA	C1A-NA	3.65	1.40	1.32
23	B	523	CLA	MG-NA	3.64	2.18	2.07
23	c	5493	CLA	C1A-NA	3.64	1.40	1.32
23	C	495	CLA	C1C-NC	-3.64	1.35	1.38
28	B	527	BCR	C5-C6	3.64	1.40	1.34
23	d	5354	CLA	C1B-C2B	3.64	1.44	1.40
23	B	518	CLA	CAA-C2A	3.64	1.60	1.54
23	c	5503	CLA	CAA-C2A	3.64	1.60	1.54
23	c	5493	CLA	MG-NA	3.64	2.18	2.07
28	h	5107	BCR	C29-C30	3.64	1.63	1.54
28	x	5130	BCR	C29-C30	3.63	1.63	1.54
32	A	568	SQD	O47-C7	3.63	1.45	1.34
25	F	51	HEM	C3B-C4B	3.62	1.48	1.44
23	b	5516	CLA	C3B-C4B	3.62	1.46	1.40
30	c	5508	DGD	O3G-C1D	3.61	1.46	1.40
23	b	5525	CLA	C1A-NA	3.61	1.40	1.32
28	h	5107	BCR	C2-C1	3.61	1.63	1.54
23	C	497	CLA	C1A-NA	3.60	1.40	1.32
23	B	511	CLA	C1A-NA	3.59	1.40	1.32
32	A	568	SQD	O3-C3	3.59	1.51	1.43
23	C	501	CLA	C4B-NB	3.59	1.39	1.34
28	c	5506	BCR	C2-C1	3.59	1.63	1.54
28	C	505	BCR	C2-C1	3.58	1.63	1.54
23	b	5526	CLA	CAA-C2A	3.58	1.60	1.54
25	f	5051	HEM	C3B-C4B	3.58	1.48	1.44
30	c	5509	DGD	O6D-C1D	3.58	1.51	1.41
23	B	522	CLA	CAA-C2A	3.57	1.60	1.54
23	b	5511	CLA	C1B-NB	3.56	1.39	1.34
23	b	5517	CLA	C4B-NB	3.56	1.39	1.34
28	t	104	BCR	C1-C6	3.55	1.58	1.53
23	b	5521	CLA	C4B-NB	3.55	1.39	1.34
23	b	5514	CLA	C1A-NA	3.55	1.40	1.32
32	A	5212	SQD	C6-S	3.55	1.81	1.77
33	T	217	LMT	O1'-C1'	3.55	1.46	1.40
30	C	507	DGD	C4D-C3D	3.55	1.61	1.52
23	D	354	CLA	C1B-C2B	3.54	1.44	1.40
23	b	5522	CLA	CAA-C2A	3.54	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	357	BCR	C29-C30	3.54	1.63	1.54
29	D	358	MGE	O6D-C1D	3.53	1.50	1.41
25	v	5552	HEM	CAA-C2A	3.53	1.58	1.52
23	a	5558	CLA	C1A-NA	3.53	1.40	1.32
23	c	5497	CLA	C1A-NA	3.53	1.40	1.32
28	d	5357	BCR	C30-C25	3.52	1.58	1.53
25	V	552	HEM	C4A-C3A	3.52	1.44	1.40
28	T	5104	BCR	C2-C1	3.52	1.63	1.54
23	c	5491	CLA	C1C-NC	-3.52	1.35	1.38
23	B	514	CLA	C1A-NA	3.52	1.40	1.32
23	B	525	CLA	C1A-NA	3.51	1.40	1.32
31	A	567	LHG	O8-C23	3.51	1.44	1.33
23	c	5496	CLA	C4B-NB	3.51	1.39	1.34
23	c	5496	CLA	CAA-C2A	3.51	1.60	1.54
23	a	5563	CLA	MG-NA	3.50	2.17	2.07
23	c	5499	CLA	CAA-C2A	3.50	1.60	1.54
23	a	5563	CLA	C4B-NB	3.49	1.38	1.34
23	b	5511	CLA	C1A-NA	3.48	1.39	1.32
23	a	5560	CLA	C4B-NB	3.48	1.38	1.34
25	V	552	HEM	C3C-C2C	-3.48	1.37	1.43
23	c	5495	CLA	C4B-NB	3.48	1.38	1.34
23	b	5517	CLA	CAA-C2A	3.47	1.60	1.54
23	C	501	CLA	C1A-NA	3.46	1.39	1.32
25	v	5552	HEM	C1A-C2A	3.45	1.49	1.43
25	f	5051	HEM	C1A-C2A	3.44	1.49	1.43
23	b	5526	CLA	C4-C3	3.44	1.59	1.50
23	c	5492	CLA	MG-NA	3.43	2.17	2.07
28	a	5566	BCR	C5-C6	3.43	1.39	1.34
31	A	567	LHG	P-O3	3.43	1.74	1.59
25	F	51	HEM	FE-NB	3.42	2.10	1.97
28	D	357	BCR	C1-C6	3.42	1.58	1.53
32	A	5212	SQD	O5-C5	3.42	1.52	1.44
32	d	5358	SQD	O5-C5	3.42	1.52	1.44
23	C	493	CLA	C3D-CAD	-3.41	1.40	1.47
28	d	5357	BCR	C29-C30	3.40	1.62	1.54
29	b	5530	MGE	O6D-C1D	3.40	1.50	1.41
25	v	5552	HEM	C4A-C3A	3.40	1.44	1.40
30	C	508	DGD	C5B-C4B	-3.40	1.53	1.55
28	X	130	BCR	C29-C30	3.40	1.62	1.54
23	C	502	CLA	C1A-NA	3.38	1.39	1.32
30	C	507	DGD	O5D-C1E	3.38	1.46	1.40
28	B	528	BCR	C29-C30	3.37	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	5517	CLA	C1A-NA	3.37	1.39	1.32
23	C	502	CLA	C5-C3	3.37	1.55	1.51
23	C	492	CLA	MG-NA	3.36	2.17	2.07
28	c	5504	BCR	C26-C25	3.36	1.39	1.34
32	A	5212	SQD	O3-C3	3.35	1.51	1.43
29	B	530	MGE	O6D-C1D	3.36	1.50	1.41
30	c	5507	DGD	CEA-CDA	-3.35	1.53	1.55
28	H	107	BCR	C2-C1	3.35	1.62	1.54
32	t	213	SQD	O47-C7	3.35	1.44	1.34
30	H	208	DGD	C4E-C5E	3.35	1.60	1.53
25	v	5552	HEM	C3B-CAB	3.35	1.50	1.40
23	A	560	CLA	MG-NA	3.35	2.17	2.07
23	C	496	CLA	C4B-NB	3.34	1.38	1.34
28	c	5504	BCR	C2-C1	3.34	1.62	1.54
23	C	492	CLA	C1A-NA	3.35	1.39	1.32
30	C	509	DGD	O3G-C1D	3.34	1.46	1.40
28	C	506	BCR	C1-C6	3.34	1.58	1.53
31	a	5567	LHG	O8-C23	3.34	1.43	1.33
23	B	521	CLA	C1A-NA	3.34	1.39	1.32
23	C	491	CLA	CAA-C2A	3.34	1.60	1.54
32	L	5213	SQD	O3-C3	3.34	1.51	1.43
25	f	5051	HEM	CHC-C1C	3.34	1.42	1.36
23	B	520	CLA	C1A-NA	3.33	1.39	1.32
25	f	5051	HEM	FE-NB	3.33	2.10	1.97
23	C	500	CLA	C4B-NB	3.33	1.38	1.34
29	D	358	MGE	O3G-C1D	3.32	1.46	1.40
28	C	504	BCR	C29-C30	3.32	1.62	1.54
29	L	210	MGE	O3G-C1D	3.32	1.46	1.40
31	a	5567	LHG	P-O6	3.31	1.74	1.59
23	c	5495	CLA	CAA-C2A	3.31	1.60	1.54
32	A	5212	SQD	C1-C2	3.31	1.62	1.52
23	c	5501	CLA	C1C-NC	-3.31	1.35	1.38
23	C	494	CLA	C1A-NA	3.31	1.39	1.32
25	v	5552	HEM	FE-NC	3.31	2.10	1.97
23	b	5514	CLA	C3B-C4B	3.31	1.45	1.40
32	a	212	SQD	O3-C3	3.30	1.50	1.43
23	B	511	CLA	C1B-NB	3.29	1.38	1.34
23	b	5516	CLA	CAA-C2A	3.29	1.60	1.54
25	f	5051	HEM	C4D-ND	-3.28	1.32	1.39
32	t	213	SQD	O3-C3	3.28	1.50	1.43
23	C	499	CLA	C4B-NB	3.27	1.38	1.34
23	b	5516	CLA	C1C-NC	-3.27	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	51	HEM	CMA-C3A	3.27	1.58	1.51
28	X	130	BCR	C26-C25	3.27	1.39	1.34
23	b	5522	CLA	C4A-NA	-3.27	1.32	1.39
26	a	5564	PQ9	C11-C2	3.26	1.54	1.51
23	b	5515	CLA	CAA-C2A	3.26	1.60	1.54
23	b	5514	CLA	CAA-C2A	3.26	1.60	1.54
28	C	505	BCR	C5-C6	3.26	1.39	1.34
23	A	558	CLA	C1A-NA	3.25	1.39	1.32
23	b	5513	CLA	C1C-NC	-3.25	1.35	1.38
28	T	5104	BCR	C1-C6	3.25	1.58	1.53
23	c	5502	CLA	C1A-NA	3.24	1.39	1.32
23	c	5497	CLA	MG-NC	3.23	2.16	2.07
30	c	5507	DGD	O6D-C1D	3.23	1.50	1.41
23	C	494	CLA	C4B-NB	3.22	1.38	1.34
25	F	51	HEM	C3B-C2B	-3.22	1.38	1.43
23	B	526	CLA	C1A-NA	3.22	1.39	1.32
23	A	560	CLA	C1B-C2B	3.22	1.44	1.40
23	b	5519	CLA	C4B-NB	3.22	1.38	1.34
28	D	357	BCR	C2-C1	3.22	1.62	1.54
30	C	508	DGD	O6D-C1D	3.22	1.50	1.41
23	C	500	CLA	CAA-C2A	3.22	1.59	1.54
23	c	5500	CLA	C4B-NB	3.22	1.38	1.34
31	A	567	LHG	O7-C7	3.22	1.44	1.34
23	c	5495	CLA	C1A-NA	3.21	1.39	1.32
23	C	493	CLA	C1A-NA	3.21	1.39	1.32
30	c	5509	DGD	O5D-C1E	3.22	1.46	1.40
23	A	563	CLA	C1B-CHB	-3.21	1.31	1.39
25	F	51	HEM	CHC-C1C	3.21	1.42	1.36
31	a	5567	LHG	O7-C7	3.21	1.44	1.34
31	A	567	LHG	P-O6	3.21	1.73	1.59
23	b	5520	CLA	C4B-NB	3.21	1.38	1.34
23	C	497	CLA	MG-NA	3.21	2.16	2.07
23	D	355	CLA	C1C-NC	-3.20	1.35	1.38
23	D	354	CLA	C1C-NC	-3.20	1.35	1.38
23	a	5563	CLA	CAA-C2A	3.20	1.59	1.54
23	c	5491	CLA	C1A-NA	3.19	1.39	1.32
28	b	5528	BCR	C29-C30	3.18	1.62	1.54
28	b	5529	BCR	C29-C30	3.18	1.62	1.54
23	D	354	CLA	C1B-CHB	-3.18	1.31	1.39
23	B	520	CLA	C3D-CAD	-3.18	1.40	1.47
29	i	5201	MGE	O6D-C5D	3.18	1.52	1.44
28	x	5130	BCR	C2-C1	3.18	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	505	BCR	C29-C30	3.18	1.62	1.54
25	v	5552	HEM	C3C-C2C	-3.18	1.38	1.43
28	x	5130	BCR	C26-C25	3.17	1.39	1.34
23	c	5496	CLA	C1A-NA	3.17	1.39	1.32
33	t	5217	LMT	O1'-C1'	3.17	1.46	1.40
28	H	107	BCR	C14-C13	3.17	1.39	1.35
23	C	496	CLA	MG-NB	3.17	2.12	2.05
23	B	517	CLA	CAA-C2A	3.17	1.59	1.54
23	C	500	CLA	C3D-CAD	-3.16	1.40	1.47
23	A	560	CLA	C3B-C4B	3.16	1.45	1.40
23	B	520	CLA	CAA-C2A	3.15	1.59	1.54
23	B	515	CLA	MG-NA	3.15	2.16	2.07
28	b	5529	BCR	C1-C6	3.15	1.58	1.53
25	V	552	HEM	FE-NC	3.15	2.09	1.97
29	D	359	MGE	O6D-C1D	3.14	1.49	1.41
23	b	5513	CLA	CAA-C2A	3.14	1.59	1.54
23	A	560	CLA	C1A-NA	3.14	1.39	1.32
23	b	5522	CLA	C4B-NB	3.14	1.38	1.34
23	c	5498	CLA	C1B-NB	3.14	1.38	1.34
28	t	104	BCR	C26-C25	3.13	1.39	1.34
23	b	5515	CLA	C4A-NA	-3.12	1.32	1.39
23	B	523	CLA	CHB-C4A	3.12	1.43	1.36
28	b	5527	BCR	C5-C6	3.12	1.39	1.34
23	a	5559	CLA	C1A-NA	3.12	1.39	1.32
28	A	566	BCR	C2-C1	3.12	1.62	1.54
23	a	5560	CLA	CAA-C2A	3.12	1.59	1.54
23	B	513	CLA	MG-NA	3.12	2.16	2.07
23	b	5519	CLA	CAA-C2A	3.12	1.59	1.54
23	c	5499	CLA	C4B-NB	3.11	1.38	1.34
23	b	5518	CLA	C4B-NB	3.12	1.38	1.34
23	B	526	CLA	CAA-C2A	3.11	1.59	1.54
28	c	5505	BCR	C2-C1	3.11	1.62	1.54
29	D	358	MGE	CCA-CBA	-3.11	1.53	1.55
28	B	527	BCR	C29-C30	3.11	1.62	1.54
23	C	502	CLA	CAA-C2A	3.11	1.59	1.54
28	H	107	BCR	C5-C6	3.11	1.39	1.34
29	l	5210	MGE	O6D-C1D	3.10	1.49	1.41
23	C	498	CLA	C1A-NA	3.09	1.39	1.32
23	B	521	CLA	CAA-C2A	3.10	1.59	1.54
28	b	5529	BCR	C2-C1	3.09	1.62	1.54
23	b	5523	CLA	C1A-NA	3.09	1.39	1.32
28	b	5527	BCR	C29-C30	3.09	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5500	CLA	C1C-NC	-3.08	1.35	1.38
23	b	5525	CLA	C3D-CAD	-3.08	1.41	1.47
23	b	5526	CLA	MG-NA	3.08	2.16	2.07
25	F	51	HEM	CAD-CBD	3.08	1.61	1.52
23	b	5523	CLA	CAA-C2A	3.08	1.59	1.54
23	b	5518	CLA	C1C-NC	-3.07	1.35	1.38
32	L	5213	SQD	O47-C7	3.07	1.43	1.34
25	F	51	HEM	C1A-NA	3.07	1.42	1.36
28	B	529	BCR	C2-C1	3.06	1.61	1.54
23	C	491	CLA	C1A-NA	3.05	1.39	1.32
23	c	5495	CLA	C1C-NC	-3.05	1.35	1.38
30	C	507	DGD	O6D-C1D	3.05	1.49	1.41
23	B	521	CLA	MG-NA	3.05	2.16	2.07
23	C	492	CLA	C1C-NC	-3.05	1.35	1.38
28	d	5357	BCR	C2-C1	3.05	1.61	1.54
32	a	212	SQD	O6-C1	3.05	1.45	1.40
23	A	563	CLA	MG-NA	3.05	2.16	2.07
28	b	5527	BCR	C26-C25	3.04	1.39	1.34
32	A	568	SQD	O5-C5	3.04	1.52	1.44
23	b	5513	CLA	C3D-CAD	-3.04	1.41	1.47
29	d	5359	MGE	O6D-C1D	3.04	1.49	1.41
23	B	523	CLA	C1C-NC	-3.03	1.35	1.38
23	A	563	CLA	C1A-NA	3.03	1.38	1.32
32	d	5358	SQD	O3-C3	3.02	1.50	1.43
23	B	522	CLA	MG-NA	3.02	2.16	2.07
23	B	524	CLA	C1A-NA	3.02	1.38	1.32
30	C	508	DGD	O5D-C1E	3.02	1.45	1.40
23	c	5491	CLA	CAA-C2A	3.02	1.59	1.54
23	B	512	CLA	C1A-NA	3.02	1.38	1.32
29	D	360	MGE	O3G-C1D	3.02	1.45	1.40
23	C	501	CLA	CHB-C4A	3.02	1.43	1.36
23	b	5519	CLA	C3D-CAD	-3.01	1.41	1.47
25	V	552	HEM	CAA-C2A	3.01	1.57	1.52
23	c	5500	CLA	CAA-C2A	3.01	1.59	1.54
23	C	497	CLA	C4B-NB	3.01	1.38	1.34
23	a	5563	CLA	C1B-CHB	-3.01	1.31	1.39
28	c	5505	BCR	C29-C30	3.00	1.61	1.54
23	b	5524	CLA	MG-NB	3.00	2.11	2.05
32	L	5213	SQD	O5-C1	3.00	1.49	1.41
24	a	5561	PHO	C4-C3	3.00	1.58	1.50
28	b	5529	BCR	C26-C25	3.00	1.39	1.34
23	A	558	CLA	MG-NA	3.00	2.16	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5493	CLA	CAA-C2A	2.99	1.59	1.54
29	b	5530	MGE	O3G-C1D	2.99	1.45	1.40
23	a	5560	CLA	C1A-NA	2.99	1.38	1.32
23	c	5501	CLA	C4B-NB	2.99	1.38	1.34
23	C	492	CLA	C4B-NB	2.99	1.38	1.34
23	B	522	CLA	C1A-NA	2.99	1.38	1.32
28	d	5357	BCR	C38-C26	2.99	1.56	1.51
23	b	5521	CLA	CAA-C2A	2.98	1.59	1.54
29	d	5359	MGE	O3G-C1D	2.98	1.45	1.40
28	b	5528	BCR	C5-C6	2.98	1.39	1.34
28	C	504	BCR	C5-C6	2.98	1.39	1.34
23	C	500	CLA	MG-NA	2.98	2.16	2.07
33	m	216	LMT	C3B-C2B	2.98	1.60	1.52
23	B	525	CLA	MG-NA	2.98	2.16	2.07
23	B	523	CLA	C1A-NA	2.97	1.38	1.32
23	a	5560	CLA	C3D-CAD	-2.98	1.41	1.47
23	d	5354	CLA	C1B-CHB	-2.97	1.31	1.39
23	b	5518	CLA	CAA-C2A	2.97	1.59	1.54
23	b	5525	CLA	CHB-C4A	2.97	1.43	1.36
23	b	5524	CLA	C1A-NA	2.97	1.38	1.32
23	C	495	CLA	CHB-C4A	2.96	1.43	1.36
25	F	51	HEM	CHB-C1B	-2.96	1.31	1.35
23	c	5500	CLA	C1A-NA	2.96	1.38	1.32
28	b	5529	BCR	C5-C6	2.96	1.39	1.34
33	a	5568	LMT	O5'-C1'	2.96	1.49	1.41
23	d	5354	CLA	C1C-NC	-2.96	1.35	1.38
23	d	5354	CLA	C1A-NA	2.95	1.38	1.32
33	t	5217	LMT	O1B-C1B	2.95	1.49	1.41
32	A	568	SQD	O6-C44	-2.95	1.38	1.43
23	B	526	CLA	C4-C3	2.95	1.58	1.50
23	c	5503	CLA	C1C-NC	-2.95	1.35	1.38
23	a	5563	CLA	C1B-NB	2.95	1.38	1.34
23	C	497	CLA	C3B-C4B	2.95	1.44	1.40
23	c	5497	CLA	C4B-NB	2.95	1.38	1.34
23	c	5503	CLA	C1B-NB	2.95	1.38	1.34
28	c	5505	BCR	C38-C26	2.95	1.56	1.51
23	b	5526	CLA	C5-C3	2.95	1.58	1.51
23	B	511	CLA	MG-NA	2.94	2.15	2.07
29	d	5361	MGE	O3G-C1D	2.94	1.45	1.40
23	C	503	CLA	C4B-NB	2.94	1.38	1.34
23	c	5494	CLA	C4B-NB	2.94	1.38	1.34
28	B	529	BCR	C14-C13	2.94	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5502	CLA	C5-C3	2.93	1.55	1.51
23	C	503	CLA	C1A-NA	2.93	1.38	1.32
29	d	5360	MGE	O6D-C1D	2.93	1.49	1.41
23	b	5525	CLA	C4B-NB	2.92	1.38	1.34
28	B	529	BCR	C5-C6	2.92	1.39	1.34
23	B	516	CLA	C4A-NA	-2.91	1.32	1.39
28	X	130	BCR	C2-C1	2.91	1.61	1.54
23	d	5355	CLA	CAA-C2A	2.91	1.59	1.54
23	c	5502	CLA	C1B-NB	2.91	1.38	1.34
28	c	5506	BCR	C29-C30	2.91	1.61	1.54
23	B	519	CLA	C3D-CAD	-2.91	1.41	1.47
28	t	104	BCR	C2-C1	2.91	1.61	1.54
23	c	5497	CLA	C3B-C4B	2.91	1.44	1.40
23	C	500	CLA	C4A-NA	-2.91	1.32	1.39
23	d	5355	CLA	C1A-NA	2.91	1.38	1.32
23	b	5518	CLA	C1A-NA	2.91	1.38	1.32
23	B	511	CLA	C3D-CAD	-2.91	1.41	1.47
33	A	569	LMT	O5'-C1'	2.90	1.49	1.41
23	b	5515	CLA	C4B-NB	2.90	1.38	1.34
23	c	5491	CLA	C3D-CAD	-2.90	1.41	1.47
25	v	5552	HEM	CAD-CBD	2.90	1.60	1.52
23	B	520	CLA	C4B-NB	2.89	1.38	1.34
28	A	566	BCR	C30-C25	2.89	1.57	1.53
23	b	5511	CLA	CHB-C4A	2.89	1.43	1.36
23	c	5492	CLA	C1A-NA	2.89	1.38	1.32
23	b	5518	CLA	C1B-NB	2.89	1.38	1.34
23	a	5563	CLA	C1A-NA	2.89	1.38	1.32
23	b	5519	CLA	C1A-NA	2.89	1.38	1.32
23	A	559	CLA	C1A-NA	2.89	1.38	1.32
28	b	5529	BCR	C14-C13	2.89	1.39	1.35
23	B	511	CLA	MG-NC	2.88	2.15	2.07
23	B	512	CLA	C1B-CHB	-2.88	1.31	1.39
23	c	5491	CLA	C4B-NB	2.88	1.38	1.34
23	c	5497	CLA	CAA-C2A	2.87	1.59	1.54
23	b	5520	CLA	C1A-NA	2.87	1.38	1.32
23	B	523	CLA	C3D-CAD	-2.87	1.41	1.47
23	C	499	CLA	CHB-C4A	2.87	1.43	1.36
23	C	501	CLA	C1B-NB	2.87	1.38	1.34
25	f	5051	HEM	C3B-CAB	2.87	1.49	1.40
23	b	5513	CLA	MG-NA	2.86	2.15	2.07
23	a	5558	CLA	C1B-CHB	-2.86	1.32	1.39
23	C	495	CLA	C1A-NA	2.86	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5503	CLA	CHB-C4A	2.86	1.43	1.36
23	b	5516	CLA	C4A-NA	-2.86	1.33	1.39
23	d	5355	CLA	CHB-C4A	2.85	1.43	1.36
23	c	5500	CLA	C3D-CAD	-2.85	1.41	1.47
23	C	498	CLA	C1C-NC	-2.85	1.36	1.38
23	B	526	CLA	C5-C3	2.84	1.58	1.51
23	D	355	CLA	C4A-NA	-2.84	1.33	1.39
23	B	518	CLA	C1A-NA	2.84	1.38	1.32
23	B	514	CLA	CAA-C2A	2.84	1.59	1.54
23	C	493	CLA	C4B-NB	2.83	1.38	1.34
23	B	525	CLA	CHB-C4A	2.83	1.43	1.36
29	D	358	MGE	O6D-C5D	2.83	1.51	1.44
23	b	5525	CLA	CAA-C2A	2.83	1.59	1.54
28	B	528	BCR	C2-C1	2.83	1.61	1.54
32	t	213	SQD	C20-C19	-2.83	1.34	1.51
28	B	529	BCR	C29-C30	2.83	1.61	1.54
23	b	5520	CLA	C1C-NC	-2.83	1.36	1.38
23	c	5502	CLA	CHB-C4A	2.83	1.43	1.36
23	C	495	CLA	CAA-C2A	2.82	1.59	1.54
23	d	5354	CLA	CAA-CBA	-2.82	1.43	1.52
23	C	497	CLA	MG-NC	2.82	2.15	2.07
33	A	569	LMT	C1'-C2'	2.81	1.60	1.52
30	C	508	DGD	O1G-C1A	2.81	1.42	1.33
23	b	5511	CLA	C1C-C2C	2.81	1.50	1.44
23	A	559	CLA	C4B-NB	2.81	1.38	1.34
23	c	5494	CLA	C3D-CAD	-2.81	1.41	1.47
23	D	354	CLA	CAA-CBA	-2.80	1.43	1.52
23	b	5511	CLA	C4C-C3C	2.80	1.50	1.45
30	C	509	DGD	O6D-C1D	2.80	1.49	1.41
23	C	491	CLA	C4B-NB	2.80	1.38	1.34
23	C	493	CLA	CAA-C2A	2.80	1.59	1.54
23	B	512	CLA	MG-NA	2.79	2.15	2.07
29	D	358	MGE	C4D-C3D	2.79	1.59	1.52
23	C	495	CLA	C1C-C2C	2.79	1.50	1.44
23	B	513	CLA	C1C-NC	-2.79	1.36	1.38
23	A	560	CLA	C1B-CHB	-2.79	1.32	1.39
23	B	519	CLA	CHB-C4A	2.79	1.43	1.36
23	b	5513	CLA	C1A-NA	2.79	1.38	1.32
29	d	5360	MGE	C4D-C3D	2.79	1.59	1.52
23	D	355	CLA	CHB-C4A	2.79	1.43	1.36
23	D	355	CLA	C4B-NB	2.78	1.38	1.34
29	i	5201	MGE	C4D-C5D	2.78	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	494	CLA	MG-NB	2.78	2.11	2.05
28	a	5566	BCR	C2-C1	2.78	1.61	1.54
23	b	5523	CLA	CHB-C4A	2.78	1.43	1.36
23	B	516	CLA	C4B-NB	2.77	1.38	1.34
23	C	494	CLA	MG-NA	2.77	2.15	2.07
23	c	5502	CLA	CAA-C2A	2.77	1.59	1.54
28	C	504	BCR	C2-C1	2.77	1.61	1.54
23	A	559	CLA	C3D-CAD	-2.77	1.41	1.47
32	L	5213	SQD	C12-C11	-2.76	1.34	1.51
28	b	5527	BCR	C2-C1	2.76	1.61	1.54
23	B	514	CLA	CHB-C4A	2.76	1.43	1.36
30	h	5208	DGD	O6E-C1E	2.76	1.48	1.41
25	F	51	HEM	C4D-ND	-2.76	1.33	1.39
30	h	5208	DGD	O6D-C5D	2.75	1.51	1.44
32	a	212	SQD	O48-C23	2.75	1.44	1.36
23	a	5558	CLA	CAA-C2A	2.75	1.59	1.54
23	C	496	CLA	CAA-C2A	2.75	1.59	1.54
23	c	5496	CLA	C4C-C3C	2.75	1.50	1.45
23	C	502	CLA	C4A-NA	-2.75	1.33	1.39
32	A	5212	SQD	O6-C1	2.75	1.45	1.40
23	C	491	CLA	MG-NA	2.74	2.15	2.07
28	A	566	BCR	C26-C25	2.75	1.38	1.34
30	c	5507	DGD	C3E-C2E	2.74	1.59	1.52
23	B	512	CLA	C4A-NA	-2.74	1.33	1.39
23	B	519	CLA	C1A-NA	2.74	1.38	1.32
23	C	503	CLA	C5-C3	2.74	1.55	1.40
32	L	5213	SQD	C17-C16	-2.74	1.34	1.51
32	L	5213	SQD	C11-C10	-2.74	1.34	1.51
23	C	498	CLA	C1B-CHB	-2.74	1.32	1.39
23	A	558	CLA	C1B-CHB	-2.73	1.32	1.39
23	b	5521	CLA	C1B-CHB	-2.73	1.32	1.39
23	B	515	CLA	C4B-NB	2.73	1.38	1.34
23	b	5526	CLA	C1A-NA	2.73	1.38	1.32
23	B	519	CLA	C1B-NB	2.73	1.38	1.34
23	b	5524	CLA	C3B-CAB	-2.73	1.46	1.49
32	L	5213	SQD	O6-C1	2.73	1.45	1.40
23	b	5526	CLA	C1C-NC	-2.73	1.36	1.38
23	a	5558	CLA	C4B-NB	2.73	1.38	1.34
30	C	508	DGD	C4E-C3E	2.73	1.59	1.52
28	D	357	BCR	C19-C18	-2.73	1.39	1.45
23	C	494	CLA	C3D-CAD	-2.72	1.41	1.47
23	C	501	CLA	CAA-C2A	2.72	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	5530	MGE	O6D-C5D	2.72	1.51	1.44
23	a	5558	CLA	C1C-NC	-2.72	1.36	1.38
23	b	5522	CLA	C1A-NA	2.72	1.38	1.32
33	t	5217	LMT	O5B-C1B	2.72	1.48	1.41
30	c	5508	DGD	C4D-C3D	2.72	1.59	1.52
32	L	5213	SQD	C20-C19	-2.71	1.34	1.51
23	A	563	CLA	C4A-NA	-2.71	1.33	1.39
28	x	5130	BCR	C14-C13	2.71	1.39	1.35
25	V	552	HEM	FE-NA	2.71	2.04	1.92
25	V	552	HEM	CAD-CBD	2.70	1.60	1.52
23	c	5496	CLA	MG-NA	2.70	2.15	2.07
25	V	552	HEM	FE-NB	2.70	2.07	1.97
32	d	5358	SQD	O6-C44	-2.70	1.38	1.43
30	H	208	DGD	O5D-C1E	2.70	1.45	1.40
25	V	552	HEM	C1A-C2A	2.70	1.48	1.43
23	B	525	CLA	CAA-C2A	2.70	1.58	1.54
23	B	517	CLA	C1C-NC	-2.70	1.36	1.38
23	B	513	CLA	C1B-CHB	-2.69	1.32	1.39
28	b	5528	BCR	C2-C1	2.69	1.61	1.54
23	b	5526	CLA	CHB-C4A	2.69	1.42	1.36
25	F	51	HEM	C1A-C2A	2.69	1.48	1.43
23	B	515	CLA	C4A-NA	-2.69	1.33	1.39
23	b	5519	CLA	CHB-C4A	2.69	1.42	1.36
30	C	508	DGD	O3G-C1D	2.69	1.45	1.40
23	D	354	CLA	MG-NB	2.69	2.11	2.05
30	H	208	DGD	O6D-C1D	2.69	1.48	1.41
23	C	496	CLA	C1A-NA	2.68	1.38	1.32
23	b	5516	CLA	C4B-NB	2.68	1.38	1.34
23	d	5354	CLA	C3D-CAD	-2.68	1.41	1.47
25	f	5051	HEM	C3D-C2D	-2.67	1.39	1.43
23	b	5515	CLA	C1B-CHB	-2.67	1.32	1.39
23	a	5559	CLA	C3D-CAD	-2.67	1.41	1.47
28	B	529	BCR	C10-C9	2.67	1.39	1.35
23	b	5512	CLA	C1B-CHB	-2.67	1.32	1.39
23	A	559	CLA	CAA-C2A	2.67	1.58	1.54
32	t	213	SQD	C19-C18	-2.67	1.35	1.51
23	b	5520	CLA	C1B-NB	2.66	1.38	1.34
28	t	104	BCR	C29-C30	2.66	1.60	1.54
32	A	5212	SQD	O5-C1	2.66	1.48	1.41
28	C	506	BCR	C29-C30	2.66	1.60	1.54
23	c	5498	CLA	MG-NB	2.66	2.10	2.05
23	A	560	CLA	C1C-NC	-2.66	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	522	CLA	CHB-C4A	2.65	1.42	1.36
23	d	5355	CLA	C5-C3	2.65	1.54	1.40
25	v	5552	HEM	C4D-ND	-2.65	1.34	1.39
23	b	5514	CLA	CHB-C4A	2.65	1.42	1.36
23	B	520	CLA	C1B-CHB	-2.65	1.32	1.39
23	A	560	CLA	C3D-CAD	-2.64	1.42	1.47
23	c	5492	CLA	C4-C3	2.64	1.57	1.50
24	a	5561	PHO	C4D-CHA	-2.64	1.41	1.45
30	C	508	DGD	C1E-C2E	2.64	1.60	1.52
23	B	517	CLA	CHB-C4A	2.64	1.42	1.36
23	B	517	CLA	C1A-NA	2.64	1.38	1.32
32	t	213	SQD	C14-C13	-2.64	1.35	1.51
29	d	5359	MGE	C4D-C3D	2.64	1.59	1.52
28	b	5529	BCR	C10-C9	2.63	1.39	1.35
23	c	5503	CLA	C1A-NA	2.63	1.38	1.32
25	F	51	HEM	C3B-CAB	2.63	1.48	1.40
30	c	5507	DGD	O3G-C1D	2.63	1.45	1.40
23	C	498	CLA	C4B-NB	2.63	1.37	1.34
33	T	217	LMT	O1B-C1B	2.63	1.48	1.41
32	L	5213	SQD	C19-C18	-2.63	1.35	1.51
23	B	524	CLA	MG-NB	2.63	2.10	2.05
23	a	5558	CLA	CHC-C1C	2.63	1.44	1.35
23	b	5520	CLA	CAA-C2A	2.63	1.58	1.54
23	c	5498	CLA	CAA-C2A	2.63	1.58	1.54
32	a	212	SQD	O5-C1	2.62	1.48	1.41
23	b	5520	CLA	C3D-CAD	-2.62	1.42	1.47
23	C	502	CLA	C1B-NB	2.62	1.37	1.34
23	B	526	CLA	C2-C3	2.62	1.38	1.32
33	T	217	LMT	O5B-C1B	2.62	1.48	1.41
23	d	5354	CLA	C3A-C4A	-2.62	1.44	1.51
30	C	507	DGD	O3G-C1D	2.62	1.44	1.40
23	B	521	CLA	CHB-C4A	2.61	1.42	1.36
28	t	104	BCR	C23-C22	-2.61	1.40	1.45
24	A	561	PHO	CAA-CBA	-2.61	1.44	1.52
23	A	559	CLA	CHB-C4A	2.61	1.42	1.36
29	i	5201	MGE	O2G-C1B	2.61	1.42	1.34
23	b	5512	CLA	C4A-NA	-2.61	1.33	1.39
23	B	526	CLA	C1B-CHB	-2.60	1.32	1.39
23	b	5514	CLA	C1C-NC	-2.60	1.36	1.38
23	B	524	CLA	C4B-NB	2.60	1.37	1.34
28	B	528	BCR	C5-C6	2.60	1.38	1.34
23	c	5503	CLA	C1C-C2C	2.60	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i	5201	MGE	O6D-C1D	2.60	1.48	1.41
29	d	5360	MGE	O6D-C5D	2.59	1.50	1.44
32	t	213	SQD	O5-C1	2.59	1.48	1.41
23	c	5503	CLA	C4B-NB	2.59	1.37	1.34
29	d	5360	MGE	O1G-C1A	2.59	1.41	1.33
23	c	5496	CLA	C1B-CHB	-2.59	1.32	1.39
25	F	51	HEM	FE-NC	2.59	2.07	1.97
23	b	5512	CLA	C1A-NA	2.59	1.37	1.32
24	A	562	PHO	C4-C3	2.59	1.57	1.50
23	B	522	CLA	CHC-C1C	2.58	1.44	1.35
23	B	518	CLA	C1C-NC	-2.58	1.36	1.38
23	C	498	CLA	C3D-CAD	-2.59	1.42	1.47
23	c	5494	CLA	MG-NB	2.58	2.10	2.05
23	B	515	CLA	C1B-CHB	-2.58	1.32	1.39
32	A	568	SQD	C17-C16	-2.58	1.35	1.51
23	b	5512	CLA	MG-NA	2.58	2.14	2.07
23	C	501	CLA	C1C-C2C	2.58	1.49	1.44
32	L	5213	SQD	C18-C17	-2.57	1.35	1.51
32	t	213	SQD	C15-C14	-2.57	1.35	1.51
28	C	505	BCR	C38-C26	2.57	1.55	1.51
25	v	5552	HEM	FE-NA	2.57	2.03	1.92
30	C	509	DGD	O6D-C5D	2.57	1.50	1.44
23	c	5500	CLA	C4A-NA	-2.57	1.33	1.39
30	C	507	DGD	C3E-C2E	2.56	1.59	1.52
30	H	208	DGD	O6D-C5D	2.56	1.50	1.44
23	c	5503	CLA	C5-C3	2.56	1.54	1.40
23	c	5493	CLA	C3D-CAD	-2.56	1.42	1.47
23	c	5500	CLA	MG-NA	2.56	2.14	2.07
28	C	506	BCR	C35-C13	2.56	1.55	1.51
23	B	526	CLA	C3B-CAB	-2.56	1.46	1.49
23	C	503	CLA	C1B-NB	2.55	1.37	1.34
23	B	511	CLA	C4C-C3C	2.55	1.49	1.45
30	c	5509	DGD	O6D-C5D	2.55	1.50	1.44
30	H	208	DGD	C1E-C2E	2.55	1.60	1.52
32	L	5213	SQD	C13-C12	-2.55	1.35	1.51
32	d	5358	SQD	O5-C1	2.55	1.48	1.41
25	f	5051	HEM	C3B-C2B	-2.55	1.39	1.43
23	D	355	CLA	C1A-NA	2.55	1.37	1.32
23	b	5525	CLA	MG-NA	2.55	2.14	2.07
30	C	508	DGD	C3D-C2D	2.55	1.59	1.52
33	t	5217	LMT	O1B-C4'	2.55	1.50	1.43
28	t	104	BCR	C35-C13	2.55	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	522	CLA	C1C-NC	-2.55	1.36	1.38
23	b	5520	CLA	CHB-C4A	2.55	1.42	1.36
30	c	5507	DGD	C1E-C2E	2.55	1.60	1.52
30	c	5508	DGD	O1G-C1A	2.55	1.41	1.33
29	I	201	MGE	O6D-C5D	2.55	1.50	1.44
23	c	5498	CLA	C1A-NA	2.55	1.37	1.32
33	m	216	LMT	O1'-C1'	2.55	1.44	1.40
23	a	5563	CLA	C4A-NA	-2.54	1.33	1.39
23	B	520	CLA	C4A-NA	-2.54	1.33	1.39
23	c	5497	CLA	MG-NB	2.54	2.10	2.05
23	d	5355	CLA	C4B-NB	2.54	1.37	1.34
23	b	5519	CLA	C1C-NC	-2.54	1.36	1.38
23	c	5494	CLA	C1B-CHB	-2.54	1.32	1.39
29	D	359	MGE	C4D-C3D	2.54	1.59	1.52
23	b	5520	CLA	MG-NC	2.53	2.14	2.07
23	B	515	CLA	C3D-CAD	-2.53	1.42	1.47
23	C	501	CLA	C3D-CAD	-2.53	1.42	1.47
23	a	5563	CLA	MG-NB	2.53	2.10	2.05
23	C	494	CLA	C1B-CHB	-2.53	1.32	1.39
24	a	5561	PHO	C1D-ND	-2.53	1.34	1.38
23	c	5500	CLA	C4-C3	2.53	1.57	1.50
25	f	5051	HEM	CMA-C3A	2.53	1.56	1.51
23	C	496	CLA	C4C-C3C	2.52	1.49	1.45
25	F	51	HEM	CMD-C2D	2.53	1.55	1.47
29	D	360	MGE	O6D-C1D	2.52	1.48	1.41
23	b	5526	CLA	C1-C2	2.52	1.57	1.49
23	B	513	CLA	C4A-NA	-2.52	1.33	1.39
33	T	217	LMT	O1B-C4'	2.52	1.50	1.43
23	C	502	CLA	MG-NB	2.52	2.10	2.05
32	t	213	SQD	C11-C10	-2.52	1.36	1.51
32	t	213	SQD	C12-C11	-2.52	1.36	1.51
29	I	201	MGE	O2G-C1B	2.52	1.41	1.34
33	A	569	LMT	O5B-C5B	2.52	1.50	1.44
29	d	5359	MGE	O6D-C5D	2.52	1.50	1.44
23	b	5526	CLA	C4B-NB	2.52	1.37	1.34
30	H	208	DGD	O6E-C1E	2.51	1.48	1.41
25	v	5552	HEM	C2C-C1C	2.51	1.50	1.43
26	A	564	PQ9	C11-C2	2.51	1.53	1.51
30	C	508	DGD	C4D-C3D	2.51	1.59	1.52
23	C	500	CLA	C1B-CHB	-2.51	1.32	1.39
25	v	5552	HEM	CMB-C2B	2.51	1.55	1.47
30	h	5208	DGD	O5D-C1E	2.51	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	5559	CLA	C1B-CHB	-2.50	1.32	1.39
23	D	355	CLA	C5-C3	2.50	1.54	1.40
23	B	511	CLA	C3C-C2C	2.50	1.42	1.36
30	c	5508	DGD	C1E-C2E	2.50	1.60	1.52
23	B	512	CLA	C4B-NB	2.50	1.37	1.34
28	h	5107	BCR	C5-C6	2.50	1.38	1.34
32	A	568	SQD	C12-C11	-2.50	1.36	1.51
23	B	525	CLA	C1B-CHB	-2.50	1.33	1.39
23	a	5560	CLA	C1B-CHB	-2.50	1.33	1.39
23	b	5519	CLA	MG-NC	2.50	2.14	2.07
32	t	213	SQD	C17-C16	-2.50	1.36	1.51
23	b	5514	CLA	C4B-NB	2.50	1.37	1.34
28	B	527	BCR	C2-C1	2.50	1.60	1.54
23	b	5522	CLA	CHB-C4A	2.49	1.42	1.36
30	C	507	DGD	O6D-C5D	2.49	1.50	1.44
23	C	496	CLA	CHB-C4A	2.49	1.42	1.36
23	c	5502	CLA	C4A-NA	-2.49	1.33	1.39
23	b	5511	CLA	C3C-C2C	2.49	1.41	1.36
23	B	521	CLA	MG-NB	2.49	2.10	2.05
23	B	516	CLA	C1A-NA	2.48	1.37	1.32
23	b	5518	CLA	CHB-C4A	2.49	1.42	1.36
23	B	523	CLA	C4A-NA	-2.49	1.33	1.39
23	c	5495	CLA	CHB-C4A	2.48	1.42	1.36
33	A	569	LMT	O5B-C1B	2.48	1.48	1.41
23	C	493	CLA	CHB-C4A	2.48	1.42	1.36
23	b	5523	CLA	C4A-NA	-2.48	1.33	1.39
23	b	5511	CLA	C3D-CAD	-2.48	1.42	1.47
23	c	5496	CLA	C1C-C2C	2.48	1.49	1.44
23	c	5493	CLA	MG-NC	2.48	2.14	2.07
23	B	513	CLA	C3D-CAD	-2.48	1.42	1.47
23	b	5523	CLA	C3D-CAD	-2.48	1.42	1.47
23	A	558	CLA	CAA-CBA	-2.48	1.44	1.52
23	c	5497	CLA	C1B-CHB	-2.47	1.33	1.39
23	A	558	CLA	C3D-CAD	-2.47	1.42	1.47
23	a	5560	CLA	C4A-NA	-2.47	1.33	1.39
23	B	518	CLA	CHB-C4A	2.47	1.42	1.36
28	a	5566	BCR	C26-C25	2.47	1.38	1.34
29	B	530	MGE	C1D-C2D	2.47	1.59	1.52
23	b	5513	CLA	C4-C3	2.46	1.57	1.50
25	v	5552	HEM	FE-NB	2.47	2.06	1.97
23	C	503	CLA	C1C-NC	-2.46	1.36	1.38
28	c	5506	BCR	C19-C18	-2.46	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	5527	BCR	C19-C18	-2.46	1.40	1.45
32	L	5213	SQD	C15-C14	-2.46	1.36	1.51
23	C	492	CLA	C1B-NB	2.46	1.37	1.34
28	A	566	BCR	C29-C30	2.46	1.60	1.54
23	B	517	CLA	C1B-CHB	-2.45	1.33	1.39
23	B	518	CLA	C4B-NB	2.45	1.37	1.34
29	B	530	MGE	O6D-C5D	2.45	1.50	1.44
23	C	498	CLA	CHC-C1C	2.45	1.43	1.35
23	b	5516	CLA	C1B-CHB	-2.45	1.33	1.39
23	B	518	CLA	C1B-NB	2.45	1.37	1.34
23	b	5526	CLA	C1B-NB	2.45	1.37	1.34
23	b	5516	CLA	OBD-CAD	2.45	1.25	1.22
32	t	213	SQD	C13-C12	-2.44	1.36	1.51
28	T	5104	BCR	C37-C22	2.44	1.55	1.51
23	C	503	CLA	CHB-C4A	2.44	1.42	1.36
32	L	5213	SQD	C16-C15	-2.44	1.36	1.51
23	a	5558	CLA	CAA-CBA	-2.44	1.44	1.52
29	I	201	MGE	O6D-C1D	2.44	1.48	1.41
32	A	568	SQD	C16-C15	-2.44	1.36	1.51
23	B	520	CLA	C4C-C3C	2.43	1.49	1.45
23	C	495	CLA	C4A-NA	-2.43	1.33	1.39
23	b	5525	CLA	MG-NB	2.43	2.10	2.05
23	b	5522	CLA	C1B-CHB	-2.43	1.33	1.39
23	b	5526	CLA	C1B-CHB	-2.43	1.33	1.39
23	B	518	CLA	MG-NB	2.43	2.10	2.05
23	c	5498	CLA	CHC-C1C	2.43	1.43	1.35
23	B	521	CLA	C4B-NB	2.43	1.37	1.34
23	B	517	CLA	C4B-NB	2.42	1.37	1.34
23	B	521	CLA	C1C-NC	-2.43	1.36	1.38
28	h	5107	BCR	C14-C13	2.42	1.38	1.35
32	A	568	SQD	O5-C1	2.42	1.48	1.41
32	d	5358	SQD	C17-C16	-2.42	1.36	1.51
23	B	515	CLA	MG-NB	2.42	2.10	2.05
23	c	5498	CLA	C4A-NA	-2.42	1.33	1.39
25	f	5051	HEM	FE-NC	2.42	2.06	1.97
32	L	5213	SQD	C14-C13	-2.42	1.36	1.51
23	C	492	CLA	CAA-C2A	2.42	1.58	1.54
23	b	5513	CLA	C4A-NA	-2.41	1.33	1.39
33	t	5217	LMT	C1B-C2B	2.41	1.59	1.52
32	A	568	SQD	C15-C14	-2.41	1.36	1.51
23	B	521	CLA	C1B-CHB	-2.41	1.33	1.39
23	B	514	CLA	C4B-NB	2.41	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	515	CLA	CHB-C4A	2.41	1.42	1.36
33	M	5216	LMT	O5'-C1'	2.41	1.48	1.41
23	A	563	CLA	C4-C3	2.41	1.56	1.50
24	A	561	PHO	C4D-CHA	-2.41	1.42	1.45
23	B	520	CLA	C4-C3	2.40	1.56	1.50
23	d	5355	CLA	MG-NB	2.40	2.10	2.05
23	c	5491	CLA	CHB-C4A	2.40	1.42	1.36
33	A	569	LMT	C1B-C2B	2.40	1.59	1.52
23	C	496	CLA	C2-C3	2.40	1.37	1.32
29	B	530	MGE	O2G-C1B	2.40	1.41	1.34
23	C	497	CLA	C4-C3	2.40	1.56	1.50
23	c	5495	CLA	C4A-NA	-2.40	1.34	1.39
25	v	5552	HEM	CMC-C2C	2.39	1.54	1.47
23	C	491	CLA	CHB-C4A	2.39	1.42	1.36
23	B	513	CLA	C5-C3	2.39	1.57	1.51
32	A	568	SQD	C11-C10	-2.39	1.36	1.51
33	a	5568	LMT	C1'-C2'	2.39	1.59	1.52
28	T	5104	BCR	C23-C22	-2.39	1.40	1.45
23	D	354	CLA	C4B-NB	2.39	1.37	1.34
33	m	216	LMT	O5'-C1'	2.39	1.48	1.41
28	c	5504	BCR	C10-C9	2.39	1.38	1.35
23	c	5503	CLA	C4-C3	2.39	1.56	1.48
23	c	5497	CLA	CHB-C4A	2.39	1.42	1.36
23	a	5559	CLA	MG-NA	2.39	2.14	2.07
23	C	502	CLA	CHB-C4A	2.39	1.42	1.36
23	b	5515	CLA	C4-C3	2.39	1.56	1.50
23	c	5493	CLA	C1B-CHB	-2.38	1.33	1.39
24	A	561	PHO	C1D-ND	-2.38	1.35	1.38
28	x	5130	BCR	C35-C13	2.38	1.55	1.51
25	f	5051	HEM	CMB-C2B	2.38	1.54	1.47
23	C	492	CLA	C1B-CHB	-2.38	1.33	1.39
23	c	5491	CLA	C4A-NA	-2.38	1.34	1.39
23	b	5522	CLA	MG-NB	2.38	2.10	2.05
23	b	5520	CLA	MG-NA	2.38	2.14	2.07
23	B	511	CLA	C1C-C2C	2.38	1.49	1.44
23	b	5526	CLA	C2-C3	2.38	1.37	1.32
32	t	213	SQD	C16-C15	-2.38	1.36	1.51
23	B	512	CLA	MG-NB	2.37	2.10	2.05
23	b	5514	CLA	CHC-C1C	2.37	1.43	1.35
28	T	5104	BCR	C29-C30	2.37	1.60	1.54
23	b	5522	CLA	C1C-NC	-2.37	1.36	1.38
28	c	5506	BCR	C10-C9	2.37	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	492	CLA	C4-C3	2.37	1.56	1.50
23	c	5501	CLA	C1C-C2C	2.37	1.49	1.44
23	b	5518	CLA	C4A-NA	-2.37	1.34	1.39
23	B	515	CLA	CAA-C2A	2.37	1.58	1.54
23	b	5522	CLA	CHC-C1C	2.37	1.43	1.35
23	c	5502	CLA	CHC-C1C	2.37	1.43	1.35
33	m	216	LMT	O5B-C1B	2.37	1.47	1.41
23	B	523	CLA	CAA-C2A	2.37	1.58	1.54
23	b	5514	CLA	C4A-NA	-2.36	1.34	1.39
23	b	5525	CLA	C1C-NC	-2.36	1.36	1.38
25	v	5552	HEM	CMD-C2D	2.36	1.54	1.47
23	c	5491	CLA	C1B-NB	2.36	1.37	1.34
23	b	5517	CLA	C1B-CHB	-2.36	1.33	1.39
23	c	5500	CLA	CHB-C4A	2.36	1.42	1.36
32	t	213	SQD	C18-C17	-2.36	1.37	1.51
23	C	499	CLA	OBD-CAD	2.36	1.25	1.22
23	c	5502	CLA	C4-C3	2.35	1.56	1.50
23	C	498	CLA	MG-NB	2.35	2.10	2.05
23	B	511	CLA	CHB-C4A	2.35	1.42	1.36
23	C	491	CLA	C4-C3	2.35	1.56	1.50
23	B	513	CLA	C4-C3	2.35	1.56	1.50
23	c	5499	CLA	C4A-NA	-2.35	1.34	1.39
23	B	514	CLA	C4-C3	2.35	1.56	1.50
23	c	5495	CLA	C1B-NB	2.35	1.37	1.34
23	d	5355	CLA	CHC-C1C	2.35	1.43	1.35
23	b	5525	CLA	C1B-CHB	-2.34	1.33	1.39
23	a	5560	CLA	MG-NB	2.34	2.10	2.05
23	c	5496	CLA	C3D-CAD	-2.34	1.42	1.47
23	B	526	CLA	CHB-C4A	2.34	1.42	1.36
23	c	5503	CLA	C3B-CAB	-2.34	1.47	1.49
25	F	51	HEM	CMB-C2B	2.34	1.54	1.47
23	c	5496	CLA	C4-C3	2.34	1.56	1.50
23	c	5501	CLA	CHB-C4A	2.34	1.42	1.36
23	c	5492	CLA	CAA-C2A	2.33	1.58	1.54
24	A	562	PHO	C1B-CHB	-2.33	1.32	1.35
24	A	562	PHO	C3D-CAD	-2.33	1.42	1.47
23	b	5517	CLA	C4A-NA	-2.33	1.34	1.39
23	C	493	CLA	C4A-NA	-2.33	1.34	1.39
23	B	524	CLA	CHB-C4A	2.33	1.42	1.36
30	c	5507	DGD	O6D-C5D	2.33	1.50	1.44
23	b	5521	CLA	MG-NB	2.33	2.10	2.05
23	c	5501	CLA	C3D-CAD	-2.33	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	5562	PHO	C4B-NB	2.33	1.39	1.36
23	d	5355	CLA	C1B-CHB	-2.33	1.33	1.39
23	C	503	CLA	C4A-NA	-2.33	1.34	1.39
23	a	5558	CLA	MG-NA	2.33	2.14	2.07
25	V	552	HEM	CHB-C1B	-2.33	1.32	1.35
23	b	5517	CLA	C2-C3	2.33	1.37	1.32
28	b	5528	BCR	C26-C25	2.33	1.38	1.34
23	b	5513	CLA	C1B-CHB	-2.33	1.33	1.39
23	C	495	CLA	CHC-C1C	2.32	1.43	1.35
23	a	5559	CLA	C4B-NB	2.32	1.37	1.34
23	B	524	CLA	CAA-C2A	2.32	1.58	1.54
23	c	5493	CLA	CHB-C4A	2.32	1.42	1.36
23	A	558	CLA	CHC-C1C	2.32	1.43	1.35
23	c	5492	CLA	C1B-NB	2.31	1.37	1.34
23	D	354	CLA	CHC-C1C	2.31	1.43	1.35
23	b	5524	CLA	C1B-CHB	-2.31	1.33	1.39
24	A	561	PHO	C4B-CHC	-2.31	1.37	1.46
23	A	563	CLA	CAA-C2A	2.31	1.58	1.54
28	X	130	BCR	C33-C5	2.31	1.54	1.51
23	C	491	CLA	C1B-CHB	-2.31	1.33	1.39
23	b	5518	CLA	CHC-C1C	2.31	1.43	1.35
25	v	5552	HEM	C2A-C3A	2.31	1.44	1.37
23	C	502	CLA	CHC-C1C	2.31	1.43	1.35
23	C	498	CLA	C4A-NA	-2.31	1.34	1.39
32	d	5358	SQD	C8-C7	2.31	1.57	1.50
32	A	5212	SQD	C44-C45	2.30	1.57	1.50
23	c	5502	CLA	MG-NC	2.30	2.14	2.07
32	a	212	SQD	C44-C45	2.30	1.57	1.50
29	d	5361	MGE	O6D-C5D	2.30	1.50	1.44
23	B	513	CLA	C1A-NA	2.30	1.37	1.32
30	c	5507	DGD	C9B-C8B	-2.30	1.54	1.55
23	C	492	CLA	C4A-NA	-2.30	1.34	1.39
28	a	5566	BCR	C14-C13	2.30	1.38	1.35
23	c	5497	CLA	C3D-CAD	-2.29	1.42	1.47
23	B	519	CLA	MG-NC	2.29	2.14	2.07
23	c	5502	CLA	C3D-CAD	-2.29	1.42	1.47
23	b	5515	CLA	MG-NA	2.29	2.14	2.07
24	a	5562	PHO	CHA-C1A	2.29	1.42	1.37
23	c	5495	CLA	C1C-C2C	2.29	1.49	1.44
24	a	5561	PHO	CAA-CBA	-2.29	1.45	1.52
23	a	5563	CLA	C5-C3	2.29	1.56	1.51
23	c	5494	CLA	CHB-C4A	2.29	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5495	CLA	CHC-C1C	2.28	1.43	1.35
25	V	552	HEM	CMA-C3A	2.29	1.56	1.51
32	L	5213	SQD	O6-C44	-2.29	1.39	1.43
29	I	201	MGE	O3G-C1D	2.28	1.44	1.40
23	C	503	CLA	C4-C3	2.28	1.56	1.48
23	C	500	CLA	C4C-C3C	2.28	1.49	1.45
23	b	5526	CLA	MG-NB	2.28	2.10	2.05
23	C	500	CLA	C1C-NC	-2.28	1.36	1.38
32	d	5358	SQD	C32-C31	-2.28	1.37	1.51
23	B	524	CLA	C1B-CHB	-2.28	1.33	1.39
23	B	517	CLA	C4A-NA	-2.28	1.34	1.39
23	c	5494	CLA	CHC-C1C	2.28	1.43	1.35
23	A	563	CLA	CHC-C1C	2.28	1.43	1.35
23	b	5516	CLA	C1A-NA	2.28	1.37	1.32
30	c	5509	DGD	C4E-C5E	2.28	1.58	1.53
23	A	563	CLA	MG-NB	2.28	2.10	2.05
23	B	525	CLA	C3D-CAD	-2.28	1.42	1.47
23	b	5512	CLA	C4B-NB	2.27	1.37	1.34
23	D	355	CLA	C4-C3	2.27	1.56	1.48
24	a	5562	PHO	C4-C3	2.27	1.56	1.50
23	b	5525	CLA	CHC-C1C	2.27	1.43	1.35
32	A	568	SQD	C13-C12	-2.27	1.37	1.51
30	C	507	DGD	C4D-C5D	2.27	1.58	1.53
28	b	5527	BCR	C1-C6	2.27	1.57	1.53
23	B	518	CLA	CHC-C1C	2.27	1.43	1.35
29	I	201	MGE	C4D-C3D	2.27	1.58	1.52
23	c	5501	CLA	CHC-C1C	2.27	1.43	1.35
30	c	5508	DGD	O5D-C1E	2.26	1.44	1.40
23	c	5493	CLA	CHC-C1C	2.26	1.43	1.35
23	A	559	CLA	C1B-CHB	-2.26	1.33	1.39
32	d	5358	SQD	C20-C19	-2.26	1.37	1.51
23	c	5497	CLA	C4-C3	2.26	1.56	1.50
23	b	5517	CLA	CHC-C1C	2.26	1.43	1.35
23	C	497	CLA	CHB-C4A	2.26	1.41	1.36
32	A	568	SQD	C14-C13	-2.26	1.37	1.51
23	B	526	CLA	C1B-NB	2.25	1.37	1.34
23	b	5523	CLA	MG-NA	2.25	2.13	2.07
33	a	5568	LMT	O5B-C1B	2.25	1.47	1.41
23	b	5512	CLA	MG-NC	2.25	2.13	2.07
25	F	51	HEM	C3D-C2D	-2.25	1.39	1.43
30	c	5507	DGD	O6E-C5E	2.25	1.50	1.44
28	a	5566	BCR	C29-C30	2.25	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	5354	CLA	MG-NB	2.25	2.10	2.05
23	B	520	CLA	MG-NA	2.25	2.13	2.07
23	B	519	CLA	C4A-NA	-2.25	1.34	1.39
24	A	561	PHO	C4-C3	2.25	1.56	1.50
29	b	5530	MGE	C4D-C5D	2.24	1.58	1.53
28	C	504	BCR	C14-C13	2.24	1.38	1.35
25	v	5552	HEM	CBA-CGA	-2.24	1.44	1.50
23	B	512	CLA	MG-NC	2.24	2.13	2.07
23	c	5496	CLA	MG-NB	2.24	2.10	2.05
23	a	5558	CLA	C3D-CAD	-2.24	1.42	1.47
23	A	558	CLA	CAA-C2A	2.24	1.58	1.54
25	F	51	HEM	O2A-CGA	2.24	1.38	1.30
23	b	5524	CLA	C4B-NB	2.24	1.37	1.34
23	c	5491	CLA	C4-C3	2.24	1.56	1.50
29	D	360	MGE	O6D-C5D	2.24	1.50	1.44
29	i	5201	MGE	C2A-C1A	2.24	1.57	1.50
24	a	5561	PHO	C4B-CHC	-2.23	1.37	1.46
28	T	5104	BCR	C26-C25	2.23	1.37	1.34
28	T	5104	BCR	C29-C28	-2.23	1.46	1.52
25	V	552	HEM	CMB-C2B	2.23	1.54	1.47
32	A	568	SQD	C8-C7	2.23	1.57	1.50
23	C	498	CLA	C1B-NB	2.23	1.37	1.34
30	h	5208	DGD	O6D-C1D	2.23	1.47	1.41
28	C	506	BCR	C14-C13	2.23	1.38	1.35
23	B	521	CLA	CHC-C1C	2.23	1.43	1.35
23	b	5520	CLA	C1B-CHB	-2.22	1.33	1.39
23	b	5516	CLA	CHB-C4A	2.23	1.41	1.36
23	a	5559	CLA	CAA-C2A	2.22	1.58	1.54
23	b	5511	CLA	MG-NC	2.22	2.13	2.07
23	C	501	CLA	CHC-C1C	2.22	1.43	1.35
23	A	563	CLA	C4B-NB	2.22	1.37	1.34
23	B	522	CLA	MG-NB	2.22	2.10	2.05
23	B	513	CLA	CHB-C4A	2.22	1.41	1.36
32	d	5358	SQD	C24-C23	2.22	1.57	1.50
23	b	5524	CLA	CHC-C1C	2.22	1.42	1.35
24	A	561	PHO	C3D-CAD	-2.22	1.42	1.47
28	X	130	BCR	C14-C13	2.22	1.38	1.35
23	c	5498	CLA	C4-C3	2.22	1.56	1.50
23	c	5492	CLA	C1B-CHB	-2.21	1.33	1.39
24	a	5561	PHO	C3D-CAD	-2.21	1.42	1.47
32	d	5358	SQD	C11-C10	-2.21	1.37	1.51
32	a	212	SQD	O6-C44	-2.21	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	499	CLA	CAA-C2A	2.21	1.58	1.54
23	C	497	CLA	CAA-C2A	2.21	1.58	1.54
23	B	524	CLA	CHC-C1C	2.21	1.42	1.35
30	c	5508	DGD	C4E-C3E	2.21	1.58	1.52
23	c	5501	CLA	MG-NC	2.21	2.13	2.07
23	B	514	CLA	C3D-CAD	-2.21	1.42	1.47
23	A	560	CLA	MG-NB	2.21	2.09	2.05
23	c	5494	CLA	MG-NC	2.21	2.13	2.07
23	c	5499	CLA	CHB-C4A	2.20	1.41	1.36
23	c	5498	CLA	C1B-CHB	-2.21	1.33	1.39
23	B	516	CLA	C1B-CHB	-2.20	1.33	1.39
23	d	5355	CLA	C4A-NA	-2.20	1.34	1.39
32	d	5358	SQD	C12-C11	-2.20	1.38	1.51
28	T	5104	BCR	C30-C25	2.20	1.56	1.53
32	d	5358	SQD	C33-C32	-2.20	1.38	1.51
30	h	5208	DGD	C1D-C2D	2.20	1.59	1.52
25	v	5552	HEM	CMA-C3A	2.20	1.56	1.51
28	c	5504	BCR	C5-C6	2.20	1.37	1.34
23	b	5519	CLA	C1B-NB	2.20	1.37	1.34
23	b	5519	CLA	C1C-C2C	2.20	1.49	1.44
30	C	509	DGD	O1G-C1A	2.20	1.40	1.33
28	B	527	BCR	C1-C6	2.20	1.56	1.53
23	B	515	CLA	C1A-NA	2.20	1.37	1.32
23	b	5524	CLA	CHB-C4A	2.20	1.41	1.36
30	C	507	DGD	O6E-C5E	2.20	1.49	1.44
25	F	51	HEM	CHD-C4C	2.20	1.40	1.36
28	t	104	BCR	C29-C28	-2.20	1.46	1.52
23	c	5501	CLA	MG-NB	2.19	2.09	2.05
23	b	5514	CLA	MG-NB	2.19	2.09	2.05
23	C	499	CLA	C4A-NA	-2.19	1.34	1.39
23	c	5492	CLA	C3D-CAD	-2.19	1.42	1.47
23	c	5502	CLA	C2-C3	2.19	1.37	1.32
23	B	523	CLA	C1B-CHB	-2.19	1.33	1.39
23	c	5496	CLA	C1B-NB	2.19	1.37	1.34
32	d	5358	SQD	C15-C14	-2.19	1.38	1.51
33	M	5216	LMT	C1B-C2B	2.19	1.59	1.52
23	b	5515	CLA	MG-NB	2.19	2.09	2.05
25	V	552	HEM	C1C-NC	-2.19	1.34	1.38
28	B	527	BCR	C19-C18	-2.19	1.41	1.45
23	D	354	CLA	CHB-C4A	2.18	1.41	1.36
23	C	493	CLA	C1B-CHB	-2.18	1.33	1.39
23	D	355	CLA	CHC-C1C	2.18	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	526	CLA	C4A-NA	-2.18	1.34	1.39
23	C	498	CLA	CAA-C2A	2.18	1.58	1.54
23	c	5503	CLA	C4A-NA	-2.18	1.34	1.39
23	c	5499	CLA	C4C-C3C	2.17	1.49	1.45
32	d	5358	SQD	C19-C18	-2.17	1.38	1.51
23	d	5355	CLA	C1C-C2C	2.17	1.49	1.44
23	C	502	CLA	MG-NC	2.17	2.13	2.07
29	l	5210	MGE	C4D-C3D	2.17	1.58	1.52
23	b	5520	CLA	C4C-C3C	2.17	1.49	1.45
23	a	5558	CLA	C4A-NA	-2.17	1.34	1.39
23	B	522	CLA	C3D-CAD	-2.16	1.42	1.47
23	B	523	CLA	C4B-NB	2.16	1.37	1.34
32	A	568	SQD	C33-C32	-2.16	1.38	1.51
28	X	130	BCR	C24-C23	2.16	1.39	1.32
29	b	5530	MGE	O1G-C1G	-2.16	1.40	1.45
28	x	5130	BCR	C24-C23	2.16	1.39	1.32
33	M	5216	LMT	C1'-C2'	2.16	1.59	1.52
23	c	5495	CLA	C4-C3	2.16	1.56	1.50
23	B	516	CLA	C1C-NC	-2.16	1.36	1.38
23	B	523	CLA	MG-NB	2.16	2.09	2.05
23	B	522	CLA	C4A-NA	-2.16	1.34	1.39
32	d	5358	SQD	C16-C15	-2.15	1.38	1.51
28	D	357	BCR	C14-C13	2.16	1.38	1.35
25	V	552	HEM	C4D-ND	-2.15	1.35	1.39
32	A	5212	SQD	O6-C44	-2.15	1.39	1.43
23	d	5354	CLA	CHC-C1C	2.15	1.42	1.35
23	D	354	CLA	C3B-CAB	-2.15	1.47	1.49
23	a	5560	CLA	C1B-NB	2.15	1.37	1.34
23	B	526	CLA	C4B-NB	2.15	1.37	1.34
26	A	564	PQ9	C30-C28	2.15	1.52	1.40
29	b	5530	MGE	C4D-C3D	2.15	1.58	1.52
23	b	5522	CLA	C3D-CAD	-2.15	1.43	1.47
23	b	5519	CLA	C4A-NA	-2.15	1.34	1.39
23	B	517	CLA	CHC-C1C	2.15	1.42	1.35
23	D	354	CLA	C3B-C2B	-2.14	1.37	1.41
28	b	5529	BCR	C35-C13	2.14	1.54	1.51
23	c	5498	CLA	C3D-CAD	-2.14	1.43	1.47
30	h	5208	DGD	C3E-C2E	2.14	1.58	1.52
23	C	497	CLA	CHC-C1C	2.14	1.42	1.35
29	B	530	MGE	C4D-C5D	2.14	1.57	1.53
29	d	5360	MGE	O3G-C1D	2.14	1.44	1.40
28	B	527	BCR	C38-C26	2.14	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	5512	CLA	CAA-CBA	-2.14	1.45	1.52
33	M	5216	LMT	C3B-C2B	2.14	1.58	1.52
23	a	5560	CLA	C4-C3	2.14	1.56	1.50
23	C	497	CLA	MG-NB	2.13	2.09	2.05
23	C	495	CLA	C3D-CAD	-2.13	1.43	1.47
29	b	5530	MGE	C1D-C2D	2.13	1.58	1.52
23	C	502	CLA	C4-C3	2.13	1.56	1.50
23	A	563	CLA	C5-C3	2.13	1.56	1.51
23	B	526	CLA	C3D-CAD	-2.13	1.43	1.47
30	c	5508	DGD	O6D-C5D	2.13	1.49	1.44
29	i	5201	MGE	O3G-C1D	2.13	1.44	1.40
23	B	521	CLA	C4A-NA	-2.13	1.34	1.39
25	V	552	HEM	CMC-C2C	2.13	1.54	1.47
23	c	5496	CLA	MG-NC	2.13	2.13	2.07
33	a	5568	LMT	C1B-C2B	2.12	1.58	1.52
29	L	210	MGE	C4D-C3D	2.12	1.58	1.52
23	B	524	CLA	C4A-NA	-2.12	1.34	1.39
23	b	5525	CLA	MG-NC	2.12	2.13	2.07
23	B	525	CLA	MG-NB	2.12	2.09	2.05
33	M	5216	LMT	O5B-C1B	2.12	1.47	1.41
23	c	5497	CLA	CHC-C1C	2.12	1.42	1.35
32	A	568	SQD	C32-C31	-2.12	1.38	1.51
29	b	5530	MGE	O2G-C1B	2.12	1.40	1.34
23	B	518	CLA	C4-C3	2.12	1.56	1.50
23	c	5493	CLA	CMB-C2B	2.12	1.56	1.51
23	c	5500	CLA	C1B-CHB	-2.11	1.34	1.39
33	m	216	LMT	O5'-C5'	2.11	1.49	1.44
23	B	525	CLA	CHC-C1C	2.11	1.42	1.35
30	H	208	DGD	C1D-C2D	2.11	1.58	1.52
23	c	5498	CLA	C1C-C2C	2.11	1.48	1.44
25	F	51	HEM	C2C-C1C	2.10	1.49	1.43
23	D	355	CLA	C1C-C2C	2.11	1.48	1.44
23	C	503	CLA	CHC-C1C	2.10	1.42	1.35
23	B	522	CLA	C1B-CHB	-2.10	1.34	1.39
23	a	5559	CLA	CHB-C4A	2.10	1.41	1.36
23	A	560	CLA	C4A-NA	-2.10	1.34	1.39
28	D	357	BCR	C38-C26	2.10	1.54	1.51
29	D	359	MGE	O6D-C5D	2.10	1.49	1.44
30	c	5507	DGD	C4D-C5D	2.10	1.57	1.53
28	X	130	BCR	C10-C9	2.10	1.38	1.35
32	t	213	SQD	O6-C1	2.10	1.44	1.40
23	b	5511	CLA	OBD-CAD	2.10	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	552	HEM	CMD-C2D	2.10	1.53	1.47
23	B	515	CLA	C4-C3	2.10	1.56	1.50
23	A	559	CLA	MG-NB	2.10	2.09	2.05
23	B	518	CLA	C4A-NA	-2.09	1.34	1.39
24	a	5562	PHO	C3D-CAD	-2.09	1.42	1.47
23	B	518	CLA	C2-C3	2.09	1.37	1.32
23	C	496	CLA	C1C-C2C	2.09	1.48	1.44
24	a	5561	PHO	C2-C3	2.09	1.37	1.32
33	a	5568	LMT	O5B-C5B	2.09	1.49	1.44
28	b	5528	BCR	C35-C13	2.09	1.54	1.51
23	b	5515	CLA	C3A-C2A	-2.09	1.48	1.54
23	b	5514	CLA	C3D-CAD	-2.08	1.43	1.47
32	d	5358	SQD	C14-C13	-2.08	1.38	1.51
25	v	5552	HEM	CHB-C1B	-2.09	1.32	1.35
30	C	509	DGD	O2G-C1B	2.08	1.40	1.34
24	a	5562	PHO	C1B-CHB	-2.08	1.33	1.35
28	c	5505	BCR	C19-C18	-2.08	1.41	1.45
29	I	201	MGE	C3G-C2G	2.08	1.56	1.50
29	d	5359	MGE	C4D-C5D	2.08	1.57	1.53
23	c	5493	CLA	C4A-NA	-2.08	1.34	1.39
23	C	491	CLA	C3D-CAD	-2.08	1.43	1.47
23	b	5520	CLA	C1C-C2C	2.08	1.48	1.44
23	c	5496	CLA	CHB-C4A	2.08	1.41	1.36
25	f	5051	HEM	CMD-C2D	2.08	1.53	1.47
23	C	502	CLA	C1B-CHB	-2.08	1.34	1.39
32	d	5358	SQD	C36-C35	-2.07	1.38	1.51
29	D	359	MGE	O1G-C1A	2.07	1.39	1.33
30	h	5208	DGD	C4E-C3E	2.07	1.57	1.52
32	A	568	SQD	C19-C18	-2.08	1.38	1.51
23	B	525	CLA	C1B-NB	2.07	1.37	1.34
23	a	5558	CLA	MG-NC	2.07	2.13	2.07
23	b	5515	CLA	CHB-C4A	2.07	1.41	1.36
23	B	521	CLA	C4-C3	2.07	1.56	1.50
23	B	511	CLA	CMC-C2C	2.07	1.55	1.51
28	c	5506	BCR	C14-C13	2.07	1.38	1.35
23	B	520	CLA	CHB-C4A	2.07	1.41	1.36
23	b	5515	CLA	C1A-NA	2.07	1.36	1.32
32	A	568	SQD	O6-C1	2.07	1.43	1.40
28	C	505	BCR	C37-C22	2.07	1.54	1.51
24	A	562	PHO	C3B-C2B	-2.07	1.37	1.41
23	c	5499	CLA	C1B-CHB	-2.07	1.34	1.39
23	a	5559	CLA	C4A-NA	-2.07	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CMB-C2B	2.07	1.56	1.51
23	b	5524	CLA	C3D-CAD	-2.07	1.43	1.47
23	c	5498	CLA	CHB-C4A	2.07	1.41	1.36
25	V	552	HEM	C2C-C1C	2.06	1.49	1.43
23	C	495	CLA	C4C-C3C	2.06	1.48	1.45
23	C	496	CLA	OBD-CAD	2.06	1.25	1.22
23	C	494	CLA	CHC-C1C	2.06	1.42	1.35
23	c	5499	CLA	C1C-C2C	2.06	1.48	1.44
23	c	5500	CLA	MG-NC	2.06	2.13	2.07
32	A	568	SQD	C18-C17	-2.06	1.38	1.51
28	b	5528	BCR	C24-C23	2.06	1.39	1.32
23	B	514	CLA	C1B-CHB	-2.06	1.34	1.39
23	B	524	CLA	C1C-NC	-2.06	1.36	1.38
23	B	520	CLA	C3B-CAB	-2.05	1.47	1.49
23	B	516	CLA	CHC-C1C	2.05	1.42	1.35
33	m	216	LMT	C4B-C3B	2.05	1.57	1.52
23	b	5516	CLA	MG-NB	2.05	2.09	2.05
23	b	5522	CLA	C4-C3	2.05	1.56	1.50
23	a	5563	CLA	C1C-NC	-2.05	1.36	1.38
30	H	208	DGD	O6E-C5E	2.05	1.49	1.44
32	t	213	SQD	C21-C20	-2.05	1.34	1.51
23	C	493	CLA	CHC-C1C	2.05	1.42	1.35
32	L	5213	SQD	C8-C7	2.05	1.56	1.50
28	B	528	BCR	C24-C23	2.05	1.39	1.32
29	d	5361	MGE	O2G-C1B	2.05	1.40	1.34
23	c	5502	CLA	C1B-CHB	-2.04	1.34	1.39
23	a	5563	CLA	C4-C3	2.04	1.55	1.50
32	A	568	SQD	C35-C34	-2.04	1.38	1.51
23	b	5512	CLA	CHB-C4A	2.04	1.41	1.36
28	c	5505	BCR	C35-C13	2.04	1.54	1.51
25	f	5051	HEM	CBD-CGD	2.04	1.55	1.50
23	a	5558	CLA	MG-NB	2.04	2.09	2.05
28	d	5357	BCR	C14-C13	2.04	1.38	1.35
23	D	354	CLA	C1C-C2C	2.04	1.48	1.44
26	D	356	PQ9	C3-C4	2.04	1.50	1.44
30	C	508	DGD	O6D-C5D	2.04	1.49	1.44
33	M	5216	LMT	C4B-C5B	2.04	1.57	1.53
23	a	5563	CLA	CHC-C1C	2.04	1.42	1.35
23	C	492	CLA	OBD-CAD	2.04	1.25	1.22
28	A	566	BCR	C19-C18	-2.04	1.41	1.45
23	d	5355	CLA	C4-C3	2.03	1.55	1.48
23	B	517	CLA	C2-C3	2.03	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	i	5201	MGE	C3G-C2G	2.03	1.56	1.50
23	c	5496	CLA	C4A-NA	-2.03	1.34	1.39
23	C	496	CLA	CHC-C1C	2.03	1.42	1.35
29	l	5210	MGE	O6D-C5D	2.03	1.49	1.44
23	b	5519	CLA	MG-NB	2.03	2.09	2.05
32	A	568	SQD	C34-C33	-2.03	1.39	1.51
23	c	5492	CLA	CHB-C4A	2.03	1.41	1.36
23	c	5503	CLA	C1-C2	2.03	1.55	1.49
25	V	552	HEM	C2A-C3A	2.03	1.43	1.37
25	f	5051	HEM	CHD-C4C	2.03	1.39	1.36
23	d	5354	CLA	C1B-NB	2.03	1.37	1.34
28	d	5357	BCR	C19-C18	-2.03	1.41	1.45
23	B	519	CLA	CHC-C1C	2.03	1.42	1.35
23	b	5526	CLA	CHC-C1C	2.02	1.42	1.35
23	b	5526	CLA	C4A-NA	-2.02	1.34	1.39
23	b	5513	CLA	C5-C3	2.02	1.56	1.51
23	C	495	CLA	C4-C3	2.02	1.55	1.50
23	C	494	CLA	CHB-C4A	2.02	1.41	1.36
33	m	216	LMT	C1'-C2'	2.02	1.58	1.52
32	d	5358	SQD	C13-C12	-2.02	1.39	1.51
25	f	5051	HEM	C2A-C3A	2.02	1.43	1.37
28	C	505	BCR	C19-C18	-2.02	1.41	1.45
23	C	492	CLA	CHB-C4A	2.02	1.41	1.36
23	C	503	CLA	MG-NC	2.02	2.13	2.07
29	D	358	MGE	O2G-C1B	2.02	1.40	1.34
23	D	354	CLA	MG-NC	2.02	2.13	2.07
23	c	5502	CLA	MG-NB	2.02	2.09	2.05
28	C	506	BCR	C19-C18	-2.02	1.41	1.45
23	B	513	CLA	C2-C3	2.02	1.37	1.32
25	v	5552	HEM	C1C-NC	-2.01	1.35	1.38
30	C	509	DGD	C3D-C2D	2.02	1.57	1.52
23	C	496	CLA	C4A-NA	-2.01	1.34	1.39
28	b	5527	BCR	C23-C22	-2.01	1.41	1.45
23	d	5355	CLA	C1C-NC	-2.01	1.36	1.38
23	a	5558	CLA	CBA-CGA	-2.01	1.44	1.50
23	b	5519	CLA	CHC-C1C	2.01	1.42	1.35
23	b	5513	CLA	C4B-NB	2.01	1.37	1.34
23	b	5523	CLA	C1B-CHB	-2.01	1.34	1.39
32	A	568	SQD	C20-C19	-2.01	1.39	1.51
29	i	5201	MGE	C3D-C2D	2.01	1.57	1.52
30	H	208	DGD	C4E-C3E	2.00	1.57	1.52
26	d	5356	PQ9	C30-C28	2.00	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	354	CLA	C3D-CAD	-2.00	1.43	1.47
32	d	5358	SQD	C35-C34	-2.00	1.39	1.51
25	F	51	HEM	C2A-C3A	2.00	1.43	1.37
23	a	5560	CLA	CHB-C4A	2.00	1.41	1.36

All (2127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	t	213	SQD	O6-C1-C2	9.46	120.22	108.18
32	L	5213	SQD	C5-C6-S	9.40	128.29	114.45
32	A	568	SQD	C5-C6-S	9.08	127.83	114.45
32	t	213	SQD	C5-C6-S	9.07	127.82	114.45
32	L	5213	SQD	O6-C1-C2	9.01	119.65	108.18
32	d	5358	SQD	O6-C1-C2	8.92	119.53	108.18
32	A	5212	SQD	O5-C1-O6	8.84	130.76	109.98
32	A	568	SQD	O6-C1-C2	8.72	119.27	108.18
32	t	213	SQD	C31-C30-C29	8.48	133.50	114.46
32	a	212	SQD	O5-C1-O6	8.47	129.88	109.98
32	A	568	SQD	O5-C1-O6	8.44	129.81	109.98
32	a	212	SQD	O6-C1-C2	8.27	118.71	108.18
32	d	5358	SQD	C5-C6-S	8.22	126.56	114.45
32	d	5358	SQD	O5-C1-O6	8.16	129.16	109.98
32	L	5213	SQD	O5-C1-O6	8.13	129.09	109.98
32	L	5213	SQD	C31-C30-C29	8.07	132.59	114.46
32	A	5212	SQD	O6-C1-C2	8.00	118.36	108.18
32	t	213	SQD	O5-C1-O6	7.79	128.28	109.98
30	c	5507	DGD	O6E-C5E-C4E	7.48	123.60	109.76
32	a	212	SQD	C5-C6-S	7.36	125.30	114.45
30	H	208	DGD	O6E-C5E-C4E	7.31	123.29	109.76
32	A	5212	SQD	C5-C6-S	7.28	125.17	114.45
30	c	5508	DGD	O6E-C5E-C4E	7.24	123.17	109.76
25	f	5051	HEM	C3B-C4B-NB	-7.15	108.88	114.00
30	C	507	DGD	O6E-C5E-C4E	7.09	122.88	109.76
30	C	508	DGD	O6E-C5E-C4E	7.08	122.87	109.76
25	f	5051	HEM	CAD-C3D-C4D	-7.08	111.81	124.53
23	C	499	CLA	C1-O2A-CGA	7.04	123.32	115.06
30	C	509	DGD	O6E-C5E-C4E	6.99	122.70	109.76
30	c	5509	DGD	O6E-C5E-C4E	6.97	122.66	109.76
30	h	5208	DGD	O6E-C5E-C4E	6.96	122.65	109.76
25	f	5051	HEM	CAD-C3D-C2D	6.92	142.66	127.25
25	F	51	HEM	CAD-C3D-C4D	-6.80	112.31	124.53
25	V	552	HEM	CAD-C3D-C4D	-6.78	112.35	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	51	HEM	CAD-C3D-C2D	6.74	142.26	127.25
25	v	5552	HEM	CAD-C3D-C4D	-6.72	112.46	124.53
25	V	552	HEM	CAD-C3D-C2D	6.68	142.12	127.25
25	v	5552	HEM	CAD-C3D-C2D	6.57	141.87	127.25
23	c	5499	CLA	C1-O2A-CGA	6.53	122.73	115.06
25	F	51	HEM	C3B-C4B-NB	-6.48	109.36	114.00
28	D	357	BCR	C38-C26-C25	6.43	131.80	124.51
28	X	130	BCR	C33-C5-C6	6.43	131.79	124.51
28	T	5104	BCR	C38-C26-C25	6.40	131.77	124.51
32	A	568	SQD	O8-S-C6	-6.33	97.49	105.64
28	d	5357	BCR	C33-C5-C6	6.24	131.58	124.51
28	c	5505	BCR	C38-C26-C25	6.21	131.55	124.51
28	d	5357	BCR	C38-C26-C25	6.20	131.54	124.51
28	B	529	BCR	C38-C26-C25	6.18	131.51	124.51
28	x	5130	BCR	C33-C5-C6	6.15	131.48	124.51
23	B	515	CLA	CAA-C2A-C3A	-6.12	98.56	113.04
25	F	51	HEM	CBD-CAD-C3D	-6.10	101.06	114.37
28	t	104	BCR	C38-C26-C25	6.07	131.39	124.51
24	A	562	PHO	C3D-C4D-CHA	6.04	115.87	109.18
32	a	212	SQD	O8-S-C6	-5.95	97.98	105.64
28	D	357	BCR	C33-C5-C6	5.92	131.22	124.51
24	a	5561	PHO	C3D-C4D-CHA	5.89	115.71	109.18
32	d	5358	SQD	O8-S-C6	-5.88	98.07	105.64
25	f	5051	HEM	CBD-CAD-C3D	-5.85	101.61	114.37
32	A	568	SQD	C10-C9-C8	5.83	135.25	113.28
28	B	527	BCR	C38-C26-C25	5.81	131.09	124.51
32	t	213	SQD	C10-C9-C8	5.78	135.07	113.28
24	a	5562	PHO	C3D-C4D-CHA	5.77	115.57	109.18
32	d	5358	SQD	C10-C9-C8	5.77	135.02	113.28
31	A	567	LHG	C25-C24-C23	5.76	136.10	113.51
32	d	5358	SQD	C25-C24-C23	5.76	136.09	113.51
32	L	5213	SQD	C10-C9-C8	5.75	134.96	113.28
24	A	561	PHO	C3D-C4D-CHA	5.74	115.54	109.18
23	b	5515	CLA	CAA-C2A-C3A	-5.74	99.47	113.04
28	B	528	BCR	C38-C26-C25	5.73	131.00	124.51
28	C	505	BCR	C38-C26-C25	5.72	131.00	124.51
31	a	5567	LHG	C25-C24-C23	5.67	135.74	113.51
28	C	506	BCR	C38-C26-C25	5.64	130.90	124.51
28	X	130	BCR	C7-C8-C9	5.62	134.63	126.22
25	v	5552	HEM	CBD-CAD-C3D	-5.62	102.11	114.37
28	h	5107	BCR	C38-C26-C25	5.61	130.87	124.51
28	c	5506	BCR	C38-C26-C25	5.53	130.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	527	BCR	C33-C5-C6	5.52	130.77	124.51
32	t	213	SQD	C25-C24-C23	5.50	135.06	113.51
28	A	566	BCR	C33-C5-C6	5.49	130.73	124.51
28	C	504	BCR	C38-C26-C25	5.49	130.73	124.51
28	x	5130	BCR	C7-C8-C9	5.47	134.40	126.22
28	b	5527	BCR	C33-C5-C6	5.47	130.71	124.51
28	b	5528	BCR	C38-C26-C25	5.46	130.70	124.51
28	t	104	BCR	C33-C5-C6	5.46	130.70	124.51
28	T	5104	BCR	C33-C5-C6	5.45	130.69	124.51
32	L	5213	SQD	C25-C24-C23	5.42	134.76	113.51
32	A	568	SQD	C25-C24-C23	5.42	134.74	113.51
28	a	5566	BCR	C38-C26-C25	5.40	130.63	124.51
28	b	5529	BCR	C38-C26-C25	5.40	130.63	124.51
28	A	566	BCR	C38-C26-C25	5.39	130.62	124.51
28	B	529	BCR	C33-C5-C6	5.37	130.59	124.51
28	a	5566	BCR	C33-C5-C6	5.35	130.57	124.51
28	H	107	BCR	C38-C26-C25	5.34	130.56	124.51
28	c	5504	BCR	C38-C26-C25	5.29	130.51	124.51
32	t	213	SQD	O8-S-C6	-5.29	98.83	105.64
28	b	5527	BCR	C38-C26-C25	5.27	130.49	124.51
28	C	506	BCR	C33-C5-C6	5.27	130.48	124.51
25	V	552	HEM	CBD-CAD-C3D	-5.25	102.91	114.37
28	X	130	BCR	C11-C10-C9	5.25	134.85	127.29
28	C	505	BCR	C33-C5-C6	5.21	130.41	124.51
28	x	5130	BCR	C38-C26-C25	5.16	130.36	124.51
28	c	5506	BCR	C33-C5-C6	5.15	130.35	124.51
23	D	354	CLA	C2B-C3B-CAB	-5.10	116.89	127.33
28	X	130	BCR	C38-C26-C25	5.10	130.29	124.51
23	B	522	CLA	C2B-C3B-CAB	-5.08	116.94	127.33
23	d	5354	CLA	C2B-C3B-CAB	-5.01	117.08	127.33
30	h	5208	DGD	O3G-C1D-C2D	4.99	114.53	108.18
32	A	5212	SQD	O8-S-C6	-4.98	99.22	105.64
26	d	5356	PQ9	C11-C2-C3	-4.97	118.97	123.77
28	H	107	BCR	C33-C5-C6	4.96	130.13	124.51
23	c	5498	CLA	C2B-C3B-CAB	-4.95	117.19	127.33
24	a	5562	PHO	C2B-C3B-CAB	-4.91	117.27	127.33
28	c	5505	BCR	C33-C5-C6	4.89	130.06	124.51
28	b	5529	BCR	C33-C5-C6	4.87	130.03	124.51
23	b	5522	CLA	C2B-C3B-CAB	-4.87	117.37	127.33
28	h	5107	BCR	C33-C5-C6	4.83	129.99	124.51
26	D	356	PQ9	C11-C2-C3	-4.82	119.12	123.77
25	f	5051	HEM	CHA-C4D-ND	4.82	130.92	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5501	CLA	C2B-C3B-CAB	-4.81	117.49	127.33
24	A	562	PHO	C2B-C3B-CAB	-4.79	117.53	127.33
28	x	5130	BCR	C11-C10-C9	4.78	134.19	127.29
28	C	504	BCR	C33-C5-C6	4.77	129.92	124.51
28	b	5528	BCR	C33-C5-C6	4.74	129.88	124.51
30	H	208	DGD	O3G-C1D-C2D	4.74	114.21	108.18
23	b	5522	CLA	C4B-C3B-CAB	4.72	136.73	127.18
25	v	5552	HEM	C3B-C4B-NB	-4.70	110.64	114.00
23	c	5502	CLA	CAA-C2A-C3A	-4.69	101.96	113.04
23	B	522	CLA	C4B-C3B-CAB	4.68	136.65	127.18
23	C	495	CLA	CAA-C2A-C3A	-4.66	102.03	113.04
23	C	498	CLA	C2B-C3B-CAB	-4.66	117.80	127.33
30	c	5508	DGD	C3G-O3G-C1D	-4.65	104.53	113.81
32	a	212	SQD	C44-O6-C1	4.65	123.07	113.81
23	c	5495	CLA	CAA-C2A-C3A	-4.63	102.09	113.04
23	D	354	CLA	C4B-C3B-CAB	4.62	136.52	127.18
25	V	552	HEM	C3B-C4B-NB	-4.60	110.71	114.00
23	C	494	CLA	CAA-C2A-C3A	-4.58	102.21	113.04
23	c	5498	CLA	C4B-C3B-CAB	4.56	136.41	127.18
23	d	5354	CLA	C4B-C3B-CAB	4.54	136.36	127.18
23	B	521	CLA	C2B-C3B-CAB	-4.54	118.05	127.33
23	c	5493	CLA	CAA-C2A-C3A	-4.53	102.32	113.04
25	V	552	HEM	CHA-C4D-ND	4.53	130.53	124.31
23	c	5494	CLA	CAA-C2A-C3A	-4.53	102.33	113.04
28	c	5504	BCR	C33-C5-C6	4.52	129.64	124.51
23	B	513	CLA	C2B-C3B-CAB	-4.52	118.08	127.33
23	C	493	CLA	CAA-C2A-C3A	-4.51	102.37	113.04
30	C	508	DGD	O5D-C1E-C2E	4.51	113.92	108.18
23	D	354	CLA	CBD-CHA-C1A	4.51	134.66	128.77
23	b	5521	CLA	C2B-C3B-CAB	-4.50	118.13	127.33
28	B	528	BCR	C33-C5-C6	4.50	129.60	124.51
23	b	5524	CLA	C2B-C3B-CAB	-4.49	118.14	127.33
23	B	515	CLA	C2B-C3B-CAB	-4.49	118.14	127.33
23	C	502	CLA	CAA-C2A-C3A	-4.47	102.47	113.04
23	B	518	CLA	C2B-C3B-CAB	-4.47	118.19	127.33
23	c	5503	CLA	C2B-C3B-CAB	-4.47	118.19	127.33
23	c	5502	CLA	C2B-C3B-CAB	-4.44	118.23	127.33
32	L	5213	SQD	O8-S-C6	-4.43	99.93	105.64
23	d	5355	CLA	C2B-C3B-CAB	-4.41	118.31	127.33
23	c	5501	CLA	C4A-NA-C1A	4.40	112.59	106.52
23	C	496	CLA	C2B-C3B-CAB	-4.40	118.32	127.33
28	X	130	BCR	C8-C9-C10	-4.40	112.22	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5526	CLA	C2B-C3B-CAB	-4.39	118.33	127.33
23	C	493	CLA	C2B-C3B-CAB	-4.38	118.36	127.33
23	b	5514	CLA	C4A-NA-C1A	4.38	112.56	106.52
24	A	561	PHO	C2B-C3B-CAB	-4.38	118.36	127.33
23	c	5491	CLA	C2B-C3B-CAB	-4.38	118.37	127.33
23	d	5354	CLA	CBD-CHA-C1A	4.38	134.49	128.77
29	D	360	MGE	O6D-C5D-C6D	4.37	117.08	106.34
23	C	501	CLA	C4A-NA-C1A	4.36	112.54	106.52
23	C	498	CLA	C4B-C3B-CAB	4.35	135.98	127.18
28	x	5130	BCR	C8-C9-C10	-4.33	112.31	118.97
23	B	514	CLA	C4A-NA-C1A	4.33	112.49	106.52
23	b	5514	CLA	C2B-C3B-CAB	-4.33	118.46	127.33
29	L	210	MGE	C3G-O3G-C1D	-4.33	105.18	113.81
23	C	502	CLA	C2B-C3B-CAB	-4.33	118.47	127.33
23	B	513	CLA	C4B-C3B-CAB	4.32	135.93	127.18
29	l	5210	MGE	C3G-O3G-C1D	-4.32	105.20	113.81
23	B	524	CLA	C2B-C3B-CAB	-4.31	118.50	127.33
25	v	5552	HEM	CHA-C4D-ND	4.31	130.23	124.31
23	C	494	CLA	CED-O2D-CGD	4.30	126.25	116.02
23	C	492	CLA	C2B-C3B-CAB	-4.28	118.57	127.33
23	C	491	CLA	C2B-C3B-CAB	-4.28	118.58	127.33
23	c	5492	CLA	C2B-C3B-CAB	-4.27	118.59	127.33
28	T	5104	BCR	C33-C5-C4	-4.26	105.51	113.34
23	B	524	CLA	C4A-NA-C1A	4.26	112.39	106.52
26	d	5356	PQ9	C11-C2-C1	4.25	121.32	117.10
28	T	5104	BCR	C38-C26-C27	-4.25	105.53	113.34
23	b	5518	CLA	C2B-C3B-CAB	-4.25	118.62	127.33
23	c	5496	CLA	C2B-C3B-CAB	-4.25	118.62	127.33
23	C	495	CLA	C2B-C3B-CAB	-4.24	118.64	127.33
23	c	5491	CLA	C4A-NA-C1A	4.23	112.35	106.52
28	x	5130	BCR	C33-C5-C4	-4.23	105.58	113.34
28	B	529	BCR	C38-C26-C27	-4.23	105.58	113.34
23	B	513	CLA	CAA-C2A-C3A	-4.22	103.06	113.04
24	a	5561	PHO	C2B-C3B-CAB	-4.22	118.69	127.33
23	B	525	CLA	C2B-C3B-CAB	-4.22	118.69	127.33
30	C	508	DGD	C3G-O3G-C1D	-4.21	105.42	113.81
30	c	5508	DGD	O5D-C1E-C2E	4.21	113.53	108.18
28	D	357	BCR	C38-C26-C27	-4.20	105.62	113.34
23	c	5503	CLA	C4A-NA-C1A	4.20	112.31	106.52
23	A	558	CLA	C2B-C3B-CAB	-4.20	118.73	127.33
28	d	5357	BCR	C38-C26-C27	-4.20	105.63	113.34
32	A	5212	SQD	C44-O6-C1	4.20	122.17	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	C2B-C3B-CAB	-4.20	118.74	127.33
28	T	5104	BCR	C29-C30-C25	4.18	117.39	110.44
23	b	5513	CLA	C2B-C3B-CAB	-4.18	118.78	127.33
23	c	5493	CLA	C2B-C3B-CAB	-4.18	118.78	127.33
23	D	355	CLA	C2B-C3B-CAB	-4.17	118.80	127.33
23	a	5560	CLA	CAA-C2A-C3A	-4.17	103.19	113.04
23	b	5516	CLA	C4A-NA-C1A	4.16	112.25	106.52
23	C	497	CLA	C4A-NA-C1A	4.16	112.25	106.52
28	D	357	BCR	C33-C5-C4	-4.15	105.72	113.34
23	C	503	CLA	C4A-NA-C1A	4.14	112.23	106.52
28	X	130	BCR	C33-C5-C4	-4.14	105.73	113.34
23	d	5355	CLA	C4B-C3B-CAB	4.14	135.56	127.18
23	A	560	CLA	CAA-C2A-C3A	-4.14	103.26	113.04
23	B	518	CLA	C4A-NA-C1A	4.13	112.22	106.52
23	B	521	CLA	C4A-NA-C1A	4.13	112.21	106.52
23	B	514	CLA	C2B-C3B-CAB	-4.12	118.89	127.33
23	B	515	CLA	C4B-C3B-CAB	4.12	135.52	127.18
23	b	5519	CLA	C2B-C3B-CAB	-4.12	118.89	127.33
23	b	5525	CLA	C4A-NA-C1A	4.12	112.20	106.52
23	c	5502	CLA	C4A-NA-C1A	4.12	112.20	106.52
23	B	517	CLA	C4A-NA-C1A	4.11	112.19	106.52
23	c	5492	CLA	C4A-NA-C1A	4.11	112.19	106.52
28	t	104	BCR	C33-C5-C4	-4.10	105.81	113.34
23	B	523	CLA	C4A-NA-C1A	4.10	112.17	106.52
23	b	5515	CLA	C2B-C3B-CAB	-4.09	118.95	127.33
30	C	509	DGD	O6D-C5D-C6D	4.09	114.84	106.61
23	b	5525	CLA	C2B-C3B-CAB	-4.09	118.96	127.33
23	b	5516	CLA	C2B-C3B-CAB	-4.09	118.96	127.33
23	c	5498	CLA	C4A-NA-C1A	4.09	112.15	106.52
23	b	5523	CLA	C4A-NA-C1A	4.08	112.15	106.52
28	d	5357	BCR	C33-C5-C4	-4.08	105.85	113.34
23	B	516	CLA	C2B-C3B-CAB	-4.08	118.98	127.33
23	c	5495	CLA	C4A-NA-C1A	4.08	112.14	106.52
23	B	516	CLA	C4A-NA-C1A	4.07	112.13	106.52
23	a	5563	CLA	C2B-C3B-CAB	-4.07	119.00	127.33
23	C	494	CLA	C4A-NA-C1A	4.05	112.11	106.52
25	V	552	HEM	C1A-CHA-C4D	-4.05	122.15	127.47
23	d	5355	CLA	C4A-NA-C1A	4.05	112.10	106.52
28	C	504	BCR	C38-C26-C27	-4.04	105.91	113.34
23	B	521	CLA	C4B-C3B-CAB	4.04	135.35	127.18
24	A	561	PHO	C1-C2-C3	4.04	133.36	126.19
23	b	5518	CLA	C4A-NA-C1A	4.02	112.07	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	505	BCR	C33-C5-C4	-4.02	105.95	113.34
23	c	5502	CLA	C4B-C3B-CAB	4.02	135.32	127.18
23	c	5495	CLA	C2B-C3B-CAB	-4.01	119.11	127.33
23	a	5560	CLA	C2B-C3B-CAB	-4.01	119.12	127.33
23	b	5521	CLA	C4B-C3B-CAB	4.01	135.29	127.18
23	b	5513	CLA	CAA-C2A-C3A	-4.00	103.57	113.04
23	A	559	CLA	C2B-C3B-CAB	-4.00	119.14	127.33
28	C	506	BCR	C38-C26-C27	-4.00	105.99	113.34
32	A	568	SQD	O7-S-C6	4.00	114.04	107.03
23	D	355	CLA	C4A-NA-C1A	3.99	112.03	106.52
23	C	503	CLA	C2B-C3B-CAB	-3.99	119.16	127.33
23	C	502	CLA	C4A-NA-C1A	3.99	112.02	106.52
30	c	5509	DGD	O6D-C5D-C6D	3.98	114.62	106.61
28	H	107	BCR	C38-C26-C27	-3.98	106.03	113.34
29	d	5361	MGE	O6D-C5D-C6D	3.98	116.12	106.34
23	C	495	CLA	C4B-C3B-CAB	3.97	135.22	127.18
23	C	493	CLA	C4A-NA-C1A	3.97	112.00	106.52
23	c	5500	CLA	C2B-C3B-CAB	-3.97	119.20	127.33
26	d	5356	PQ9	C24-C23-C25	3.97	121.42	115.39
23	b	5512	CLA	CAA-C2A-C3A	-3.97	103.65	113.04
23	B	526	CLA	C2B-C3B-CAB	-3.97	119.21	127.33
23	a	5558	CLA	C2B-C3B-CAB	-3.96	119.22	127.33
23	b	5511	CLA	C4A-NA-C1A	3.95	111.97	106.52
28	B	528	BCR	C38-C26-C27	-3.95	106.08	113.34
23	C	492	CLA	C4A-NA-C1A	3.95	111.96	106.52
23	b	5526	CLA	CAA-C2A-C3A	-3.94	103.72	113.04
23	A	563	CLA	C2B-C3B-CAB	-3.94	119.26	127.33
23	C	498	CLA	C4A-NA-C1A	3.94	111.95	106.52
23	b	5517	CLA	CBD-CHA-C1A	3.94	133.91	128.77
23	C	496	CLA	C4A-NA-C1A	3.94	111.94	106.52
23	c	5494	CLA	CBD-CHA-C1A	3.93	133.91	128.77
23	a	5559	CLA	C2B-C3B-CAB	-3.93	119.28	127.33
28	c	5505	BCR	C23-C24-C25	3.93	138.93	127.32
23	b	5524	CLA	C4A-NA-C1A	3.93	111.94	106.52
23	B	525	CLA	C4A-NA-C1A	3.93	111.94	106.52
23	B	517	CLA	CBD-CHA-C1A	3.93	133.90	128.77
23	b	5517	CLA	C2B-C3B-CAB	-3.93	119.29	127.33
29	D	360	MGE	O2G-C1B-C2B	3.93	120.16	111.56
23	C	499	CLA	C4A-NA-C1A	3.92	111.92	106.52
23	d	5354	CLA	CAA-C2A-C3A	-3.92	103.78	113.04
26	D	356	PQ9	C11-C2-C1	3.92	120.98	117.10
23	C	500	CLA	C2B-C3B-CAB	-3.92	119.31	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	511	CLA	C2A-C1A-CHA	3.91	127.60	123.57
28	C	504	BCR	C24-C23-C22	3.91	132.07	126.22
30	c	5508	DGD	O5D-C6D-C5D	3.91	115.68	108.97
23	c	5494	CLA	CED-O2D-CGD	3.91	125.33	116.02
28	C	504	BCR	C33-C5-C4	-3.91	106.16	113.34
28	b	5529	BCR	C29-C30-C25	3.91	116.94	110.44
23	c	5501	CLA	C4B-C3B-CAB	3.91	135.09	127.18
23	b	5521	CLA	C4A-NA-C1A	3.90	111.89	106.52
23	C	493	CLA	C4B-C3B-CAB	3.90	135.07	127.18
23	b	5517	CLA	C4A-NA-C1A	3.89	111.89	106.52
23	D	355	CLA	C4B-C3B-CAB	3.89	135.05	127.18
23	B	519	CLA	C2B-C3B-CAB	-3.88	119.38	127.33
23	c	5499	CLA	C2B-C3B-CAB	-3.88	119.38	127.33
23	b	5526	CLA	CED-O2D-CGD	3.88	125.26	116.02
23	B	512	CLA	CAA-C2A-C3A	-3.88	103.86	113.04
23	C	494	CLA	CBD-CHA-C1A	3.88	133.84	128.77
23	c	5493	CLA	C4A-NA-C1A	3.88	111.87	106.52
23	C	495	CLA	C4A-NA-C1A	3.88	111.87	106.52
23	b	5511	CLA	C2A-C1A-CHA	3.88	127.56	123.57
23	B	524	CLA	C4B-C3B-CAB	3.87	135.02	127.18
23	A	563	CLA	OBD-CAD-CBD	-3.87	120.10	125.94
23	B	518	CLA	C4B-C3B-CAB	3.87	135.01	127.18
23	B	517	CLA	C2B-C3B-CAB	-3.87	119.41	127.33
26	D	356	PQ9	C24-C23-C25	3.86	121.26	115.39
23	B	512	CLA	C2B-C3B-CAB	-3.86	119.42	127.33
28	C	506	BCR	C33-C5-C4	-3.86	106.25	113.34
28	C	505	BCR	C23-C24-C25	3.86	138.71	127.32
23	C	502	CLA	C4B-C3B-CAB	3.86	134.99	127.18
23	B	517	CLA	OBD-CAD-CBD	-3.86	120.12	125.94
23	b	5513	CLA	C4B-C3B-CAB	3.85	134.97	127.18
28	c	5506	BCR	C38-C26-C27	-3.85	106.27	113.34
23	B	526	CLA	C4A-NA-C1A	3.85	111.82	106.52
28	c	5504	BCR	C38-C26-C27	-3.83	106.30	113.34
23	A	558	CLA	CBD-CHA-C1A	3.83	133.77	128.77
23	c	5499	CLA	C4A-NA-C1A	3.82	111.79	106.52
25	v	5552	HEM	C1A-CHA-C4D	-3.82	122.45	127.47
28	C	506	BCR	C8-C7-C6	3.82	138.60	127.32
28	t	104	BCR	C29-C30-C25	3.82	116.79	110.44
23	c	5493	CLA	C4B-C3B-CAB	3.82	134.91	127.18
32	L	5213	SQD	O48-C23-C24	3.81	123.94	111.94
23	c	5496	CLA	C4A-NA-C1A	3.81	111.77	106.52
28	A	566	BCR	C38-C26-C27	-3.81	106.34	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5514	CLA	C4B-C3B-CAB	3.81	134.89	127.18
23	b	5512	CLA	C2B-C3B-CAB	-3.81	119.53	127.33
23	A	559	CLA	CAA-C2A-C3A	-3.81	104.04	113.04
29	d	5361	MGE	O2G-C1B-C2B	3.81	119.90	111.56
28	b	5527	BCR	C38-C26-C27	-3.81	106.35	113.34
23	C	497	CLA	C2B-C3B-CAB	-3.80	119.54	127.33
23	B	519	CLA	C4A-NA-C1A	3.80	111.75	106.52
28	A	566	BCR	C33-C5-C4	-3.80	106.37	113.34
25	F	51	HEM	CHA-C4D-ND	3.80	129.52	124.31
28	a	5566	BCR	C38-C26-C27	-3.79	106.37	113.34
28	h	5107	BCR	C38-C26-C27	-3.79	106.37	113.34
23	b	5518	CLA	C4B-C3B-CAB	3.79	134.85	127.18
23	b	5524	CLA	C4B-C3B-CAB	3.79	134.86	127.18
23	b	5522	CLA	C4A-NA-C1A	3.79	111.75	106.52
23	a	5559	CLA	C4B-C3B-CAB	3.79	134.85	127.18
23	B	520	CLA	C2B-C3B-CAB	-3.79	119.57	127.33
23	b	5520	CLA	C2B-C3B-CAB	-3.79	119.57	127.33
23	D	354	CLA	CAA-C2A-C3A	-3.79	104.08	113.04
28	c	5505	BCR	C38-C26-C27	-3.78	106.39	113.34
32	a	212	SQD	O7-S-C6	3.79	113.66	107.03
28	c	5506	BCR	C33-C5-C4	-3.78	106.39	113.34
30	C	507	DGD	O5D-C1E-C2E	3.78	112.99	108.18
30	C	508	DGD	O5D-C6D-C5D	3.78	115.45	108.97
23	b	5523	CLA	CBD-CHA-C1A	3.78	133.71	128.77
23	b	5523	CLA	C1D-CHD-C4C	3.78	128.46	122.60
23	a	5559	CLA	CAA-C2A-C3A	-3.77	104.11	113.04
23	c	5494	CLA	C2B-C3B-CAB	-3.77	119.60	127.33
23	b	5519	CLA	C4A-NA-C1A	3.77	111.72	106.52
28	T	5104	BCR	C24-C23-C22	3.77	131.85	126.22
23	a	5560	CLA	C4A-NA-C1A	3.77	111.71	106.52
32	t	213	SQD	O48-C23-C24	3.77	123.78	111.94
23	C	491	CLA	C4B-C3B-CAB	3.76	134.79	127.18
23	A	560	CLA	C2B-C3B-CAB	-3.76	119.64	127.33
23	A	558	CLA	C4B-C3B-CAB	3.76	134.78	127.18
23	C	496	CLA	C4B-C3B-CAB	3.75	134.77	127.18
28	c	5504	BCR	C24-C23-C22	3.75	131.83	126.22
23	B	514	CLA	C4B-C3B-CAB	3.75	134.77	127.18
33	a	5568	LMT	C1-O1'-C1'	-3.75	107.21	113.96
23	c	5497	CLA	C4A-NA-C1A	3.75	111.68	106.52
23	B	517	CLA	C2D-C1D-ND	3.75	112.24	109.41
26	A	564	PQ9	C11-C12-C13	-3.74	120.43	126.76
23	c	5496	CLA	C4B-C3B-CAB	3.74	134.75	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	525	CLA	C4B-C3B-CAB	3.74	134.75	127.18
23	c	5491	CLA	C4B-C3B-CAB	3.74	134.75	127.18
28	c	5505	BCR	C33-C5-C4	-3.73	106.48	113.34
28	B	527	BCR	C38-C26-C27	-3.73	106.49	113.34
23	B	511	CLA	CBD-CHA-C1A	3.73	133.64	128.77
23	B	511	CLA	C4A-NA-C1A	3.73	111.66	106.52
28	X	130	BCR	C38-C26-C27	-3.73	106.49	113.34
28	b	5529	BCR	C38-C26-C27	-3.72	106.51	113.34
33	A	569	LMT	C1-O1'-C1'	-3.72	107.27	113.96
23	C	500	CLA	C4A-NA-C1A	3.72	111.64	106.52
28	b	5527	BCR	C33-C5-C4	-3.71	106.52	113.34
23	b	5526	CLA	C4A-NA-C1A	3.71	111.64	106.52
23	B	526	CLA	CAA-C2A-C3A	-3.71	104.27	113.04
28	B	528	BCR	C30-C25-C26	-3.71	117.23	122.60
28	H	107	BCR	C33-C5-C4	-3.71	106.53	113.34
28	t	104	BCR	C38-C26-C27	-3.70	106.54	113.34
23	C	493	CLA	CBD-CHA-C1A	3.70	133.60	128.77
29	d	5360	MGE	O6D-C5D-C6D	3.70	115.42	106.34
28	B	527	BCR	C33-C5-C4	-3.69	106.55	113.34
23	b	5517	CLA	OBD-CAD-CBD	-3.69	120.37	125.94
23	c	5500	CLA	C4A-NA-C1A	3.69	111.61	106.52
30	c	5507	DGD	O5D-C1E-C2E	3.69	112.88	108.18
23	b	5513	CLA	CBD-CHA-C1A	3.68	133.58	128.77
28	d	5357	BCR	C29-C30-C25	3.68	116.56	110.44
28	x	5130	BCR	C38-C26-C27	-3.68	106.58	113.34
23	b	5525	CLA	C4B-C3B-CAB	3.68	134.62	127.18
23	c	5492	CLA	C4B-C3B-CAB	3.67	134.62	127.18
23	A	559	CLA	C4B-C3B-CAB	3.67	134.61	127.18
23	B	512	CLA	C4B-C3B-CAB	3.67	134.60	127.18
23	b	5511	CLA	C2B-C3B-CAB	-3.67	119.82	127.33
23	B	522	CLA	C4A-NA-C1A	3.67	111.57	106.52
23	D	354	CLA	C1-C2-C3	3.67	132.70	126.19
28	x	5130	BCR	C23-C24-C25	3.66	138.13	127.32
23	a	5558	CLA	CBD-CHA-C1A	3.66	133.55	128.77
23	b	5526	CLA	C4B-C3B-CAB	3.65	134.57	127.18
28	b	5529	BCR	C33-C5-C4	-3.65	106.63	113.34
29	B	530	MGE	C3G-O3G-C1D	-3.65	106.53	113.81
23	b	5515	CLA	C4B-C3B-CAB	3.65	134.57	127.18
23	C	492	CLA	C4B-C3B-CAB	3.65	134.57	127.18
28	x	5130	BCR	C29-C30-C25	3.65	116.50	110.44
28	X	130	BCR	C23-C24-C25	3.65	138.10	127.32
30	h	5208	DGD	C1E-O6E-C5E	3.64	120.81	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5511	CLA	CBD-CHA-C1A	3.64	133.53	128.77
23	C	501	CLA	C2D-C1D-ND	3.64	112.16	109.41
23	A	563	CLA	C4B-C3B-CAB	3.63	134.54	127.18
23	c	5494	CLA	O2A-CGA-CBA	3.63	121.67	110.52
23	c	5503	CLA	C4B-C3B-CAB	3.63	134.52	127.18
31	A	567	LHG	O8-C23-C24	3.63	123.35	111.94
23	A	560	CLA	C4A-NA-C1A	3.63	111.52	106.52
28	B	529	BCR	C33-C5-C4	-3.62	106.69	113.34
32	d	5358	SQD	C31-C30-C29	3.62	134.21	114.61
23	c	5494	CLA	C4A-NA-C1A	3.62	111.52	106.52
28	h	5107	BCR	C11-C10-C9	3.62	132.51	127.29
23	b	5519	CLA	CED-O2D-CGD	3.62	124.63	116.02
28	H	107	BCR	C11-C10-C9	3.61	132.50	127.29
23	B	520	CLA	C4A-NA-C1A	3.61	111.50	106.52
23	B	516	CLA	C4B-C3B-CAB	3.61	134.49	127.18
23	C	495	CLA	CBD-CHA-C1A	3.61	133.49	128.77
23	C	494	CLA	O2A-CGA-CBA	3.61	121.61	110.52
23	c	5498	CLA	C2D-C1D-ND	3.61	112.13	109.41
28	a	5566	BCR	C33-C5-C4	-3.60	106.72	113.34
28	c	5506	BCR	C8-C7-C6	3.60	137.95	127.32
23	c	5495	CLA	C4B-C3B-CAB	3.59	134.46	127.18
28	h	5107	BCR	C29-C30-C25	3.59	116.41	110.44
24	a	5562	PHO	CBD-CHA-C1A	3.59	132.83	126.57
23	c	5497	CLA	C2B-C3B-CAB	-3.59	119.98	127.33
23	B	518	CLA	O2A-CGA-CBA	3.59	123.22	111.94
28	X	130	BCR	C2-C1-C6	3.59	116.40	110.44
28	c	5504	BCR	C33-C5-C4	-3.58	106.76	113.34
24	A	562	PHO	CBD-CHA-C1A	3.58	132.82	126.57
23	b	5519	CLA	C4B-C3B-CAB	3.58	134.43	127.18
23	a	5559	CLA	C4A-NA-C1A	3.58	111.45	106.52
28	d	5357	BCR	C30-C25-C26	-3.57	117.42	122.60
23	a	5558	CLA	C4B-C3B-CAB	3.58	134.42	127.18
28	T	5104	BCR	C30-C25-C26	-3.57	117.43	122.60
23	C	497	CLA	C7-C6-C5	-3.57	102.48	113.01
23	b	5525	CLA	CBD-CHA-C1A	3.57	133.44	128.77
30	C	507	DGD	C1E-O6E-C5E	3.57	120.66	113.73
23	c	5491	CLA	CED-O2D-CGD	3.57	124.50	116.02
23	b	5518	CLA	O2A-CGA-CBA	3.56	123.15	111.94
28	t	104	BCR	C8-C7-C6	3.56	137.84	127.32
23	C	491	CLA	C4A-NA-C1A	3.56	111.43	106.52
28	d	5357	BCR	C1-C6-C5	-3.55	117.46	122.60
32	d	5358	SQD	O48-C23-C24	3.55	123.12	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	519	CLA	C4B-C3B-CAB	3.55	134.36	127.18
23	a	5563	CLA	C4B-C3B-CAB	3.55	134.36	127.18
23	B	523	CLA	CBD-CHA-C1A	3.55	133.41	128.77
23	b	5520	CLA	C4A-NA-C1A	3.54	111.41	106.52
23	B	518	CLA	CAA-C2A-C3A	-3.54	104.67	113.04
32	A	568	SQD	C31-C30-C29	3.54	133.77	114.61
23	A	559	CLA	C4A-NA-C1A	3.54	111.40	106.52
23	C	494	CLA	C2B-C3B-CAB	-3.54	120.09	127.33
23	b	5517	CLA	C4B-C3B-CAB	3.54	134.34	127.18
23	C	503	CLA	C4B-C3B-CAB	3.53	134.33	127.18
23	C	496	CLA	CED-O2D-CGD	3.53	124.42	116.02
25	f	5051	HEM	C1A-CHA-C4D	-3.53	122.83	127.47
28	h	5107	BCR	C33-C5-C4	-3.53	106.86	113.34
23	b	5516	CLA	O2A-CGA-CBA	3.53	123.03	111.94
30	C	507	DGD	O5D-C6D-C5D	3.53	115.02	108.97
23	C	500	CLA	C4B-C3B-CAB	3.52	134.31	127.18
28	x	5130	BCR	C16-C17-C18	3.52	132.36	127.29
23	b	5512	CLA	C4B-C3B-CAB	3.51	134.29	127.18
23	c	5492	CLA	CED-O2D-CGD	3.51	124.37	116.02
23	c	5493	CLA	CBD-CHA-C1A	3.51	133.36	128.77
23	A	563	CLA	C4A-NA-C1A	3.51	111.36	106.52
28	b	5528	BCR	C38-C26-C27	-3.51	106.90	113.34
23	b	5526	CLA	OBD-CAD-CBD	-3.51	120.65	125.94
28	C	505	BCR	C38-C26-C27	-3.51	106.90	113.34
28	X	130	BCR	C29-C30-C25	3.51	116.27	110.44
28	C	505	BCR	C2-C1-C6	3.50	116.26	110.44
23	B	523	CLA	C2D-C1D-ND	3.50	112.06	109.41
23	c	5492	CLA	C2D-C1D-ND	3.50	112.06	109.41
28	b	5528	BCR	C33-C5-C4	-3.50	106.91	113.34
23	c	5503	CLA	CED-O2D-CGD	3.50	124.34	116.02
28	C	505	BCR	C29-C30-C25	3.50	116.25	110.44
23	B	513	CLA	C4A-NA-C1A	3.49	111.34	106.52
28	c	5505	BCR	C29-C30-C25	3.49	116.25	110.44
28	b	5528	BCR	C29-C30-C25	3.49	116.24	110.44
23	c	5494	CLA	C4B-C3B-CAB	3.49	134.25	127.18
28	c	5504	BCR	C1-C6-C5	-3.49	117.55	122.60
23	b	5516	CLA	C4B-C3B-CAB	3.48	134.23	127.18
23	c	5498	CLA	CAA-C2A-C3A	-3.48	104.80	113.04
28	D	357	BCR	C1-C6-C5	-3.48	117.56	122.60
29	d	5359	MGE	O2G-C1B-C2B	3.48	119.19	111.56
23	c	5495	CLA	CBD-CHA-C1A	3.48	133.32	128.77
23	b	5521	CLA	CBD-CHA-C1A	3.48	133.32	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	494	CLA	C4B-C3B-CAB	3.48	134.22	127.18
28	a	5566	BCR	C29-C30-C25	3.48	116.22	110.44
23	C	501	CLA	C4B-C3B-CAB	3.48	134.22	127.18
23	B	515	CLA	C4A-NA-C1A	3.48	111.31	106.52
28	x	5130	BCR	C2-C1-C6	3.47	116.21	110.44
23	c	5496	CLA	CAA-C2A-C3A	-3.47	104.83	113.04
32	A	568	SQD	C11-C10-C9	3.47	133.38	114.61
23	d	5354	CLA	C4A-NA-C1A	3.47	111.30	106.52
23	b	5518	CLA	CAA-C2A-C3A	-3.46	104.85	113.04
28	H	107	BCR	C30-C25-C26	-3.46	117.58	122.60
28	C	504	BCR	C1-C6-C5	-3.46	117.59	122.60
23	c	5500	CLA	C4B-C3B-CAB	3.46	134.18	127.18
23	B	517	CLA	O2A-CGA-CBA	3.45	122.80	111.94
28	D	357	BCR	C30-C25-C26	-3.45	117.60	122.60
23	d	5355	CLA	C1-C2-C3	3.45	132.32	126.19
28	b	5529	BCR	C2-C1-C6	3.45	116.17	110.44
30	C	508	DGD	C3G-C2G-C1G	-3.45	104.00	111.86
30	c	5508	DGD	O2G-C1B-C2B	3.45	119.11	111.56
30	c	5509	DGD	C1E-O6E-C5E	3.44	120.42	113.73
30	c	5507	DGD	O5D-C6D-C5D	3.44	114.86	108.97
28	b	5528	BCR	C30-C25-C26	-3.44	117.63	122.60
23	A	563	CLA	CAA-C2A-C3A	-3.43	104.92	113.04
23	C	499	CLA	C2B-C3B-CAB	-3.44	120.30	127.33
30	C	507	DGD	O6D-C5D-C6D	3.43	113.50	106.61
23	b	5514	CLA	OBD-CAD-CBD	-3.42	120.77	125.94
23	B	511	CLA	C2B-C3B-CAB	-3.42	120.32	127.33
23	B	517	CLA	C4B-C3B-CAB	3.42	134.11	127.18
28	T	5104	BCR	C8-C7-C6	3.42	137.42	127.32
30	c	5507	DGD	O6D-C5D-C6D	3.42	113.49	106.61
28	b	5528	BCR	C2-C1-C6	3.42	116.12	110.44
23	a	5560	CLA	C4B-C3B-CAB	3.41	134.09	127.18
23	c	5499	CLA	C4B-C3B-CAB	3.41	134.07	127.18
28	c	5506	BCR	C30-C25-C26	-3.41	117.67	122.60
28	A	566	BCR	C29-C30-C25	3.41	116.10	110.44
23	B	526	CLA	C4B-C3B-CAB	3.40	134.07	127.18
32	t	213	SQD	C11-C10-C9	3.40	133.00	114.61
24	a	5561	PHO	CBD-CHA-C1A	3.40	132.50	126.57
23	B	512	CLA	C4A-NA-C1A	3.40	111.20	106.52
32	d	5358	SQD	C11-C10-C9	3.39	132.98	114.61
23	B	513	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
23	b	5523	CLA	C2D-C1D-ND	3.39	111.97	109.41
23	b	5524	CLA	CBD-CHA-C1A	3.39	133.20	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	5508	DGD	C3G-C2G-C1G	-3.39	104.14	111.86
31	a	5567	LHG	O8-C23-C24	3.39	122.60	111.94
32	A	568	SQD	O48-C23-C24	3.38	122.58	111.94
23	C	492	CLA	CED-O2D-CGD	3.38	124.07	116.02
28	X	130	BCR	C30-C25-C26	-3.37	117.71	122.60
28	t	104	BCR	C30-C25-C26	-3.38	117.71	122.60
28	x	5130	BCR	C30-C25-C26	-3.37	117.72	122.60
29	D	359	MGE	O6D-C5D-C6D	3.37	114.62	106.34
28	D	357	BCR	C2-C1-C6	3.37	116.04	110.44
23	C	497	CLA	C1-C2-C3	3.37	132.17	126.19
23	c	5497	CLA	C7-C6-C5	-3.37	103.09	113.01
28	H	107	BCR	C29-C30-C25	3.37	116.03	110.44
29	b	5530	MGE	C3G-O3G-C1D	-3.36	107.10	113.81
30	C	509	DGD	C1E-O6E-C5E	3.36	120.27	113.73
23	B	517	CLA	C1-C2-C3	3.36	132.16	126.19
23	B	522	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
23	D	354	CLA	OBD-CAD-CBD	-3.36	120.86	125.94
23	C	503	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
28	x	5130	BCR	C12-C13-C14	-3.36	113.81	118.97
23	B	520	CLA	C4B-C3B-CAB	3.36	133.97	127.18
23	B	526	CLA	OBD-CAD-CBD	-3.35	120.88	125.94
23	C	501	CLA	CBD-CHA-C1A	3.35	133.15	128.77
23	C	498	CLA	C2D-C1D-ND	3.35	111.94	109.41
28	a	5566	BCR	C24-C23-C22	3.35	131.22	126.22
28	B	529	BCR	C29-C30-C25	3.35	116.00	110.44
23	b	5515	CLA	C4A-NA-C1A	3.35	111.13	106.52
23	B	516	CLA	O2A-CGA-CBA	3.34	122.46	111.94
30	h	5208	DGD	O6D-C5D-C6D	3.34	113.33	106.61
29	B	530	MGE	O3G-C1D-C2D	3.34	112.43	108.18
23	B	523	CLA	C1D-CHD-C4C	3.34	127.77	122.60
28	B	529	BCR	C2-C1-C6	3.33	115.98	110.44
29	l	5210	MGE	O6D-C5D-C6D	3.33	114.52	106.34
28	c	5506	BCR	C29-C30-C25	3.33	115.97	110.44
23	c	5501	CLA	C2D-C1D-ND	3.33	111.92	109.41
28	a	5566	BCR	C30-C25-C26	-3.33	117.78	122.60
23	C	494	CLA	C2D-C1D-ND	3.32	111.92	109.41
23	a	5563	CLA	C4A-NA-C1A	3.32	111.09	106.52
25	f	5051	HEM	C4C-NC-C1C	3.32	108.98	105.53
23	b	5520	CLA	C7-C6-C5	-3.31	103.25	113.01
23	B	524	CLA	CBD-CHA-C1A	3.31	133.10	128.77
24	A	561	PHO	CBD-CHA-C1A	3.31	132.34	126.57
28	d	5357	BCR	C24-C23-C22	3.31	131.16	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	5107	BCR	C30-C25-C26	-3.31	117.81	122.60
24	a	5561	PHO	C1-C2-C3	3.31	132.06	126.19
23	A	560	CLA	CBD-CHA-C1A	3.30	133.09	128.77
30	C	508	DGD	O2G-C1B-C2B	3.30	118.80	111.56
28	t	104	BCR	C24-C23-C22	3.30	131.16	126.22
23	b	5517	CLA	O2A-CGA-CBA	3.30	122.33	111.94
23	A	560	CLA	C4B-C3B-CAB	3.30	133.86	127.18
23	c	5496	CLA	CED-O2D-CGD	3.30	123.87	116.02
24	A	562	PHO	CAA-C2A-C3A	-3.30	105.25	113.04
23	b	5513	CLA	C4A-NA-C1A	3.29	111.06	106.52
23	c	5493	CLA	CED-O2D-CGD	3.29	123.85	116.02
23	C	500	CLA	CBD-CHA-C1A	3.29	133.06	128.77
23	B	521	CLA	CBD-CHA-C1A	3.28	133.06	128.77
32	t	213	SQD	O7-S-C6	3.28	112.78	107.03
23	c	5492	CLA	CBD-CHA-C1A	3.27	133.05	128.77
23	C	502	CLA	O2A-CGA-CBA	3.28	122.24	111.94
23	b	5522	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
23	a	5563	CLA	CAA-C2A-C3A	-3.27	105.30	113.04
24	a	5562	PHO	CAA-C2A-C3A	-3.28	105.30	113.04
28	C	506	BCR	C23-C24-C25	3.27	136.99	127.32
23	A	558	CLA	C4A-NA-C1A	3.27	111.03	106.52
23	B	517	CLA	C1D-CHD-C4C	3.27	127.67	122.60
23	B	521	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
24	a	5562	PHO	C7-C6-C5	-3.27	103.37	113.01
23	B	516	CLA	C1-C2-C3	3.27	131.99	126.19
28	A	566	BCR	C24-C23-C22	3.26	131.10	126.22
28	A	566	BCR	C30-C25-C26	-3.26	117.88	122.60
30	H	208	DGD	O2G-C1B-C2B	3.26	118.71	111.56
29	I	201	MGE	O2G-C1B-C2B	3.26	118.70	111.56
29	i	5201	MGE	O2G-C1B-C2B	3.26	118.70	111.56
23	C	503	CLA	CED-O2D-CGD	3.26	123.78	116.02
23	B	522	CLA	O2A-CGA-CBA	3.26	122.19	111.94
23	B	519	CLA	CED-O2D-CGD	3.26	123.77	116.02
28	C	506	BCR	C2-C1-C6	3.26	115.86	110.44
28	d	5357	BCR	C2-C1-C6	3.26	115.85	110.44
23	A	558	CLA	C1-C2-C3	3.26	131.97	126.19
23	B	526	CLA	CED-O2D-CGD	3.25	123.76	116.02
23	b	5516	CLA	CED-O2D-CGD	3.25	123.75	116.02
23	a	5563	CLA	OBD-CAD-CBD	-3.25	121.04	125.94
32	L	5213	SQD	C11-C10-C9	3.25	132.18	114.61
23	b	5520	CLA	C4B-C3B-CAB	3.25	133.75	127.18
23	a	5558	CLA	CED-O2D-CGD	3.24	123.74	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5512	CLA	CBD-CHA-C1A	3.24	133.01	128.77
26	a	5564	PQ9	C11-C12-C13	-3.24	121.28	126.76
23	B	515	CLA	C2A-C3A-C4A	3.24	106.39	101.40
23	C	498	CLA	CAA-C2A-C3A	-3.24	105.37	113.04
23	B	513	CLA	O2A-CGA-CBA	3.24	122.13	111.94
23	c	5500	CLA	CBD-CHA-C1A	3.24	133.00	128.77
23	c	5502	CLA	CBD-CHA-C1A	3.24	133.00	128.77
23	C	492	CLA	C2D-C1D-ND	3.24	111.86	109.41
23	C	496	CLA	CAA-C2A-C3A	-3.23	105.40	113.04
23	b	5512	CLA	C4A-NA-C1A	3.23	110.98	106.52
23	b	5514	CLA	C2D-C1D-ND	3.23	111.85	109.41
28	b	5529	BCR	C30-C25-C26	-3.23	117.93	122.60
23	D	355	CLA	C1-C2-C3	3.23	131.93	126.19
28	c	5505	BCR	C2-C1-C6	3.22	115.80	110.44
32	t	213	SQD	C44-O6-C1	3.22	120.23	113.81
28	B	529	BCR	C30-C25-C26	-3.22	117.94	122.60
23	c	5502	CLA	O2A-CGA-CBA	3.22	122.07	111.94
23	c	5501	CLA	CBD-CHA-C1A	3.22	132.98	128.77
23	c	5495	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
26	A	564	PQ9	C16-C17-C18	-3.22	120.86	127.80
30	H	208	DGD	O5D-C1E-C2E	3.22	112.27	108.18
23	c	5493	CLA	O2A-CGA-CBA	3.22	122.06	111.94
28	h	5107	BCR	C23-C24-C25	3.22	136.82	127.32
25	F	51	HEM	C4C-NC-C1C	3.22	108.88	105.53
23	C	493	CLA	O2A-CGA-CBA	3.22	122.06	111.94
23	b	5512	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
29	B	530	MGE	O2G-C1B-C2B	3.21	118.60	111.56
32	d	5358	SQD	O7-S-C6	3.21	112.66	107.03
32	A	5212	SQD	O7-S-C6	3.21	112.66	107.03
23	B	514	CLA	CBD-CHA-C1A	3.21	132.97	128.77
29	D	359	MGE	O2G-C1B-C2B	3.21	118.59	111.56
23	b	5519	CLA	CBD-CHA-C1A	3.21	132.96	128.77
28	C	506	BCR	C29-C30-C25	3.21	115.77	110.44
29	D	358	MGE	O2G-C1B-C2B	3.20	118.58	111.56
23	c	5503	CLA	OBD-CAD-CBD	-3.20	121.10	125.94
23	b	5513	CLA	O2A-CGA-CBA	3.20	122.01	111.94
23	c	5497	CLA	O2A-CGA-CBA	3.20	122.00	111.94
23	C	491	CLA	CBD-CHA-C1A	3.20	132.95	128.77
28	b	5527	BCR	C2-C1-C6	3.20	115.76	110.44
23	c	5500	CLA	C1D-CHD-C4C	3.20	127.56	122.60
23	C	502	CLA	CBD-CHA-C1A	3.20	132.95	128.77
29	I	201	MGE	O6D-C5D-C6D	3.20	114.19	106.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	210	MGE	O6D-C5D-C6D	3.19	114.19	106.34
24	a	5562	PHO	O2A-CGA-CBA	3.19	121.98	111.94
23	A	558	CLA	CAA-C2A-C3A	-3.19	105.51	113.04
23	a	5559	CLA	CED-O2D-CGD	3.18	123.59	116.02
26	a	5564	PQ9	C16-C17-C18	-3.18	120.94	127.80
23	b	5523	CLA	C2A-C3A-C4A	3.18	106.29	101.40
30	c	5508	DGD	C1E-O6E-C5E	3.17	119.90	113.73
23	B	517	CLA	CAA-C2A-C3A	-3.17	105.54	113.04
28	B	528	BCR	C33-C5-C4	-3.17	107.52	113.34
23	a	5558	CLA	CAA-C2A-C3A	-3.17	105.55	113.04
24	A	562	PHO	O2A-CGA-CBA	3.16	121.89	111.94
29	b	5530	MGE	O2G-C1B-C2B	3.16	118.48	111.56
23	b	5521	CLA	C7-C6-C5	-3.16	103.69	113.01
23	D	354	CLA	C4A-NA-C1A	3.16	110.88	106.52
30	C	507	DGD	O2G-C1B-C2B	3.16	118.48	111.56
30	c	5507	DGD	C1E-O6E-C5E	3.16	119.87	113.73
28	H	107	BCR	C24-C23-C22	3.15	130.93	126.22
23	C	492	CLA	OBD-CAD-CBD	-3.15	121.18	125.94
24	A	561	PHO	CED-O2D-CGD	3.15	123.51	116.02
28	C	504	BCR	C30-C25-C26	-3.15	118.04	122.60
23	B	512	CLA	OBD-CAD-CBD	-3.15	121.19	125.94
23	B	520	CLA	CBD-CHA-C1A	3.15	132.88	128.77
23	B	513	CLA	CBD-CHA-C1A	3.14	132.88	128.77
23	B	511	CLA	CMB-C2B-C1B	-3.15	123.78	128.62
23	C	502	CLA	C2A-C3A-C4A	3.14	106.24	101.40
23	C	495	CLA	CMB-C2B-C1B	-3.14	123.79	128.62
23	B	513	CLA	C1D-CHD-C4C	3.14	127.47	122.60
23	b	5515	CLA	O2A-CGA-CBA	3.14	121.81	111.94
23	B	522	CLA	C1D-CHD-C4C	3.14	127.46	122.60
28	c	5504	BCR	C2-C1-C6	3.14	115.65	110.44
23	c	5494	CLA	C2D-C1D-ND	3.14	111.78	109.41
23	C	499	CLA	C4B-C3B-CAB	3.14	133.53	127.18
23	B	516	CLA	C2D-C1D-ND	3.13	111.78	109.41
23	B	521	CLA	C7-C6-C5	-3.13	103.78	113.01
28	D	357	BCR	C29-C30-C25	3.13	115.64	110.44
23	B	525	CLA	C2D-C1D-ND	3.13	111.77	109.41
28	H	107	BCR	C15-C14-C13	3.13	131.80	127.29
23	b	5522	CLA	O2A-CGA-CBA	3.13	121.77	111.94
23	B	525	CLA	C1D-C2D-C3D	-3.13	104.23	106.78
28	H	107	BCR	C12-C13-C14	-3.13	114.17	118.97
23	c	5494	CLA	OBD-CAD-CBD	-3.12	121.23	125.94
28	C	506	BCR	C30-C25-C26	-3.12	118.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	520	CLA	C7-C6-C5	-3.12	103.82	113.01
28	C	505	BCR	C16-C17-C18	3.12	131.78	127.29
23	a	5558	CLA	C4A-NA-C1A	3.12	110.82	106.52
23	b	5512	CLA	CED-O2D-CGD	3.12	123.43	116.02
23	B	524	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
28	H	107	BCR	C23-C24-C25	3.11	136.52	127.32
23	b	5520	CLA	CBD-CHA-C1A	3.11	132.84	128.77
23	C	500	CLA	C2A-C3A-C4A	3.11	106.19	101.40
23	A	560	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
28	D	357	BCR	C23-C24-C25	3.11	136.51	127.32
23	b	5518	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
23	b	5514	CLA	CBD-CHA-C1A	3.11	132.83	128.77
32	d	5358	SQD	C45-O47-C7	3.11	125.58	117.92
23	c	5496	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
23	B	519	CLA	CAA-C2A-C3A	-3.10	105.70	113.04
28	H	107	BCR	C1-C6-C5	-3.10	118.11	122.60
23	A	559	CLA	CBD-CHA-C1A	3.10	132.83	128.77
23	c	5497	CLA	CBD-CHA-C1A	3.10	132.82	128.77
23	c	5499	CLA	C2A-C3A-C4A	3.10	106.17	101.40
30	c	5507	DGD	O2G-C1B-C2B	3.10	118.35	111.56
23	b	5521	CLA	C2A-C3A-C4A	3.10	106.17	101.40
23	b	5521	CLA	C6-C5-C3	3.10	120.15	112.78
23	d	5354	CLA	C1-C2-C3	3.10	131.69	126.19
28	B	529	BCR	C24-C23-C22	3.10	130.85	126.22
23	c	5500	CLA	C7-C6-C5	-3.10	103.88	113.01
30	h	5208	DGD	O2G-C1B-C2B	3.10	118.34	111.56
26	a	5564	PQ9	C19-C18-C20	3.10	120.10	115.39
26	a	5564	PQ9	C24-C23-C25	3.10	120.10	115.39
23	B	523	CLA	C2B-C3B-CAB	-3.10	120.99	127.33
28	B	528	BCR	C2-C1-C6	3.10	115.59	110.44
28	b	5527	BCR	C23-C24-C25	3.09	136.46	127.32
23	b	5514	CLA	C2A-C3A-C4A	3.09	106.15	101.40
23	c	5501	CLA	C7-C6-C5	-3.09	103.91	113.01
23	a	5559	CLA	CBD-CHA-C1A	3.09	132.80	128.77
23	b	5517	CLA	C1-C2-C3	3.08	131.67	126.19
28	b	5528	BCR	C1-C6-C5	-3.09	118.13	122.60
23	d	5355	CLA	OBD-CAD-CBD	-3.08	121.28	125.94
30	H	208	DGD	O6D-C5D-C6D	3.08	112.81	106.61
23	b	5517	CLA	C2D-C1D-ND	3.08	111.74	109.41
28	h	5107	BCR	C1-C6-C5	-3.08	118.14	122.60
23	A	560	CLA	C2A-C3A-C4A	3.08	106.14	101.40
23	B	511	CLA	C2D-C1D-ND	3.08	111.73	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	C1D-CHD-C4C	3.07	127.36	122.60
28	B	528	BCR	C29-C30-C25	3.07	115.55	110.44
23	b	5521	CLA	CAA-C2A-C3A	-3.07	105.78	113.04
23	b	5517	CLA	CAA-C2A-C3A	-3.07	105.79	113.04
23	C	502	CLA	C1D-CHD-C4C	3.07	127.36	122.60
23	C	494	CLA	CMB-C2B-C1B	-3.06	123.91	128.62
28	h	5107	BCR	C8-C7-C6	3.07	136.37	127.32
23	B	511	CLA	C1D-C2D-C3D	-3.06	104.28	106.78
23	b	5511	CLA	C4B-C3B-CAB	3.06	133.38	127.18
28	C	506	BCR	C16-C17-C18	3.06	131.71	127.29
30	C	508	DGD	C1E-O6E-C5E	3.06	119.68	113.73
28	h	5107	BCR	C24-C23-C22	3.06	130.79	126.22
23	b	5511	CLA	C2D-C1D-ND	3.06	111.72	109.41
23	C	492	CLA	C6-C5-C3	3.06	120.04	112.78
23	C	500	CLA	C1D-CHD-C4C	3.05	127.34	122.60
23	C	495	CLA	C6-C5-C3	3.05	120.04	112.78
23	c	5502	CLA	C2A-C3A-C4A	3.05	106.09	101.40
28	C	504	BCR	C2-C1-C6	3.05	115.51	110.44
23	C	497	CLA	O2A-CGA-CBA	3.05	121.53	111.94
28	B	527	BCR	C30-C25-C26	-3.05	118.19	122.60
23	a	5560	CLA	CBD-CHA-C1A	3.04	132.75	128.77
28	b	5528	BCR	C23-C24-C25	3.04	136.29	127.32
23	D	355	CLA	C1D-CHD-C4C	3.04	127.31	122.60
23	b	5513	CLA	OBD-CAD-CBD	-3.03	121.36	125.94
28	b	5529	BCR	C1-C6-C5	-3.03	118.21	122.60
28	H	107	BCR	C2-C1-C6	3.03	115.48	110.44
29	i	5201	MGE	O6D-C5D-C6D	3.03	113.80	106.34
32	A	5212	SQD	C3-C4-C5	-3.03	104.79	110.20
23	c	5495	CLA	CBA-CAA-C2A	3.03	123.00	114.01
23	C	496	CLA	C2D-C1D-ND	3.03	111.70	109.41
23	c	5502	CLA	CED-O2D-CGD	3.03	123.22	116.02
28	B	528	BCR	C23-C24-C25	3.03	136.26	127.32
26	D	356	PQ9	C19-C18-C20	3.02	119.99	115.39
23	C	497	CLA	CBD-CHA-C1A	3.03	132.72	128.77
23	b	5521	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
23	d	5354	CLA	O2A-CGA-CBA	3.02	121.45	111.94
26	A	564	PQ9	C19-C18-C20	3.02	119.98	115.39
23	b	5520	CLA	O2A-CGA-CBA	3.02	121.45	111.94
23	B	511	CLA	C4B-C3B-CAB	3.02	133.30	127.18
30	H	208	DGD	C1E-O6E-C5E	3.02	119.60	113.73
26	A	564	PQ9	C24-C23-C25	3.02	119.98	115.39
23	B	524	CLA	CED-O2D-CGD	3.02	123.20	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	506	BCR	C35-C13-C12	3.02	122.98	118.09
28	B	529	BCR	C23-C24-C25	3.02	136.24	127.32
30	c	5509	DGD	O2G-C1B-C2B	3.02	118.18	111.56
23	a	5560	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
23	b	5522	CLA	C1D-CHD-C4C	3.02	127.28	122.60
23	A	563	CLA	C1-C2-C3	3.02	131.55	126.19
28	x	5130	BCR	C1-C6-C5	-3.02	118.23	122.60
23	B	524	CLA	C2D-C1D-ND	3.01	111.69	109.41
29	d	5360	MGE	O2G-C1B-C2B	3.01	118.16	111.56
23	b	5514	CLA	O2A-CGA-CBA	3.01	121.42	111.94
23	b	5515	CLA	CED-O2D-CGD	3.01	123.18	116.02
23	c	5491	CLA	O2A-CGA-CBA	3.01	121.41	111.94
28	c	5505	BCR	C35-C13-C12	3.01	122.96	118.09
28	c	5506	BCR	C23-C24-C25	3.01	136.21	127.32
23	c	5495	CLA	C1D-CHD-C4C	3.00	127.26	122.60
23	C	495	CLA	CBA-CAA-C2A	3.00	122.93	114.01
32	L	5213	SQD	C44-O6-C1	3.00	119.80	113.81
23	B	525	CLA	C1D-CHD-C4C	3.00	127.26	122.60
23	C	496	CLA	C1-C2-C3	3.00	131.52	126.19
32	a	212	SQD	C3-C4-C5	-3.00	104.84	110.20
23	C	499	CLA	C2A-C3A-C4A	3.00	106.01	101.40
23	B	514	CLA	OBD-CAD-CBD	-3.00	121.42	125.94
23	C	496	CLA	C1D-CHD-C4C	2.99	127.24	122.60
28	X	130	BCR	C1-C6-C5	-2.99	118.27	122.60
23	B	512	CLA	CBD-CHA-C1A	2.99	132.68	128.77
23	C	491	CLA	CED-O2D-CGD	2.99	123.13	116.02
23	c	5494	CLA	CMB-C2B-C1B	-2.99	124.02	128.62
28	c	5506	BCR	C2-C1-C6	2.99	115.41	110.44
23	c	5497	CLA	C1-C2-C3	2.99	131.49	126.19
30	C	509	DGD	O2G-C1B-C2B	2.99	118.10	111.56
23	D	355	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
28	t	104	BCR	C11-C10-C9	2.98	131.59	127.29
23	B	520	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
23	B	525	CLA	CBD-CHA-C1A	2.98	132.67	128.77
28	b	5527	BCR	C1-C6-C5	-2.98	118.28	122.60
28	x	5130	BCR	C34-C9-C8	2.98	122.91	118.09
23	A	563	CLA	C1D-CHD-C4C	2.98	127.22	122.60
23	A	560	CLA	C1D-CHD-C4C	2.98	127.22	122.60
23	b	5516	CLA	C1-C2-C3	2.98	131.48	126.19
23	C	495	CLA	C1D-CHD-C4C	2.98	127.21	122.60
23	B	523	CLA	C6-C5-C3	2.97	119.85	112.78
28	c	5504	BCR	C32-C1-C6	2.97	115.25	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5524	CLA	CAA-C2A-C3A	-2.97	106.02	113.04
23	b	5517	CLA	C1D-CHD-C4C	2.97	127.20	122.60
23	b	5523	CLA	C2B-C3B-CAB	-2.97	121.25	127.33
23	b	5513	CLA	C1D-CHD-C4C	2.97	127.20	122.60
23	B	518	CLA	CED-O2D-CGD	2.96	123.07	116.02
23	b	5519	CLA	CAA-C2A-C3A	-2.96	106.04	113.04
28	b	5529	BCR	C23-C24-C25	2.96	136.07	127.32
24	A	562	PHO	C7-C6-C5	-2.96	104.28	113.01
23	C	494	CLA	C2A-C3A-C4A	2.96	105.95	101.40
28	B	528	BCR	C24-C23-C22	2.96	130.64	126.22
23	B	518	CLA	C1D-CHD-C4C	2.96	127.19	122.60
23	b	5516	CLA	C2D-C1D-ND	2.96	111.64	109.41
23	C	494	CLA	C2A-C1A-NA	-2.96	107.97	111.24
23	c	5499	CLA	CBD-CHA-C1A	2.96	132.63	128.77
23	C	495	CLA	O2A-CGA-CBA	2.95	121.23	111.94
23	b	5523	CLA	OBD-CAD-CBD	-2.96	121.48	125.94
23	A	558	CLA	C2A-C3A-C4A	2.95	105.94	101.40
23	C	499	CLA	CBD-CHA-C1A	2.95	132.63	128.77
23	c	5503	CLA	C2D-C1D-ND	2.95	111.64	109.41
31	A	567	LHG	O7-C7-C8	2.95	118.02	111.56
28	c	5504	BCR	C1-C6-C7	2.95	123.86	115.69
23	b	5521	CLA	C2D-C1D-ND	2.95	111.64	109.41
28	C	504	BCR	C29-C30-C25	2.95	115.34	110.44
28	h	5107	BCR	C2-C1-C6	2.95	115.34	110.44
23	b	5521	CLA	C1D-CHD-C4C	2.95	127.17	122.60
23	b	5516	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
23	B	521	CLA	C1D-CHD-C4C	2.94	127.17	122.60
28	B	529	BCR	C1-C6-C5	-2.94	118.34	122.60
26	D	356	PQ9	C16-C17-C18	-2.94	121.46	127.80
28	h	5107	BCR	C32-C1-C6	2.94	115.20	110.33
23	c	5491	CLA	C1D-CHD-C4C	2.94	127.16	122.60
23	C	497	CLA	C4B-C3B-CAB	2.94	133.12	127.18
28	h	5107	BCR	C12-C13-C14	-2.94	114.46	118.97
23	B	522	CLA	CED-O2D-CGD	2.93	123.00	116.02
23	c	5501	CLA	C1D-CHD-C4C	2.93	127.15	122.60
23	C	502	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
23	b	5522	CLA	CED-O2D-CGD	2.93	123.00	116.02
23	B	516	CLA	CED-O2D-CGD	2.93	122.99	116.02
23	B	520	CLA	C2D-C1D-ND	2.93	111.62	109.41
23	c	5496	CLA	CBD-CHA-C1A	2.93	132.59	128.77
23	C	499	CLA	C1D-CHD-C4C	2.93	127.14	122.60
23	B	514	CLA	C2A-C3A-C4A	2.93	105.90	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	514	CLA	C1D-CHD-C4C	2.92	127.13	122.60
23	B	512	CLA	CED-O2D-CGD	2.92	122.97	116.02
23	b	5512	CLA	O2A-CGA-CBA	2.92	121.13	111.94
28	B	527	BCR	C2-C1-C6	2.92	115.29	110.44
23	b	5518	CLA	C1D-CHD-C4C	2.92	127.13	122.60
24	A	561	PHO	OBD-CAD-CBD	-2.92	121.53	125.94
30	h	5208	DGD	O5D-C1E-C2E	2.92	111.90	108.18
23	B	521	CLA	C2A-C3A-C4A	2.92	105.89	101.40
23	c	5495	CLA	CMB-C2B-C1B	-2.92	124.13	128.62
23	c	5503	CLA	C1D-CHD-C4C	2.92	127.12	122.60
28	X	130	BCR	C34-C9-C8	2.92	122.81	118.09
28	D	357	BCR	C8-C7-C6	2.92	135.93	127.32
23	c	5492	CLA	CAA-C2A-C3A	-2.91	106.15	113.04
23	b	5522	CLA	C7-C6-C5	-2.91	104.42	113.01
23	b	5515	CLA	C6-C5-C3	2.91	119.71	112.78
23	B	520	CLA	CED-O2D-CGD	2.91	122.95	116.02
23	B	516	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
29	D	358	MGE	O6D-C5D-C6D	2.91	113.49	106.34
28	B	527	BCR	C35-C13-C12	2.91	122.80	118.09
28	B	529	BCR	C7-C8-C9	2.91	130.57	126.22
28	X	130	BCR	C12-C13-C14	-2.91	114.50	118.97
23	C	497	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
23	C	493	CLA	CED-O2D-CGD	2.91	122.94	116.02
28	D	357	BCR	C12-C13-C14	-2.91	114.50	118.97
23	B	525	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
23	B	521	CLA	CED-O2D-CGD	2.90	122.93	116.02
23	B	521	CLA	CAA-C2A-C3A	-2.90	106.17	113.04
23	C	503	CLA	CAA-C2A-C3A	-2.90	106.18	113.04
23	B	521	CLA	C2D-C1D-ND	2.90	111.60	109.41
23	B	513	CLA	C2D-C1D-ND	2.90	111.60	109.41
28	c	5504	BCR	C30-C25-C26	-2.90	118.40	122.60
23	D	354	CLA	C2A-C3A-C4A	2.90	105.86	101.40
23	D	354	CLA	O2A-CGA-CBA	2.89	121.05	111.94
23	b	5525	CLA	O2A-CGA-CBA	2.89	121.04	111.94
28	c	5505	BCR	C1-C6-C5	-2.89	118.41	122.60
23	a	5560	CLA	CMB-C2B-C1B	-2.89	124.17	128.62
23	d	5354	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
23	a	5563	CLA	C1-C2-C3	2.89	131.32	126.19
23	b	5524	CLA	CED-O2D-CGD	2.89	122.90	116.02
28	t	104	BCR	C35-C13-C12	2.89	122.77	118.09
23	C	496	CLA	O2A-CGA-CBA	2.89	121.03	111.94
23	b	5519	CLA	C1D-CHD-C4C	2.89	127.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	514	CLA	C2D-C1D-ND	2.89	111.59	109.41
23	c	5502	CLA	C1D-CHD-C4C	2.88	127.07	122.60
28	b	5529	BCR	C24-C23-C22	2.88	130.53	126.22
23	A	559	CLA	C2A-C3A-C4A	2.88	105.83	101.40
28	d	5357	BCR	C23-C24-C25	2.88	135.83	127.32
23	b	5524	CLA	C1D-CHD-C4C	2.88	127.07	122.60
24	a	5561	PHO	CED-O2D-CGD	2.88	122.86	116.02
23	b	5514	CLA	C1D-CHD-C4C	2.88	127.06	122.60
23	a	5558	CLA	C2A-C3A-C4A	2.88	105.83	101.40
23	B	523	CLA	C4B-C3B-CAB	2.88	133.00	127.18
23	B	520	CLA	O2A-CGA-CBA	2.87	120.98	111.94
23	C	499	CLA	OBD-CAD-CBD	-2.88	121.60	125.94
23	b	5511	CLA	CMB-C2B-C1B	-2.87	124.20	128.62
23	C	503	CLA	C1D-CHD-C4C	2.87	127.05	122.60
23	A	558	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
23	C	499	CLA	O2A-CGA-CBA	2.87	120.97	111.94
24	a	5562	PHO	CED-O2D-CGD	2.87	122.85	116.02
23	c	5499	CLA	O2A-CGA-CBA	2.87	120.97	111.94
23	C	502	CLA	CED-O2D-CGD	2.87	122.85	116.02
23	a	5559	CLA	C1D-CHD-C4C	2.87	127.05	122.60
23	c	5493	CLA	C2A-C3A-C4A	2.87	105.81	101.40
23	c	5499	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
23	b	5519	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
23	C	501	CLA	C7-C6-C5	-2.87	104.56	113.01
23	d	5355	CLA	CED-O2D-CGD	2.86	122.83	116.02
23	C	502	CLA	C2D-C1D-ND	2.86	111.57	109.41
29	I	201	MGE	O1G-C1G-C2G	-2.86	101.33	108.83
23	B	521	CLA	C6-C5-C3	2.86	119.58	112.78
23	B	523	CLA	C2A-C3A-C4A	2.86	105.80	101.40
29	i	5201	MGE	O1G-C1G-C2G	-2.86	101.33	108.83
23	B	524	CLA	CAA-C2A-C3A	-2.86	106.28	113.04
28	H	107	BCR	C8-C7-C6	2.86	135.76	127.32
23	C	492	CLA	O2A-CGA-CBA	2.86	120.93	111.94
23	A	560	CLA	CMB-C2B-C1B	-2.86	124.23	128.62
23	B	524	CLA	C1D-CHD-C4C	2.86	127.03	122.60
23	B	515	CLA	O2A-CGA-CBA	2.86	120.92	111.94
28	b	5527	BCR	C29-C30-C25	2.85	115.18	110.44
28	B	527	BCR	C23-C24-C25	2.85	135.75	127.32
23	c	5495	CLA	O2A-CGA-CBA	2.85	120.91	111.94
25	V	552	HEM	C4A-NA-C1A	2.85	110.52	106.76
24	A	562	PHO	OBD-CAD-CBD	-2.85	121.64	125.94
23	b	5511	CLA	C1D-C2D-C3D	-2.85	104.45	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	5355	CLA	C1D-CHD-C4C	2.85	127.01	122.60
23	a	5563	CLA	CED-O2D-CGD	2.85	122.79	116.02
25	v	5552	HEM	C4A-NA-C1A	2.85	110.51	106.76
23	c	5495	CLA	C2D-C1D-ND	2.84	111.56	109.41
23	a	5560	CLA	C2A-C3A-C4A	2.84	105.77	101.40
31	a	5567	LHG	O7-C7-C8	2.84	117.79	111.56
23	D	355	CLA	CBD-CHA-C1A	2.84	132.49	128.77
23	c	5498	CLA	C1D-CHD-C4C	2.84	127.01	122.60
23	C	491	CLA	C1D-CHD-C4C	2.84	127.01	122.60
23	C	499	CLA	CMB-C2B-C1B	-2.84	124.25	128.62
23	c	5493	CLA	C1-C2-C3	2.84	131.23	126.19
28	C	506	BCR	C1-C6-C5	-2.84	118.49	122.60
23	B	514	CLA	O2A-CGA-CBA	2.84	120.87	111.94
23	B	519	CLA	CBD-CHA-C1A	2.84	132.48	128.77
23	c	5500	CLA	C1-C2-C3	2.84	131.23	126.19
32	A	568	SQD	C32-C31-C30	2.84	129.96	114.61
23	c	5492	CLA	C6-C5-C3	2.83	119.52	112.78
23	b	5520	CLA	C2D-C1D-ND	2.83	111.55	109.41
23	b	5522	CLA	C2A-C3A-C4A	2.83	105.76	101.40
23	a	5559	CLA	C2A-C3A-C4A	2.83	105.75	101.40
23	c	5499	CLA	C2D-C1D-ND	2.83	111.55	109.41
23	b	5513	CLA	C2D-C1D-ND	2.83	111.55	109.41
28	B	527	BCR	C29-C30-C25	2.82	115.13	110.44
24	a	5561	PHO	OBD-CAD-CBD	-2.82	121.68	125.94
28	A	566	BCR	C23-C24-C25	2.82	135.65	127.32
28	b	5529	BCR	C8-C7-C6	2.82	135.65	127.32
23	C	497	CLA	C1D-CHD-C4C	2.82	126.97	122.60
23	b	5513	CLA	CMB-C2B-C1B	-2.82	124.29	128.62
23	c	5497	CLA	C4B-C3B-CAB	2.81	132.87	127.18
28	T	5104	BCR	C23-C22-C21	-2.81	114.65	118.97
23	c	5496	CLA	C1-C2-C3	2.81	131.19	126.19
28	H	107	BCR	C28-C27-C26	2.81	118.00	113.74
23	c	5495	CLA	C6-C5-C3	2.81	119.46	112.78
28	B	528	BCR	C1-C6-C5	-2.81	118.53	122.60
23	C	499	CLA	C2A-C1A-CHA	2.81	128.70	123.83
23	b	5526	CLA	C1D-CHD-C4C	2.81	126.95	122.60
23	c	5491	CLA	CAA-C2A-C3A	-2.81	106.40	113.04
23	B	512	CLA	O2A-CGA-CBA	2.81	120.77	111.94
23	B	519	CLA	C1D-C2D-C3D	-2.81	104.49	106.78
28	d	5357	BCR	C8-C7-C6	2.80	135.60	127.32
23	C	495	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
23	b	5525	CLA	C1D-CHD-C4C	2.80	126.94	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	5527	BCR	C30-C25-C26	-2.80	118.55	122.60
23	D	354	CLA	C1D-CHD-C4C	2.80	126.94	122.60
23	c	5496	CLA	C1D-CHD-C4C	2.80	126.94	122.60
23	b	5519	CLA	C2D-C1D-ND	2.80	111.53	109.41
23	a	5563	CLA	O2A-CGA-CBA	2.80	120.75	111.94
23	b	5515	CLA	C2A-C3A-C4A	2.80	105.71	101.40
23	c	5498	CLA	CED-O2D-CGD	2.80	122.68	116.02
23	d	5355	CLA	CBD-CHA-C1A	2.80	132.43	128.77
32	A	568	SQD	O8-S-O7	2.80	117.83	111.78
23	c	5491	CLA	CBD-CHA-C1A	2.80	132.43	128.77
23	C	503	CLA	O2A-CGA-CBA	2.80	120.74	111.94
23	B	526	CLA	C2A-C3A-C4A	2.80	105.70	101.40
23	a	5559	CLA	O2A-CGA-CBA	2.80	120.74	111.94
23	c	5498	CLA	C1D-C2D-C3D	-2.80	104.50	106.78
23	C	496	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
28	T	5104	BCR	C35-C13-C12	2.80	122.61	118.09
30	c	5509	DGD	C3G-C2G-C1G	-2.80	105.49	111.86
32	A	568	SQD	C45-O47-C7	2.79	124.81	117.92
29	B	530	MGE	O1G-C1G-C2G	-2.79	101.51	108.83
23	B	525	CLA	O2A-CGA-CBA	2.79	120.73	111.94
25	F	51	HEM	C1A-CHA-C4D	-2.79	123.79	127.47
23	B	520	CLA	C1D-CHD-C4C	2.79	126.93	122.60
23	c	5499	CLA	CED-O2D-CGD	2.79	122.66	116.02
23	c	5496	CLA	C2A-C3A-C4A	2.79	105.69	101.40
23	C	498	CLA	CMB-C2B-C1B	-2.79	124.33	128.62
23	b	5523	CLA	O2A-CGA-CBA	2.79	120.71	111.94
23	A	563	CLA	O2A-CGA-CBA	2.79	120.71	111.94
28	c	5504	BCR	C40-C30-C25	2.79	114.94	110.33
23	B	526	CLA	O2A-CGA-CBA	2.78	120.70	111.94
23	C	493	CLA	C2A-C3A-C4A	2.78	105.68	101.40
23	C	492	CLA	CBD-CHA-C1A	2.78	132.41	128.77
23	B	515	CLA	C6-C5-C3	2.78	119.39	112.78
23	A	558	CLA	C2D-C1D-ND	2.78	111.51	109.41
28	C	504	BCR	C35-C13-C12	2.78	122.58	118.09
23	C	495	CLA	C7-C6-C5	-2.78	104.83	113.01
23	c	5494	CLA	C1D-CHD-C4C	2.78	126.91	122.60
28	a	5566	BCR	C23-C24-C25	2.77	135.51	127.32
23	c	5498	CLA	OBD-CAD-CBD	-2.77	121.75	125.94
23	C	495	CLA	C1-C2-C3	2.77	131.11	126.19
23	b	5520	CLA	C1D-C2D-C3D	-2.77	104.52	106.78
23	c	5493	CLA	C1D-CHD-C4C	2.77	126.90	122.60
28	t	104	BCR	C2-C1-C6	2.77	115.04	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5515	CLA	CBD-CHA-C1A	2.77	132.39	128.77
23	C	492	CLA	CAA-C2A-C3A	-2.77	106.50	113.04
23	B	519	CLA	C2A-C3A-C4A	2.77	105.66	101.40
26	d	5356	PQ9	C14-C13-C15	2.76	119.59	115.39
23	B	519	CLA	CMB-C2B-C1B	-2.76	124.37	128.62
23	C	501	CLA	C1-C2-C3	2.76	131.10	126.19
28	c	5505	BCR	C16-C17-C18	2.76	131.27	127.29
23	b	5518	CLA	CED-O2D-CGD	2.76	122.59	116.02
23	c	5503	CLA	CAA-C2A-C3A	-2.76	106.51	113.04
33	m	216	LMT	C1-O1'-C1'	-2.76	108.99	113.96
23	a	5558	CLA	C7-C6-C5	-2.76	104.87	113.01
23	C	498	CLA	C1D-C2D-C3D	-2.76	104.53	106.78
23	B	525	CLA	C7-C6-C5	-2.76	104.87	113.01
23	c	5500	CLA	C2A-C3A-C4A	2.76	105.64	101.40
23	c	5495	CLA	C1-C2-C3	2.76	131.08	126.19
24	a	5561	PHO	C7-C6-C5	-2.76	104.89	113.01
28	D	357	BCR	C24-C23-C22	2.76	130.34	126.22
23	C	492	CLA	C2A-C3A-C4A	2.76	105.64	101.40
23	C	492	CLA	C1D-C2D-C3D	-2.76	104.53	106.78
23	b	5523	CLA	C6-C5-C3	2.75	119.33	112.78
23	A	558	CLA	O2A-CGA-CBA	2.75	120.61	111.94
23	B	522	CLA	C7-C6-C5	-2.75	104.90	113.01
23	B	518	CLA	C6-C7-C8	2.75	123.07	115.14
23	C	498	CLA	C1D-CHD-C4C	2.75	126.87	122.60
23	b	5520	CLA	OBD-CAD-CBD	-2.75	121.78	125.94
28	B	527	BCR	C24-C23-C22	2.75	130.33	126.22
23	B	522	CLA	C2A-C3A-C4A	2.75	105.63	101.40
23	A	560	CLA	CMB-C2B-C3B	2.75	129.30	124.97
23	C	492	CLA	C1D-CHD-C4C	2.75	126.87	122.60
28	d	5357	BCR	C37-C22-C23	2.75	122.54	118.09
23	C	493	CLA	C1D-CHD-C4C	2.75	126.86	122.60
23	c	5500	CLA	CAA-C2A-C3A	-2.75	106.54	113.04
28	c	5504	BCR	C23-C24-C25	2.75	135.44	127.32
23	a	5563	CLA	CMB-C2B-C1B	-2.75	124.39	128.62
23	B	515	CLA	CBD-CHA-C1A	2.75	132.36	128.77
23	A	559	CLA	C1D-CHD-C4C	2.75	126.86	122.60
23	D	355	CLA	CED-O2D-CGD	2.75	122.55	116.02
23	C	494	CLA	C1D-CHD-C4C	2.75	126.86	122.60
23	C	495	CLA	CMB-C2B-C3B	2.74	129.29	124.97
23	B	526	CLA	C1D-CHD-C4C	2.74	126.85	122.60
28	b	5527	BCR	C16-C17-C18	2.74	131.24	127.29
23	a	5558	CLA	C2D-C1D-ND	2.74	111.48	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	5354	CLA	C2A-C3A-C4A	2.74	105.61	101.40
28	h	5107	BCR	C28-C27-C26	2.74	117.89	113.74
28	B	528	BCR	C8-C7-C6	2.74	135.42	127.32
23	B	520	CLA	CMB-C2B-C1B	-2.74	124.41	128.62
28	C	504	BCR	C23-C24-C25	2.74	135.40	127.32
23	C	496	CLA	CBD-CHA-C1A	2.74	132.35	128.77
28	C	505	BCR	C19-C18-C17	-2.74	114.77	118.97
28	H	107	BCR	C32-C1-C6	2.74	114.86	110.33
23	D	355	CLA	O2A-CGA-CBA	2.73	120.54	111.94
23	a	5558	CLA	C1-C2-C3	2.73	131.04	126.19
28	C	504	BCR	C1-C6-C7	2.73	123.26	115.69
28	h	5107	BCR	C15-C14-C13	2.73	131.23	127.29
23	b	5525	CLA	CED-O2D-CGD	2.73	122.52	116.02
23	b	5518	CLA	CMB-C2B-C1B	-2.73	124.42	128.62
28	T	5104	BCR	C11-C10-C9	2.73	131.22	127.29
25	v	5552	HEM	C2A-C1A-NA	-2.73	105.94	109.73
23	b	5520	CLA	C1D-CHD-C4C	2.73	126.83	122.60
23	B	519	CLA	C1D-CHD-C4C	2.73	126.83	122.60
23	B	525	CLA	CED-O2D-CGD	2.73	122.51	116.02
23	C	495	CLA	C2D-C1D-ND	2.73	111.47	109.41
23	b	5523	CLA	CMB-C2B-C1B	-2.73	124.43	128.62
29	L	210	MGE	O2G-C1B-C2B	2.72	117.53	111.56
29	b	5530	MGE	O6D-C5D-C6D	2.72	113.03	106.34
28	c	5505	BCR	C30-C25-C26	-2.72	118.66	122.60
23	b	5525	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
23	C	491	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
23	B	525	CLA	C2A-C3A-C4A	2.72	105.59	101.40
23	c	5497	CLA	C2A-C3A-C4A	2.72	105.59	101.40
23	b	5523	CLA	C1-C2-C3	2.72	131.02	126.19
23	c	5493	CLA	C7-C6-C5	-2.72	104.99	113.01
23	A	558	CLA	C7-C6-C5	-2.72	104.99	113.01
28	c	5504	BCR	C29-C30-C25	2.72	114.96	110.44
28	C	504	BCR	C32-C1-C6	2.72	114.83	110.33
23	B	518	CLA	CBD-CHA-C1A	2.72	132.32	128.77
23	C	500	CLA	CMB-C2B-C1B	-2.72	124.44	128.62
28	b	5528	BCR	C24-C23-C22	2.72	130.28	126.22
23	a	5560	CLA	C1D-CHD-C4C	2.72	126.81	122.60
23	a	5558	CLA	O2A-CGA-CBA	2.72	120.49	111.94
23	C	495	CLA	C2A-C3A-C4A	2.72	105.58	101.40
26	d	5356	PQ9	C16-C17-C18	-2.71	121.94	127.80
23	B	515	CLA	C2D-C1D-ND	2.72	111.46	109.41
23	A	563	CLA	C2A-C3A-C4A	2.71	105.58	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	558	CLA	CED-O2D-CGD	2.71	122.48	116.02
23	c	5491	CLA	C2A-C3A-C4A	2.71	105.58	101.40
23	B	522	CLA	CBD-CHA-C1A	2.71	132.32	128.77
23	d	5354	CLA	C2A-C1A-NA	-2.71	108.24	111.24
23	b	5523	CLA	CMB-C2B-C3B	2.71	129.24	124.97
23	c	5500	CLA	C2D-C1D-ND	2.71	111.46	109.41
23	b	5513	CLA	CMB-C2B-C3B	2.71	129.24	124.97
23	B	512	CLA	C2D-C1D-ND	2.71	111.46	109.41
23	a	5563	CLA	C2A-C3A-C4A	2.71	105.56	101.40
23	b	5512	CLA	C1D-CHD-C4C	2.70	126.79	122.60
23	b	5513	CLA	CED-O2D-CGD	2.70	122.45	116.02
23	B	512	CLA	C2A-C3A-C4A	2.70	105.55	101.40
23	C	491	CLA	O2A-CGA-CBA	2.70	120.44	111.94
23	D	355	CLA	C2D-C1D-ND	2.70	111.45	109.41
28	d	5357	BCR	C12-C13-C14	-2.70	114.82	118.97
28	c	5506	BCR	C30-C25-C24	2.70	123.17	115.69
23	C	497	CLA	CED-O2D-CGD	2.70	122.44	116.02
28	C	505	BCR	C1-C6-C5	-2.70	118.69	122.60
23	B	516	CLA	CBA-CAA-C2A	2.70	122.02	114.01
23	A	559	CLA	CED-O2D-CGD	2.70	122.44	116.02
23	C	493	CLA	C1-C2-C3	2.70	130.98	126.19
30	C	509	DGD	C3G-C2G-C1G	-2.69	105.72	111.86
23	c	5497	CLA	CED-O2D-CGD	2.69	122.42	116.02
23	B	515	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
23	B	511	CLA	C1D-CHD-C4C	2.69	126.77	122.60
28	t	104	BCR	C1-C6-C5	-2.69	118.70	122.60
23	c	5494	CLA	C2A-C3A-C4A	2.69	105.54	101.40
23	c	5492	CLA	C1D-C2D-C3D	-2.69	104.59	106.78
23	C	494	CLA	CMB-C2B-C3B	2.69	129.20	124.97
23	B	519	CLA	OBD-CAD-CBD	-2.69	121.89	125.94
23	c	5501	CLA	CED-O2D-CGD	2.69	122.41	116.02
23	c	5495	CLA	C7-C6-C5	-2.68	105.10	113.01
28	C	506	BCR	C19-C18-C17	-2.68	114.85	118.97
28	X	130	BCR	C16-C17-C18	2.68	131.16	127.29
26	A	564	PQ9	C26-C27-C28	-2.68	122.13	128.63
23	b	5524	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
23	B	519	CLA	C2D-C1D-ND	2.68	111.44	109.41
23	D	354	CLA	C2D-C1D-ND	2.68	111.44	109.41
28	C	505	BCR	C35-C13-C12	2.68	122.43	118.09
30	c	5508	DGD	O6D-C5D-C6D	2.68	112.00	106.61
24	a	5562	PHO	OBD-CAD-CBD	-2.68	121.89	125.94
23	c	5492	CLA	C1D-CHD-C4C	2.68	126.75	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	527	BCR	C1-C6-C5	-2.68	118.72	122.60
24	A	562	PHO	C1D-C2D-C3D	-2.68	104.59	106.89
23	C	500	CLA	C1-C2-C3	2.68	130.95	126.19
26	D	356	PQ9	C21-C22-C23	-2.68	122.03	127.80
23	b	5518	CLA	C6-C7-C8	2.68	122.85	115.14
28	b	5528	BCR	C8-C7-C6	2.68	135.22	127.32
28	T	5104	BCR	C1-C6-C5	-2.67	118.73	122.60
23	d	5354	CLA	C1D-CHD-C4C	2.67	126.75	122.60
29	l	5210	MGE	O2G-C1B-C2B	2.67	117.42	111.56
28	t	104	BCR	C23-C22-C21	-2.67	114.86	118.97
23	B	511	CLA	CMB-C2B-C3B	2.67	129.18	124.97
23	b	5518	CLA	CBD-CHA-C1A	2.67	132.26	128.77
28	C	506	BCR	C12-C13-C14	-2.67	114.86	118.97
28	t	104	BCR	C7-C8-C9	2.67	130.21	126.22
28	d	5357	BCR	C36-C18-C19	2.67	122.41	118.09
23	B	513	CLA	CED-O2D-CGD	2.67	122.37	116.02
23	B	511	CLA	C4D-CHA-CBD	-2.67	103.08	109.37
23	c	5500	CLA	C1D-C2D-C3D	-2.67	104.60	106.78
23	A	560	CLA	CED-O2D-CGD	2.66	122.36	116.02
28	C	504	BCR	C23-C22-C21	-2.66	114.88	118.97
23	b	5526	CLA	O2A-CGA-CBA	2.66	120.31	111.94
25	F	51	HEM	C4A-NA-C1A	2.66	110.27	106.76
23	b	5520	CLA	CMB-C2B-C1B	-2.66	124.53	128.62
23	b	5520	CLA	CED-O2D-CGD	2.66	122.35	116.02
23	b	5517	CLA	CMB-C2B-C1B	-2.66	124.53	128.62
32	d	5358	SQD	C32-C31-C30	2.66	129.01	114.61
23	C	503	CLA	CMB-C2B-C1B	-2.66	124.54	128.62
23	B	520	CLA	CMB-C2B-C3B	2.66	129.15	124.97
23	C	500	CLA	C7-C6-C5	-2.65	105.19	113.01
26	A	564	PQ9	C14-C13-C15	2.65	119.42	115.39
29	d	5360	MGE	C3G-O3G-C1D	-2.65	108.52	113.81
26	a	5564	PQ9	C14-C13-C15	2.65	119.42	115.39
23	C	493	CLA	C7-C6-C5	-2.65	105.20	113.01
23	b	5511	CLA	C4D-CHA-CBD	-2.65	103.13	109.37
33	T	217	LMT	C1-O1'-C1'	-2.65	109.19	113.96
23	a	5558	CLA	C1D-CHD-C4C	2.64	126.70	122.60
23	b	5516	CLA	CBA-CAA-C2A	2.64	121.86	114.01
28	c	5506	BCR	C35-C13-C12	2.64	122.36	118.09
23	c	5497	CLA	C6-C5-C3	2.64	119.06	112.78
30	h	5208	DGD	O6D-C5D-C4D	2.64	114.64	109.76
29	d	5359	MGE	O6D-C5D-C6D	2.64	112.83	106.34
23	c	5497	CLA	C1D-CHD-C4C	2.64	126.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	5357	BCR	C7-C8-C9	2.64	130.16	126.22
29	b	5530	MGE	O1G-C1G-C2G	-2.63	101.92	108.83
23	a	5558	CLA	CMB-C2B-C1B	-2.63	124.57	128.62
23	b	5526	CLA	C2A-C3A-C4A	2.63	105.45	101.40
26	a	5564	PQ9	C26-C27-C28	-2.64	122.24	128.63
23	B	512	CLA	C1D-CHD-C4C	2.63	126.68	122.60
23	c	5495	CLA	CMB-C2B-C3B	2.63	129.12	124.97
23	B	516	CLA	CBD-CHA-C1A	2.63	132.21	128.77
30	H	208	DGD	O6D-C5D-C4D	2.63	114.63	109.76
23	c	5494	CLA	CMB-C2B-C3B	2.63	129.12	124.97
28	B	529	BCR	C8-C7-C6	2.63	135.09	127.32
23	c	5497	CLA	CAA-C2A-C3A	-2.63	106.82	113.04
23	B	513	CLA	C6-C5-C3	2.63	119.03	112.78
33	t	5217	LMT	C1-O1'-C1'	-2.63	109.23	113.96
23	b	5514	CLA	C1-C2-C3	2.63	130.86	126.19
23	B	524	CLA	O2A-CGA-CBA	2.63	120.20	111.94
29	l	5210	MGE	O1G-C1G-C2G	-2.63	101.94	108.83
28	c	5506	BCR	C24-C23-C22	2.63	130.14	126.22
23	B	512	CLA	CMB-C2B-C1B	-2.62	124.59	128.62
23	b	5518	CLA	O2A-C1-C2	2.62	114.23	108.55
23	C	501	CLA	CED-O2D-CGD	2.62	122.26	116.02
23	c	5498	CLA	C2A-C3A-C4A	2.62	105.43	101.40
23	B	515	CLA	CED-O2D-CGD	2.62	122.25	116.02
24	A	562	PHO	CED-O2D-CGD	2.62	122.25	116.02
23	C	494	CLA	OBD-CAD-CBD	-2.62	121.98	125.94
23	b	5526	CLA	C1-C2-C3	2.62	130.84	126.19
23	B	514	CLA	CAA-C2A-C3A	-2.62	106.85	113.04
23	B	518	CLA	C2D-C1D-ND	2.62	111.39	109.41
23	B	524	CLA	C7-C6-C5	-2.62	105.30	113.01
23	b	5525	CLA	C2A-C3A-C4A	2.62	105.42	101.40
23	b	5523	CLA	C4B-C3B-CAB	2.62	132.48	127.18
28	b	5529	BCR	C35-C13-C12	2.61	122.32	118.09
23	C	497	CLA	C6-C5-C3	2.61	119.00	112.78
23	A	558	CLA	C1D-CHD-C4C	2.61	126.65	122.60
23	B	523	CLA	O2A-CGA-CBA	2.61	120.15	111.94
28	T	5104	BCR	C2-C1-C6	2.61	114.78	110.44
23	B	515	CLA	C7-C6-C5	-2.61	105.32	113.01
23	b	5512	CLA	C2A-C3A-C4A	2.61	105.41	101.40
28	A	566	BCR	C16-C17-C18	2.61	131.05	127.29
28	X	130	BCR	C24-C23-C22	2.61	130.11	126.22
23	C	493	CLA	OBD-CAD-CBD	-2.60	122.01	125.94
23	b	5519	CLA	CMB-C2B-C1B	-2.60	124.62	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5511	CLA	C1D-CHD-C4C	2.60	126.64	122.60
23	B	513	CLA	C2A-C3A-C4A	2.60	105.40	101.40
23	c	5498	CLA	CMB-C2B-C1B	-2.60	124.62	128.62
23	C	498	CLA	CBD-CHA-C1A	2.60	132.17	128.77
23	c	5491	CLA	C7-C6-C5	-2.60	105.36	113.01
23	C	501	CLA	C1D-C2D-C3D	-2.60	104.66	106.78
23	A	559	CLA	O2A-CGA-CBA	2.60	120.11	111.94
23	C	494	CLA	C1D-C2D-C3D	-2.59	104.66	106.78
23	b	5520	CLA	C2A-C3A-C4A	2.59	105.39	101.40
23	C	498	CLA	CED-O2D-CGD	2.59	122.19	116.02
25	F	51	HEM	O2A-CGA-CBA	2.59	123.38	114.22
23	b	5514	CLA	CAA-C2A-C3A	-2.59	106.91	113.04
28	B	527	BCR	C16-C17-C18	2.59	131.03	127.29
23	c	5492	CLA	C2A-C1A-NA	-2.59	108.38	111.24
23	b	5512	CLA	CMB-C2B-C1B	-2.59	124.64	128.62
28	D	357	BCR	C35-C13-C12	2.59	122.28	118.09
23	a	5563	CLA	C1D-CHD-C4C	2.59	126.61	122.60
23	a	5560	CLA	CAA-CBA-CGA	2.59	121.60	113.27
23	a	5559	CLA	C2D-C1D-ND	2.58	111.36	109.41
23	b	5517	CLA	C7-C6-C5	-2.58	105.39	113.01
32	A	5212	SQD	C45-O47-C7	2.58	124.50	116.68
23	B	516	CLA	C2A-C3A-C4A	2.58	105.38	101.40
23	b	5522	CLA	CBD-CHA-C1A	2.58	132.15	128.77
23	B	523	CLA	CMB-C2B-C1B	-2.58	124.65	128.62
23	C	498	CLA	C2A-C3A-C4A	2.58	105.37	101.40
23	b	5520	CLA	CMB-C2B-C3B	2.58	129.03	124.97
28	A	566	BCR	C7-C8-C9	2.58	130.08	126.22
32	d	5358	SQD	C36-C35-C34	2.58	128.58	114.61
23	b	5515	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
28	c	5506	BCR	C16-C17-C18	2.58	131.01	127.29
29	L	210	MGE	O1G-C1G-C2G	-2.58	102.07	108.83
23	A	559	CLA	CMB-C2B-C1B	-2.58	124.65	128.62
26	D	356	PQ9	C26-C27-C28	-2.58	122.38	128.63
23	C	493	CLA	C2D-C1D-ND	2.58	111.36	109.41
24	a	5561	PHO	C1D-C2D-C3D	-2.57	104.68	106.89
28	x	5130	BCR	C35-C13-C12	2.57	122.26	118.09
23	B	526	CLA	C1-C2-C3	2.57	130.76	126.19
23	d	5355	CLA	C2A-C3A-C4A	2.57	105.36	101.40
23	B	524	CLA	CMB-C2B-C1B	-2.57	124.66	128.62
23	B	520	CLA	CAA-C2A-C3A	-2.57	106.96	113.04
23	B	515	CLA	C1D-CHD-C4C	2.57	126.58	122.60
23	b	5524	CLA	C7-C6-C5	-2.57	105.43	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5525	CLA	C2D-C1D-ND	2.57	111.35	109.41
32	L	5213	SQD	C3-C4-C5	-2.57	105.62	110.20
28	C	505	BCR	C30-C25-C26	-2.57	118.88	122.60
23	C	500	CLA	O2A-CGA-CBA	2.57	120.01	111.94
23	c	5502	CLA	C1-C2-C3	2.56	130.74	126.19
32	A	568	SQD	C36-C35-C34	2.56	128.47	114.61
23	c	5494	CLA	C1D-C2D-C3D	-2.56	104.69	106.78
26	A	564	PQ9	C21-C22-C23	-2.56	122.28	127.80
23	b	5512	CLA	CMB-C2B-C3B	2.56	129.00	124.97
23	b	5525	CLA	CMB-C2B-C1B	-2.56	124.69	128.62
28	A	566	BCR	C36-C18-C19	2.56	122.23	118.09
23	A	563	CLA	CMB-C2B-C1B	-2.56	124.69	128.62
23	C	501	CLA	O2A-CGA-CBA	2.56	119.98	111.94
23	b	5515	CLA	C1D-CHD-C4C	2.55	126.56	122.60
28	h	5107	BCR	C1-C6-C7	2.55	122.77	115.69
28	c	5506	BCR	C37-C22-C23	2.55	122.22	118.09
23	a	5559	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
23	c	5496	CLA	C2D-C1D-ND	2.55	111.34	109.41
23	b	5524	CLA	C2A-C1A-NA	-2.55	108.42	111.24
23	B	520	CLA	C2A-C3A-C4A	2.55	105.32	101.40
23	c	5496	CLA	O2A-CGA-CBA	2.55	119.96	111.94
28	A	566	BCR	C35-C13-C12	2.55	122.21	118.09
23	C	496	CLA	C7-C6-C5	-2.54	105.51	113.01
28	c	5504	BCR	C35-C13-C12	2.55	122.21	118.09
23	a	5560	CLA	CMB-C2B-C3B	2.55	128.98	124.97
28	h	5107	BCR	C35-C13-C12	2.54	122.21	118.09
23	C	499	CLA	C2D-C1D-ND	2.54	111.33	109.41
24	A	561	PHO	C4A-NA-C1A	2.54	111.77	108.42
23	c	5499	CLA	C1D-CHD-C4C	2.54	126.54	122.60
28	b	5529	BCR	C7-C8-C9	2.54	130.01	126.22
23	b	5517	CLA	C2A-C3A-C4A	2.54	105.31	101.40
23	B	517	CLA	C2A-C1A-CHA	2.54	128.23	123.83
23	B	526	CLA	CBD-CHA-C1A	2.54	132.09	128.77
23	b	5518	CLA	C16-C15-C13	2.54	122.45	115.14
23	b	5525	CLA	C7-C6-C5	-2.54	105.53	113.01
28	c	5506	BCR	C40-C30-C29	-2.54	98.46	108.73
23	D	355	CLA	CMB-C2B-C1B	-2.54	124.72	128.62
28	a	5566	BCR	C8-C7-C6	2.54	134.81	127.32
23	C	499	CLA	CAA-C2A-C3A	-2.54	107.04	113.04
23	c	5498	CLA	O2A-CGA-CBA	2.54	119.92	111.94
28	a	5566	BCR	C37-C22-C23	2.54	122.19	118.09
32	A	568	SQD	C44-O6-C1	2.53	118.86	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	523	CLA	CMB-C2B-C3B	2.53	128.96	124.97
26	d	5356	PQ9	C19-C18-C20	2.53	119.23	115.39
23	A	559	CLA	C2D-C1D-ND	2.53	111.32	109.41
23	d	5355	CLA	O2A-CGA-CBA	2.53	119.89	111.94
32	d	5358	SQD	O8-S-O7	2.53	117.25	111.78
23	b	5516	CLA	CBD-CHA-C1A	2.53	132.07	128.77
23	c	5495	CLA	C2A-C3A-C4A	2.52	105.28	101.40
23	B	518	CLA	CMB-C2B-C1B	-2.52	124.74	128.62
23	C	491	CLA	CAA-C2A-C3A	-2.52	107.08	113.04
23	B	519	CLA	C1-C2-C3	2.52	130.67	126.19
28	C	505	BCR	C12-C13-C14	-2.52	115.10	118.97
23	C	498	CLA	O2D-CGD-CBD	2.52	116.47	111.33
28	B	529	BCR	C35-C13-C12	2.52	122.17	118.09
23	B	512	CLA	C1-C2-C3	2.51	130.66	126.19
23	c	5495	CLA	C2A-C1A-CHA	2.51	128.19	123.83
25	f	5051	HEM	C4A-NA-C1A	2.52	110.08	106.76
28	H	107	BCR	C16-C17-C18	2.52	130.92	127.29
24	a	5561	PHO	C4A-NA-C1A	2.51	111.73	108.42
28	A	566	BCR	C1-C6-C5	-2.51	118.96	122.60
23	C	496	CLA	C1D-C2D-C3D	-2.51	104.73	106.78
23	a	5560	CLA	C7-C6-C5	-2.51	105.60	113.01
23	C	494	CLA	CBA-CAA-C2A	2.51	121.47	114.01
28	B	527	BCR	C8-C7-C6	2.51	134.74	127.32
23	b	5518	CLA	C2A-C3A-C4A	2.51	105.26	101.40
30	C	508	DGD	O6D-C5D-C6D	2.51	111.66	106.61
23	b	5521	CLA	CED-O2D-CGD	2.51	121.99	116.02
23	b	5516	CLA	CMB-C2B-C1B	-2.51	124.76	128.62
23	b	5524	CLA	C2D-C1D-ND	2.51	111.31	109.41
23	C	496	CLA	C2A-C3A-C4A	2.51	105.26	101.40
23	B	512	CLA	C7-C6-C5	-2.51	105.62	113.01
23	c	5493	CLA	OBD-CAD-CBD	-2.51	122.16	125.94
23	A	563	CLA	C1D-C2D-C3D	-2.51	104.73	106.78
28	c	5506	BCR	C19-C18-C17	-2.50	115.12	118.97
28	t	104	BCR	C12-C13-C14	-2.50	115.12	118.97
23	B	518	CLA	C2A-C3A-C4A	2.50	105.25	101.40
23	b	5518	CLA	C6-C5-C3	2.50	118.73	112.78
23	c	5496	CLA	C1D-C2D-C3D	-2.50	104.74	106.78
28	C	504	BCR	C37-C22-C23	2.50	122.14	118.09
28	c	5506	BCR	C1-C6-C5	-2.50	118.98	122.60
23	c	5492	CLA	OBD-CAD-CBD	-2.50	122.16	125.94
23	b	5513	CLA	C6-C5-C3	2.50	118.73	112.78
23	B	524	CLA	C2A-C1A-NA	-2.50	108.48	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	499	CLA	CED-O2D-CGD	2.50	121.97	116.02
24	A	562	PHO	C4D-CHA-CBD	-2.50	103.73	107.53
23	c	5503	CLA	CBD-CHA-C1A	2.50	132.04	128.77
23	B	512	CLA	C1D-C2D-C3D	-2.50	104.74	106.78
23	B	524	CLA	C2A-C3A-C4A	2.50	105.24	101.40
32	a	212	SQD	C45-O47-C7	2.50	124.24	116.68
25	V	552	HEM	C2A-C1A-NA	-2.50	106.27	109.73
28	X	130	BCR	C30-C25-C24	2.50	122.61	115.69
28	x	5130	BCR	C28-C27-C26	2.50	117.52	113.74
23	c	5500	CLA	CMB-C2B-C1B	-2.49	124.79	128.62
23	c	5496	CLA	C7-C6-C5	-2.49	105.67	113.01
23	B	518	CLA	C7-C6-C5	-2.49	105.68	113.01
24	A	562	PHO	C4A-NA-C1A	2.49	111.69	108.42
28	T	5104	BCR	C7-C8-C9	2.49	129.93	126.22
23	A	560	CLA	C6-C7-C8	2.49	122.30	115.14
23	b	5516	CLA	C1D-CHD-C4C	2.49	126.46	122.60
28	c	5504	BCR	C37-C22-C23	2.49	122.11	118.09
28	C	504	BCR	C7-C8-C9	2.49	129.94	126.22
23	A	558	CLA	CMB-C2B-C1B	-2.49	124.80	128.62
29	d	5359	MGE	C3G-C2G-C1G	-2.49	106.20	111.86
26	d	5356	PQ9	C26-C27-C28	-2.48	122.61	128.63
23	D	355	CLA	C2A-C3A-C4A	2.48	105.22	101.40
23	c	5503	CLA	C1D-C2D-C3D	-2.48	104.75	106.78
23	C	494	CLA	C2A-C1A-CHA	2.48	128.13	123.83
28	C	506	BCR	C30-C25-C24	2.48	122.57	115.69
23	B	516	CLA	C7-C6-C5	-2.48	105.70	113.01
28	C	506	BCR	C40-C30-C29	-2.48	98.68	108.73
23	C	502	CLA	C2A-C1A-CHA	2.48	128.13	123.83
23	A	560	CLA	CAA-CBA-CGA	2.48	121.26	113.27
23	b	5526	CLA	CBD-CHA-C1A	2.48	132.01	128.77
23	B	523	CLA	C1-C2-C3	2.48	130.59	126.19
23	b	5519	CLA	C7-C6-C5	-2.48	105.71	113.01
26	a	5564	PQ9	C21-C22-C23	-2.48	122.45	127.80
23	b	5517	CLA	OBD-CAD-C3D	2.48	132.52	127.91
23	B	512	CLA	CMB-C2B-C3B	2.48	128.87	124.97
23	b	5526	CLA	C1-O2A-CGA	2.48	123.92	116.98
23	b	5511	CLA	CMB-C2B-C3B	2.48	128.87	124.97
24	a	5562	PHO	C4A-NA-C1A	2.48	111.68	108.42
23	b	5513	CLA	C2A-C3A-C4A	2.47	105.21	101.40
23	C	497	CLA	C2A-C3A-C4A	2.47	105.21	101.40
23	A	558	CLA	C16-C15-C13	2.47	122.26	115.14
23	B	521	CLA	C1D-C2D-C3D	-2.47	104.76	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	526	CLA	C6-C5-C3	2.47	118.65	112.78
23	B	515	CLA	C1D-C2D-C3D	-2.47	104.76	106.78
29	B	530	MGE	C3G-C2G-C1G	-2.47	106.24	111.86
23	B	523	CLA	OBD-CAD-CBD	-2.47	122.21	125.94
23	c	5502	CLA	C2A-C1A-CHA	2.47	128.11	123.83
23	b	5518	CLA	C2D-C1D-ND	2.47	111.27	109.41
23	B	516	CLA	C1D-C2D-C3D	-2.46	104.77	106.78
28	a	5566	BCR	C1-C6-C5	-2.46	119.03	122.60
23	a	5563	CLA	CMB-C2B-C3B	2.46	128.85	124.97
29	B	530	MGE	O6D-C5D-C6D	2.46	112.39	106.34
29	i	5201	MGE	C3G-O3G-C1D	-2.46	108.90	113.81
28	a	5566	BCR	C36-C18-C19	2.46	122.07	118.09
23	a	5560	CLA	CED-O2D-CGD	2.46	121.87	116.02
23	b	5526	CLA	C6-C5-C3	2.46	118.63	112.78
28	t	104	BCR	C8-C9-C10	-2.46	115.19	118.97
32	d	5358	SQD	C44-O6-C1	2.46	118.70	113.81
33	t	5217	LMT	C3'-C4'-C5'	-2.46	105.33	110.85
23	b	5517	CLA	C2A-C1A-NA	-2.45	108.53	111.24
23	c	5502	CLA	CMB-C2B-C1B	-2.45	124.85	128.62
23	b	5524	CLA	O2A-CGA-CBA	2.45	119.66	111.94
28	h	5107	BCR	C16-C17-C18	2.45	130.83	127.29
23	C	493	CLA	C4D-CHA-CBD	-2.45	103.60	109.37
23	b	5519	CLA	C1-C2-C3	2.45	130.54	126.19
23	B	514	CLA	C7-C6-C5	-2.45	105.79	113.01
23	B	520	CLA	C1D-C2D-C3D	-2.45	104.78	106.78
23	B	519	CLA	C7-C6-C5	-2.45	105.79	113.01
23	C	498	CLA	O2A-CGA-CBA	2.45	119.65	111.94
23	b	5525	CLA	C1D-C2D-C3D	-2.45	104.78	106.78
23	C	498	CLA	C7-C6-C5	-2.45	105.80	113.01
23	C	500	CLA	CAA-C2A-C3A	-2.44	107.26	113.04
23	c	5500	CLA	O2A-CGA-CBA	2.44	119.63	111.94
23	B	517	CLA	C7-C6-C5	-2.44	105.81	113.01
25	V	552	HEM	C4A-C3A-C2A	2.44	108.69	107.00
23	B	513	CLA	CMB-C2B-C1B	-2.44	124.87	128.62
23	B	513	CLA	C1-C2-C3	2.44	130.53	126.19
28	a	5566	BCR	C16-C17-C18	2.44	130.81	127.29
23	C	497	CLA	O2D-CGD-CBD	2.44	116.30	111.33
28	B	528	BCR	C1-C6-C7	2.44	122.45	115.69
28	c	5504	BCR	C30-C25-C24	2.43	122.44	115.69
23	b	5516	CLA	C16-C15-C13	2.44	122.15	115.14
23	a	5558	CLA	CMB-C2B-C3B	2.43	128.80	124.97
23	B	517	CLA	C2A-C3A-C4A	2.43	105.14	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	5357	BCR	C16-C17-C18	2.43	130.79	127.29
23	b	5520	CLA	C1-C2-C3	2.43	130.51	126.19
23	b	5523	CLA	C1D-C2D-C3D	-2.43	104.80	106.78
28	b	5529	BCR	C32-C1-C6	2.43	114.35	110.33
28	D	357	BCR	C16-C17-C18	2.43	130.79	127.29
28	D	357	BCR	C37-C22-C23	2.43	122.02	118.09
23	A	558	CLA	CBA-CAA-C2A	2.43	121.22	114.01
23	c	5501	CLA	C2A-C3A-C4A	2.43	105.13	101.40
23	C	503	CLA	CMB-C2B-C3B	2.43	128.79	124.97
23	B	520	CLA	C1-C2-C3	2.43	130.50	126.19
23	C	491	CLA	C2D-C1D-ND	2.43	111.24	109.41
29	D	360	MGE	O1G-C1G-C2G	-2.43	102.47	108.83
28	b	5527	BCR	C35-C13-C12	2.42	122.01	118.09
23	c	5499	CLA	CMB-C2B-C1B	-2.42	124.89	128.62
23	c	5499	CLA	O2D-CGD-CBD	2.42	116.27	111.33
28	c	5504	BCR	C23-C22-C21	-2.42	115.25	118.97
23	c	5502	CLA	C2D-C1D-ND	2.42	111.24	109.41
23	c	5497	CLA	OBD-CAD-CBD	-2.42	122.28	125.94
28	c	5505	BCR	C12-C13-C14	-2.42	115.25	118.97
23	B	515	CLA	C6-C7-C8	2.42	122.11	115.14
23	b	5512	CLA	C7-C6-C5	-2.42	105.89	113.01
32	d	5358	SQD	C15-C14-C13	2.42	127.69	114.61
23	a	5563	CLA	CBD-CHA-C1A	2.42	131.93	128.77
23	B	517	CLA	C4D-CHA-CBD	-2.42	103.68	109.37
23	C	501	CLA	C4D-CHA-CBD	-2.42	103.68	109.37
23	A	563	CLA	CED-O2D-CGD	2.42	121.77	116.02
24	A	561	PHO	C7-C6-C5	-2.42	105.89	113.01
23	d	5354	CLA	CED-O2D-CGD	2.41	121.76	116.02
23	B	518	CLA	OBD-CAD-CBD	-2.41	122.29	125.94
23	b	5520	CLA	C6-C7-C8	2.41	122.09	115.14
28	T	5104	BCR	C40-C30-C29	-2.41	98.95	108.73
28	B	527	BCR	C12-C13-C14	-2.41	115.26	118.97
28	b	5528	BCR	C1-C6-C7	2.41	122.38	115.69
28	c	5504	BCR	C12-C13-C14	-2.41	115.26	118.97
23	c	5498	CLA	CBD-CHA-C1A	2.41	131.93	128.77
23	b	5519	CLA	C2A-C3A-C4A	2.41	105.11	101.40
32	A	568	SQD	C3-C4-C5	-2.41	105.89	110.20
23	c	5499	CLA	C2A-C1A-CHA	2.41	128.01	123.83
23	C	503	CLA	C2A-C3A-C4A	2.41	105.11	101.40
23	d	5354	CLA	C2D-C1D-ND	2.41	111.23	109.41
23	b	5513	CLA	C1-C2-C3	2.41	130.47	126.19
23	c	5493	CLA	CMB-C2B-C1B	-2.41	124.92	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	5559	CLA	CMB-C2B-C1B	-2.41	124.92	128.62
23	b	5513	CLA	C1D-C2D-C3D	-2.41	104.81	106.78
28	c	5505	BCR	C8-C7-C6	2.40	134.42	127.32
23	c	5491	CLA	C2A-C1A-NA	-2.40	108.58	111.24
23	B	520	CLA	C6-C7-C8	2.40	122.05	115.14
23	B	516	CLA	C1D-CHD-C4C	2.40	126.32	122.60
23	b	5515	CLA	C6-C7-C8	2.40	122.06	115.14
23	B	517	CLA	OBD-CAD-C3D	2.40	132.38	127.91
23	B	522	CLA	CAA-C2A-C3A	-2.40	107.37	113.04
28	B	527	BCR	C36-C18-C19	2.40	121.97	118.09
25	v	5552	HEM	C1B-NB-C4B	2.40	107.62	105.16
23	c	5492	CLA	O2A-CGA-CBA	2.40	119.48	111.94
23	B	517	CLA	CMB-C2B-C1B	-2.40	124.93	128.62
23	c	5497	CLA	CMB-C2B-C1B	-2.40	124.94	128.62
32	t	213	SQD	C3-C4-C5	-2.39	105.93	110.20
32	d	5358	SQD	C3-C4-C5	-2.39	105.93	110.20
23	c	5502	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
23	c	5493	CLA	C2D-C1D-ND	2.39	111.22	109.41
23	c	5491	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
24	a	5562	PHO	C4D-CHA-CBD	-2.39	103.90	107.53
28	b	5527	BCR	C8-C7-C6	2.39	134.38	127.32
32	A	5212	SQD	O8-S-O7	2.39	116.95	111.78
23	C	499	CLA	CMB-C2B-C3B	2.39	128.73	124.97
23	C	499	CLA	O2D-CGD-CBD	2.39	116.20	111.33
28	x	5130	BCR	C30-C25-C24	2.39	122.30	115.69
23	b	5519	CLA	C1D-C2D-C3D	-2.39	104.83	106.78
28	H	107	BCR	C1-C6-C7	2.39	122.31	115.69
23	c	5494	CLA	CBA-CAA-C2A	2.39	121.10	114.01
23	b	5518	CLA	C7-C6-C5	-2.38	105.98	113.01
23	a	5558	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
23	b	5522	CLA	C2D-C1D-ND	2.38	111.21	109.41
28	c	5506	BCR	C12-C13-C14	-2.38	115.31	118.97
28	a	5566	BCR	C30-C25-C24	2.38	122.29	115.69
28	b	5529	BCR	C12-C13-C14	-2.38	115.31	118.97
28	X	130	BCR	C35-C13-C12	2.38	121.94	118.09
23	c	5492	CLA	C4D-CHA-CBD	-2.38	103.77	109.37
23	c	5503	CLA	C2A-C3A-C4A	2.38	105.06	101.40
23	b	5526	CLA	C7-C6-C5	-2.38	106.01	113.01
23	B	518	CLA	C16-C15-C13	2.37	121.98	115.14
28	B	529	BCR	C12-C13-C14	-2.37	115.32	118.97
23	c	5494	CLA	C2A-C1A-NA	-2.38	108.61	111.24
25	V	552	HEM	O2A-CGA-CBA	2.37	122.61	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	5558	CLA	CBA-CAA-C2A	2.37	121.06	114.01
23	c	5501	CLA	C1D-C2D-C3D	-2.37	104.84	106.78
23	C	503	CLA	C1-C2-C3	2.37	130.40	126.19
23	b	5519	CLA	C6-C5-C3	2.37	118.42	112.78
23	A	563	CLA	CBD-CHA-C1A	2.37	131.87	128.77
23	c	5492	CLA	C2A-C3A-C4A	2.37	105.04	101.40
23	b	5515	CLA	C7-C6-C5	-2.37	106.03	113.01
23	A	559	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
28	X	130	BCR	C37-C22-C23	2.37	121.92	118.09
23	c	5501	CLA	C4D-CHA-CBD	-2.37	103.79	109.37
28	T	5104	BCR	C12-C13-C14	-2.37	115.33	118.97
28	A	566	BCR	C37-C22-C23	2.37	121.92	118.09
23	b	5526	CLA	OBD-CAD-C3D	2.37	132.31	127.91
32	L	5213	SQD	O7-S-C6	2.37	111.17	107.03
33	t	5217	LMT	O1B-C1B-C2B	2.36	113.79	108.12
23	c	5501	CLA	O2A-CGA-CBA	2.36	119.38	111.94
26	D	356	PQ9	C14-C13-C15	2.36	118.98	115.39
28	C	505	BCR	C36-C18-C19	2.36	121.91	118.09
23	b	5516	CLA	C7-C6-C5	-2.36	106.06	113.01
23	C	495	CLA	CED-O2D-CGD	2.36	121.63	116.02
23	b	5515	CLA	C1D-C2D-C3D	-2.36	104.85	106.78
28	B	528	BCR	C32-C1-C6	2.36	114.24	110.33
23	C	503	CLA	C2D-C1D-ND	2.36	111.19	109.41
23	B	515	CLA	CMB-C2B-C1B	-2.36	125.00	128.62
23	C	502	CLA	CMB-C2B-C1B	-2.36	125.00	128.62
23	A	560	CLA	C1-C2-C3	2.35	130.37	126.19
23	b	5525	CLA	C4D-CHA-CBD	-2.35	103.83	109.37
23	b	5517	CLA	C4D-CHA-CBD	-2.35	103.83	109.37
28	T	5104	BCR	C37-C22-C23	2.35	121.90	118.09
29	b	5530	MGE	O3G-C1D-C2D	2.35	111.17	108.18
23	b	5521	CLA	C1D-C2D-C3D	-2.35	104.86	106.78
23	c	5499	CLA	C1D-C2D-C3D	-2.35	104.86	106.78
23	c	5500	CLA	CMB-C2B-C3B	2.35	128.67	124.97
28	C	506	BCR	C36-C18-C19	2.35	121.89	118.09
23	c	5491	CLA	C2D-C1D-ND	2.35	111.19	109.41
28	X	130	BCR	C28-C27-C26	2.35	117.30	113.74
23	d	5354	CLA	O2D-CGD-CBD	2.35	116.11	111.33
23	c	5502	CLA	C1D-C2D-C3D	-2.35	104.86	106.78
23	a	5563	CLA	C1D-C2D-C3D	-2.35	104.86	106.78
25	f	5051	HEM	CBA-CAA-C2A	-2.35	108.56	112.69
23	b	5517	CLA	CMB-C2B-C3B	2.34	128.66	124.97
23	b	5523	CLA	C4D-CHA-CBD	-2.34	103.86	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	561	PHO	O2A-CGA-CBA	2.34	119.31	111.94
23	B	526	CLA	C1D-C2D-C3D	-2.34	104.87	106.78
28	A	566	BCR	C19-C18-C17	-2.34	115.37	118.97
23	b	5512	CLA	C1-C2-C3	2.34	130.34	126.19
23	b	5515	CLA	C2D-C1D-ND	2.34	111.18	109.41
23	b	5520	CLA	CAA-C2A-C3A	-2.34	107.52	113.04
29	d	5361	MGE	O1G-C1G-C2G	-2.34	102.70	108.83
23	D	355	CLA	C1D-C2D-C3D	-2.34	104.87	106.78
23	B	519	CLA	CMB-C2B-C3B	2.34	128.65	124.97
23	d	5355	CLA	CMB-C2B-C1B	-2.34	125.03	128.62
24	A	561	PHO	C1D-C2D-C3D	-2.34	104.89	106.89
23	B	516	CLA	CMB-C2B-C1B	-2.33	125.03	128.62
23	A	560	CLA	C7-C6-C5	-2.33	106.13	113.01
24	A	562	PHO	C6-C5-C3	2.33	118.33	112.78
23	b	5514	CLA	C4D-CHA-CBD	-2.33	103.88	109.37
23	A	560	CLA	C6-C5-C3	2.33	118.32	112.78
23	b	5523	CLA	C7-C6-C5	-2.33	106.14	113.01
23	C	498	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
23	C	497	CLA	C2D-C1D-ND	2.33	111.17	109.41
23	b	5516	CLA	C2A-C3A-C4A	2.33	104.98	101.40
23	C	501	CLA	C2A-C1A-CHA	2.33	127.86	123.83
23	c	5501	CLA	C2A-C1A-NA	-2.33	108.67	111.24
23	C	494	CLA	C4D-CHA-CBD	-2.33	103.89	109.37
23	b	5518	CLA	CMB-C2B-C3B	2.33	128.63	124.97
24	a	5562	PHO	C2A-C1A-NA	-2.33	108.34	111.93
23	c	5497	CLA	C4D-CHA-CBD	-2.32	103.90	109.37
23	B	519	CLA	C2A-C1A-CHA	2.32	127.86	123.83
23	b	5511	CLA	C2A-C1A-NA	-2.32	108.67	111.24
28	C	506	BCR	C37-C22-C23	2.32	121.85	118.09
23	a	5563	CLA	C2D-C1D-ND	2.32	111.16	109.41
23	B	522	CLA	C6-C7-C8	2.32	121.82	115.14
23	b	5525	CLA	CMB-C2B-C3B	2.32	128.62	124.97
28	C	504	BCR	C32-C1-C2	-2.32	99.33	108.73
23	c	5497	CLA	CMB-C2B-C3B	2.32	128.62	124.97
33	T	217	LMT	O1B-C1B-C2B	2.32	113.68	108.12
23	A	558	CLA	C4D-CHA-CBD	-2.32	103.92	109.37
28	a	5566	BCR	C2-C1-C6	2.32	114.29	110.44
28	c	5506	BCR	C23-C22-C21	-2.32	115.41	118.97
28	d	5357	BCR	C35-C13-C12	2.31	121.83	118.09
26	D	356	PQ9	C11-C12-C13	-2.31	122.85	126.76
23	C	501	CLA	C2A-C1A-NA	-2.31	108.68	111.24
23	C	493	CLA	C2A-C1A-CHA	2.31	127.84	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	500	CLA	C2D-C1D-ND	2.31	111.15	109.41
23	b	5519	CLA	C4D-CHA-CBD	-2.31	103.94	109.37
23	b	5519	CLA	O2A-CGA-CBA	2.31	119.19	111.94
23	c	5495	CLA	C2A-C1A-NA	-2.30	108.69	111.24
23	c	5493	CLA	C4D-CHA-CBD	-2.30	103.94	109.37
23	B	514	CLA	C4D-CHA-CBD	-2.30	103.95	109.37
23	C	495	CLA	C2A-C1A-CHA	2.30	127.82	123.83
23	c	5503	CLA	O2A-CGA-CBA	2.30	119.18	111.94
23	b	5524	CLA	CMB-C2B-C1B	-2.30	125.08	128.62
23	c	5503	CLA	CMB-C2B-C1B	-2.30	125.08	128.62
23	C	491	CLA	C7-C6-C5	-2.30	106.23	113.01
23	B	519	CLA	C4D-CHA-CBD	-2.30	103.96	109.37
23	C	502	CLA	C1-C2-C3	2.30	130.27	126.19
23	B	525	CLA	CMB-C2B-C1B	-2.30	125.09	128.62
28	D	357	BCR	C23-C22-C21	-2.30	115.44	118.97
23	A	558	CLA	CMB-C2B-C3B	2.30	128.58	124.97
23	b	5521	CLA	CMB-C2B-C1B	-2.29	125.09	128.62
28	X	130	BCR	C32-C1-C2	-2.29	99.44	108.73
23	B	517	CLA	C1D-C2D-C3D	-2.29	104.91	106.78
23	b	5512	CLA	C2D-C1D-ND	2.29	111.14	109.41
23	c	5499	CLA	CMB-C2B-C3B	2.29	128.58	124.97
23	C	500	CLA	CMB-C2B-C3B	2.29	128.58	124.97
29	I	201	MGE	C3G-O3G-C1D	-2.29	109.25	113.81
28	H	107	BCR	C35-C13-C12	2.29	121.79	118.09
32	a	212	SQD	O8-S-O7	2.29	116.73	111.78
25	v	5552	HEM	O2A-CGA-CBA	2.29	122.30	114.22
23	C	496	CLA	CMB-C2B-C1B	-2.28	125.11	128.62
23	B	523	CLA	C7-C6-C5	-2.28	106.28	113.01
30	H	208	DGD	C3G-C2G-C1G	-2.28	106.66	111.86
23	B	512	CLA	C6-C5-C3	2.28	118.20	112.78
23	c	5497	CLA	O2D-CGD-CBD	2.28	115.98	111.33
25	V	552	HEM	C1B-NB-C4B	2.28	107.50	105.16
23	B	517	CLA	C2A-C1A-NA	-2.28	108.72	111.24
23	b	5522	CLA	CMB-C2B-C1B	-2.28	125.12	128.62
23	c	5491	CLA	C1D-C2D-C3D	-2.28	104.92	106.78
28	C	504	BCR	C40-C30-C25	2.28	114.10	110.33
28	A	566	BCR	C2-C1-C6	2.28	114.22	110.44
23	B	517	CLA	C6-C5-C3	2.28	118.19	112.78
23	C	501	CLA	C2A-C3A-C4A	2.28	104.90	101.40
23	B	514	CLA	C6-C7-C8	2.28	121.69	115.14
23	C	503	CLA	CBD-CHA-C1A	2.27	131.74	128.77
28	X	130	BCR	C19-C18-C17	-2.27	115.48	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	t	104	BCR	C36-C18-C19	2.27	121.77	118.09
23	b	5514	CLA	CMB-C2B-C1B	-2.27	125.13	128.62
23	b	5516	CLA	C1D-C2D-C3D	-2.27	104.92	106.78
28	C	506	BCR	C24-C23-C22	2.27	129.62	126.22
28	C	506	BCR	C23-C22-C21	-2.27	115.48	118.97
28	t	104	BCR	C37-C22-C23	2.27	121.77	118.09
28	B	529	BCR	C40-C30-C25	2.27	114.09	110.33
23	D	354	CLA	CED-O2D-CGD	2.27	121.42	116.02
23	B	526	CLA	CMB-C2B-C1B	-2.27	125.13	128.62
23	c	5502	CLA	C4D-CHA-CBD	-2.27	104.03	109.37
28	a	5566	BCR	C32-C1-C6	2.27	114.08	110.33
28	a	5566	BCR	C12-C13-C14	-2.27	115.49	118.97
23	C	497	CLA	C4D-CHA-CBD	-2.27	104.03	109.37
23	C	497	CLA	CMB-C2B-C1B	-2.27	125.14	128.62
23	d	5354	CLA	C4D-CHA-CBD	-2.26	104.04	109.37
28	C	505	BCR	C8-C7-C6	2.26	134.00	127.32
28	h	5107	BCR	C37-C22-C23	2.26	121.75	118.09
28	B	529	BCR	C15-C14-C13	2.26	130.55	127.29
23	C	491	CLA	C1D-C2D-C3D	-2.26	104.93	106.78
28	A	566	BCR	C8-C7-C6	2.26	133.99	127.32
23	B	526	CLA	CMB-C2B-C3B	2.26	128.52	124.97
28	C	504	BCR	C12-C13-C14	-2.26	115.50	118.97
24	A	561	PHO	C4B-C3B-C2B	-2.26	105.96	107.60
23	a	5559	CLA	C1D-C2D-C3D	-2.25	104.94	106.78
28	A	566	BCR	C12-C13-C14	-2.26	115.50	118.97
28	C	504	BCR	C11-C10-C9	2.25	130.54	127.29
23	C	501	CLA	CMB-C2B-C1B	-2.26	125.15	128.62
23	D	354	CLA	C2A-C1A-NA	-2.25	108.75	111.24
28	c	5506	BCR	C36-C18-C19	2.25	121.74	118.09
23	C	496	CLA	C2A-C1A-NA	-2.25	108.75	111.24
29	D	359	MGE	C3G-O3G-C1D	-2.25	109.32	113.81
23	b	5517	CLA	C2A-C1A-CHA	2.25	127.73	123.83
23	b	5514	CLA	C2A-C1A-CHA	2.25	127.73	123.83
28	T	5104	BCR	C36-C18-C19	2.25	121.73	118.09
33	T	217	LMT	C3'-C4'-C5'	-2.25	105.80	110.85
28	B	529	BCR	C32-C1-C6	2.25	114.05	110.33
23	D	354	CLA	C4D-CHA-CBD	-2.25	104.07	109.37
28	H	107	BCR	C7-C8-C9	2.25	129.58	126.22
23	B	525	CLA	CMB-C2B-C3B	2.25	128.51	124.97
23	c	5492	CLA	CMD-C2D-C3D	2.25	128.51	124.97
32	A	568	SQD	C15-C14-C13	2.25	126.76	114.61
23	B	525	CLA	O2D-CGD-CBD	2.25	115.91	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5498	CLA	C7-C6-C5	-2.25	106.39	113.01
23	d	5355	CLA	C2D-C1D-ND	2.25	111.11	109.41
25	f	5051	HEM	C2A-C1A-NA	-2.25	106.62	109.73
28	b	5528	BCR	C32-C1-C6	2.25	114.05	110.33
23	c	5502	CLA	CMB-C2B-C3B	2.24	128.50	124.97
23	B	514	CLA	C2A-C1A-CHA	2.24	127.72	123.83
23	B	517	CLA	CMB-C2B-C3B	2.24	128.50	124.97
23	b	5516	CLA	CAA-C2A-C1A	-2.24	106.03	111.62
23	b	5522	CLA	CAA-C2A-C3A	-2.24	107.75	113.04
23	b	5523	CLA	C6-C7-C8	2.24	121.59	115.14
28	d	5357	BCR	C19-C18-C17	-2.24	115.53	118.97
25	f	5051	HEM	O2A-CGA-CBA	2.24	122.12	114.22
28	D	357	BCR	C7-C8-C9	2.24	129.56	126.22
23	a	5560	CLA	C2A-C1A-NA	-2.23	108.77	111.24
28	c	5505	BCR	C36-C18-C19	2.23	121.70	118.09
23	b	5524	CLA	C2A-C3A-C4A	2.23	104.83	101.40
28	c	5505	BCR	C7-C8-C9	2.23	129.55	126.22
23	B	521	CLA	O2A-CGA-CBA	2.23	118.96	111.94
23	c	5495	CLA	CED-O2D-CGD	2.23	121.32	116.02
23	B	521	CLA	C6-C7-C8	2.23	121.56	115.14
23	B	524	CLA	C1-C2-C3	2.23	130.15	126.19
23	C	502	CLA	C1D-C2D-C3D	-2.23	104.96	106.78
28	H	107	BCR	C36-C18-C19	2.23	121.70	118.09
23	b	5519	CLA	CMB-C2B-C3B	2.23	128.48	124.97
28	a	5566	BCR	C35-C13-C12	2.23	121.69	118.09
23	c	5501	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
24	a	5562	PHO	C1D-C2D-C3D	-2.23	104.98	106.89
23	c	5493	CLA	C2A-C1A-CHA	2.23	127.69	123.83
23	c	5494	CLA	C4D-CHA-CBD	-2.23	104.13	109.37
23	c	5497	CLA	C6-C7-C8	2.22	121.55	115.14
23	b	5519	CLA	C2A-C1A-CHA	2.22	127.69	123.83
28	c	5504	BCR	C7-C8-C9	2.22	129.54	126.22
28	t	104	BCR	C40-C30-C29	-2.22	99.73	108.73
23	c	5498	CLA	O2D-CGD-CBD	2.22	115.86	111.33
23	C	503	CLA	C1D-C2D-C3D	-2.22	104.97	106.78
23	b	5521	CLA	C6-C7-C8	2.22	121.53	115.14
23	c	5491	CLA	C16-C15-C13	2.22	121.53	115.14
23	c	5498	CLA	C4D-CHA-CBD	-2.22	104.15	109.37
23	C	493	CLA	CMB-C2B-C1B	-2.22	125.21	128.62
23	c	5500	CLA	CED-O2D-CGD	2.21	121.29	116.02
24	A	561	PHO	O2D-CGD-CBD	2.22	115.84	111.33
23	C	492	CLA	C1-C2-C3	2.21	130.12	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5513	CLA	O2D-CGD-CBD	2.21	115.84	111.33
23	B	516	CLA	C4D-CHA-CBD	-2.21	104.17	109.37
28	C	504	BCR	C30-C25-C24	2.21	121.81	115.69
25	F	51	HEM	CBA-CAA-C2A	-2.21	108.80	112.69
23	B	514	CLA	CED-O2D-CGD	2.21	121.28	116.02
28	b	5527	BCR	C12-C13-C14	-2.21	115.58	118.97
23	A	559	CLA	C1D-C2D-C3D	-2.21	104.98	106.78
28	t	104	BCR	C34-C9-C8	2.21	121.66	118.09
23	b	5521	CLA	O2A-CGA-CBA	2.21	118.88	111.94
30	C	508	DGD	C6E-C5E-C4E	-2.21	107.67	113.00
23	B	514	CLA	CMB-C2B-C1B	-2.21	125.23	128.62
23	c	5503	CLA	CMB-C2B-C3B	2.20	128.44	124.97
28	c	5504	BCR	C11-C10-C9	2.20	130.47	127.29
23	b	5524	CLA	C3A-C2A-C1A	2.20	104.20	101.08
23	a	5558	CLA	C16-C15-C13	2.20	121.48	115.14
23	b	5516	CLA	CMB-C2B-C3B	2.20	128.44	124.97
23	B	514	CLA	C2A-C1A-NA	-2.20	108.81	111.24
23	B	518	CLA	O2A-C1-C2	2.20	113.32	108.55
23	b	5514	CLA	CED-O2D-CGD	2.20	121.25	116.02
24	a	5561	PHO	CMB-C2B-C3B	2.20	128.43	124.97
25	v	5552	HEM	CBA-CAA-C2A	2.20	116.57	112.69
23	c	5493	CLA	CMB-C2B-C3B	2.20	128.44	124.97
23	B	515	CLA	C2A-C1A-CHA	2.20	127.64	123.83
30	h	5208	DGD	C3G-C2G-C1G	-2.20	106.85	111.86
23	B	526	CLA	C7-C6-C5	-2.20	106.53	113.01
23	B	518	CLA	C6-C5-C3	2.20	118.00	112.78
23	b	5517	CLA	C6-C5-C3	2.20	118.01	112.78
24	a	5561	PHO	C4D-CHA-CBD	-2.20	104.19	107.53
28	c	5504	BCR	C28-C27-C26	2.20	117.07	113.74
23	b	5519	CLA	C1-O2A-CGA	2.20	123.13	116.98
23	D	355	CLA	O2D-CGD-CBD	2.20	115.81	111.33
23	d	5355	CLA	C1D-C2D-C3D	-2.19	104.99	106.78
23	c	5497	CLA	C2D-C1D-ND	2.19	111.07	109.41
28	B	527	BCR	C19-C18-C17	-2.19	115.60	118.97
28	a	5566	BCR	C8-C9-C10	-2.19	115.60	118.97
28	h	5107	BCR	C34-C9-C8	2.19	121.64	118.09
23	b	5526	CLA	C2D-C1D-ND	2.19	111.07	109.41
28	b	5529	BCR	C1-C6-C7	2.19	121.77	115.69
23	B	523	CLA	CED-O2D-CGD	2.19	121.24	116.02
23	A	563	CLA	CMB-C2B-C3B	2.19	128.42	124.97
23	b	5524	CLA	CMB-C2B-C3B	2.19	128.43	124.97
23	B	519	CLA	O2A-CGA-CBA	2.19	118.84	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	5528	BCR	C7-C8-C9	2.19	129.50	126.22
23	B	525	CLA	C2A-C1A-CHA	2.19	127.63	123.83
23	C	499	CLA	C4D-CHA-CBD	-2.19	104.21	109.37
29	D	358	MGE	C3G-C2G-C1G	-2.19	106.87	111.86
23	C	495	CLA	C4D-CHA-CBD	-2.19	104.21	109.37
31	A	567	LHG	P-O6-C4	-2.19	106.26	122.03
23	a	5560	CLA	O2A-CGA-CBA	2.19	118.83	111.94
23	B	526	CLA	C2D-C1D-ND	2.19	111.06	109.41
24	A	562	PHO	C6-C7-C8	2.19	121.44	115.14
23	B	520	CLA	C4D-CHA-CBD	-2.19	104.22	109.37
23	A	560	CLA	C11-C12-C13	2.19	121.44	115.14
23	d	5354	CLA	C7-C6-C5	-2.19	106.57	113.01
28	d	5357	BCR	C23-C22-C21	-2.19	115.61	118.97
23	C	491	CLA	C2A-C3A-C4A	2.19	104.76	101.40
23	c	5499	CLA	CAA-C2A-C3A	-2.19	107.87	113.04
28	C	505	BCR	C28-C27-C26	2.19	117.06	113.74
29	D	359	MGE	C6A-C5A-C4A	-2.19	109.55	114.46
23	c	5500	CLA	C6-C5-C3	2.18	117.97	112.78
23	B	523	CLA	C4D-CHA-CBD	-2.18	104.24	109.37
23	A	559	CLA	C6-C7-C8	2.18	121.42	115.14
23	C	497	CLA	CAA-C2A-C3A	-2.18	107.89	113.04
23	C	497	CLA	CMB-C2B-C3B	2.18	128.40	124.97
28	b	5529	BCR	C28-C27-C26	2.18	117.04	113.74
23	B	526	CLA	OBD-CAD-C3D	2.18	131.96	127.91
24	A	561	PHO	C6-C5-C3	2.18	117.96	112.78
25	f	5051	HEM	C4D-ND-C1D	2.17	107.39	105.16
23	C	502	CLA	CMB-C2B-C3B	2.17	128.39	124.97
23	B	523	CLA	C1D-C2D-C3D	-2.18	105.00	106.78
23	c	5501	CLA	C6-C7-C8	2.18	121.40	115.14
24	a	5562	PHO	C16-C15-C13	2.18	121.40	115.14
23	b	5512	CLA	C1D-C2D-C3D	-2.17	105.01	106.78
28	X	130	BCR	C36-C18-C19	2.17	121.61	118.09
32	t	213	SQD	O8-S-O7	2.17	116.48	111.78
28	h	5107	BCR	C30-C25-C24	2.17	121.71	115.69
23	C	501	CLA	OBD-CAD-CBD	-2.17	122.66	125.94
23	d	5354	CLA	CHB-C4A-NA	2.17	127.15	124.58
23	B	513	CLA	C7-C6-C5	-2.17	106.62	113.01
28	D	357	BCR	C40-C30-C25	2.17	113.92	110.33
23	a	5560	CLA	C4D-CHA-CBD	-2.17	104.27	109.37
28	c	5504	BCR	C32-C1-C2	-2.17	99.96	108.73
23	C	498	CLA	C6-C5-C3	2.17	117.93	112.78
25	F	51	HEM	C2A-C1A-NA	-2.17	106.73	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5494	CLA	C2A-C1A-CHA	2.17	127.58	123.83
23	C	497	CLA	C2A-C1A-NA	-2.17	108.85	111.24
26	D	356	PQ9	C24-C23-C22	-2.16	119.23	123.52
28	a	5566	BCR	C7-C8-C9	2.16	129.45	126.22
28	x	5130	BCR	C37-C22-C23	2.16	121.59	118.09
23	b	5526	CLA	CMB-C2B-C1B	-2.16	125.30	128.62
24	A	561	PHO	C4D-CHA-CBD	-2.16	104.25	107.53
24	a	5561	PHO	O2A-CGA-CBA	2.16	118.73	111.94
23	b	5521	CLA	C2A-C1A-NA	-2.16	108.85	111.24
23	B	511	CLA	CED-O2D-CGD	2.16	121.16	116.02
25	V	552	HEM	C4D-ND-C1D	2.16	107.37	105.16
28	T	5104	BCR	C23-C24-C25	2.16	133.69	127.32
28	C	505	BCR	C7-C8-C9	2.16	129.44	126.22
23	B	518	CLA	C2A-C1A-NA	-2.16	108.86	111.24
23	B	516	CLA	C16-C15-C13	2.16	121.35	115.14
28	b	5528	BCR	C30-C25-C24	2.16	121.67	115.69
28	x	5130	BCR	C36-C18-C19	2.16	121.58	118.09
23	B	522	CLA	C2D-C1D-ND	2.15	111.04	109.41
23	C	491	CLA	C16-C15-C13	2.15	121.34	115.14
23	D	354	CLA	CMB-C2B-C1B	-2.15	125.31	128.62
23	A	560	CLA	C4D-CHA-CBD	-2.15	104.30	109.37
23	B	524	CLA	CMB-C2B-C3B	2.15	128.36	124.97
23	a	5558	CLA	C4D-CHA-CBD	-2.15	104.30	109.37
28	H	107	BCR	C30-C25-C24	2.16	121.66	115.69
23	c	5496	CLA	C4D-CHA-CBD	-2.15	104.30	109.37
23	b	5516	CLA	OBD-CAD-C3D	2.15	131.91	127.91
23	C	492	CLA	C4D-CHA-CBD	-2.15	104.31	109.37
28	t	104	BCR	C23-C24-C25	2.15	133.67	127.32
29	i	5201	MGE	O3G-C1D-C2D	2.15	110.91	108.18
23	b	5526	CLA	C1D-C2D-C3D	-2.14	105.03	106.78
23	B	522	CLA	C1D-C2D-C3D	-2.14	105.03	106.78
23	C	500	CLA	CED-O2D-CGD	2.14	121.12	116.02
23	A	559	CLA	C4D-CHA-CBD	-2.14	104.32	109.37
24	A	562	PHO	C2A-C1A-NA	-2.14	108.63	111.93
23	B	524	CLA	C1D-C2D-C3D	-2.14	105.03	106.78
23	A	563	CLA	OBD-CAD-C3D	2.14	131.90	127.91
24	A	561	PHO	CAA-C2A-C3A	-2.14	107.97	113.04
30	C	508	DGD	O3G-C3G-C2G	2.14	116.08	110.99
23	B	514	CLA	C1D-C2D-C3D	-2.14	105.03	106.78
24	a	5561	PHO	C4B-C3B-C2B	-2.14	106.05	107.60
23	b	5518	CLA	OBD-CAD-C3D	2.14	131.89	127.91
23	C	502	CLA	C4D-CHA-CBD	-2.14	104.33	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5498	CLA	C6-C5-C3	2.14	117.87	112.78
23	C	492	CLA	OBD-CAD-C3D	2.14	131.89	127.91
23	C	498	CLA	CMB-C2B-C3B	2.14	128.33	124.97
28	A	566	BCR	C1-C6-C7	2.14	121.61	115.69
23	b	5525	CLA	C2A-C1A-CHA	2.13	127.53	123.83
23	b	5511	CLA	CED-O2D-CGD	2.13	121.09	116.02
23	c	5491	CLA	C2A-C1A-CHA	2.13	127.53	123.83
32	A	5212	SQD	O47-C45-C44	2.13	116.23	108.40
23	C	500	CLA	CMA-C3A-C2A	-2.13	104.98	114.14
28	T	5104	BCR	C8-C9-C10	-2.13	115.69	118.97
28	a	5566	BCR	C34-C9-C8	2.13	121.54	118.09
23	b	5515	CLA	C12-C11-C10	-2.13	102.08	113.02
23	c	5501	CLA	C1-C2-C3	2.13	129.97	126.19
23	c	5495	CLA	C4D-CHA-CBD	-2.13	104.36	109.37
29	b	5530	MGE	C3G-C2G-C1G	-2.13	107.01	111.86
32	d	5358	SQD	C6-C5-C4	-2.13	107.37	111.86
23	c	5493	CLA	C12-C11-C10	-2.13	102.09	113.02
23	C	493	CLA	C1D-C2D-C3D	-2.13	105.04	106.78
23	c	5496	CLA	CBA-CAA-C2A	2.13	120.33	114.01
23	c	5496	CLA	CMB-C2B-C1B	-2.13	125.35	128.62
23	C	502	CLA	C2A-C1A-NA	-2.13	108.89	111.24
30	C	509	DGD	O5D-C6D-C5D	2.13	112.62	108.97
23	d	5354	CLA	CMB-C2B-C1B	-2.13	125.35	128.62
23	C	498	CLA	C4D-CHA-CBD	-2.13	104.36	109.37
23	b	5518	CLA	CBA-CAA-C2A	2.13	120.32	114.01
28	x	5130	BCR	C32-C1-C2	-2.12	100.12	108.73
23	b	5525	CLA	O2D-CGD-CBD	2.12	115.66	111.33
25	v	5552	HEM	C4A-C3A-C2A	2.12	108.47	107.00
23	b	5515	CLA	C1-C2-C3	2.12	129.96	126.19
23	C	497	CLA	C6-C7-C8	2.12	121.26	115.14
23	B	522	CLA	CMB-C2B-C1B	-2.12	125.36	128.62
26	A	564	PQ9	C6-C5-C4	2.12	119.44	114.80
23	C	493	CLA	CMB-C2B-C3B	2.12	128.31	124.97
23	D	354	CLA	C7-C6-C5	-2.12	106.76	113.01
23	c	5500	CLA	CBA-CAA-C2A	2.12	120.31	114.01
23	b	5519	CLA	C2A-C1A-NA	-2.12	108.90	111.24
28	C	504	BCR	C16-C17-C18	2.12	130.35	127.29
23	B	515	CLA	C4D-CHA-CBD	-2.12	104.38	109.37
23	b	5525	CLA	C2A-C1A-NA	-2.12	108.90	111.24
23	c	5501	CLA	C2A-C1A-CHA	2.12	127.50	123.83
23	c	5500	CLA	C4D-CHA-CBD	-2.12	104.39	109.37
23	c	5502	CLA	CBA-CAA-C2A	2.12	120.30	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	563	CLA	C2D-C1D-ND	2.12	111.01	109.41
23	B	521	CLA	O2D-CGD-CBD	2.12	115.64	111.33
23	B	520	CLA	C2A-C1A-CHA	2.12	127.50	123.83
23	c	5492	CLA	C7-C6-C5	-2.11	106.78	113.01
32	L	5213	SQD	C15-C14-C13	2.11	126.05	114.61
28	H	107	BCR	C37-C22-C23	2.11	121.51	118.09
23	c	5495	CLA	OBD-CAD-C3D	2.11	131.84	127.91
23	b	5526	CLA	CMB-C2B-C3B	2.11	128.30	124.97
24	A	562	PHO	C2A-C3A-C4A	2.11	105.87	101.11
23	C	500	CLA	C4D-CHA-CBD	-2.11	104.40	109.37
25	F	51	HEM	C3A-C4A-NA	-2.11	107.82	109.41
24	A	561	PHO	C2A-C3A-C4A	2.11	105.87	101.11
28	t	104	BCR	C16-C17-C18	2.11	130.34	127.29
23	a	5559	CLA	C6-C7-C8	2.11	121.21	115.14
23	C	496	CLA	C2A-C1A-CHA	2.11	127.48	123.83
23	b	5523	CLA	CAA-C2A-C3A	-2.11	108.05	113.04
23	b	5514	CLA	C7-C6-C5	-2.11	106.80	113.01
28	A	566	BCR	C30-C25-C24	2.11	121.53	115.69
23	b	5526	CLA	C4D-CHA-CBD	-2.11	104.41	109.37
23	D	355	CLA	CAA-C2A-C3A	-2.11	108.06	113.04
30	C	509	DGD	C3G-O3G-C1D	-2.11	109.61	113.81
23	B	517	CLA	C6-C7-C8	2.11	121.20	115.14
23	b	5521	CLA	C4D-CHA-CBD	-2.10	104.41	109.37
23	B	513	CLA	CMB-C2B-C3B	2.10	128.28	124.97
33	M	5216	LMT	C1-O1'-C1'	-2.10	110.17	113.96
23	b	5515	CLA	CBA-CAA-C2A	2.10	120.25	114.01
28	c	5505	BCR	C19-C18-C17	-2.10	115.74	118.97
28	c	5505	BCR	C28-C27-C26	2.10	116.93	113.74
23	A	560	CLA	O2A-CGA-CBA	2.10	118.55	111.94
30	C	508	DGD	O3G-C1D-C2D	2.10	110.86	108.18
24	A	561	PHO	C3D-C4D-ND	2.10	110.47	106.97
29	d	5360	MGE	C6A-C5A-C4A	-2.10	109.74	114.46
23	B	518	CLA	CBA-CAA-C2A	2.10	120.24	114.01
23	B	517	CLA	CBA-CAA-C2A	2.10	120.24	114.01
23	C	492	CLA	CMB-C2B-C1B	-2.10	125.39	128.62
23	b	5520	CLA	C4D-CHA-CBD	-2.10	104.44	109.37
23	b	5521	CLA	C1-C2-C3	2.10	129.91	126.19
23	c	5495	CLA	C6-C7-C8	2.09	121.17	115.14
24	A	562	PHO	O2D-CGD-CBD	2.09	115.60	111.33
23	b	5514	CLA	C6-C7-C8	2.10	121.17	115.14
28	b	5529	BCR	C15-C14-C13	2.10	130.31	127.29
23	C	495	CLA	C16-C15-C13	2.09	121.17	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	T	217	LMT	C1B-O1B-C4'	-2.09	112.65	117.99
24	A	561	PHO	C3A-C4A-NA	-2.09	109.98	113.57
23	B	521	CLA	C1-C2-C3	2.09	129.91	126.19
23	b	5512	CLA	C6-C5-C3	2.09	117.75	112.78
23	c	5499	CLA	CAA-C2A-C1A	2.09	116.84	111.62
30	c	5508	DGD	O2D-C2D-C1D	2.09	114.60	110.04
23	c	5503	CLA	C4D-CHA-CBD	-2.09	104.45	109.37
28	T	5104	BCR	C34-C9-C8	2.09	121.47	118.09
23	C	501	CLA	C6-C7-C8	2.09	121.16	115.14
23	B	523	CLA	CAA-C2A-C3A	-2.09	108.11	113.04
29	D	360	MGE	O1G-C1A-C2A	2.09	118.50	111.94
23	b	5513	CLA	C4D-CHA-CBD	-2.08	104.46	109.37
23	A	563	CLA	C6-C5-C3	2.09	117.74	112.78
28	B	529	BCR	C1-C6-C7	2.08	121.46	115.69
28	T	5104	BCR	C19-C18-C17	-2.08	115.77	118.97
23	b	5521	CLA	OBD-CAD-C3D	2.08	131.79	127.91
23	B	518	CLA	CMB-C2B-C3B	2.08	128.25	124.97
28	x	5130	BCR	C24-C23-C22	2.08	129.33	126.22
23	d	5354	CLA	C2A-C1A-CHA	2.08	127.44	123.83
23	B	526	CLA	C4D-CHA-CBD	-2.08	104.47	109.37
28	B	529	BCR	C11-C10-C9	2.08	130.29	127.29
23	C	499	CLA	OBD-CAD-C3D	2.08	131.78	127.91
23	B	513	CLA	C1D-C2D-C3D	-2.08	105.08	106.78
23	b	5517	CLA	C6-C7-C8	2.08	121.12	115.14
28	c	5505	BCR	C34-C9-C8	2.08	121.45	118.09
29	D	359	MGE	O1G-C1G-C2G	-2.08	103.38	108.83
32	d	5358	SQD	C34-C33-C32	2.08	125.85	114.61
23	a	5558	CLA	C1D-C2D-C3D	-2.08	105.08	106.78
23	b	5516	CLA	C4D-CHA-CBD	-2.08	104.48	109.37
28	h	5107	BCR	C36-C18-C19	2.08	121.45	118.09
23	a	5560	CLA	C6-C5-C3	2.08	117.72	112.78
24	a	5561	PHO	C3D-C4D-ND	2.08	110.43	106.97
30	c	5508	DGD	O3G-C1D-C2D	2.07	110.82	108.18
23	B	523	CLA	C6-C7-C8	2.07	121.11	115.14
23	B	519	CLA	C6-C5-C3	2.07	117.71	112.78
23	d	5355	CLA	CAA-C2A-C3A	-2.07	108.14	113.04
32	L	5213	SQD	O8-S-O7	2.07	116.26	111.78
25	f	5051	HEM	C3A-C4A-NA	-2.07	107.85	109.41
23	b	5511	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
23	D	355	CLA	CMB-C2B-C3B	2.07	128.24	124.97
23	b	5513	CLA	C16-C15-C13	2.07	121.11	115.14
23	b	5514	CLA	C2A-C1A-NA	-2.07	108.95	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	504	BCR	C28-C27-C26	2.07	116.88	113.74
23	C	501	CLA	CMB-C2B-C3B	2.07	128.23	124.97
28	b	5527	BCR	C19-C18-C17	-2.07	115.79	118.97
28	b	5528	BCR	C35-C13-C12	2.07	121.44	118.09
31	a	5567	LHG	P-O6-C4	-2.07	107.14	122.03
23	A	563	CLA	CMA-C3A-C2A	-2.07	105.25	114.14
23	b	5524	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
23	c	5491	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
23	B	526	CLA	C1-O2A-CGA	2.06	122.76	116.98
28	a	5566	BCR	C19-C18-C17	-2.07	115.80	118.97
32	a	212	SQD	O47-C45-C44	2.07	115.99	108.40
28	b	5529	BCR	C30-C25-C24	2.07	121.41	115.69
25	v	5552	HEM	CMA-C3A-C4A	-2.06	125.45	128.62
28	B	529	BCR	C36-C18-C19	2.06	121.43	118.09
23	C	496	CLA	CMB-C2B-C3B	2.06	128.22	124.97
23	B	515	CLA	CMB-C2B-C3B	2.06	128.22	124.97
23	c	5499	CLA	C4D-CHA-CBD	-2.06	104.52	109.37
23	c	5495	CLA	C16-C15-C13	2.06	121.07	115.14
24	A	562	PHO	C16-C15-C13	2.06	121.07	115.14
29	d	5360	MGE	C3G-C2G-C1G	-2.06	107.17	111.86
32	d	5358	SQD	C17-C16-C15	2.06	125.75	114.61
28	b	5528	BCR	C32-C1-C2	-2.06	100.39	108.73
23	B	515	CLA	C12-C11-C10	-2.06	102.46	113.02
28	C	506	BCR	C32-C1-C6	2.06	113.74	110.33
24	a	5562	PHO	C2A-C3A-C4A	2.06	105.75	101.11
23	C	500	CLA	C1D-C2D-C3D	-2.06	105.10	106.78
23	B	524	CLA	C4D-CHA-CBD	-2.06	104.53	109.37
32	t	213	SQD	C15-C14-C13	2.06	125.74	114.61
28	d	5357	BCR	C34-C9-C8	2.05	121.41	118.09
23	c	5496	CLA	C2A-C1A-NA	-2.05	108.97	111.24
23	b	5522	CLA	C1D-C2D-C3D	-2.05	105.10	106.78
23	C	499	CLA	CAA-C2A-C1A	2.05	116.75	111.62
25	V	552	HEM	CBA-CAA-C2A	2.05	116.31	112.69
28	B	528	BCR	C30-C25-C24	2.05	121.38	115.69
23	c	5493	CLA	CBA-CAA-C2A	2.05	120.10	114.01
28	B	528	BCR	C40-C30-C25	2.05	113.73	110.33
23	a	5560	CLA	C11-C12-C13	2.05	121.04	115.14
23	a	5559	CLA	C4D-CHA-CBD	-2.05	104.55	109.37
23	C	502	CLA	CBA-CAA-C2A	2.05	120.09	114.01
23	B	512	CLA	C2A-C1A-CHA	2.05	127.38	123.83
23	c	5492	CLA	C2A-C1A-CHA	2.05	127.38	123.83
23	b	5515	CLA	C4D-CHA-CBD	-2.05	104.55	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	5107	BCR	C8-C9-C10	-2.05	115.82	118.97
23	B	517	CLA	C11-C12-C13	2.05	121.04	115.14
29	d	5360	MGE	O1G-C1A-C2A	2.04	118.37	111.94
23	B	516	CLA	CAA-C2A-C3A	-2.04	108.21	113.04
28	x	5130	BCR	C3-C4-C5	2.04	116.84	113.74
23	b	5513	CLA	C2A-C1A-NA	-2.04	108.98	111.24
23	b	5513	CLA	C6-C7-C8	2.04	121.02	115.14
23	b	5523	CLA	C4B-NB-C1B	2.04	109.45	106.76
23	B	521	CLA	CMB-C2B-C1B	-2.04	125.48	128.62
25	f	5051	HEM	C1B-NB-C4B	2.04	107.25	105.16
23	b	5515	CLA	CMA-C3A-C2A	-2.04	105.36	114.14
23	b	5515	CLA	CMB-C2B-C1B	-2.04	125.48	128.62
23	A	558	CLA	CMA-C3A-C2A	-2.04	105.36	114.14
23	d	5354	CLA	C3A-C2A-C1A	2.04	103.97	101.08
23	D	355	CLA	CBA-CAA-C2A	2.04	120.07	114.01
26	a	5564	PQ9	C6-C5-C4	2.04	119.26	114.80
26	d	5356	PQ9	C24-C23-C22	-2.04	119.48	123.52
23	b	5523	CLA	CHB-C4A-NA	2.04	126.99	124.58
23	b	5515	CLA	C2A-C1A-CHA	2.04	127.36	123.83
23	c	5501	CLA	CAA-C2A-C3A	-2.04	108.22	113.04
24	a	5562	PHO	C1-C2-C3	2.04	129.81	126.19
23	B	522	CLA	OBD-CAD-C3D	2.04	131.70	127.91
28	c	5504	BCR	C34-C9-C8	2.03	121.38	118.09
30	C	507	DGD	O6D-C1D-C2D	2.03	114.48	110.31
23	C	492	CLA	CMD-C2D-C3D	2.03	128.17	124.97
23	b	5514	CLA	C16-C15-C13	2.03	120.99	115.14
23	B	513	CLA	C4D-CHA-CBD	-2.03	104.58	109.37
23	C	497	CLA	C2A-C1A-CHA	2.03	127.35	123.83
28	x	5130	BCR	C19-C18-C17	-2.03	115.85	118.97
28	d	5357	BCR	C32-C1-C6	2.03	113.69	110.33
23	C	491	CLA	C6-C5-C3	2.03	117.61	112.78
23	b	5514	CLA	OBD-CAD-C3D	2.03	131.69	127.91
23	b	5516	CLA	C2A-C1A-NA	-2.03	109.00	111.24
30	c	5508	DGD	O1G-C1A-C2A	2.03	118.33	111.94
32	A	568	SQD	C34-C33-C32	2.03	125.59	114.61
23	C	499	CLA	C2A-C1A-NA	-2.03	109.00	111.24
23	a	5559	CLA	CMB-C2B-C3B	2.03	128.16	124.97
23	C	500	CLA	C6-C5-C3	2.03	117.60	112.78
23	C	491	CLA	CBA-CAA-C2A	2.03	120.03	114.01
26	d	5356	PQ9	C21-C22-C23	-2.02	123.43	127.80
23	b	5513	CLA	C2A-C1A-CHA	2.03	127.34	123.83
23	b	5523	CLA	C2A-C1A-NA	-2.02	109.00	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5497	CLA	C2A-C1A-NA	-2.02	109.00	111.24
23	b	5512	CLA	C4D-CHA-CBD	-2.02	104.61	109.37
30	c	5508	DGD	O3G-C3G-C2G	2.02	115.80	110.99
28	D	357	BCR	C34-C9-C8	2.02	121.36	118.09
23	A	559	CLA	CMB-C2B-C3B	2.02	128.15	124.97
25	F	51	HEM	O1A-CGA-CBA	-2.02	116.08	123.03
23	C	500	CLA	C2A-C1A-NA	-2.02	109.01	111.24
28	h	5107	BCR	C11-C12-C13	2.02	132.15	126.38
23	B	524	CLA	C2A-C1A-CHA	2.02	127.33	123.83
32	t	213	SQD	O6-C44-C45	-2.02	106.19	110.99
28	T	5104	BCR	C30-C25-C24	2.02	121.28	115.69
25	f	5051	HEM	C4A-C3A-C2A	2.02	108.40	107.00
23	c	5503	CLA	C1-C2-C3	2.01	129.77	126.19
23	D	354	CLA	O2D-CGD-CBD	2.01	115.44	111.33
23	B	516	CLA	CAA-C2A-C1A	-2.02	106.60	111.62
23	B	515	CLA	CBA-CAA-C2A	2.01	119.99	114.01
23	C	496	CLA	C4D-CHA-CBD	-2.01	104.63	109.37
23	C	491	CLA	O2D-CGD-CBD	2.01	115.43	111.33
23	C	493	CLA	CBA-CAA-C2A	2.01	119.99	114.01
28	D	357	BCR	C36-C18-C19	2.01	121.35	118.09
28	H	107	BCR	C34-C9-C8	2.01	121.35	118.09
23	A	559	CLA	CAA-CBA-CGA	2.01	119.75	113.27
24	a	5562	PHO	C6-C7-C8	2.01	120.93	115.14
23	c	5500	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
23	c	5492	CLA	C1-C2-C3	2.01	129.75	126.19
28	A	566	BCR	C34-C9-C8	2.01	121.34	118.09
23	B	521	CLA	CHB-C4A-NA	2.01	126.95	124.58
28	B	528	BCR	C7-C8-C9	2.00	129.21	126.22
28	t	104	BCR	C30-C25-C24	2.00	121.24	115.69
23	C	493	CLA	O2D-CGD-CBD	2.00	115.41	111.33
28	C	505	BCR	C1-C6-C7	2.00	121.24	115.69
23	b	5513	CLA	CMA-C3A-C2A	-2.00	105.53	114.14
23	c	5498	CLA	CMB-C2B-C3B	2.00	128.12	124.97
25	V	552	HEM	C3A-C4A-NA	-2.00	107.90	109.41
23	c	5501	CLA	C12-C11-C10	-2.00	102.75	113.02

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	562	PHO	C2A
24	A	562	PHO	C13
24	A	562	PHO	C8

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Mol	Chain	Res	Type	Atom
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D
30	c	5507	DGD	C5E
24	a	5561	PHO	C2A
24	a	5561	PHO	C13
24	a	5561	PHO	C8
30	h	5208	DGD	C2D
30	h	5208	DGD	C5D
30	h	5208	DGD	C5E
30	C	508	DGD	C2D
30	C	508	DGD	C5D
30	C	508	DGD	C5E
30	C	507	DGD	C2D
30	C	507	DGD	C5D
30	C	507	DGD	C5E
30	c	5509	DGD	C2D
30	c	5509	DGD	C5D
30	c	5509	DGD	C5E
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
30	c	5508	DGD	C2D
30	c	5508	DGD	C5D
30	c	5508	DGD	C5E
30	C	509	DGD	C2D
30	C	509	DGD	C5D
30	C	509	DGD	C5E
24	A	561	PHO	C2A
24	A	561	PHO	C13
24	A	561	PHO	C8
24	a	5562	PHO	C2A
24	a	5562	PHO	C13
24	a	5562	PHO	C8

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	D	354	CLA	C1-C2-C3-C4
23	d	5354	CLA	C1-C2-C3-C4
23	C	503	CLA	C1-C2-C3-C4
23	c	5503	CLA	C1-C2-C3-C4

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	335/344 (97%)	-0.39	0	100	100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.36	0	100	100	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.36	0	100	100	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.36	0	100	100	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.34	0	100	100	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.24	1 (0%)	93	54	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.37	0	100	100	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.38	0	100	100	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.15	1 (1%)	75	20	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.06	1 (1%)	75	20	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.20	0	100	100	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	0	100	100	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.28	0	100	100	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.17	0	100	100	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.29	0	100	100	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.23	0	100	100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.40	0	100	100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.30	0	100	100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.36	0	100	100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.29	0	100	100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.11	0	100	100	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.21	1 (2%)	52	10	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.35	0	100	100	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.29	0	100	100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.29	0 100 100	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.24	1 (0%) 90 41	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.26	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.45	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.25	1 (1%) 79 22	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.34	0 100 100	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.36	0 100 100	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.20	0 100 100	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.19	0 100 100	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.16	0 100 100	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.31	6 (0%) 93 63	35, 66, 85, 101	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	l	5001	MET	3.9
5	E	84	LYS	3.2
13	o	5049	ASP	2.7
3	c	5029	GLU	2.5
15	U	37	GLU	2.3
5	e	5003	GLY	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
22	UNK	c	5486	8/-	0.39	29.92	63,64,65,66	0
22	UNK	C	486	8/-	0.27	28.09	55,56,59,60	0
22	UNK	c	5484	5/-	0.76	12.72	69,69,70,72	0
22	UNK	c	5489	7/-	0.38	9.65	73,73,74,74	0
22	UNK	C	478	11/-	0.35	9.32	58,65,66,66	0
33	LMT	A	569	35/35	0.46	9.04	80,89,92,93	0
22	UNK	c	5485	5/-	0.44	8.96	68,69,69,70	0
28	BCR	H	107	40/40	0.34	7.10	77,83,88,89	0
33	LMT	a	5568	35/35	0.47	6.95	79,92,94,96	0
19	CA	K	56	1/1	0.14	6.16	119,119,119,119	0
33	LMT	t	5217	35/35	0.42	5.68	76,95,104,105	0
22	UNK	c	5479	11/-	0.33	5.47	76,77,77,77	0
22	UNK	c	5478	11/-	0.47	5.41	76,79,81,81	0
22	UNK	C	489	7/-	0.34	5.30	75,76,77,78	0
33	LMT	T	217	35/35	0.35	5.19	83,93,96,97	0
28	BCR	x	5130	40/40	0.48	5.07	77,81,85,86	0
22	UNK	c	5490	4/-	0.38	4.94	91,92,92,92	0
28	BCR	h	5107	40/40	0.35	4.89	74,79,82,83	0
26	PQ9	A	564	30/45	0.36	4.69	54,57,63,64	30
22	UNK	c	5474	15/-	0.26	4.43	39,50,56,56	0
23	CLA	B	511	41/65	0.34	4.20	88,90,92,98	0
22	UNK	C	483	13/-	0.29	4.12	61,68,78,78	0
23	CLA	b	5511	41/65	0.40	4.11	88,92,95,96	0
28	BCR	C	505	40/40	0.41	3.91	75,81,91,92	0
28	BCR	X	130	40/40	0.35	3.45	68,71,80,81	0
28	BCR	b	5529	40/40	0.41	3.37	69,72,74,74	0
22	UNK	c	5488	5/-	0.27	3.11	59,59,59,60	0
28	BCR	d	5357	40/40	0.37	3.09	61,72,86,88	0
28	BCR	D	357	40/40	0.28	3.05	61,66,78,80	0
28	BCR	c	5505	40/40	0.39	3.01	84,87,91,92	0
22	UNK	C	481	13/-	0.36	2.94	61,64,68,69	0
23	CLA	a	5560	65/65	0.22	2.76	62,68,100,101	0
26	PQ9	a	5564	30/45	0.28	2.69	51,55,62,62	30
29	MGE	d	5359	47/48	0.31	2.66	72,81,96,98	0
22	UNK	c	5475	12/-	0.42	2.66	74,78,84,84	0
22	UNK	C	474	15/-	0.22	2.65	26,37,40,40	0
22	UNK	c	5477	7/-	0.29	2.60	67,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	a	5563	55/65	0.34	2.57	59,65,102,103	0
28	BCR	c	5504	40/40	0.30	2.39	73,80,88,89	0
29	MGE	D	359	41/48	0.26	2.28	60,67,76,79	0
22	UNK	C	479	11/-	0.30	2.26	58,64,67,67	0
23	CLA	b	5516	65/65	0.28	2.20	62,66,84,86	0
23	CLA	c	5503	50/65	0.28	2.14	88,91,92,93	0
21	BCT	D	353	4/4	0.24	2.13	72,73,73,74	0
23	CLA	C	495	65/65	0.24	2.03	58,68,74,76	0
28	BCR	A	566	40/40	0.28	2.02	50,57,64,66	0
23	CLA	B	519	65/65	0.25	1.99	73,82,85,87	0
22	UNK	C	485	5/-	0.29	1.92	57,59,61,61	0
23	CLA	c	5501	65/65	0.26	1.91	82,91,94,95	0
23	CLA	b	5515	65/65	0.22	1.88	46,51,74,76	0
22	UNK	C	475	12/-	0.38	1.88	68,69,72,73	0
29	MGE	D	358	47/48	0.25	1.86	65,72,79,81	0
28	BCR	B	528	40/40	0.22	1.86	54,68,74,75	0
23	CLA	B	526	65/65	0.29	1.83	71,82,97,98	0
23	CLA	A	563	55/65	0.25	1.76	43,49,75,78	0
26	PQ9	D	356	30/45	0.24	1.76	49,67,80,83	0
32	SQD	A	568	54/54	0.33	1.75	76,82,90,90	0
30	DGD	C	507	53/66	0.26	1.73	55,66,86,88	0
33	LMT	m	216	35/35	0.29	1.69	62,87,89,91	0
23	CLA	c	5497	65/65	0.26	1.67	66,82,84,87	0
28	BCR	C	504	40/40	0.21	1.65	57,64,70,70	0
23	CLA	c	5498	65/65	0.27	1.62	81,90,93,93	0
33	LMT	M	5216	35/35	0.28	1.61	58,83,90,90	0
29	MGE	b	5530	48/48	0.18	1.54	59,64,71,73	0
22	UNK	C	482	13/-	0.23	1.53	64,66,67,67	0
22	UNK	c	5487	7/-	0.28	1.49	57,57,58,58	0
22	UNK	c	5476	9/-	0.30	1.49	58,60,62,62	0
24	PHO	a	5562	64/64	0.22	1.46	70,75,81,82	0
28	BCR	T	5104	40/40	0.23	1.42	67,71,78,79	0
23	CLA	B	512	65/65	0.25	1.41	68,75,78,79	0
23	CLA	B	515	65/65	0.21	1.41	55,66,71,72	0
28	BCR	t	104	40/40	0.21	1.40	65,72,84,85	0
23	CLA	D	355	50/65	0.22	1.38	63,65,68,70	0
28	BCR	b	5527	40/40	0.21	1.35	58,63,72,72	0
28	BCR	B	527	40/40	0.19	1.34	58,65,68,69	0
28	BCR	B	529	40/40	0.27	1.34	62,69,80,80	0
25	HEM	F	51	43/43	0.26	1.31	78,84,92,95	0
29	MGE	l	5210	48/48	0.22	1.29	59,69,78,81	0
28	BCR	c	5506	40/40	0.32	1.29	75,81,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CLA	B	516	65/65	0.27	1.28	61,76,92,97	0
23	CLA	b	5512	65/65	0.24	1.28	68,72,75,76	0
29	MGE	d	5361	48/48	0.20	1.28	61,68,78,83	0
23	CLA	C	497	65/65	0.27	1.27	74,78,80,82	0
23	CLA	b	5513	65/65	0.21	1.25	54,61,84,90	0
31	LHG	A	567	39/49	0.22	1.25	57,73,79,81	0
23	CLA	C	501	65/65	0.24	1.21	70,78,83,85	0
23	CLA	c	5495	65/65	0.23	1.20	74,81,86,88	0
22	UNK	C	487	7/-	0.28	1.18	49,52,52,53	0
22	UNK	C	476	9/-	0.31	1.16	61,62,63,64	0
30	DGD	c	5509	57/66	0.28	1.16	67,72,77,78	0
22	UNK	C	477	7/-	0.17	1.14	47,49,51,51	0
23	CLA	d	5354	65/65	0.18	1.12	39,47,64,65	0
23	CLA	b	5519	65/65	0.22	1.11	70,75,80,81	0
28	BCR	a	5566	40/40	0.25	1.10	59,75,78,79	0
30	DGD	C	508	47/66	0.20	1.09	61,71,80,83	0
29	MGE	i	5201	48/48	0.28	1.08	67,83,88,90	0
23	CLA	b	5520	65/65	0.23	1.08	63,72,74,76	0
25	HEM	f	5051	43/43	0.28	1.06	80,84,97,101	0
30	DGD	H	208	54/66	0.21	1.04	61,69,75,76	0
23	CLA	B	522	65/65	0.23	1.04	54,65,75,77	0
32	SQD	t	213	47/54	0.31	1.03	61,95,116,117	0
30	DGD	c	5507	53/66	0.23	1.01	66,74,90,91	0
31	LHG	a	5567	39/49	0.28	1.00	65,68,74,80	0
32	SQD	L	5213	47/54	0.31	1.00	52,85,106,108	0
29	MGE	D	360	48/48	0.20	0.99	52,60,63,68	0
29	MGE	d	5360	41/48	0.22	0.94	68,72,78,80	0
23	CLA	B	520	65/65	0.24	0.93	62,67,76,79	0
23	CLA	c	5496	65/65	0.25	0.93	79,83,95,97	0
22	UNK	c	5483	13/-	0.29	0.93	71,75,80,82	0
32	SQD	a	212	26/54	0.29	0.91	82,94,101,103	0
23	CLA	A	560	65/65	0.20	0.90	49,57,86,88	0
25	HEM	V	552	43/43	0.19	0.88	37,54,58,59	0
22	UNK	C	484	5/-	0.30	0.83	47,51,52,53	0
29	MGE	L	210	48/48	0.22	0.83	59,68,73,75	0
22	UNK	c	5482	13/-	0.22	0.82	60,61,71,72	0
23	CLA	C	493	65/65	0.21	0.81	67,71,77,79	0
24	PHO	A	561	64/64	0.18	0.78	32,52,55,59	0
26	PQ9	d	5356	30/45	0.18	0.77	51,57,66,66	0
24	PHO	a	5561	64/64	0.18	0.75	51,55,66,68	0
23	CLA	C	503	50/65	0.27	0.75	83,86,88,94	0
23	CLA	C	498	65/65	0.21	0.70	64,74,98,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	UNK	c	5481	13/-	0.22	0.65	60,62,66,66	0
23	CLA	c	5500	65/65	0.21	0.65	64,69,82,83	0
30	DGD	h	5208	54/66	0.20	0.65	57,68,73,75	0
28	BCR	b	5528	40/40	0.18	0.62	61,64,72,73	0
23	CLA	C	496	65/65	0.24	0.62	71,78,88,89	0
23	CLA	d	5355	50/65	0.23	0.59	74,77,80,81	0
25	HEM	v	5552	43/43	0.19	0.58	65,67,70,70	0
32	SQD	A	5212	26/54	0.25	0.56	75,100,107,107	0
23	CLA	c	5502	51/65	0.26	0.53	93,96,97,98	0
23	CLA	B	525	65/65	0.21	0.51	67,84,91,92	0
32	SQD	d	5358	54/54	0.29	0.49	74,85,106,107	0
23	CLA	C	502	51/65	0.22	0.49	74,80,83,84	0
23	CLA	b	5526	65/65	0.30	0.46	66,71,92,95	0
23	CLA	b	5514	65/65	0.18	0.41	41,51,74,75	0
30	DGD	C	509	57/66	0.20	0.40	52,60,69,70	0
23	CLA	B	514	65/65	0.19	0.39	59,64,82,83	0
29	MGE	B	530	48/48	0.18	0.37	55,64,70,72	0
28	BCR	C	506	40/40	0.24	0.37	68,72,79,80	0
23	CLA	b	5522	65/65	0.19	0.37	60,66,75,76	0
23	CLA	c	5499	47/65	0.22	0.33	60,69,76,78	0
23	CLA	B	513	65/65	0.18	0.30	56,61,67,67	0
24	PHO	A	562	64/64	0.16	0.27	47,53,63,66	0
29	MGE	I	201	48/48	0.20	0.19	73,81,89,90	0
23	CLA	b	5517	65/65	0.16	0.15	54,58,66,71	0
23	CLA	b	5525	65/65	0.20	0.09	71,77,80,82	0
23	CLA	C	491	65/65	0.18	0.04	63,70,77,79	0
23	CLA	c	5493	65/65	0.22	0.02	67,81,86,86	0
23	CLA	B	521	65/65	0.18	0.02	58,63,66,68	0
23	CLA	C	499	47/65	0.17	0.01	57,60,66,69	0
27	OEC	a	5565	5/9	0.15	-0.03	63,64,71,87	0
30	DGD	c	5508	47/66	0.17	-0.06	66,76,82,84	0
23	CLA	a	5559	65/65	0.15	-0.11	42,49,60,60	0
23	CLA	A	559	65/65	0.15	-0.11	39,43,49,52	0
23	CLA	C	492	60/65	0.17	-0.14	53,58,76,77	0
23	CLA	B	524	56/65	0.18	-0.19	67,72,77,80	0
23	CLA	D	354	65/65	0.15	-0.22	35,43,63,66	0
23	CLA	B	518	65/65	0.18	-0.23	53,64,79,79	0
27	OEC	A	565	5/9	0.14	-0.24	62,63,65,66	0
23	CLA	b	5523	65/65	0.15	-0.25	45,52,74,75	0
23	CLA	b	5524	56/65	0.18	-0.26	63,68,89,91	0
23	CLA	B	523	65/65	0.16	-0.28	47,56,73,74	0
23	CLA	b	5518	65/65	0.17	-0.30	60,64,69,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	5491	65/65	0.17	-0.35	70,78,81,86	0
23	CLA	a	5558	65/65	0.15	-0.36	41,50,55,61	0
23	CLA	c	5494	46/65	0.17	-0.39	72,77,86,88	0
23	CLA	C	494	46/65	0.14	-0.40	59,66,68,72	0
23	CLA	c	5492	60/65	0.16	-0.40	57,61,83,84	0
23	CLA	C	500	65/65	0.15	-0.42	59,63,73,74	0
22	UNK	C	488	5/-	0.14	-0.46	41,45,47,47	0
23	CLA	B	517	65/65	0.14	-0.56	37,44,56,57	0
23	CLA	b	5521	65/65	0.16	-0.57	48,57,63,64	0
23	CLA	A	558	65/65	0.13	-0.69	41,46,50,51	0
22	UNK	C	490	4/-	0.11	-1.54	67,67,68,68	0
19	CA	k	5056	1/1	0.14	-1.62	119,119,119,119	0
21	BCT	d	5353	4/4	0.12	-2.37	75,75,76,77	0
20	FE2	a	5557	1/1	0.09	-3.13	75,75,75,75	0
20	FE2	A	557	1/1	0.05	-3.80	60,60,60,60	0
22	UNK	c	5480	7/-	0.26	-	65,66,66,67	0
22	UNK	C	480	7/-	0.22	-	35,36,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.