



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 05:04 PM EST

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 : unknown  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

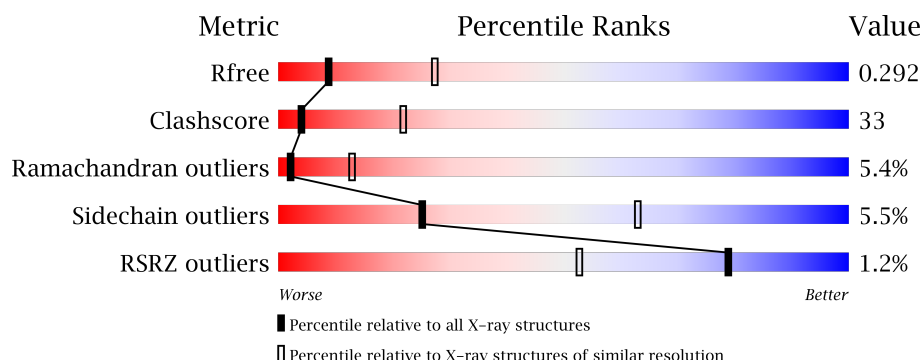
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



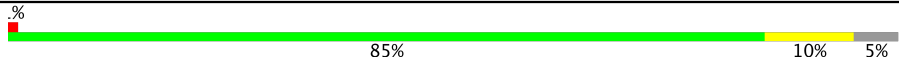
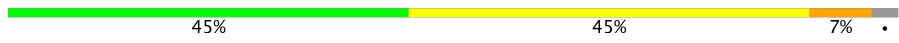

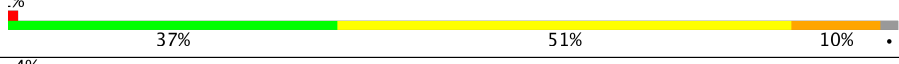
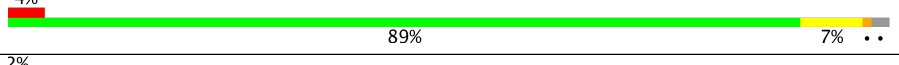
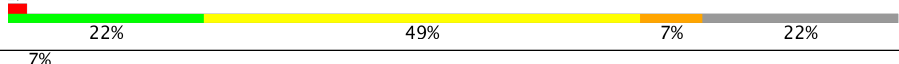
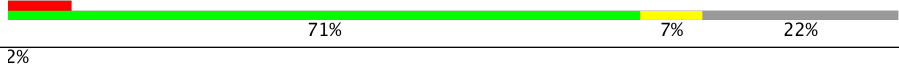
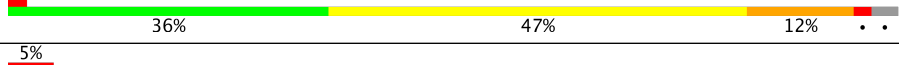
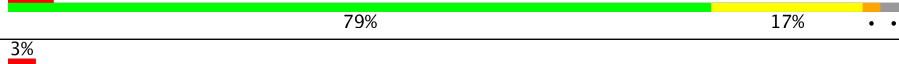
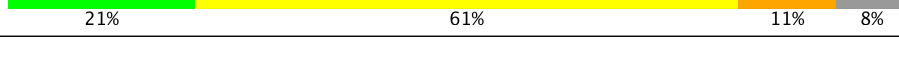

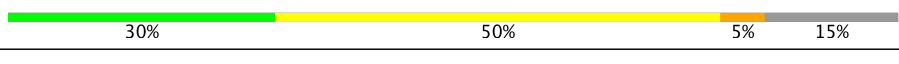
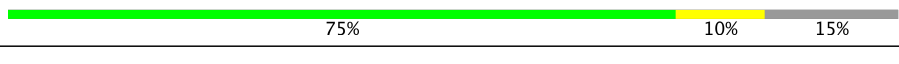

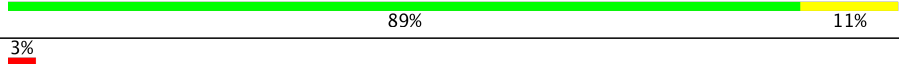


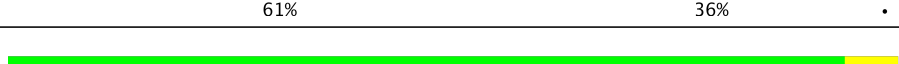
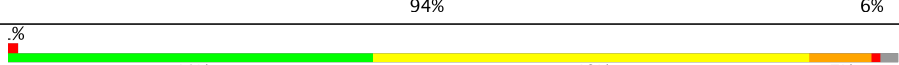
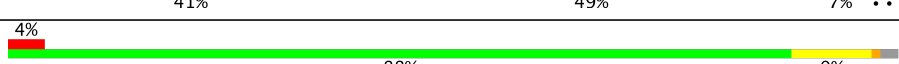

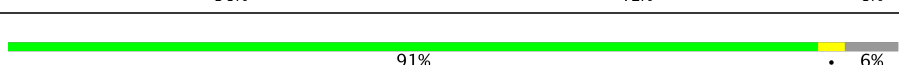
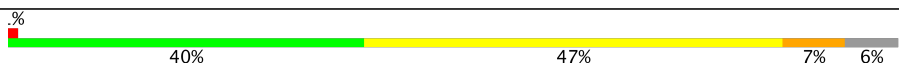
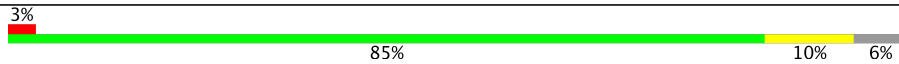

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	473	

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Mol	Chain	Length	Quality of chain
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
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	

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	X
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	498	X	-	-	-
20	CLA	C	499	X	-	-	-
20	CLA	C	500	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	D	354	X	-	-	-
20	CLA	D	355	X	-	-	-
20	CLA	a	5558	X	-	-	-
20	CLA	a	5559	X	-	-	-
20	CLA	a	5560	X	-	-	X
20	CLA	a	5563	X	-	-	X
20	CLA	b	5511	X	-	-	X
20	CLA	b	5512	X	-	-	-
20	CLA	b	5513	X	-	-	-
20	CLA	b	5514	X	-	-	-
20	CLA	b	5515	X	-	-	-
20	CLA	b	5516	X	-	-	-
20	CLA	b	5517	X	-	-	-
20	CLA	b	5518	X	-	-	-
20	CLA	b	5519	X	-	-	-
20	CLA	b	5520	X	-	-	-
20	CLA	b	5521	X	-	-	-
20	CLA	b	5522	X	-	-	-
20	CLA	b	5523	X	-	-	-
20	CLA	b	5524	X	-	-	-
20	CLA	b	5525	X	-	-	-
20	CLA	b	5526	X	-	-	-
20	CLA	c	5491	X	-	-	-
20	CLA	c	5492	X	-	-	-
20	CLA	c	5493	X	-	-	-
20	CLA	c	5494	X	-	-	-
20	CLA	c	5495	X	-	-	-
20	CLA	c	5496	X	-	-	-
20	CLA	c	5497	X	-	-	-
20	CLA	c	5498	X	-	-	-
20	CLA	c	5499	X	-	-	-
20	CLA	c	5500	X	-	-	-
20	CLA	c	5501	X	-	-	-
20	CLA	c	5502	X	-	-	-
20	CLA	c	5503	X	-	-	X
20	CLA	d	5354	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	5355	X	-	-	-
22	PQ9	A	564	-	-	-	X
22	PQ9	a	5564	-	-	-	X
24	BCR	B	528	-	-	-	X
24	BCR	C	504	-	-	-	X
24	BCR	C	505	-	-	-	X
24	BCR	D	357	-	-	-	X
24	BCR	H	107	-	-	-	X
24	BCR	X	130	-	-	-	X
24	BCR	b	5529	-	-	-	X
24	BCR	c	5504	-	-	-	X
24	BCR	d	5357	-	-	-	X
24	BCR	h	5107	-	-	-	X
24	BCR	x	5130	-	-	-	X
27	LMT	A	569	-	-	-	X
27	LMT	M	5216	-	-	-	X
27	LMT	T	217	-	-	-	X
27	LMT	a	5568	-	-	-	X
27	LMT	t	5217	-	-	-	X
28	MGE	d	5359	-	-	-	X
29	UNK	C	481	-	-	-	X
29	UNK	C	482	-	-	-	X
29	UNK	C	489	-	-	-	X
29	UNK	c	5474	-	-	-	X
29	UNK	c	5477	-	-	-	X
29	UNK	c	5484	-	-	-	X
29	UNK	c	5485	-	-	-	X
29	UNK	c	5489	-	-	-	X
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			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	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

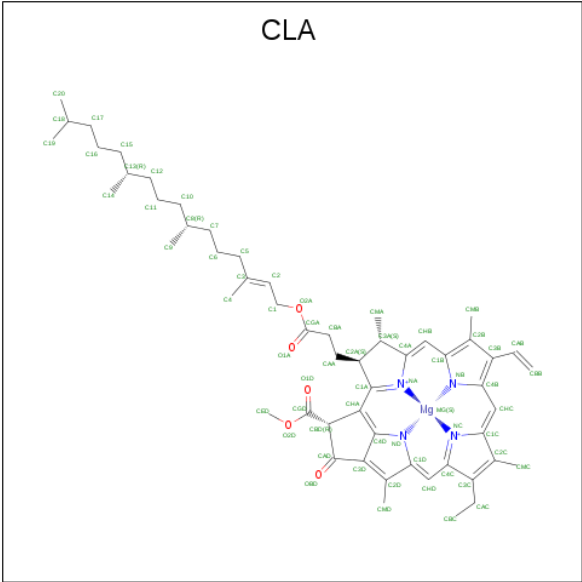
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

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

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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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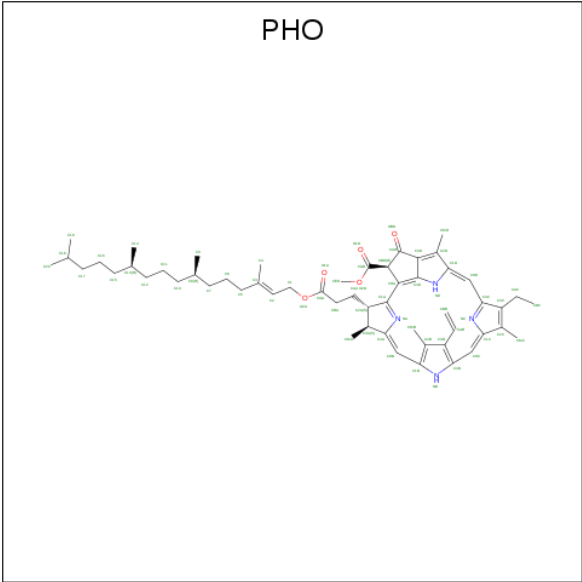
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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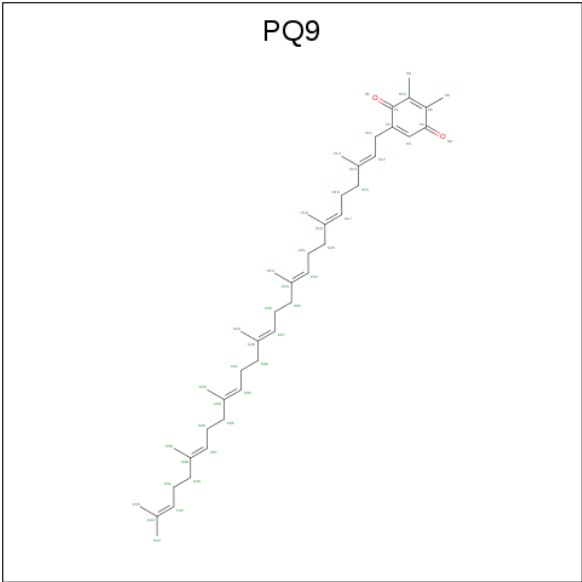
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



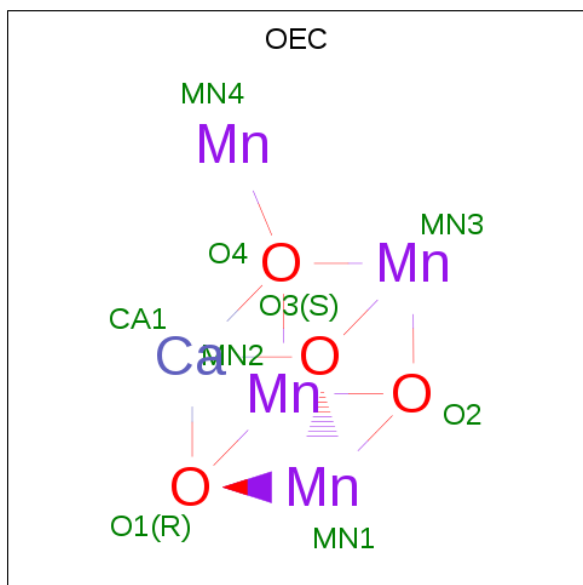
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: C<sub>43</sub>H<sub>64</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

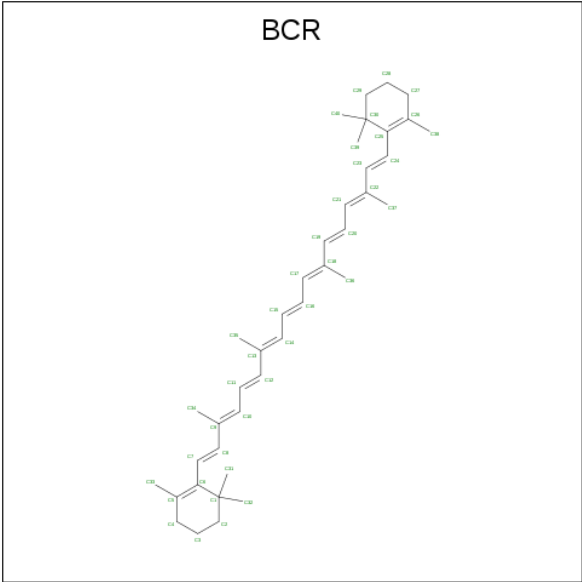
- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).





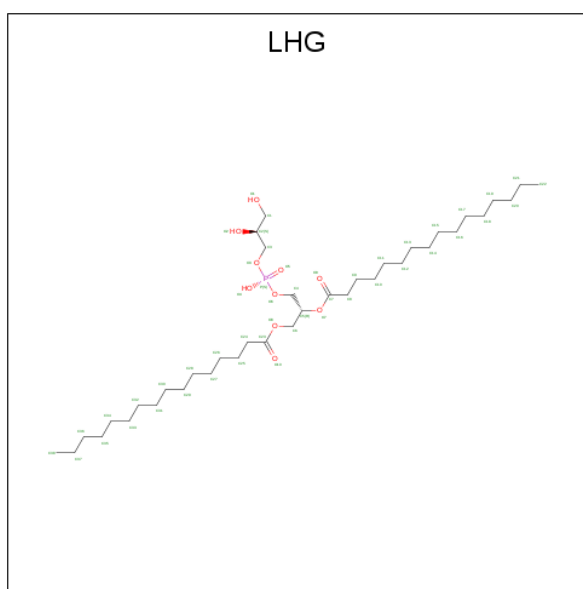
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

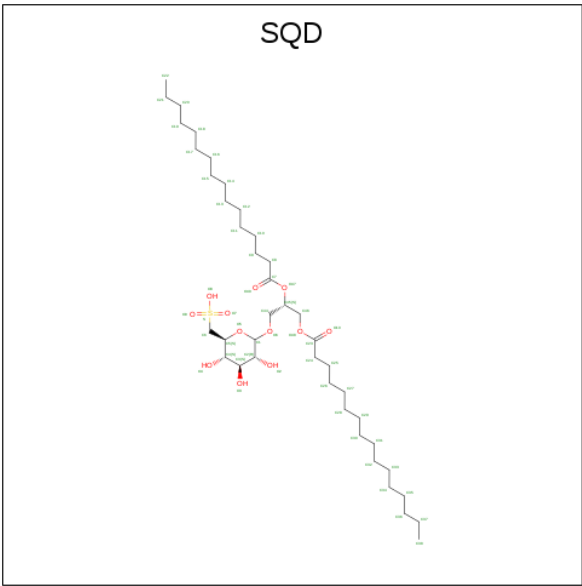
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

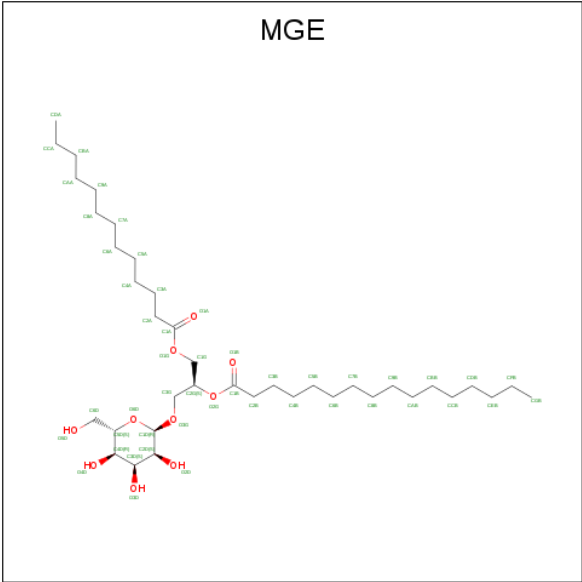
L]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



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

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



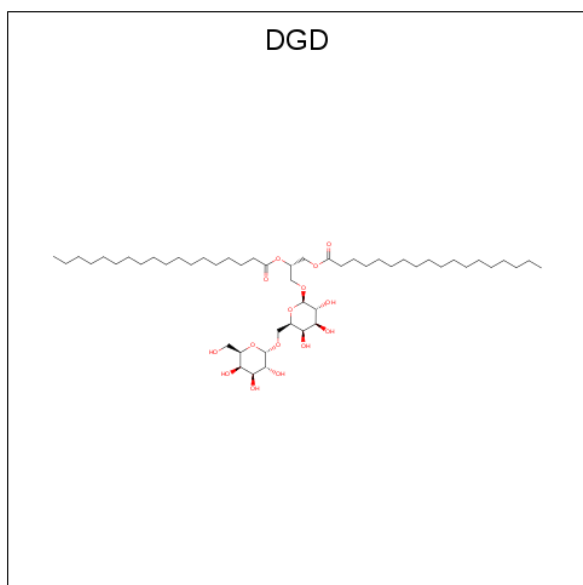


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total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

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).

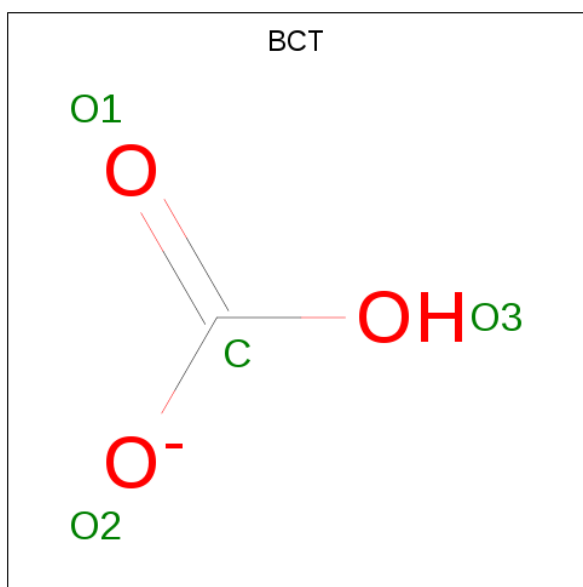
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

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



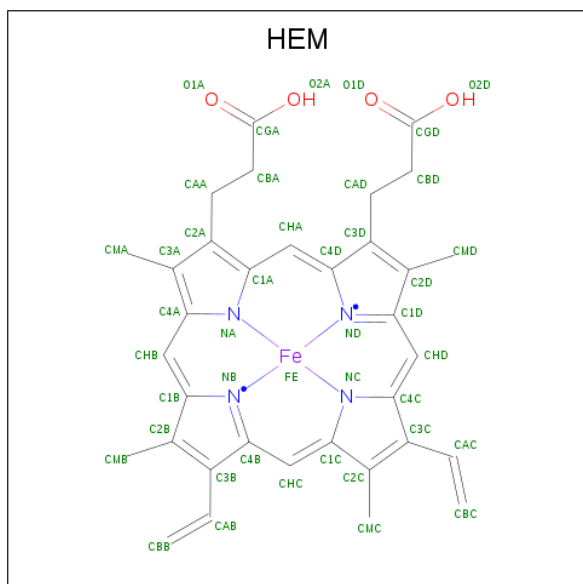
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

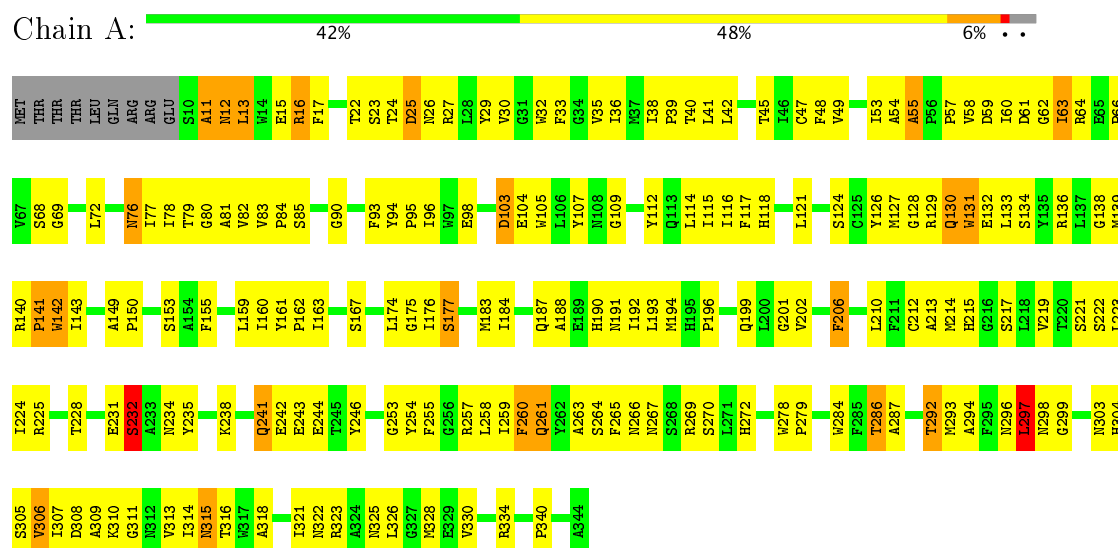
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total	Ca	0	0
			1	1		
33	k	1	Total	Ca	0	0
			1	1		



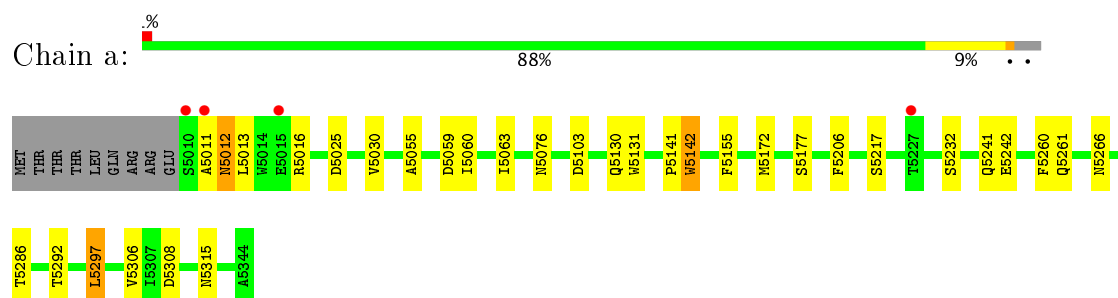
### 3 Residue-property plots

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

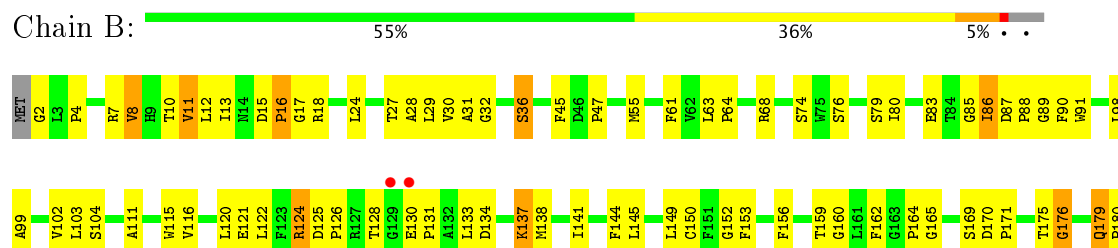
- Molecule 1: Photosystem Q(B) protein

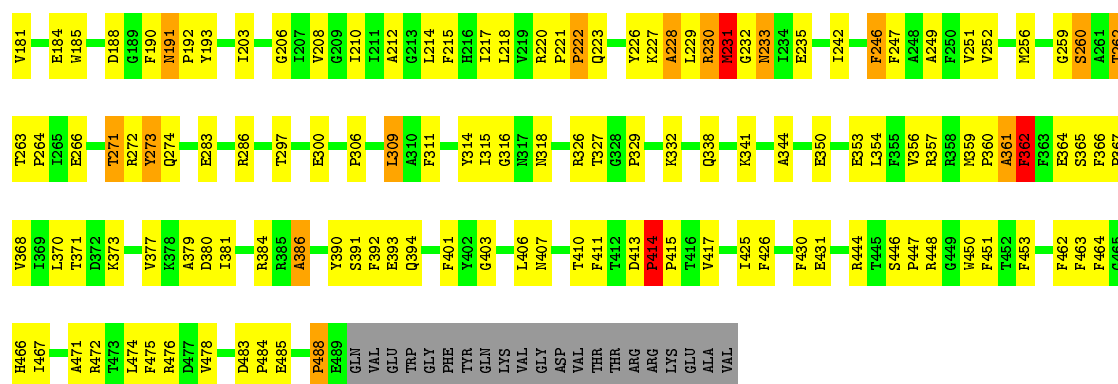


- Molecule 1: Photosystem Q(B) protein



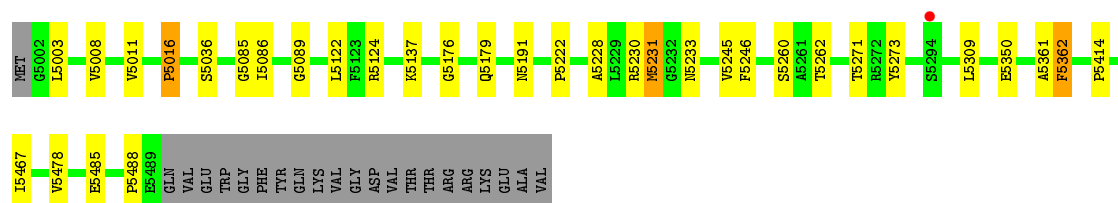
- Molecule 2: CP47 protein





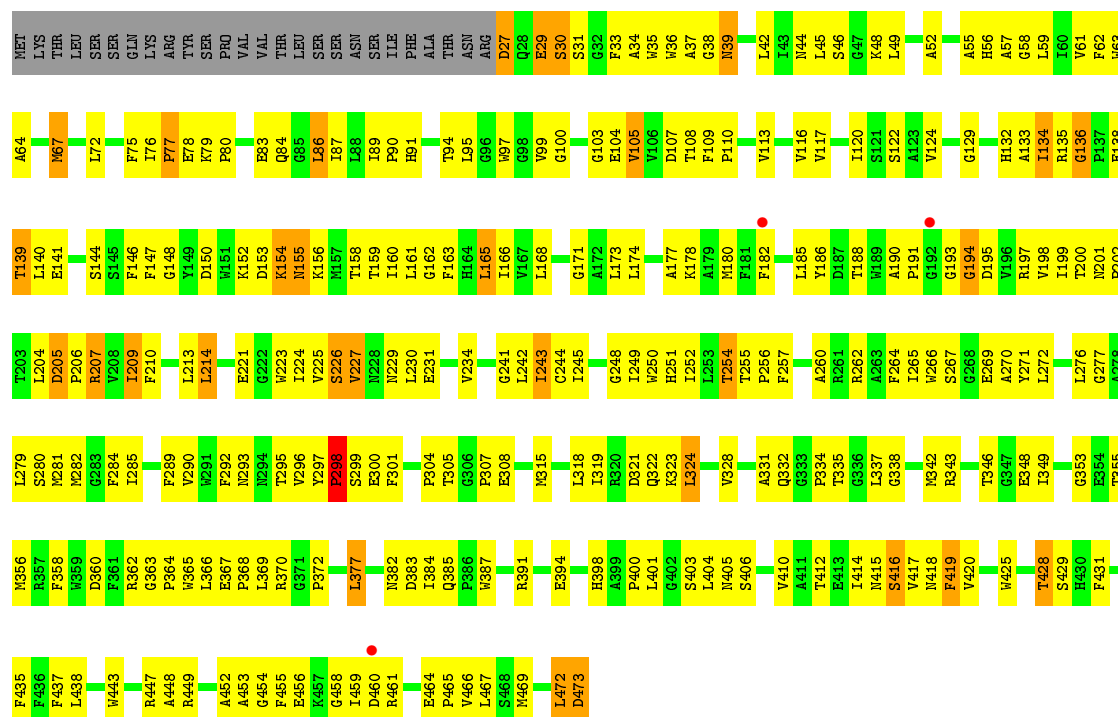
• Molecule 2: CP47 protein

Chain b: 89% 6% . .



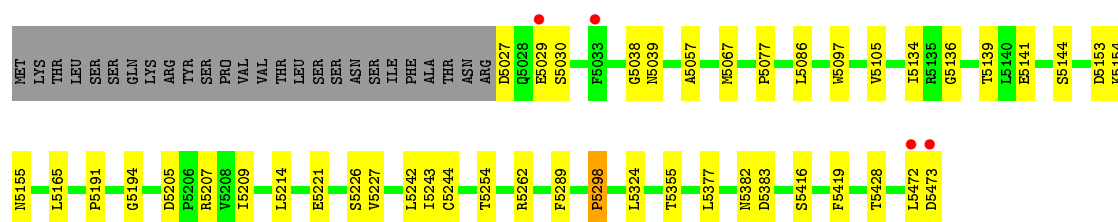
• Molecule 3: photosystem II CP43 protein

Chain C: 40% 48% 6% 5%



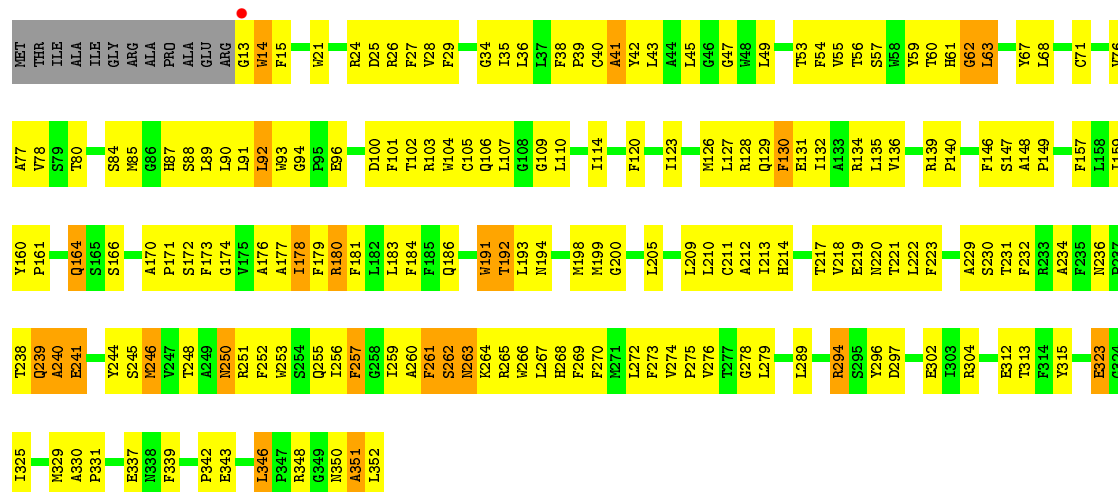
• Molecule 3: photosystem II CP43 protein

Chain c: 85% 10% 5%



• Molecule 4: photosystem II reaction center D2 protein

Chain D: 45% 45% 7% .



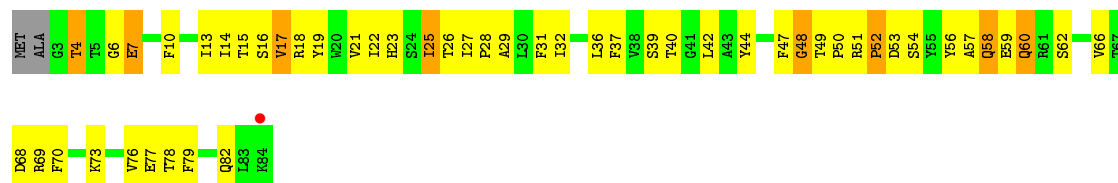
• Molecule 4: photosystem II reaction center D2 protein

Chain d: 88% 9% .



• Molecule 5: Cytochrome b559 alpha subunit

Chain E: 37% 51% 10% .

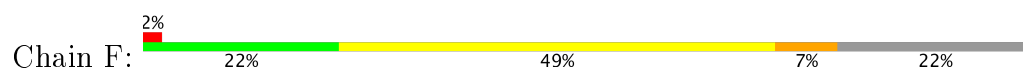


• Molecule 5: Cytochrome b559 alpha subunit

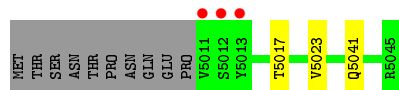
Chain e: 4% 89% 7% .



- Molecule 6: Cytochrome b559 beta subunit



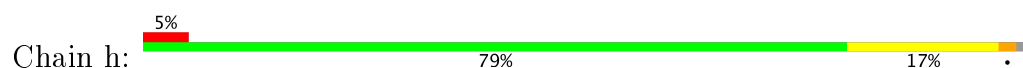
- Molecule 6: Cytochrome b559 beta subunit



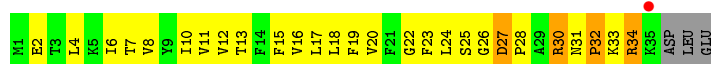
- Molecule 7: Photosystem II reaction center H protein



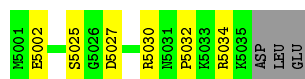
- Molecule 7: Photosystem II reaction center H protein



- Molecule 8: Photosystem II reaction center I protein



- Molecule 8: Photosystem II reaction center I protein



- Molecule 9: Photosystem II reaction center J protein





- Molecule 9: Photosystem II reaction center J protein

Chain j: 75% 10% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 35% 59% 5%



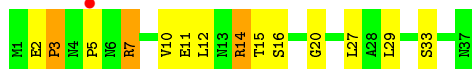
- Molecule 10: Photosystem II reaction center protein K

Chain k: 89% 11%



- Molecule 11: Photosystem II reaction center L protein

Chain L: 3% 62% 30% 8%



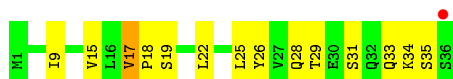
- Molecule 11: Photosystem II reaction center L protein

Chain l: 8% 84% 16%



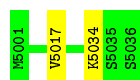
- Molecule 12: Photosystem II reaction center M protein

Chain M: 3% 61% 36% .

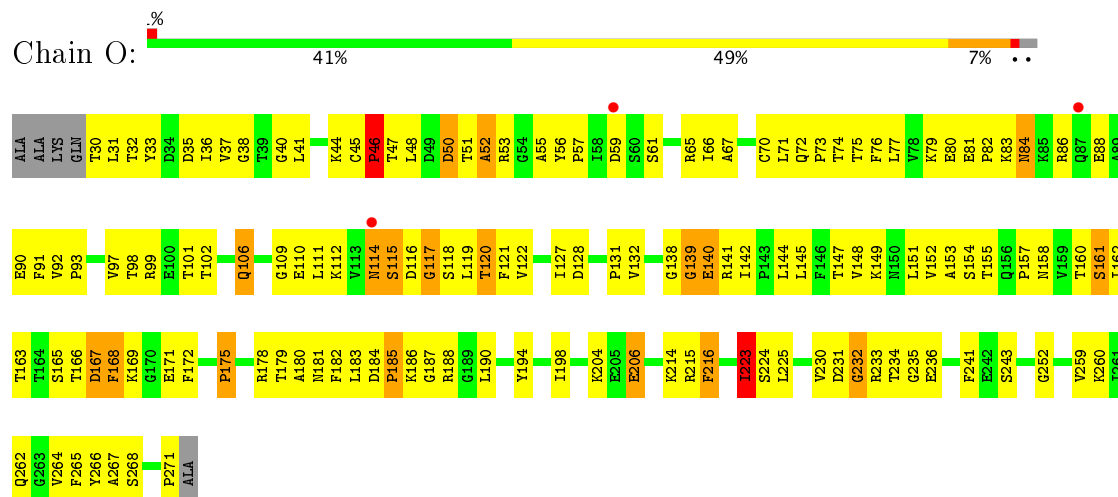


- Molecule 12: Photosystem II reaction center M protein

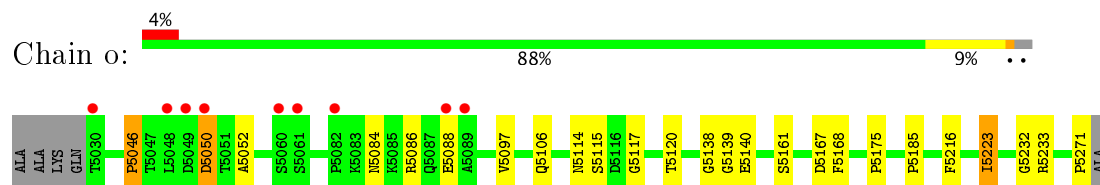
Chain m: 94% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



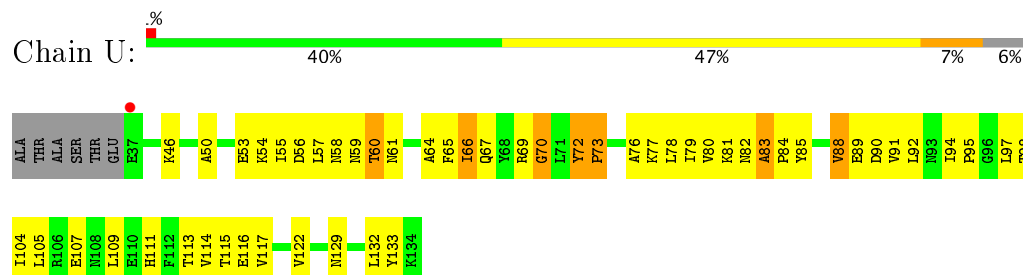
- Molecule 14: Photosystem II reaction center T protein



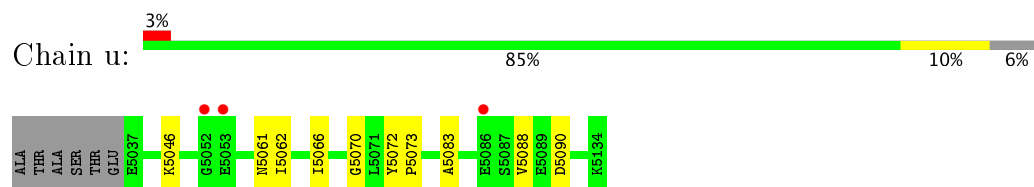
- Molecule 14: Photosystem II reaction center T protein



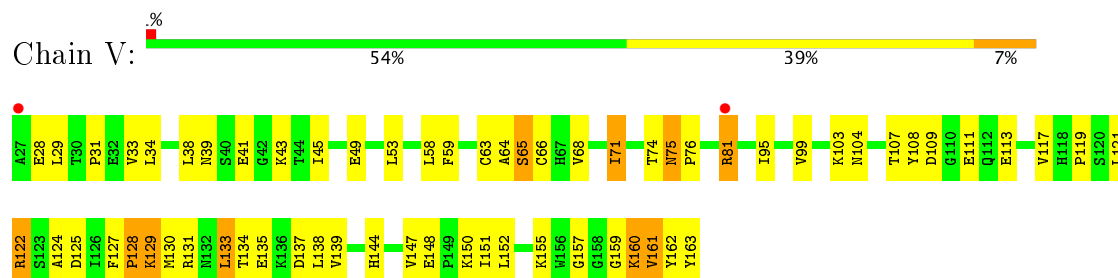
- Molecule 15: Photosystem II 12 kDa extrinsic protein



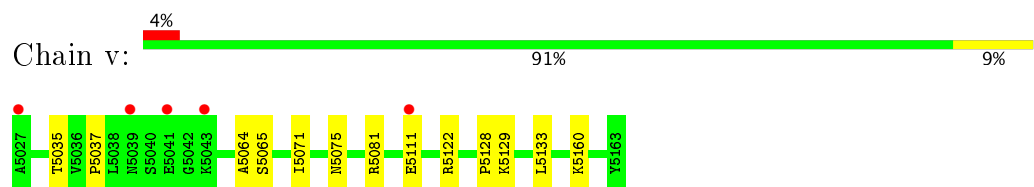
- Molecule 15: Photosystem II 12 kDa extrinsic protein



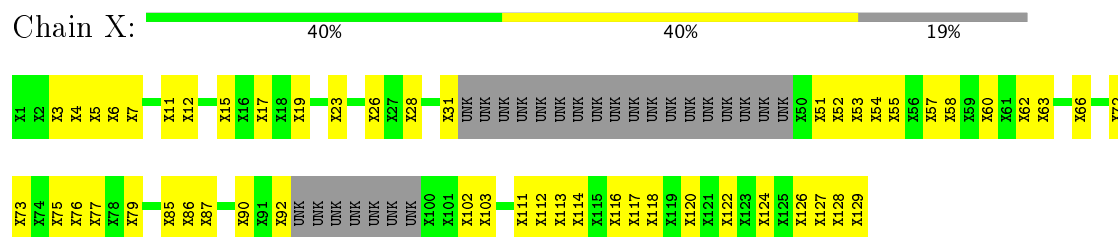
- Molecule 16: Cytochrome c-550



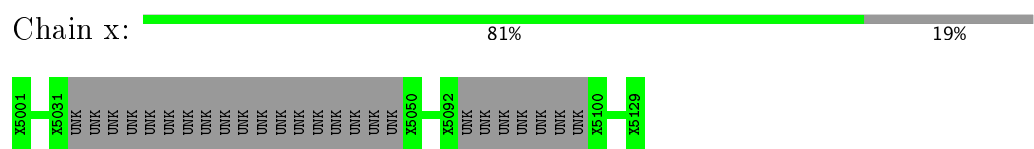
- Molecule 16: Cytochrome c-550



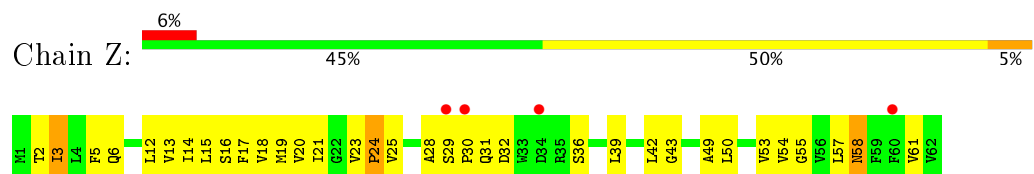
- Molecule 17: Unassigned subunits



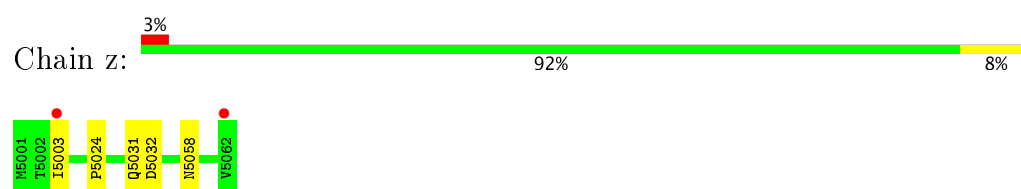
- Molecule 17: Unassigned subunits



- Molecule 18: Photosystem II reaction center Z protein



- Molecule 18: Photosystem II reaction center Z protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.234 , 0.286 0.242 , 0.292	Depositor DCC
$R_{free}$ test set	1733 reflections (1.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, MGE, DGD, 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 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	57	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	a	1	0	0	0	0
20	A	250	0	265	15	0
20	B	1007	0	1088	74	0
20	C	774	0	783	51	0
20	D	115	0	111	8	0
20	a	250	0	265	0	0
20	b	1007	0	1088	0	0
20	c	774	0	783	0	0
20	d	115	0	111	0	0
21	A	128	0	148	12	0
21	a	128	0	148	0	0
22	A	30	0	37	2	0
22	D	30	0	37	7	0
22	a	30	0	37	0	0
22	d	30	0	37	0	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	6	0
24	C	120	0	168	20	0
24	D	40	0	56	4	0
24	H	40	0	56	3	0
24	T	40	0	56	5	0
24	X	40	0	56	9	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	t	40	0	56	0	0
24	x	40	0	56	0	0
25	A	39	0	51	4	0
25	a	39	0	51	0	0
26	A	80	0	92	0	0
26	L	47	0	60	0	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	0	0
27	A	35	0	46	0	0
27	M	35	0	46	0	0
27	T	35	0	46	3	0
27	a	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	m	35	0	46	0	0
27	t	35	0	46	0	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	0	0
28	d	136	0	194	0	0
28	i	48	0	72	0	0
28	l	48	0	72	0	0
29	C	152	0	17	2	0
29	c	152	0	17	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	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	0	0
32	v	43	0	30	0	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47107	1538	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1538) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:CD	17:X:26:UNK:NE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:PRO:HB3	20: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	20: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	20: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
20:C:493:CLA:H191	20: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
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
20:B:515:CLA:H141	20:B:520:CLA:HMA2	1.54	0.90
24: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	20: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
8:I:34:ARG:HE	8:I:34:ARG:H	0.92	0.89
15:U:50:ALA:CB	15:U:113:THR:HG21	2.04	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
20: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
2:B:271:THR:H	2:B:274:GLN:HE21	1.17	0.86
28:D:360:MGE:H6D2	11:L:15:THR:HG21	1.57	0.86
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.04	0.86
2:B:327:THR:HG22	20:B:517:CLA:H12	1.58	0.86
13:O:145:LEU:HD23	13:O:175:PRO:HG2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:159:GLY:O	16:V:161:VAL:N	2.08	0.86
13:O:145:LEU:CD2	13:O:175:PRO:HG2	2.06	0.86
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.05	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:306:VAL:O	1:A:306:VAL:HG23	1.77	0.84
1:A:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
14:T:29:ILE:HD12	14:T:29:ILE:H	1.43	0.84
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
20:C:493:CLA:HBA1	20:C:493:CLA:HBD	1.59	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
1:A:279:PRO:HB2	21:A:561:PHO:HBC1	1.58	0.83
7:H:38:PHE:HB2	24:H:107:BCR:H10C	1.61	0.83
3:C:209:ILE:HG23	24: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
20: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:166:ILE:HG23	3:C:245:ILE:HG23	1.62	0.82
3:C:293:ASN:ND2	3:C:296:VAL:HG22	1.94	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
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.62	0.81
3:C:406:SER:O	3:C:418:ASN:HB2	1.78	0.81
4:D:192:THR:HG23	20:D:354:CLA:HBC2	1.60	0.81
5:E:18:ARG:HG2	5:E:22:ILE:HD11	1.62	0.81
24:C:504:BCR:H353	24:X:130:BCR:H321	1.62	0.81
3:C:116:VAL:HG11	24:C:505:BCR:H323	1.62	0.80
6:F:21:VAL:O	6:F:25:THR:HG23	1.80	0.80
3:C:464:GLU:HB2	3:C:467:LEU:HD12	1.61	0.80
4:D:351:ALA:O	4:D:352:LEU:OXT	1.99	0.80
20:C:491:CLA:HMB3	24: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
4:D:27:PHE:HD2	4:D:28:VAL:HG23	1.45	0.80
1:A:60:ILE:HG23	1:A:61:ASP:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:49:ALA:O	18:Z:53:VAL:HG23	1.82	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	20: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	20:C:501:CLA:H2A	1.66	0.78
3:C:405:ASN:HD22	30:C:509:DGD:HD5	1.48	0.78
3:C:346:THR:O	13:O:40:GLY:HA2	1.84	0.78
14:T:4:ILE:HG13	24:T:5104:BCR:H383	1.65	0.78
4:D:266:TRP:HD1	28:D:360:MGE:H3D	1.48	0.77
8:I:16:VAL:O	8:I:20:VAL:HG23	1.82	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	20: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	24: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
15:U:88:VAL:O	15:U:91:VAL:HG23	1.85	0.76
17:X:126:UNK:O	17:X:127:UNK:HB2	1.86	0.76
2:B:68:ARG:NH2	20: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
2:B:263:THR:HG21	2:B:448:ARG:NH1	1.99	0.76
15:U:113:THR:CG2	15:U:114:VAL:H	1.94	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	20:C:498:CLA:HBB1	1.69	0.75
4:D:266:TRP:CD1	28:D:360:MGE:H3D	2.22	0.75
6:F:34:LEU:HD22	9:J:24:ILE:HD13	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	20:B:513:CLA:HMC3	1.69	0.74
20:A:558:CLA:HBB1	20:D:354:CLA:NB	2.02	0.74
3:C:204:LEU:O	3:C:205:ASP:HB3	1.85	0.74
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	0.73
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.70	0.73
3:C:449:ARG:HH22	8:I:27:ASP:HB3	1.51	0.73
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.53	0.73
15:U:50:ALA:HB3	15:U:113:THR:HG21	1.70	0.73
1:A:309:ALA:HB3	16:V:28:GLU:HG3	1.68	0.73
2:B:27:THR:O	20: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
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	0.72
21: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
20:B:518:CLA:HMD1	20: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
24:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	0.72
3:C:293:ASN:ND2	3:C:296:VAL:H	1.87	0.71
3:C:334:PRO:HA	13:O:179:THR:HB	1.72	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
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.25	0.71
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.55	0.71
4:D:36:LEU:O	4:D:39:PRO:HD2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:M:25:LEU:O	12:M:28:GLN:HG3	1.92	0.69
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.56	0.69
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.07	0.69
21: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	20:C:501:CLA:HMA3	1.74	0.69
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.74	0.69
10:K:17:ILE:CD1	18:Z:6:GLN:HE21	2.05	0.69
3:C:241:GLY:C	3:C:243:ILE:H	1.96	0.69
18:Z:21:ILE:O	18:Z:25:VAL:HG23	1.91	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
20:C:495:CLA:HBD	20:C:495:CLA:HBA1	1.75	0.69
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
3:C:214:LEU:H	3:C:214:LEU:HD23	1.58	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
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
20:A:559:CLA:HED2	4:D:198:MET:SD	2.33	0.68
3:C:84:GLN:HB2	3:C:86:LEU:HD22	1.75	0.68
2:B:126:PRO:HG3	7:H:12:ARG:NH2	2.09	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
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	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
5:E:58:GLN:HE22	16:V:28:GLU:HA	1.58	0.68
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.11	0.68
24:C:505:BCR:H312	18:Z:55:GLY:HA2	1.75	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	20:B:520:CLA:HAC2	1.75	0.67
20:B:515:CLA:HMB3	20:B:516:CLA:H11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PRO:HG3	7:H:27:THR:H	1.60	0.67
3:C:124:VAL:HB	24:C:505:BCR:H362	1.77	0.67
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	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
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	0.67
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.75	0.67
3:C:150:ASP:O	3:C:153:ASP:HB3	1.96	0.67
5:E:40:THR:HG21	17:X:102:UNK:CB	2.25	0.67
17:X:54:UNK:HB1	17:X:57:UNK:CG2	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
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.78	0.66
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.78	0.66
3:C:56:HIS:C	3:C:58:GLY:H	1.99	0.66
14:T:4:ILE:HD13	14:T:4:ILE:C	2.16	0.66
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.11	0.66
2:B:297:THR:CB	2:B:300:GLU:HG3	2.26	0.65
2:B:463:PHE:HZ	20:B:518:CLA:HBB1	1.61	0.65
4:D:267:LEU:HD23	4:D:267:LEU:C	2.17	0.65
5:E:10:PHE:O	5:E:13:ILE:HG22	1.95	0.65
13:O:77:LEU:N	13:O:77:LEU:HD12	2.10	0.65
24:X:130:BCR:H331	24:X:130:BCR:HC8	1.78	0.65
10:K:23:ASP:OD2	17:X:6:UNK:NE2	2.34	0.65
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.25	0.65
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.25	0.65
5:E:22:ILE:HG23	17:X:116:UNK:HA	1.78	0.65
1:A:270:SER:HA	4:D:232:PHE:HE2	1.61	0.65
3:C:466:VAL:HA	3:C:469:MET:HE3	1.79	0.65
10:K:28:ILE:O	10:K:31:LEU:HB2	1.97	0.65
1:A:76:ASN:ND2	1:A:79:THR:H	1.95	0.65
2:B:176:GLY:HA3	2:B:266:GLU:OE1	1.96	0.65
17:X:51:UNK:O	17:X:52:UNK:C	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:558:CLA:H143	21: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
1:A:94:TYR:OH	1:A:104:GLU:HG2	1.97	0.65
5:E:78:THR:O	5:E:82:GLN:HG2	1.97	0.65
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.80	0.64
20:C:501:CLA:H151	18:Z:20:VAL:HG13	1.78	0.64
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.33	0.64
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.80	0.64
3:C:265:ILE:HD13	20: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	22:D:356:PQ9:H17	1.80	0.64
6:F:37:ILE:HG22	9:J:28:PHE:CE1	2.33	0.64
20:C:495:CLA:CMD	20:C:497:CLA:HAB	2.27	0.64
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.33	0.64
2:B:223:GLN:HE22	2:B:227:LYS:CD	2.10	0.64
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.80	0.64
1:A:134:SER:HB2	1:A:139:MET:HG3	1.79	0.63
1:A:187:GLN:HG3	1:A:325:ASN:OD1	1.98	0.63
16:V:95:ILE:O	16:V:99:VAL:HG23	1.97	0.63
24:C:504:BCR:H311	24:C:504:BCR:H343	1.81	0.63
24:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	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
2:B:120:LEU:HD13	20: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
20:B:519:CLA:HMC2	24:H:107:BCR:H343	1.81	0.63
16:V:49:GLU:O	16:V:53:LEU:HG	1.98	0.63
4:D:36:LEU:C	4:D:39:PRO:HD2	2.19	0.63
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	0.63
3:C:248:GLY:O	3:C:252:ILE:HG13	1.97	0.63
3:C:343:ARG:HB2	13:O:101:THR:HG23	1.80	0.63
2:B:208:VAL:HG21	20:B:512:CLA:HMC1	1.81	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	0.63
4:D:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63
7:H:43:LEU:HD23	17:X:60:UNK:CZ	2.29	0.63
16:V:38:LEU:HD13	16:V:45:ILE:CD1	2.29	0.63
1:A:16:ARG:HD3	1:A:17:PHE:N	2.14	0.63
3:C:417:VAL:O	3:C:417:VAL:HG22	1.99	0.63
3:C:52:ALA:HA	20:C:501:CLA:HMB3	1.80	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
3:C:158:THR:HG22	3:C:251:HIS:O	1.99	0.63
7:H:6:TRP:O	7:H:10:ILE:HG13	1.99	0.63
2:B:246:PHE:CD1	2:B:246:PHE:C	2.72	0.62
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
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
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.81	0.62
13:O:110:GLU:O	13:O:110:GLU:HG3	1.99	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
20:C:501:CLA:H171	18:Z:20:VAL:HA	1.79	0.62
4:D:103:ARG:NH1	5:E:77:GLU:HG3	2.15	0.62
2:B:2:GLY:HA3	11:L:11:GLU:OE1	2.00	0.62
13:O:183:LEU:HD22	13:O:187:GLY:O	1.99	0.62
1:A:72:LEU:HD23	14:T:3:THR:HG21	1.82	0.62
3:C:55:ALA:HB1	24:C:504:BCR:H373	1.82	0.62
4:D:90:LEU:HD23	4:D:109:GLY:HA2	1.81	0.62
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.30	0.62
13:O:46:PRO:HB2	13:O:266:TYR:CG	2.35	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
2:B:329:PRO:CB	20:B:517:CLA:HED1	2.26	0.61
3:C:35:TRP:NE1	3:C:36:TRP:HD1	1.99	0.61
17:X:26:UNK:HG2	17:X:26:UNK:NE2	2.20	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	32:F:51:HEM:HMC2	1.82	0.61
16:V:39:ASN:HD21	16:V:41:GLU:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:O	2:B:251:VAL:HG23	2.00	0.61
3:C:298:PRO:O	3:C:299:SER:CB	2.48	0.61
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
5:E:10:PHE:HA	5:E:13:ILE:HG22	1.83	0.61
7:H:21:VAL:HG22	7:H:22:ALA:O	2.01	0.61
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.01	0.61
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.82	0.61
2:B:31:ALA:HB2	20:B:515:CLA:HBC3	1.83	0.61
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	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
29:C:474:UNK:C15	22:D:356:PQ9:H293	2.31	0.61
13:O:128:ASP:OD2	13:O:149:LYS:HG2	2.01	0.60
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.31	0.60
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.16	0.60
2:B:271:THR:HG22	2:B:274:GLN:H	1.64	0.60
5:E:56:TYR:HB3	5:E:60:GLN:HG3	1.83	0.60
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	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
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
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.15	0.60
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	0.60
9:J:8:ILE:H	9:J:8:ILE:HD12	1.66	0.60
14:T:21:ILE:HD12	24:T:5104:BCR:H332	1.83	0.60
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	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
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
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
5:E:60:GLN:O	5:E:60:GLN:HG3	2.01	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:55:ALA:O	13:O:57:PRO:HD3	2.02	0.59
3:C:428:THR:HG22	3:C:429:SER:N	2.17	0.59
3:C:458:GLY:HA2	4:D:222:LEU:O	2.02	0.59
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.32	0.59
13:O:112:LYS:HE2	13:O:114:ASN:HB3	1.84	0.59
13:O:179:THR:CG2	13:O:180:ALA:N	2.65	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
7:H:29:PRO:O	7:H:33:VAL:HG23	2.02	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
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.38	0.59
1:A:307:ILE:HD11	1:A:311:GLY:O	2.00	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD22	20:D:354:CLA:HBA2	1.85	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:315:MET:O	3:C:319:ILE:HG13	2.04	0.58
3:C:465:PRO:C	3:C:469:MET:HE2	2.23	0.58
1:A:131:TRP:CE3	1:A:132:GLU:N	2.72	0.58
3:C:456:GLU:N	3:C:456:GLU:OE1	2.35	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
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
2:B:24:LEU:HD21	20:B:526:CLA:HAB	1.86	0.58
21:A:562:PHO:CMC	4:D:279:LEU:HD11	2.34	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58
2:B:149:LEU:HG	20:B:513:CLA:CBC	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:O:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
1:A:54:ALA:O	1:A:55:ALA:HB2	2.03	0.57
1:A:62:GLY:HA3	3:C:356:MET:SD	2.44	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
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.69	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	0.57
3:C:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
5:E:60:GLN:C	5:E:62:SER:H	2.07	0.57
1:A:217:SER:HA	4:D:272:LEU:HD12	1.86	0.57
6:F:34:LEU:HD22	9:J:24:ILE:CD1	2.32	0.57
13:O:142:ILE:HD12	13:O:142:ILE:N	2.19	0.57
4:D:343:GLU:HG2	16:V:161:VAL:HG11	1.86	0.57
8:I:27:ASP:N	8:I:28:PRO:CD	2.67	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	1.85	0.57
9:J:14:ALA:HB1	24:X:130:BCR:H393	1.85	0.57
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.57
2:B:150:CYS:HA	20:B:513:CLA:HBC2	1.87	0.57
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.04	0.57
18:Z:39:LEU:O	18:Z:42:LEU:HB3	2.05	0.57
3:C:44:ASN:O	3:C:45:LEU:HG	2.04	0.57
3:C:428:THR:CG2	30:C:508:DGD:HA91	2.35	0.57
4:D:239:GLN:O	4:D:240:ALA:HB3	2.05	0.57
4:D:273:PHE:CZ	28:L:210:MGE:H3B2	2.40	0.57
4:D:261:PHE:HB2	22:D:356:PQ9:H92	1.84	0.57
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	0.57
4:D:239:GLN:O	4:D:240:ALA:CB	2.53	0.57
5:E:15:THR:HG23	9:J:8:ILE:O	2.04	0.57
10:K:18:PHE:O	10:K:19:ASP:C	2.43	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	0.57
13:O:168:PHE:CD1	13:O:168:PHE:N	2.71	0.57
14:T:4:ILE:O	14:T:4:ILE:HD13	2.04	0.57
20: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
13:O:172:PHE:CE2	13:O:223:ILE:HG12	2.39	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:MET:HA	6:F:43:ILE:HG13	1.84	0.57
9:J:15:THR:HG22	10:K:38:VAL:HG22	1.85	0.57
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.35	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
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
2:B:138:MET:SD	20:B:525:CLA:HAC1	2.45	0.56
2:B:391:SER:OG	2:B:394:GLN:HB2	2.05	0.56
13:O:145:LEU:O	13:O:147:THR:HG22	2.05	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	0.56
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	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
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.26	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
16:V:39:ASN:ND2	16:V:41:GLU:HB2	2.20	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:27:ASP:O	10:K:46:ARG:HD3	2.06	0.56
3:C:56:HIS:C	3:C:58:GLY:N	2.59	0.56
1:A:29:TYR:HD1	1:A:133:LEU:HB2	1.69	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
3:C:315:MET:CE	3:C:319:ILE:HD11	2.35	0.56
8:I:11:VAL:O	8:I:15:PHE:HD1	1.89	0.56
15:U:77:LYS:O	15:U:81:LYS:HB2	2.06	0.56
16:V:81:ARG:HH11	16:V:81:ARG:HG3	1.71	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
1:A:13:LEU:N	1:A:13:LEU:HD23	2.21	0.56
3:C:293:ASN:HD21	3:C:296:VAL:H	1.51	0.56
4:D:178:ILE:HG22	4:D:179:PHE:N	2.21	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
2:B:467:ILE:HD13	4:D:126:MET:SD	2.46	0.56
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
16:V:107:THR:HG22	16:V:108:TYR:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.41	0.55
3:C:260:ALA:O	3:C:264:PHE:HD2	1.89	0.55
3:C:348:GLU:OE2	13:O:37:VAL:HA	2.06	0.55
3:C:400:PRO:C	3:C:401:LEU:HD23	2.26	0.55
10:K:39:TRP:O	10:K:43:VAL:HG23	2.05	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: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
1:A:38:ILE:O	1:A:42:LEU:HG	2.07	0.55
2:B:283:GLU:OE1	2:B:286:ARG:HD2	2.07	0.55
4:D:176:ALA:C	4:D:178:ILE:H	2.10	0.55
5:E:13:ILE:HD13	32:F:51:HEM:O1D	2.07	0.55
6:F:18:VAL:HG13	6:F:19:ARG:N	2.22	0.55
15:U:72:TYR:CB	15:U:73:PRO:CD	2.84	0.55
1:A:224:ILE:CG2	2:B:484:PRO:HG3	2.35	0.55
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.34	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
2:B:233:ASN:C	2:B:233:ASN:HD22	2.10	0.55
1:A:264:SER:OG	1:A:265:PHE:N	2.40	0.55
2:B:229:LEU:O	2:B:230:ARG:C	2.44	0.55
3:C:42:LEU:CD1	20:C:501:CLA:HMA3	2.36	0.55
3:C:209:ILE:CG2	24:C:506:BCR:H382	2.35	0.55
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.89	0.55
2:B:18:ARG:HG3	2:B:18:ARG:HH11	1.70	0.55
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.55
20:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
13:O:47:THR:HG22	13:O:48:LEU:N	2.22	0.55
16:V:159:GLY:O	16:V:160:LYS:C	2.45	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
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.70	0.55
3:C:37:ALA:HA	20:C:498:CLA:O1A	2.06	0.55
3:C:466:VAL:HA	3:C:469:MET:CE	2.36	0.55
13:O:145:LEU:HD23	13:O:175:PRO:CG	2.34	0.55
3:C:416:SER:O	3:C:417:VAL:CG1	2.55	0.54
9:J:14:ALA:CB	24:X:130:BCR:H393	2.38	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.71	0.54
2:B:10:THR:C	2:B:12:LEU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:346:LEU:O	4:D:348:ARG:HG3	2.07	0.54
13:O:75:THR:HG22	13:O:77:LEU:HD11	1.88	0.54
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.82	0.54
24:B:527:BCR:H322	28:B:530:MGE:H2G	1.89	0.54
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.37	0.54
30:C:509:DGD:HD2	9:J:32:ALA:O	2.06	0.54
3:C:91:HIS:HB3	20:C:493:CLA:HBA2	1.88	0.54
10:K:43:VAL:HG12	10:K:46:ARG:HG3	1.90	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	24:C:504:BCR:C37	2.37	0.54
4:D:325:ILE:O	4:D:329:MET:HB3	2.08	0.54
5:E:25:ILE:O	5:E:29:ALA:HB2	2.08	0.54
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.35	0.54
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	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:418:ASN:HB3	30:C:509:DGD:HE2	1.89	0.54
3:C:52:ALA:HB1	20:C:499:CLA:HAB	1.89	0.54
3:C:75:PHE:CE2	3:C:77:PRO:HA	2.43	0.54
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	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
1:A:174:LEU:HD22	21:A:561:PHO:H152	1.89	0.54
5:E:76:VAL:O	5:E:79:PHE:HB2	2.07	0.54
10:K:45:PHE:O	10:K:46:ARG:C	2.46	0.54
3:C:201:ASN:N	3:C:202:PRO:HD3	2.22	0.54
4:D:100:ASP:OD1	4:D:102:THR:HG22	2.07	0.54
3:C:276:LEU:CD2	20:C:498:CLA:HBB1	2.37	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	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
3:C:99:VAL:HG23	3:C:100:GLY:H	1.72	0.53
4:D:45:LEU:HD13	4:D:49:LEU:HD12	1.90	0.53
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.89	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.89	0.53
1:A:159:LEU:O	1:A:163:ILE:HG13	2.08	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.53
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53
1:A:76:ASN:HD22	1:A:76:ASN:C	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	0.53
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.44	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
3:C:158:THR:O	3:C:251:HIS:HB3	2.07	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.90	0.53
3:C:84:GLN:HB2	3:C:86:LEU:CD2	2.37	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
14:T:29:ILE:CD1	14:T:29:ILE:H	2.18	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.28	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
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
1:A:286:THR:HB	20:A:558:CLA:O1D	2.09	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CD2	2.44	0.53
2:B:12:LEU:HB2	20:B:522:CLA:HMC2	1.90	0.53
3:C:48:LYS:HE2	3:C:133:ALA:HA	1.90	0.53
13:O:162:ILE:HA	13:O:166:THR:HG21	1.90	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
1:A:124:SER:O	1:A:127:MET:HB3	2.09	0.53
1:A:238:LYS:O	1:A:241:GLN:HB3	2.09	0.53
3:C:29:GLU:HG3	3:C:30:SER:N	2.22	0.53
4:D:221:THR:HG22	4:D:221:THR:O	2.08	0.53
15:U:72:TYR:O	15:U:73:PRO:C	2.46	0.53
1:A:183:MET:HA	20: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:141:PRO:O	1:A:143:ILE:N	2.38	0.53
1:A:176:ILE:HD13	20:A:559:CLA:HED3	1.91	0.53
21:A:561:PHO:NC	4:D:209:LEU:HD12	2.24	0.53
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.75	0.52
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HA	24:B:528:BCR:C40	2.39	0.52
2:B:152:GLY:C	20:B:516:CLA:HMC3	2.30	0.52
2:B:476:ARG:HG3	2:B:476:ARG:HH11	1.74	0.52
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.71	0.52
20:C:492:CLA:H111	20:C:493:CLA:HMB2	1.90	0.52
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
5:E:32:ILE:O	5:E:36:LEU:HG	2.10	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.09	0.52
10:K:31:LEU:HB3	24:X:130:BCR:C15	2.39	0.52
13:O:33:TYR:C	13:O:35:ASP:H	2.12	0.52
28:D:360:MGE:H241	14:T:13:ILE:HG21	1.90	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
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
2:B:263:THR:O	2:B:263:THR:HG22	2.08	0.52
2:B:391:SER:OG	2:B:394:GLN:NE2	2.43	0.52
3:C:103:GLY:HA3	3:C:301:PHE:CE1	2.37	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
1:A:103:ASP:OD1	1:A:103:ASP:N	2.40	0.52
3:C:56:HIS:O	3:C:58:GLY:N	2.42	0.52
4:D:93:TRP:HZ2	20:D:355:CLA:O1A	1.93	0.52
5:E:69:ARG:O	5:E:70:PHE:HB2	2.09	0.52
17:X:12:UNK:CG	18:Z:17:PHE:CE1	2.90	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
2:B:220:ARG:HD2	7:H:20:LYS:O	2.10	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	0.52
3:C:29:GLU:C	3:C:31:SER:H	2.13	0.52
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.52
13:O:206:GLU:CD	13:O:206:GLU:H	2.13	0.52
14:T:1:MET:C	14:T:4:ILE:HG22	2.30	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
8:I:13:THR:O	8:I:17:LEU:HG	2.09	0.52
16:V:134:THR:HG23	16:V:137:ASP:OD2	2.10	0.52
1:A:63:ILE:CG2	3:C:335:THR:HG21	2.40	0.52
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
1:A:27:ARG:NH1	1:A:27:ARG:O	2.43	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
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
3:C:116:VAL:HG21	24:C:505:BCR:C32	2.40	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
20:C:503:CLA:HMC2	24:C:505:BCR:H372	1.91	0.52
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.91	0.52
11:L:2:GLU:HB3	11:L:3:PRO:HD2	1.92	0.52
13:O:118:SER:HB3	13:O:157:PRO:HA	1.90	0.52
16:V:33:VAL:HG12	16:V:33:VAL:O	2.10	0.52
1:A:257:ARG:HH12	1:A:261:GLN:CD	2.13	0.51
4:D:14:TRP:CD1	4:D:15:PHE:N	2.78	0.51
9:J:24:ILE:HG23	9:J:25:VAL:N	2.24	0.51
13:O:110:GLU:OE2	13:O:112:LYS:HB2	2.10	0.51
18:Z:57:LEU:O	18:Z:61:VAL:HG23	2.10	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:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
2:B:463:PHE:CZ	20:B:518:CLA:HBB1	2.43	0.51
13:O:172:PHE:HE2	13:O:223:ILE:HG12	1.75	0.51
16:V:59:PHE:HA	16:V:63:CYS:SG	2.50	0.51
1:A:192:ILE:HG23	1:A:193:LEU:N	2.25	0.51
2:B:212:ALA:HB2	20:B:519:CLA:HMC3	1.91	0.51
20:C:493:CLA:HBA1	20:C:493:CLA:CBD	2.37	0.51
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.91	0.51
17:X:76:UNK:O	17:X:77:UNK:C	2.57	0.51
2:B:380:ASP:OD2	2:B:380:ASP:C	2.47	0.51
2:B:229:LEU:HD11	20:B:519:CLA:O1A	2.11	0.51
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	0.51
1:A:326:LEU:HD21	3:C:412:THR:HB	1.93	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
14:T:4:ILE:HB	27:T:217:LMT:O6'	2.11	0.51
15:U:69:ARG:O	15:U:70:GLY:C	2.47	0.51
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.45	0.51
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:T:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
3:C:438:LEU:HD11	20:C:495:CLA:HBB1	1.92	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
20:C:495:CLA:HMD3	20:C:497:CLA:HAB	1.92	0.51
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.93	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
6:F:11:VAL:HG12	6:F:12:SER:N	2.26	0.51
2:B:175:THR:O	2:B:175:THR:HG22	2.11	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
8:I:4:LEU:O	8:I:8:VAL:HG23	2.11	0.51
2:B:233:ASN:C	2:B:233:ASN:ND2	2.64	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HH11	1.75	0.50
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.09	0.50
20:B:517:CLA:H202	11:L:27:LEU:HD11	1.93	0.50
17:X:85:UNK:C	17:X:86:UNK:OD1	2.59	0.50
20:B:525:CLA:H112	20:B:525:CLA:H162	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
4:D:63:LEU:N	4:D:63:LEU:HD12	2.26	0.50
6:F:45:ARG:HG2	6:F:45:ARG:OXT	2.11	0.50
3:C:372:PRO:O	13:O:36:ILE:HD12	2.11	0.50
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
3:C:150:ASP:HB3	3:C:153:ASP:CB	2.32	0.50
3:C:241:GLY:C	3:C:243:ILE:N	2.64	0.50
20:A:560:CLA:HAB	20:D:354:CLA:H72	1.93	0.50
15:U:64:ALA:O	15:U:67:GLN:HG2	2.10	0.50
29:C:484:UNK:HG1	29:C:485:UNK:C	2.40	0.50
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.32	0.50
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:145:LEU:CD2	13:O:175:PRO:CG	2.86	0.50
14:T:15:ALA:HB2	24:T:5104:BCR:H14C	1.92	0.50
1:A:22:THR:HG23	1:A:136:ARG:NH1	2.26	0.50
1:A:62:GLY:O	1:A:63:ILE:O	2.29	0.50
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.93	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
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.93	0.50
10:K:19:ASP:N	10:K:20:PRO:HD2	2.26	0.50
10:K:37:PHE:HB3	24:X:130:BCR:C40	2.42	0.50
2:B:231:MET:C	2:B:233:ASN:H	2.15	0.50
12:M:15:VAL:O	12:M:19:SER:HB2	2.12	0.50
10:K:43:VAL:HG21	17:X:31:UNK:HG3	1.93	0.50
18:Z:36:SER:CA	18:Z:39:LEU:HD12	2.35	0.50
2:B:15:ASP:O	2:B:17:GLY:N	2.45	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
3:C:178:LYS:HD2	3:C:182:PHE:O	2.11	0.50
4:D:60:THR:HG23	4:D:61:HIS:H	1.77	0.50
13:O:147:THR:HG21	13:O:175:PRO:HD2	1.93	0.50
1:A:72:LEU:HD22	27:T:217:LMT:O3'	2.12	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
13:O:216:PHE:C	13:O:216:PHE:CD2	2.85	0.50
16:V:128:PRO:O	16:V:130:MET:N	2.45	0.50
2:B:31:ALA:HB2	20:B:515:CLA:CBC	2.42	0.49
4:D:176:ALA:C	4:D:178:ILE:N	2.66	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.11	0.49
4:D:35:ILE:O	4:D:35:ILE:HG22	2.12	0.49
7:H:59:ASN:OD1	7:H:59:ASN:O	2.29	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
2:B:246:PHE:HD1	2:B:246:PHE:C	2.15	0.49
2:B:286:ARG:HD3	2:B:286:ARG:C	2.33	0.49
3:C:416:SER:O	3:C:417:VAL:HG12	2.11	0.49
13:O:73:PRO:CG	13:O:102:THR:CB	2.90	0.49
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.46	0.49
16:V:144:HIS:CE1	16:V:148:GLU:OE2	2.65	0.49
2:B:474:LEU:HD11	20:B:518:CLA:HAA1	1.94	0.49
3:C:46:SER:HA	3:C:49:LEU:HB3	1.93	0.49
3:C:67:MET:HE1	20:C:494:CLA:NC	2.26	0.49
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:VAL:HG12	4:D:56:THR:N	2.26	0.49
5:E:47:PHE:O	5:E:49:THR:N	2.45	0.49
9:J:12:ILE:O	9:J:16:VAL:HG23	2.12	0.49
16:V:104:ASN:HD21	16:V:113:GLU:CD	2.14	0.49
3:C:277:GLY:C	20:C:495:CLA:HBC2	2.33	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
13:O:51:THR:O	13:O:52:ALA:O	2.30	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:13:ILE:HG22	2:B:13:ILE:O	2.11	0.49
2:B:145:LEU:CD1	20:B:525:CLA:HMB2	2.43	0.49
2:B:165:GLY:HA3	2:B:179:GLN:O	2.11	0.49
2:B:222:PRO:HG3	7:H:27:THR:N	2.26	0.49
3:C:199:ILE:N	3:C:199:ILE:HD12	2.27	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.92	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	0.49
13:O:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	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
2:B:271:THR:HB	2:B:274:GLN:HG3	1.95	0.49
3:C:78:GLU:OE2	3:C:78:GLU:HA	2.12	0.49
13:O:65:ARG:HG2	13:O:66:ILE:N	2.27	0.49
1:A:232:SER:OG	1:A:235:TYR:CD1	2.65	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
3:C:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
10:K:43:VAL:O	10:K:43:VAL:HG12	2.13	0.49
13:O:101:THR:O	13:O:101:THR:HG22	2.13	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.32	0.49
3:C:281:MET:HG3	28:I:201:MGE:H231	1.94	0.49
3:C:250:TRP:HE1	20:C:496:CLA:HED1	1.78	0.49
8:I:24:LEU:C	8:I:26:GLY:H	2.16	0.49
18:Z:28:ALA:O	18:Z:30:PRO:HD3	2.12	0.49
6:F:40:MET:O	6:F:42:PHE:N	2.46	0.49
24:T:5104:BCR:H403	24:T:5104:BCR:H23C	1.95	0.49
15:U:73:PRO:HD2	16:V:109:ASP:HB3	1.94	0.49
1:A:58:VAL:O	1:A:60:ILE:N	2.46	0.49
2:B:28:ALA:O	2:B:104:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:PHE:N	20:B:516:CLA:HMC3	2.27	0.49
3:C:162:GLY:O	3:C:166:ILE:HG13	2.12	0.49
3:C:269:GLU:CG	3:C:448:ALA:HB2	2.34	0.49
16:V:128:PRO:O	16:V:129:LYS:C	2.51	0.49
1:A:153:SER:CB	20:A:558:CLA:H43	2.43	0.48
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.48
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	0.48
3:C:342:MET:HE3	3:C:353:GLY:H	1.78	0.48
3:C:369:LEU:HD21	3:C:384:ILE:HG12	1.95	0.48
4:D:57:SER:O	4:D:63:LEU:O	2.31	0.48
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.30	0.48
13:O:154:SER:O	13:O:168:PHE:HA	2.13	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
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
1:A:140:ARG:NH2	25:A:567:LHG:O5	2.46	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.94	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
12:M:33:GLN:C	12:M:35:SER:H	2.16	0.48
15:U:72:TYR:CG	15:U:73:PRO:N	2.79	0.48
11:L:14:ARG:HG2	12:M:26:TYR:CE1	2.44	0.48
1:A:228:THR:OG1	1:A:231:GLU:HG2	2.13	0.48
2:B:18:ARG:NH1	2:B:18:ARG:HG3	2.28	0.48
20:B:520:CLA:OBD	20:B:520:CLA:H151	2.13	0.48
10:K:15:TYR:C	10:K:17:ILE:H	2.17	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
20:B:513:CLA:H2	20:B:515:CLA:H91	1.95	0.48
3:C:48:LYS:HB3	20:C:501:CLA:HMA2	1.95	0.48
4:D:312:GLU:HB2	13:O:185:PRO:HB3	1.96	0.48
16:V:39:ASN:OD1	16:V:43:LYS:N	2.46	0.48
18:Z:15:LEU:O	18:Z:19:MET:HG2	2.13	0.48
2:B:124:ARG:HD3	2:B:130:GLU:C	2.33	0.48
4:D:180:ARG:HD3	4:D:180:ARG:C	2.33	0.48
4:D:246:MET:HE3	4:D:263:ASN:H	1.78	0.48
28:L:210:MGE:H5A2	12:M:22:LEU:HD21	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:116:VAL:HG13	3:C:117:VAL:N	2.29	0.48
4:D:126:MET:HE1	4:D:147:SER:HA	1.95	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.49	0.48
28:D:358:MGE:O3D	9:J:37:GLY:HA3	2.14	0.48
16:V:160:LYS:O	16:V:161:VAL:C	2.52	0.48
17:X:86:UNK:N	17:X:86:UNK:OD1	2.45	0.48
1:A:153:SER:HB3	20:A:558:CLA:H43	1.96	0.48
3:C:229:ASN:HD22	3:C:231:GLU:HG2	1.79	0.48
3:C:254:THR:HG22	3:C:255:THR:N	2.19	0.48
3:C:435:PHE:O	3:C:438:LEU:N	2.47	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.13	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	0.48
13:O:33:TYR:C	13:O:35:ASP:N	2.66	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
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
2:B:61:PHE:CZ	20:B:517:CLA:HBB1	2.49	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48
7:H:45:ILE:O	7:H:46:LEU:C	2.51	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
15:U:73:PRO:HG2	16:V:109:ASP:N	2.29	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
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
4:D:272:LEU:HD23	4:D:272:LEU:C	2.35	0.47
13:O:67:ALA:HB3	13:O:268:SER:OG	2.14	0.47
17:X:3:UNK:C	17:X:5:UNK:N	2.76	0.47
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.48	0.47
3:C:59:LEU:HD13	20:C:500:CLA:HMD2	1.96	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.47	0.47
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	0.47
9:J:18:GLY:O	9:J:22:ILE:HG12	2.14	0.47
11:L:14:ARG:HG3	11:L:14:ARG:HH11	1.78	0.47
13:O:73:PRO:HG2	13:O:102:THR:CB	2.45	0.47
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:LEU:HD12	20:B:522:CLA:HBB1	1.96	0.47
25:A:567:LHG:HC61	3:C:443:TRP:HH2	1.77	0.47
2:B:191:ASN:HD22	2:B:192:PRO:N	2.12	0.47
2:B:262:THR:O	2:B:262:THR:CG2	2.61	0.47
3:C:152:LYS:O	3:C:154:LYS:N	2.47	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
3:C:449:ARG:HD3	20:C:495:CLA:HED1	1.95	0.47
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.36	0.47
4:D:213:ILE:HG23	4:D:214:HIS:N	2.28	0.47
6:F:11:VAL:HG12	6:F:12:SER:H	1.79	0.47
3:C:62:PHE:CE2	10:K:28:ILE:HB	2.50	0.47
11:L:12:LEU:HD12	12:M:25:LEU:HD12	1.95	0.47
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.28	0.47
1:A:213:ALA:O	1:A:217:SER:CB	2.63	0.47
1:A:314:ILE:HG22	1:A:314:ILE:O	2.14	0.47
2:B:228:ALA:O	2:B:230:ARG:NH1	2.47	0.47
4:D:49:LEU:HD13	24:D:357:BCR:C15	2.45	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
7:H:12:ARG:HG3	7:H:12:ARG:NH1	2.30	0.47
11:L:14:ARG:HD3	12:M:26:TYR:OH	2.15	0.47
13:O:147:THR:OG1	13:O:148:VAL:N	2.47	0.47
13:O:169:LYS:HG2	13:O:224:SER:HB2	1.96	0.47
14:T:4:ILE:HB	27:T:217:LMT:C6'	2.44	0.47
15:U:105:LEU:O	15:U:109:LEU:HG	2.15	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
1:A:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
2:B:179:GLN:HE21	2:B:179:GLN:HA	1.78	0.47
20: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
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.47
1:A:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:7:ARG:NH2	28:D:359:MGE:O3D	2.47	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47
20:A:558:CLA:H201	28:D:360:MGE:H232	1.96	0.47
7:H:12:ARG:HH11	7:H:12:ARG:HG3	1.80	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:111:UNK:C	17:X:113:UNK:N	2.76	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	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
20:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47
13:O:79:LYS:HA	13:O:90:GLU:O	2.15	0.47
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.91	0.47
17:X:75:UNK:O	17:X:79:UNK:HG2	2.15	0.47
1:A:29:TYR:CD1	1:A:133:LEU:HB2	2.49	0.47
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.15	0.47
2:B:145:LEU:HD11	20:B:525:CLA:HMB2	1.96	0.47
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.30	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
16:V:162:TYR:O	16:V:163:TYR:OXT	2.33	0.47
1:A:306:VAL:O	1:A:306:VAL:CG2	2.49	0.47
1:A:140:ARG:HH22	25:A:567:LHG:P	2.38	0.47
2:B:29:LEU:HD12	20:B:524:CLA:HBB2	1.95	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	0.47
3:C:55:ALA:C	24:C:504:BCR:H373	2.35	0.47
4:D:40:CYS:O	4:D:41:ALA:C	2.53	0.47
4:D:68:LEU:HD21	5:E:44:TYR:CD1	2.50	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
4:D:214:HIS:HA	22:D:356:PQ9:O4	2.15	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
16:V:133:LEU:H	16:V:133:LEU:HD23	1.80	0.47
17:X:114:UNK:O	17:X:117:UNK:HB1	2.15	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
2:B:169:SER:HA	2:B:176:GLY:HA2	1.97	0.46
3:C:255:THR:HG23	3:C:256:PRO:CD	2.41	0.46
8:I:6:ILE:O	8:I:10:ILE:HG12	2.15	0.46
13:O:225:LEU:HD12	13:O:225:LEU:N	2.29	0.46
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.46
2:B:390:TYR:CD1	2:B:390:TYR:N	2.83	0.46
3:C:180:MET:CE	3:C:202:PRO:HG2	2.45	0.46
3:C:415:ASN:O	3:C:416:SER:CB	2.64	0.46
3:C:453:ALA:CB	8:I:31:ASN:ND2	2.76	0.46
3:C:460:ASP:O	3:C:461:ARG:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:513:CLA:H162	7:H:38:PHE:HE2	1.80	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
13:O:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	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
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.50	0.46
4:D:222:LEU:HA	4:D:244:TYR:HA	1.97	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
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.46
1:A:60:ILE:CG2	1:A:61:ASP:H	2.23	0.46
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.51	0.46
6:F:25:THR:O	6:F:29:PRO:HG2	2.15	0.46
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	0.46
13:O:47:THR:HG22	13:O:48:LEU:H	1.80	0.46
13:O:80:GLU:O	13:O:81:GLU:C	2.53	0.46
15:U:98:THR:C	15:U:100:ARG:H	2.16	0.46
17:X:126:UNK:N	17:X:126:UNK:CD	2.77	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
1:A:183:MET:HB3	20:A:558:CLA:HBC2	1.98	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
15:U:113:THR:O	15:U:114:VAL:HG23	2.16	0.46
18:Z:5:PHE:HA	18:Z:57:LEU:CD1	2.40	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
2:B:263:THR:CG2	2:B:448:ARG:NH1	2.70	0.46
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
3:C:39:ASN:OD1	20:C:499:CLA:HBB2	2.16	0.46
6:F:45:ARG:CG	6:F:45:ARG:OXT	2.64	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
12:M:9:ILE:N	12:M:9:ILE:HD12	2.30	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
14:T:11:ALA:HB3	24:T:5104:BCR:H363	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.46
20:C:497:CLA:H142	24:C:506:BCR:H362	1.96	0.46
5:E:23:HIS:C	5:E:25:ILE:N	2.69	0.46
4:D:106:GLN:NE2	5:E:48:GLY:HA3	2.31	0.46
5:E:59:GLU:O	5:E:60:GLN:C	2.53	0.46
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
15:U:59:ASN:O	15:U:60:THR:C	2.54	0.46
17:X:112:UNK:C	17:X:114:UNK:N	2.79	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
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
2:B:10:THR:O	2:B:12:LEU:N	2.49	0.46
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.46	0.46
2:B:462:PHE:CE1	20:B:523:CLA:HMB3	2.50	0.46
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
17:X:117:UNK:NZ	17:X:117:UNK:HB1	2.31	0.46
2:B:149:LEU:HB2	20:B:514:CLA:H203	1.97	0.46
2:B:249:ALA:O	2:B:252:VAL:HG22	2.16	0.46
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.46
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.97	0.46
1:A:26:ASN:O	1:A:27:ARG:C	2.54	0.46
1:A:60:ILE:CG2	1:A:61:ASP:N	2.79	0.46
20:B:518:CLA:H51	20:B:519:CLA:H101	1.97	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
13:O:116:ASP:O	13:O:158:ASN:N	2.35	0.46
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
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
2:B:356:VAL:HA	2:B:370:LEU:HD23	1.96	0.45
3:C:400:PRO:O	3:C:401:LEU:HD23	2.15	0.45
3:C:410:VAL:HG12	3:C:412:THR:H	1.80	0.45
20:D:355:CLA:H3A	20:D:355:CLA:HBA2	1.53	0.45
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.45
7:H:44:ILE:O	7:H:48:ILE:HG13	2.16	0.45
13:O:114:ASN:O	13:O:115:SER:O	2.33	0.45
13:O:151:LEU:HD12	13:O:171:GLU:O	2.17	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:PRO:HD3	20:B:517:CLA:HED2	1.98	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
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
13:O:70:CYS:SG	13:O:71:LEU:N	2.89	0.45
13:O:98:THR:CG2	13:O:99:ARG:H	2.04	0.45
1:A:306:VAL:HG21	1:A:316:THR:CG2	2.42	0.45
22:A:564:PQ9:H91	22:A:564:PQ9:H61	1.69	0.45
2:B:156:PHE:HB2	20:B:516:CLA:HAC1	1.99	0.45
2:B:215:PHE:C	2:B:215:PHE:CD2	2.89	0.45
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.45
20:B:511:CLA:CAA	24:H:107:BCR:H19C	2.47	0.45
3:C:331:ALA:O	3:C:338:GLY:HA2	2.17	0.45
3:C:453:ALA:HB1	8:I:31:ASN:HD22	1.81	0.45
11:L:14:ARG:CG	11:L:14:ARG:HH11	2.29	0.45
15:U:115:THR:HG22	15:U:116:GLU:N	2.32	0.45
1:A:22:THR:HG22	1:A:22:THR:O	2.16	0.45
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.52	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
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	20:C:495:CLA:HAA1	2.51	0.45
2:B:193:TYR:CE1	2:B:260:SER:N	2.84	0.45
3:C:139:THR:O	3:C:139:THR:HG23	2.16	0.45
3:C:299:SER:OG	3:C:304:PRO:HA	2.17	0.45
4:D:213:ILE:CG2	4:D:214:HIS:N	2.79	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	0.45
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.45
9:J:8:ILE:N	9:J:8:ILE:HD12	2.30	0.45
1:A:210:LEU:HD13	21:A:562:PHO:ND	2.31	0.45
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.97	0.45
3:C:250:TRP:HE1	20:C:496:CLA:CED	2.30	0.45
4:D:179:PHE:O	4:D:183:LEU:HG	2.17	0.45
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	0.45
13:O:70:CYS:O	13:O:265:PHE:HB2	2.16	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
10:K:46:ARG:HH22	17:X:31:UNK:CG2	2.30	0.45
15:U:92:LEU:HD11	15:U:109:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:50:ALA:O	15:U:53:GLU:HB2	2.17	0.45
18:Z:2:THR:O	18:Z:3:ILE:C	2.55	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.78	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
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
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
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
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	0.45
1:A:40:THR:CG2	1:A:118:HIS:O	2.65	0.45
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.99	0.45
20:A:559:CLA:H61	21:A:561:PHO:HMB3	1.99	0.45
20:B:514:CLA:O1A	20:B:515:CLA:HBA1	2.16	0.45
3:C:305:THR:CG2	3:C:307:PRO:HD2	2.31	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	0.45
4:D:68:LEU:HB2	6:F:40:MET:HE1	1.99	0.45
13:O:59:ASP:C	13:O:61:SER:H	2.21	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.82	0.45
2:B:10:THR:HG23	2:B:13:ILE:HD11	1.99	0.45
2:B:297:THR:H	2:B:300:GLU:CD	2.20	0.45
20: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
2:B:171:PRO:HD3	7:H:65:LEU:C	2.37	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.52	0.44
20:B:517:CLA:HBA2	20:B:517:CLA:H3A	1.71	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
32:F:51:HEM:HAD2	32:F:51:HEM:HHA	1.67	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
4:D:100:ASP:C	4:D:100:ASP:OD1	2.55	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
8:I:17:LEU:O	8:I:18:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:31:SER:C	12:M:33:GLN:H	2.21	0.44
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.44
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.51	0.44
12:M:33:GLN:O	12:M:35:SER:N	2.50	0.44
4:D:302:GLU:OE1	13:O:186:LYS:CE	2.65	0.44
1:A:323:ARG:HD2	1:A:323:ARG:HA	1.64	0.44
1:A:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
2:B:124:ARG:HA	2:B:131:PRO:HA	1.99	0.44
3:C:265:ILE:HB	20:C:495:CLA:HED3	1.98	0.44
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.52	0.44
5:E:60:GLN:C	5:E:62:SER:N	2.71	0.44
13:O:81:GLU:O	13:O:82:PRO:C	2.56	0.44
15:U:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	0.44
24:C:504:BCR:H11C	24:X:130:BCR:H322	1.99	0.44
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.19	0.44
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.00	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.44
3:C:116:VAL:O	3:C:117:VAL:C	2.56	0.44
3:C:257:PHE:CD1	3:C:257:PHE:N	2.85	0.44
4:D:85:MET:HE3	4:D:107:LEU:HB3	1.99	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
5:E:28:PRO:O	5:E:32:ILE:HG13	2.18	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.82	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
16:V:63:CYS:SG	32:V:552:HEM:HAB	2.57	0.44
16:V:64:ALA:O	16:V:66:CYS:N	2.51	0.44
17:X:126:UNK:HB2	17:X:127:UNK:H	1.41	0.44
20:A:558:CLA:HBD	20:A:559:CLA:HAC2	1.99	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	0.44
3:C:42:LEU:HD11	20:C:501:CLA:C1A	2.48	0.44
3:C:292:PHE:HB3	30:C:507:DGD:HD62	1.99	0.44
4:D:60:THR:CG2	4:D:61:HIS:H	2.31	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
17:X:128:UNK:O	17:X:129:UNK:C	2.66	0.44
10:K:21:LEU:HD11	24:X:130:BCR:HC42	1.99	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
21:A:561:PHO:HED2	4:D:257:PHE:CE2	2.52	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:ALA:C	3:C:454:GLY:H	2.21	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
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
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.44
2:B:450:TRP:O	2:B:451:PHE:C	2.55	0.44
2:B:476:ARG:HG3	2:B:476:ARG:NH1	2.33	0.44
3:C:135:ARG:O	3:C:136:GLY:O	2.35	0.44
5:E:51:ARG:O	5:E:54:SER:N	2.48	0.44
15:U:98:THR:C	15:U:100:ARG:N	2.71	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.44	0.44
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.99	0.44
3:C:405:ASN:HB2	30:C:509:DGD:HG32	2.00	0.44
20:C:501:CLA:HMD2	10:K:40:GLN:CD	2.37	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.48	0.44
13:O:52:ALA:HA	13:O:230:VAL:O	2.18	0.44
2:B:341:LYS:HB3	2:B:406:LEU:HD12	2.00	0.43
2:B:450:TRP:O	2:B:453:PHE:N	2.51	0.43
3:C:225:VAL:O	3:C:225:VAL:HG12	2.18	0.43
3:C:321:ASP:OD2	15:U:129:ASN:HB2	2.18	0.43
4:D:21:TRP:CE2	4:D:26:ARG:NH2	2.78	0.43
10:K:15:TYR:OH	18:Z:58:ASN:HB2	2.17	0.43
11:L:7:ARG:HA	11:L:7:ARG:HD2	1.69	0.43
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	0.43
1:A:48:PHE:HA	1:A:115:ILE:CD1	2.48	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.91	0.43
2:B:193:TYR:HE1	2:B:260:SER:N	2.17	0.43
2:B:217:ILE:HG22	2:B:218:LEU:HD23	1.99	0.43
2:B:36:SER:OG	24:B:528:BCR:H362	2.18	0.43
20:C:498:CLA:H122	20:C:500:CLA:HED1	2.00	0.43
3:C:134:ILE:HD11	20:C:501:CLA:H92	2.00	0.43
4:D:256:ILE:HG12	4:D:256:ILE:O	2.19	0.43
4:D:263:ASN:HB3	28:D:360:MGE:O3D	2.19	0.43
4:D:93:TRP:CZ2	20:D:355:CLA:O1A	2.71	0.43
7:H:19:GLY:O	7:H:21:VAL:HG12	2.17	0.43
16:V:117:VAL:O	16:V:117:VAL:HG12	2.17	0.43
2:B:31:ALA:N	20:B:515:CLA:HBC3	2.33	0.43
20:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:HB	3:C:308:GLU:HB2	1.99	0.43
24:D:357:BCR:H383	28:D:358:MGE:H6B1	2.00	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.54	0.43
13:O:231:ASP:O	13:O:232:GLY:C	2.56	0.43
15:U:78:LEU:HD13	15:U:97:LEU:HD21	2.01	0.43
18:Z:12:LEU:HA	18:Z:50:LEU:HD13	1.99	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.43
1:A:76:ASN:HD21	1:A:79:THR:H	1.66	0.43
2:B:318:ASN:ND2	2:B:361:ALA:HB2	2.34	0.43
2:B:332:LYS:HG3	2:B:444:ARG:HH21	1.84	0.43
20:B:520:CLA:H122	20:B:522:CLA:H43	2.00	0.43
20:C:491:CLA:H42	20:C:492:CLA:HMD1	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
22:D:356:PQ9:H61	22:D:356:PQ9:H91	1.75	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
3:C:33:PHE:HE1	4:D:229:ALA:HB2	1.82	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
13:O:153:ALA:HB1	13:O:168:PHE:HB3	2.00	0.43
17:X:102:UNK:O	17:X:103:UNK:C	2.66	0.43
24:X:130:BCR:HC31	18:Z:13:VAL:HG13	2.00	0.43
1:A:225:ARG:NH1	2:B:484:PRO:HD3	2.34	0.43
1:A:25:ASP:HA	4:D:251:ARG:NH2	2.32	0.43
1:A:284:TRP:O	1:A:287:ALA:HB3	2.18	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
2:B:271:THR:HG22	2:B:273:TYR:N	2.34	0.43
20:C:498:CLA:H191	30:C:509:DGD:HA91	2.00	0.43
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: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
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
1:A:35:VAL:HG22	24:A:566:BCR:HC42	2.00	0.43
2:B:208:VAL:HG21	20:B:512:CLA:CMC	2.48	0.43
2:B:403:GLY:O	2:B:407:ASN:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:127:UNK:CG	17:X:128:UNK:N	2.81	0.43
2:B:360:PRO:O	2:B:362:PHE:N	2.51	0.43
2:B:368:VAL:O	2:B:368:VAL:HG13	2.19	0.43
3:C:205:ASP:OD2	3:C:205:ASP:C	2.57	0.43
3:C:214:LEU:HD23	3:C:214:LEU:N	2.31	0.43
20:C:491:CLA:CAD	20:C:493:CLA:H12	2.49	0.43
4:D:178:ILE:CG2	4:D:179:PHE:N	2.81	0.43
13:O:231:ASP:OD1	13:O:231:ASP:O	2.37	0.43
14:T:4:ILE:CD1	14:T:4:ILE:C	2.85	0.43
3:C:180:MET:SD	3:C:202:PRO:HG2	2.57	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	0.43
3:C:385:GLN:HB2	3:C:387:TRP:CD1	2.54	0.43
3:C:168:LEU:HD13	20:C:497:CLA:H2	2.01	0.43
4:D:134:ARG:HA	4:D:134:ARG:NE	2.34	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	0.43
24:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
2:B:221:PRO:O	2:B:222:PRO:C	2.56	0.43
20:B:515:CLA:CHA	20:B:515:CLA:HBA1	2.48	0.43
2:B:464:PHE:HD2	20:B:521:CLA:HAC2	1.83	0.43
3:C:323:LYS:O	3:C:324:LEU:HB2	2.19	0.43
3:C:394:GLU:O	3:C:398:HIS:HD2	2.02	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
13:O:32:THR:H	13:O:35:ASP:CB	2.28	0.43
14:T:22:PHE:O	14:T:23:PHE:CD2	2.71	0.43
15:U:66:ILE:HD11	15:U:72:TYR:CZ	2.54	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.00	0.42
3:C:201:ASN:O	3:C:202:PRO:C	2.58	0.42
3:C:417:VAL:O	3:C:417:VAL:HG13	2.18	0.42
3:C:87:ILE:C	3:C:90:PRO:HD2	2.39	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.79	0.42
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.54	0.42
1:A:206:PHE:CD1	21: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
2:B:31:ALA:CA	20:B:515:CLA:HBC3	2.49	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
3:C:104:GLU:O	3:C:105:VAL:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.01	0.42
4:D:313:THR:C	4:D:315:TYR:N	2.72	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.42
13:O:120:THR:OG1	13:O:154:SER:HB3	2.19	0.42
17:X:118:UNK:C	17:X:120:UNK:N	2.80	0.42
2:B:314:TYR:CZ	2:B:316:GLY:HA3	2.55	0.42
20:B:518:CLA:HBD	20:B:518:CLA:HBA1	2.00	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
4:D:246:MET:CE	4:D:264:LYS:HG3	2.49	0.42
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.85	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
13:O:30:THR:HG22	13:O:31:LEU:N	2.33	0.42
1:A:225:ARG:HH12	2:B:483:ASP:CA	2.19	0.42
1:A:261:GLN:O	1:A:264:SER:HB3	2.19	0.42
1:A:69:GLY:O	1:A:80:GLY:HA2	2.19	0.42
20:B:524:CLA:H102	24:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:N	3:C:147:PHE:CD1	2.85	0.42
4:D:103:ARG:HA	4:D:103:ARG:HD3	1.81	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
2:B:125:ASP:O	2:B:128:THR:O	2.38	0.42
2:B:214:LEU:O	2:B:217:ILE:HB	2.18	0.42
2:B:271:THR:HG22	2:B:274:GLN:HG3	2.02	0.42
4:D:47:GLY:HA2	24:D:357:BCR:H332	2.01	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	0.42
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.42
20:B:516:CLA:H72	24: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
3:C:171:GLY:HA3	20:C:502:CLA:H41	2.01	0.42
3:C:472:LEU:H	3:C:472:LEU:HD12	1.84	0.42
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.79	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	0.42
16:V:64:ALA:O	16:V:65:SER:C	2.57	0.42
17:X:54:UNK:O	17:X:55:UNK:C	2.66	0.42
17:X:23:UNK:CG2	18:Z:25:VAL:HG11	2.50	0.42
1:A:33:PHE:CE1	1:A:128:GLY:HA3	2.55	0.42
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.42
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	0.42
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.49	0.42
1:A:184:ILE:HA	20:A:558:CLA:HBC1	2.02	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:103:LEU:HD21	20:B:515:CLA:HMC3	2.01	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
3:C:168:LEU:CD1	20:C:497:CLA:H2	2.49	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42
7:H:54:ILE:O	7:H:55:LEU:HD23	2.20	0.42
12:M:15:VAL:O	12:M:19:SER:CB	2.68	0.42
14:T:2:GLU:O	14:T:3:THR:C	2.57	0.42
32:V:552:HEM:HAD2	32:V:552:HEM:HHA	1.56	0.42
1:A:257:ARG:HH12	1:A:261:GLN:NE2	2.18	0.42
2:B:30:VAL:O	2:B:30:VAL:HG12	2.19	0.42
20:B:515:CLA:H152	20:B:520:CLA:HED1	2.02	0.42
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.82	0.42
7:H:12:ARG:N	7:H:13:PRO:CD	2.82	0.42
11:L:12:LEU:HD13	12:M:25:LEU:HB2	2.02	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.83	0.42
16:V:29:LEU:O	16:V:29:LEU:HG	2.18	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
3:C:138:GLU:O	3:C:139:THR:HB	2.20	0.42
3:C:405:ASN:ND2	30:C:509:DGD:HD5	2.26	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.20	0.42
4:D:274:VAL:HG13	22:D:356:PQ9:H251	2.02	0.42
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
5:E:37:PHE:CD1	5:E:42:LEU:HD23	2.55	0.42
13:O:44:LYS:HA	13:O:72:GLN:CD	2.40	0.42
13:O:98:THR:CG2	13:O:99:ARG:N	2.70	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	0.42
1:A:314:ILE:O	1:A:315:ASN:O	2.38	0.41
2:B:462:PHE:CZ	20:B:523:CLA:HMB3	2.55	0.41
20:C:493:CLA:H171	20:C:500:CLA:HBB2	2.01	0.41
20:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:PHE:HZ	22:D:356:PQ9:H243	1.85	0.41
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
25:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.41
3:C:322:GLN:O	3:C:324:LEU:N	2.49	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
3:C:61:VAL:O	3:C:62:PHE:C	2.57	0.41
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
4:D:267:LEU:CD2	4:D:267:LEU:C	2.88	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	0.41
2:B:10:THR:C	2:B:12:LEU:N	2.73	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
6:F:40:MET:C	6:F:42:PHE:N	2.74	0.41
8:I:33:LYS:HA	8:I:34:ARG:NH2	2.16	0.41
13:O:106:GLN:HE21	13:O:106:GLN:N	2.18	0.41
15:U:69:ARG:HG3	15:U:70:GLY:N	2.33	0.41
16:V:75:ASN:N	16:V:76:PRO:HD3	2.35	0.41
1:A:76:ASN:ND2	1:A:76:ASN:C	2.73	0.41
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.55	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.52	0.41
3:C:334:PRO:O	13:O:182:PHE:HB2	2.19	0.41
17:X:52:UNK:O	17:X:54:UNK:N	2.54	0.41
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.41
1:A:292:THR:C	1:A:294:ALA:H	2.23	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.20	0.41
2:B:208:VAL:HG12	2:B:208:VAL:O	2.20	0.41
20:B:513:CLA:H3A	20:B:513:CLA:CGA	2.50	0.41
3:C:166:ILE:HG23	3:C:245:ILE:CG2	2.42	0.41
3:C:190:ALA:HB3	3:C:193:GLY:C	2.41	0.41
3:C:419:PHE:CD1	3:C:419:PHE:C	2.93	0.41
4:D:178:ILE:O	4:D:181:PHE:N	2.54	0.41
4:D:259:ILE:HG22	4:D:260:ALA:N	2.34	0.41
8:I:27:ASP:O	8:I:28:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:UNK:C	17:X:122:UNK:N	2.82	0.41
1:A:54:ALA:O	1:A:55:ALA:CB	2.69	0.41
2:B:359:MET:HB2	2:B:425:ILE:HG23	2.02	0.41
20:B:521:CLA:C4	20: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
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
24:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
13:O:77:LEU:N	13:O:77:LEU:CD1	2.81	0.41
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.01	0.41
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.41
7:H:46:LEU:HD11	30:H:208:DGD:HA22	2.02	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
2:B:61:PHE:HZ	20:B:517:CLA:HBB1	1.85	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	0.41
3:C:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
3:C:418:ASN:HB3	30:C:509:DGD:C2E	2.51	0.41
4:D:159:ILE:O	4:D:160:TYR:C	2.58	0.41
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.20	0.41
17:X:4:UNK:O	17:X:5:UNK:C	2.69	0.41
3:C:229:ASN:HD22	3:C:231:GLU:CG	2.34	0.41
3:C:416:SER:C	3:C:417:VAL:HG12	2.41	0.41
3:C:56:HIS:O	3:C:59:LEU:N	2.53	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	0.41
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
1:A:321:ILE:HG22	1:A:322:ASN:N	2.35	0.41
2:B:272:ARG:HH12	4:D:164:GLN:HG3	1.86	0.41
3:C:42:LEU:HG	20:C:501:CLA:O1D	2.20	0.41
20:C:502:CLA:HBA2	20:C:502:CLA:O2D	2.20	0.41
10:K:17:ILE:HD11	18:Z:6:GLN:NE2	2.31	0.41
10:K:43:VAL:HG21	17:X:31:UNK:CG	2.51	0.41
1:A:13:LEU:CD2	1:A:13:LEU:H	2.33	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
3:C:109:PHE:O	3:C:110:PRO:C	2.59	0.41
3:C:146:PHE:CD2	3:C:147:PHE:CE1	3.09	0.41
3:C:438:LEU:HD21	30:C:507:DGD:HAH2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:SER:OG	5:E:19:TYR:HB2	2.21	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
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.40
1:A:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	0.40
2:B:68:ARG:HH12	20:B:514:CLA:CED	2.33	0.40
20:B:518:CLA:CHA	20:B:518:CLA:HBA1	2.51	0.40
2:B:87:ASP:O	2:B:88:PRO:C	2.58	0.40
3:C:173:LEU:HD23	3:C:173:LEU:HA	1.86	0.40
20:C:494:CLA:CHA	20:C:494:CLA:HBA1	2.52	0.40
4:D:38:PHE:HZ	4:D:128:ARG:NH2	2.18	0.40
12:M:17:VAL:HG12	12:M:18:PRO:N	2.35	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
21:A:561:PHO:HND	4:D:209:LEU:HD12	1.87	0.40
2:B:12:LEU:CD1	20:B:522:CLA:HBB1	2.51	0.40
2:B:74:SER:C	2:B:76:SER:N	2.74	0.40
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.89	0.40
8:I:31:ASN:HB2	8:I:32:PRO:HD2	2.03	0.40
10:K:45:PHE:C	10:K:46:ARG:OXT	2.58	0.40
13:O:142:ILE:CD1	13:O:142:ILE:N	2.84	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.40
8:I:30:ARG:HG2	8:I:30:ARG:H	1.60	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
15:U:69:ARG:HB2	15:U:69:ARG:HE	1.69	0.40
1:A:206:PHE:HD2	1:A:206:PHE:HA	1.75	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.40
2:B:164:PRO:HD3	20:B:516:CLA:O1D	2.22	0.40
2:B:230:ARG:NH1	2:B:474:LEU:HD22	2.36	0.40
2:B:450:TRP:HB3	20:B:517:CLA:HMB2	2.04	0.40
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.79	0.40
20:C:491:CLA:HMA1	24:C:506:BCR:H401	2.02	0.40
4:D:103:ARG:O	4:D:106:GLN:N	2.55	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
28:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:22:PHE:O	14:T:23:PHE:CG	2.75	0.40
17:X:62:UNK:O	17:X:66:UNK:N	2.55	0.40
17:X:85:UNK:N	17:X:85:UNK:OD1	2.54	0.40
1:A:131:TRP:CD2	1:A:132:GLU:N	2.89	0.40
1:A:255:PHE:CE2	22:A:564:PQ9:H151	2.57	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
3:C:252:ILE:HG22	3:C:252:ILE:O	2.21	0.40
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.40
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
4:D:34:GLY:C	4:D:36:LEU:H	2.25	0.40
8:I:24:LEU:O	8:I:26:GLY:N	2.48	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	3	17
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	14
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	3	20
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	4	23
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	12
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	2	11
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	3	16
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	19
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	6
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	6

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

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

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Mol	Chain	Res	Type
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
3	c	5154	LYS
3	c	5226	SER
3	c	5324	LEU
3	c	5416	SER
4	d	5239	GLN

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Mol	Chain	Res	Type
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
5	E	48	GLY
7	H	26	GLY
8	I	25	SER
9	J	35	GLY
10	K	13	GLU

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Mol	Chain	Res	Type
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
13	o	5138	GLY
13	o	5161	SER
13	o	5233	ARG
15	u	5070	GLY
18	z	5031	GLN

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Mol	Chain	Res	Type
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
7	h	5059	ASN
9	j	5011	TRP
11	l	5005	PRO
11	l	5007	ARG
13	o	5167	ASP

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Mol	Chain	Res	Type
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
13	O	139	GLY
16	V	129	LYS
1	a	5172	MET
1	a	5217	SER
2	b	5089	GLY

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Mol	Chain	Res	Type
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
6	f	5023	VAL
7	h	5058	VAL
18	z	5024	PRO
2	B	86	ILE
2	B	232	GLY

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Mol	Chain	Res	Type
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%)	19	54
1	a	269/280 (96%)	252 (94%)	17 (6%)	21	57
2	B	378/407 (93%)	361 (96%)	17 (4%)	32	71
2	b	378/407 (93%)	360 (95%)	18 (5%)	30	69
3	C	341/374 (91%)	320 (94%)	21 (6%)	21	58
3	c	341/374 (91%)	320 (94%)	21 (6%)	21	58
4	D	273/283 (96%)	259 (95%)	14 (5%)	28	66
4	d	273/283 (96%)	258 (94%)	15 (6%)	25	63
5	E	68/73 (93%)	65 (96%)	3 (4%)	33	72
5	e	68/73 (93%)	66 (97%)	2 (3%)	48	82
6	F	27/39 (69%)	26 (96%)	1 (4%)	39	76
6	f	27/39 (69%)	26 (96%)	1 (4%)	39	76
7	H	50/55 (91%)	42 (84%)	8 (16%)	3	14
7	h	50/55 (91%)	43 (86%)	7 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	27 (84%)	5 (16%)	3	15
8	i	32/35 (91%)	27 (84%)	5 (16%)	3	15
9	J	22/28 (79%)	21 (96%)	1 (4%)	32	71
9	j	22/28 (79%)	21 (96%)	1 (4%)	32	71
10	K	29/30 (97%)	28 (97%)	1 (3%)	42	78
10	k	29/30 (97%)	28 (97%)	1 (3%)	42	78
11	L	34/35 (97%)	31 (91%)	3 (9%)	12	41
11	l	34/35 (97%)	31 (91%)	3 (9%)	12	41
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%)	25	63
13	o	181/208 (87%)	172 (95%)	9 (5%)	28	67
14	T	26/29 (90%)	25 (96%)	1 (4%)	38	75
14	t	26/29 (90%)	25 (96%)	1 (4%)	38	75
15	U	83/89 (93%)	80 (96%)	3 (4%)	40	77
15	u	83/89 (93%)	80 (96%)	3 (4%)	40	77
16	V	117/117 (100%)	113 (97%)	4 (3%)	42	78
16	v	117/117 (100%)	111 (95%)	6 (5%)	28	66
18	Z	43/52 (83%)	42 (98%)	1 (2%)	56	85
18	z	43/52 (83%)	42 (98%)	1 (2%)	56	85
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	25	63

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
1	A	103	ASP
1	A	131	TRP
1	A	155	PHE

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Mol	Chain	Res	Type
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
3	C	355	THR
3	C	377	LEU
3	C	383	ASP

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Mol	Chain	Res	Type
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
11	L	16	SER
13	O	46	PRO
13	O	50	ASP

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Mol	Chain	Res	Type
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
2	b	5191	ASN
2	b	5222	PRO
2	b	5231	MET

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Mol	Chain	Res	Type
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
4	d	5241	GLU
4	d	5246	MET
4	d	5250	ASN

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Mol	Chain	Res	Type
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
16	v	5081	ARG
16	v	5111	GLU
16	v	5122	ARG

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Mol	Chain	Res	Type
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
4	D	224	GLN
4	D	250	ASN
4	D	255	GLN

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Mol	Chain	Res	Type
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
3	c	5398	HIS
3	c	5415	ASN
4	d	5061	HIS

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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
26	SQD	A	5212	-	25,26,54	2.82	12 (48%)	35,37,65	3.15	13 (37%)
20	CLA	A	558	1	56,73,73	1.32	5 (8%)	65,113,113	1.54	14 (21%)
20	CLA	A	559	-	56,73,73	1.36	4 (7%)	65,113,113	1.44	9 (13%)
20	CLA	A	560	-	56,73,73	1.35	5 (8%)	65,113,113	1.56	15 (23%)
21	PHO	A	561	-	67,69,69	1.01	4 (5%)	87,99,99	1.42	16 (18%)
21	PHO	A	562	-	67,69,69	1.03	6 (8%)	87,99,99	1.48	15 (17%)
20	CLA	A	563	-	46,63,73	1.42	6 (13%)	53,101,113	1.65	14 (26%)
22	PQ9	A	564	-	30,30,45	0.85	1 (3%)	39,39,57	1.45	8 (20%)
23	OEC	A	565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
24	BCR	A	566	-	41,41,41	1.57	7 (17%)	56,56,56	2.09	21 (37%)
25	LHG	A	567	-	38,38,48	1.87	5 (13%)	39,44,54	1.49	4 (10%)
26	SQD	A	568	-	53,54,54	2.45	28 (52%)	63,65,65	3.02	20 (31%)
27	LMT	A	569	-	36,36,36	1.53	6 (16%)	47,47,47	1.09	2 (4%)
20	CLA	B	511	-	32,49,73	1.88	9 (28%)	37,84,113	1.75	9 (24%)
20	CLA	B	512	2	56,73,73	1.31	3 (5%)	65,113,113	1.52	14 (21%)
20	CLA	B	513	2	56,73,73	1.42	6 (10%)	65,113,113	1.57	13 (20%)
20	CLA	B	514	2	56,73,73	1.44	5 (8%)	65,113,113	1.47	13 (20%)
20	CLA	B	515	-	56,73,73	1.37	6 (10%)	65,113,113	1.64	14 (21%)
20	CLA	B	516	-	56,73,73	1.31	4 (7%)	65,113,113	1.53	11 (16%)
20	CLA	B	517	-	56,73,73	1.41	5 (8%)	65,113,113	1.67	15 (23%)
20	CLA	B	518	2	56,73,73	1.38	5 (8%)	65,113,113	1.59	14 (21%)
20	CLA	B	519	-	56,73,73	1.48	4 (7%)	65,113,113	1.49	14 (21%)
20	CLA	B	520	-	56,73,73	1.37	7 (12%)	65,113,113	1.48	13 (20%)
20	CLA	B	521	2	56,73,73	1.44	7 (12%)	65,113,113	1.56	13 (20%)
20	CLA	B	522	-	56,73,73	1.36	4 (7%)	65,113,113	1.50	9 (13%)
20	CLA	B	523	-	56,73,73	1.49	4 (7%)	65,113,113	1.53	13 (20%)
20	CLA	B	524	2	47,64,73	1.45	4 (8%)	54,102,113	1.63	12 (22%)
20	CLA	B	525	-	56,73,73	1.39	4 (7%)	65,113,113	1.53	12 (18%)
20	CLA	B	526	-	56,73,73	1.53	8 (14%)	65,113,113	1.55	13 (20%)
24	BCR	B	527	-	41,41,41	1.70	8 (19%)	56,56,56	2.03	16 (28%)
24	BCR	B	528	-	41,41,41	1.86	6 (14%)	56,56,56	1.97	15 (26%)
24	BCR	B	529	-	41,41,41	1.79	8 (19%)	56,56,56	2.17	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.21	6 (10%)
20	CLA	C	491	3	56,73,73	1.39	5 (8%)	65,113,113	1.40	10 (15%)
20	CLA	C	492	3	51,68,73	1.36	7 (13%)	59,107,113	1.58	13 (22%)
20	CLA	C	493	3	56,73,73	1.36	4 (7%)	65,113,113	1.56	15 (23%)
20	CLA	C	494	-	37,54,73	1.62	4 (10%)	43,90,113	1.81	11 (25%)
20	CLA	C	495	-	56,73,73	1.52	6 (10%)	65,113,113	1.65	14 (21%)
20	CLA	C	496	3	56,73,73	1.46	7 (12%)	65,113,113	1.55	15 (23%)
20	CLA	C	497	-	56,73,73	1.34	5 (8%)	65,113,113	1.61	13 (20%)
20	CLA	C	498	3	56,73,73	1.29	4 (7%)	65,113,113	1.50	13 (20%)
20	CLA	C	499	-	38,55,73	1.64	4 (10%)	44,91,113	1.73	14 (31%)
20	CLA	C	500	-	56,73,73	1.29	6 (10%)	65,113,113	1.47	12 (18%)
20	CLA	C	501	3	56,73,73	1.50	4 (7%)	65,113,113	1.48	11 (16%)
20	CLA	C	502	-	42,59,73	1.66	8 (19%)	48,96,113	1.79	13 (27%)
20	CLA	C	503	3	41,58,73	1.63	4 (9%)	47,95,113	1.68	12 (25%)
24	BCR	C	504	-	41,41,41	1.83	7 (17%)	56,56,56	2.16	22 (39%)
24	BCR	C	505	-	41,41,41	1.91	8 (19%)	56,56,56	2.08	16 (28%)
24	BCR	C	506	-	41,41,41	1.71	9 (21%)	56,56,56	2.17	21 (37%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.51	7 (10%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.72	11 (17%)
30	DGD	C	509	-	58,58,67	1.11	6 (10%)	72,72,81	1.43	7 (9%)
31	BCT	D	353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	D	354	4	56,73,73	1.36	6 (10%)	65,113,113	1.53	12 (18%)
20	CLA	D	355	-	41,58,73	1.71	5 (12%)	47,95,113	1.73	12 (25%)
22	PQ9	D	356	-	30,30,45	0.86	1 (3%)	39,39,57	1.61	8 (20%)
24	BCR	D	357	-	41,41,41	1.90	9 (21%)	56,56,56	2.22	20 (35%)
28	MGE	D	358	-	47,47,48	1.21	5 (10%)	55,55,56	1.00	3 (5%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.07	5 (10%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.16	4 (7%)
32	HEM	F	51	5,6	28,50,50	1.95	10 (35%)	17,82,82	2.55	6 (35%)
24	BCR	H	107	-	41,41,41	2.07	7 (17%)	56,56,56	2.24	24 (42%)
30	DGD	H	208	-	55,55,67	1.47	10 (18%)	69,69,81	1.55	8 (11%)
28	MGE	I	201	-	48,48,48	1.10	6 (12%)	56,56,56	1.12	5 (8%)
28	MGE	L	210	-	48,48,48	0.98	3 (6%)	56,56,56	1.19	5 (8%)
26	SQD	L	5213	-	46,47,54	2.70	24 (52%)	56,58,65	2.84	15 (26%)
27	LMT	M	5216	-	36,36,36	1.46	8 (22%)	47,47,47	0.94	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMT	T	217	-	36,36,36	1.41	7 (19%)	47,47,47	1.06	4 (8%)
24	BCR	T	5104	-	41,41,41	1.51	9 (21%)	56,56,56	2.26	22 (39%)
32	HEM	V	552	16	28,50,50	1.86	10 (35%)	17,82,82	2.19	5 (29%)
24	BCR	X	130	-	41,41,41	1.89	10 (24%)	56,56,56	2.49	24 (42%)
26	SQD	a	212	-	25,26,54	3.07	13 (52%)	35,37,65	3.30	15 (42%)
20	CLA	a	5558	1	56,73,73	1.32	7 (12%)	65,113,113	1.48	12 (18%)
20	CLA	a	5559	-	56,73,73	1.27	3 (5%)	65,113,113	1.44	10 (15%)
20	CLA	a	5560	-	56,73,73	1.31	5 (8%)	65,113,113	1.55	14 (21%)
21	PHO	a	5561	-	67,69,69	1.02	5 (7%)	87,99,99	1.36	13 (14%)
21	PHO	a	5562	-	67,69,69	1.03	5 (7%)	87,99,99	1.47	15 (17%)
20	CLA	a	5563	-	46,63,73	1.46	6 (13%)	53,101,113	1.59	12 (22%)
22	PQ9	a	5564	-	30,30,45	0.89	1 (3%)	39,39,57	1.42	8 (20%)
23	OEC	a	5565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
24	BCR	a	5566	-	41,41,41	1.64	7 (17%)	56,56,56	2.09	22 (39%)
25	LHG	a	5567	-	38,38,48	1.91	5 (13%)	39,44,54	1.45	3 (7%)
27	LMT	a	5568	-	36,36,36	1.45	6 (16%)	47,47,47	1.12	1 (2%)
20	CLA	b	5511	-	32,49,73	2.03	8 (25%)	37,84,113	1.76	10 (27%)
20	CLA	b	5512	2	56,73,73	1.32	5 (8%)	65,113,113	1.52	13 (20%)
20	CLA	b	5513	2	56,73,73	1.34	5 (8%)	65,113,113	1.56	14 (21%)
20	CLA	b	5514	2	56,73,73	1.40	4 (7%)	65,113,113	1.51	12 (18%)
20	CLA	b	5515	-	56,73,73	1.37	7 (12%)	65,113,113	1.62	14 (21%)
20	CLA	b	5516	-	56,73,73	1.40	5 (8%)	65,113,113	1.59	12 (18%)
20	CLA	b	5517	-	56,73,73	1.34	5 (8%)	65,113,113	1.58	13 (20%)
20	CLA	b	5518	2	56,73,73	1.34	4 (7%)	65,113,113	1.60	17 (26%)
20	CLA	b	5519	-	56,73,73	1.44	5 (8%)	65,113,113	1.52	13 (20%)
20	CLA	b	5520	-	56,73,73	1.42	6 (10%)	65,113,113	1.48	13 (20%)
20	CLA	b	5521	2	56,73,73	1.25	4 (7%)	65,113,113	1.55	15 (23%)
20	CLA	b	5522	-	56,73,73	1.38	5 (8%)	65,113,113	1.48	9 (13%)
20	CLA	b	5523	-	56,73,73	1.45	5 (8%)	65,113,113	1.59	13 (20%)
20	CLA	b	5524	2	47,64,73	1.42	3 (6%)	54,102,113	1.57	11 (20%)
20	CLA	b	5525	-	56,73,73	1.44	4 (7%)	65,113,113	1.51	12 (18%)
20	CLA	b	5526	-	56,73,73	1.64	8 (14%)	65,113,113	1.61	14 (21%)
24	BCR	b	5527	-	41,41,41	1.52	8 (19%)	56,56,56	1.95	14 (25%)
24	BCR	b	5528	-	41,41,41	1.68	6 (14%)	56,56,56	2.00	17 (30%)
24	BCR	b	5529	-	41,41,41	1.67	8 (19%)	56,56,56	2.09	18 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.15	6 (10%)
20	CLA	c	5491	3	56,73,73	1.35	5 (8%)	65,113,113	1.50	11 (16%)
20	CLA	c	5492	3	51,68,73	1.37	6 (11%)	59,107,113	1.53	11 (18%)
20	CLA	c	5493	3	56,73,73	1.37	5 (8%)	65,113,113	1.56	15 (23%)
20	CLA	c	5494	-	37,54,73	1.63	4 (10%)	43,90,113	1.72	11 (25%)
20	CLA	c	5495	-	56,73,73	1.45	6 (10%)	65,113,113	1.66	16 (24%)
20	CLA	c	5496	-	56,73,73	1.47	8 (14%)	65,113,113	1.50	12 (18%)
20	CLA	c	5497	-	56,73,73	1.43	6 (10%)	65,113,113	1.57	14 (21%)
20	CLA	c	5498	3	56,73,73	1.36	6 (10%)	65,113,113	1.51	14 (21%)
20	CLA	c	5499	-	38,55,73	1.61	6 (15%)	44,91,113	1.65	10 (22%)
20	CLA	c	5500	-	56,73,73	1.37	5 (8%)	65,113,113	1.50	14 (21%)
20	CLA	c	5501	3	56,73,73	1.39	4 (7%)	65,113,113	1.44	10 (15%)
20	CLA	c	5502	-	42,59,73	1.73	7 (16%)	48,96,113	1.76	12 (25%)
20	CLA	c	5503	3	41,58,73	1.78	6 (14%)	47,95,113	1.64	9 (19%)
24	BCR	c	5504	-	41,41,41	2.11	6 (14%)	56,56,56	2.13	22 (39%)
24	BCR	c	5505	-	41,41,41	1.93	8 (19%)	56,56,56	2.09	18 (32%)
24	BCR	c	5506	-	41,41,41	1.92	9 (21%)	56,56,56	2.10	20 (35%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.50	6 (8%)
30	DGD	c	5508	-	48,48,67	1.48	9 (18%)	62,62,81	1.76	12 (19%)
30	DGD	c	5509	-	58,58,67	1.34	7 (12%)	72,72,81	1.42	6 (8%)
31	BCT	d	5353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	d	5354	4	56,73,73	1.32	7 (12%)	65,113,113	1.53	12 (18%)
20	CLA	d	5355	-	41,58,73	1.81	7 (17%)	47,95,113	1.68	11 (23%)
22	PQ9	d	5356	-	30,30,45	0.78	0	39,39,57	1.60	6 (15%)
24	BCR	d	5357	-	41,41,41	1.95	8 (19%)	56,56,56	2.28	21 (37%)
26	SQD	d	5358	-	53,54,54	2.44	27 (50%)	63,65,65	2.90	20 (31%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	1.00	3 (5%)
28	MGE	d	5360	-	41,41,48	1.20	6 (14%)	49,49,56	1.09	5 (10%)
28	MGE	d	5361	-	48,48,48	1.05	4 (8%)	56,56,56	1.10	3 (5%)
32	HEM	f	5051	5,6	28,50,50	1.99	10 (35%)	17,82,82	2.54	8 (47%)
24	BCR	h	5107	-	41,41,41	1.97	7 (17%)	56,56,56	2.24	25 (44%)
30	DGD	h	5208	-	55,55,67	1.38	9 (16%)	69,69,81	1.56	8 (11%)
28	MGE	i	5201	-	48,48,48	1.25	8 (16%)	56,56,56	1.13	4 (7%)
28	MGE	l	5210	-	48,48,48	0.90	3 (6%)	56,56,56	1.16	5 (8%)
27	LMT	m	216	-	36,36,36	1.47	7 (19%)	47,47,47	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	t	104	-	41,41,41	1.63	9 (21%)	56,56,56	2.22	22 (39%)
26	SQD	t	213	-	46,47,54	2.69	22 (47%)	56,58,65	2.95	17 (30%)
27	LMT	t	5217	-	36,36,36	1.46	5 (13%)	47,47,47	1.04	3 (6%)
32	HEM	v	5552	16	28,50,50	2.01	9 (32%)	17,82,82	2.26	6 (35%)
24	BCR	x	5130	-	41,41,41	1.93	8 (19%)	56,56,56	2.48	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
26	SQD	A	5212	-	-	0/19/39/69	0/1/1/1
20	CLA	A	558	1	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	559	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	560	-	3/3/20/25	0/37/135/135	0/0/9/9
21	PHO	A	561	-	-	0/53/103/103	0/1/6/6
21	PHO	A	562	-	-	0/53/103/103	0/1/6/6
20	CLA	A	563	-	3/3/18/25	0/25/123/135	0/0/9/9
22	PQ9	A	564	-	-	0/23/43/61	0/1/1/1
23	OEC	A	565	1,3	-	0/0/0/54	0/0/0/5
24	BCR	A	566	-	-	0/29/63/63	0/2/2/2
25	LHG	A	567	-	-	0/43/43/53	0/0/0/0
26	SQD	A	568	-	-	0/49/69/69	0/1/1/1
27	LMT	A	569	-	-	0/21/61/61	0/2/2/2
20	CLA	B	511	-	3/3/15/25	0/8/106/135	0/0/9/9
20	CLA	B	512	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	513	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	514	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	515	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	516	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	517	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	518	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	519	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	520	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	521	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	522	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	523	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	524	2	3/3/18/25	0/27/125/135	0/0/9/9
20	CLA	B	525	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	526	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	527	-	-	0/29/63/63	0/2/2/2
24	BCR	B	528	-	-	0/29/63/63	0/2/2/2
24	BCR	B	529	-	-	0/29/63/63	0/2/2/2
28	MGE	B	530	-	-	0/43/63/63	0/1/1/1
20	CLA	C	491	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	492	3	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	C	493	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	494	-	3/3/16/25	0/15/113/135	0/0/9/9
20	CLA	C	495	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	496	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	497	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	498	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	499	-	3/3/16/25	0/16/114/135	0/0/9/9
20	CLA	C	500	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	501	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	502	-	3/3/17/25	0/21/119/135	0/0/9/9
20	CLA	C	503	3	3/3/17/25	0/19/117/135	0/0/9/9
24	BCR	C	504	-	-	0/29/63/63	0/2/2/2
24	BCR	C	505	-	-	0/29/63/63	0/2/2/2
24	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
31	BCT	D	353	19	-	0/0/0/0	0/0/0/0
20	CLA	D	354	4	3/3/20/25	1/37/135/135	0/0/9/9
20	CLA	D	355	-	3/3/17/25	0/19/117/135	0/0/9/9
22	PQ9	D	356	-	-	0/23/43/61	0/1/1/1
24	BCR	D	357	-	-	0/29/63/63	0/2/2/2
28	MGE	D	358	-	-	0/42/62/63	0/1/1/1
28	MGE	D	359	-	-	0/36/56/63	0/1/1/1
28	MGE	D	360	-	-	0/43/63/63	0/1/1/1
32	HEM	F	51	5,6	-	0/6/54/54	0/0/8/8
24	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	MGE	I	201	-	-	0/43/63/63	0/1/1/1
28	MGE	L	210	-	-	0/43/63/63	0/1/1/1
26	SQD	L	5213	-	-	0/42/62/69	0/1/1/1
27	LMT	M	5216	-	-	0/21/61/61	0/2/2/2
27	LMT	T	217	-	-	0/21/61/61	0/2/2/2
24	BCR	T	5104	-	-	0/29/63/63	0/2/2/2
32	HEM	V	552	16	-	0/6/54/54	0/0/8/8
24	BCR	X	130	-	-	0/29/63/63	0/2/2/2
26	SQD	a	212	-	-	0/19/39/69	0/1/1/1
20	CLA	a	5558	1	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	5559	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	5560	-	3/3/20/25	0/37/135/135	0/0/9/9
21	PHO	a	5561	-	-	0/53/103/103	0/1/6/6
21	PHO	a	5562	-	-	0/53/103/103	0/1/6/6
20	CLA	a	5563	-	3/3/18/25	0/25/123/135	0/0/9/9
22	PQ9	a	5564	-	-	0/23/43/61	0/1/1/1
23	OEC	a	5565	1,3	-	0/0/0/54	0/0/0/5
24	BCR	a	5566	-	-	0/29/63/63	0/2/2/2
25	LHG	a	5567	-	-	0/43/43/53	0/0/0/0
27	LMT	a	5568	-	-	0/21/61/61	0/2/2/2
20	CLA	b	5511	-	3/3/15/25	0/8/106/135	0/0/9/9
20	CLA	b	5512	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5513	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5514	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5515	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5516	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5517	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5518	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5519	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5520	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5521	2	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5522	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5523	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5524	2	3/3/18/25	0/27/125/135	0/0/9/9
20	CLA	b	5525	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	5526	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	5527	-	-	0/29/63/63	0/2/2/2
24	BCR	b	5528	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	5529	-	-	0/29/63/63	0/2/2/2
28	MGE	b	5530	-	-	0/43/63/63	0/1/1/1
20	CLA	c	5491	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5492	3	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	c	5493	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5494	-	3/3/16/25	0/15/113/135	0/0/9/9
20	CLA	c	5495	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5496	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5497	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5498	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5499	-	3/3/16/25	0/16/114/135	0/0/9/9
20	CLA	c	5500	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5501	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	5502	-	3/3/17/25	0/21/119/135	0/0/9/9
20	CLA	c	5503	3	3/3/17/25	0/19/117/135	0/0/9/9
24	BCR	c	5504	-	-	0/29/63/63	0/2/2/2
24	BCR	c	5505	-	-	0/29/63/63	0/2/2/2
24	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
31	BCT	d	5353	19	-	0/0/0/0	0/0/0/0
20	CLA	d	5354	4	3/3/20/25	1/37/135/135	0/0/9/9
20	CLA	d	5355	-	3/3/17/25	0/19/117/135	0/0/9/9
22	PQ9	d	5356	-	-	0/23/43/61	0/1/1/1
24	BCR	d	5357	-	-	0/29/63/63	0/2/2/2
26	SQD	d	5358	-	-	0/49/69/69	0/1/1/1
28	MGE	d	5359	-	-	0/42/62/63	0/1/1/1
28	MGE	d	5360	-	-	0/36/56/63	0/1/1/1
28	MGE	d	5361	-	-	0/43/63/63	0/1/1/1
32	HEM	f	5051	5,6	-	0/6/54/54	0/0/8/8
24	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
28	MGE	i	5201	-	-	0/43/63/63	0/1/1/1
28	MGE	l	5210	-	-	0/43/63/63	0/1/1/1
27	LMT	m	216	-	-	0/21/61/61	0/2/2/2
24	BCR	t	104	-	-	0/29/63/63	0/2/2/2
26	SQD	t	213	-	-	0/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
32	HEM	v	5552	16	-	0/6/54/54	0/0/8/8
24	BCR	x	5130	-	-	0/29/63/63	0/2/2/2

All (915) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	v	5552	HEM	CAD-C3D	-4.12	1.44	1.52
32	V	552	HEM	CAD-C3D	-3.60	1.45	1.52
20	A	563	CLA	C1B-CHB	-3.46	1.31	1.40
20	D	354	CLA	C1B-CHB	-3.42	1.31	1.40
32	f	5051	HEM	C4D-ND	-3.37	1.32	1.36
32	f	5051	HEM	CAD-C3D	-3.34	1.46	1.52
32	F	51	HEM	CAD-C3D	-3.34	1.46	1.52
26	A	568	SQD	O6-C44	-3.25	1.38	1.43
20	a	5563	CLA	C1B-CHB	-3.24	1.31	1.40
20	d	5354	CLA	C1B-CHB	-3.21	1.31	1.40
21	A	562	PHO	CHB-C1B	-3.16	1.32	1.38
20	B	512	CLA	C1B-CHB	-3.11	1.31	1.40
20	a	5558	CLA	C1B-CHB	-3.09	1.32	1.40
26	t	213	SQD	C20-C19	-3.06	1.34	1.51
20	A	560	CLA	C1B-CHB	-3.02	1.32	1.40
21	a	5562	PHO	CHB-C1B	-3.01	1.33	1.38
26	L	5213	SQD	C12-C11	-2.99	1.34	1.51
26	d	5358	SQD	O6-C44	-2.98	1.38	1.43
26	L	5213	SQD	C17-C16	-2.96	1.34	1.51
20	C	498	CLA	C1B-CHB	-2.96	1.32	1.40
26	L	5213	SQD	C11-C10	-2.96	1.34	1.51
20	A	558	CLA	C1B-CHB	-2.96	1.32	1.40
20	b	5521	CLA	C1B-CHB	-2.96	1.32	1.40
26	L	5213	SQD	C20-C19	-2.93	1.34	1.51
20	B	513	CLA	C1B-CHB	-2.92	1.32	1.40
20	d	5354	CLA	CAA-CBA	-2.90	1.43	1.52
20	b	5515	CLA	C1B-CHB	-2.90	1.32	1.40
20	b	5512	CLA	C1B-CHB	-2.89	1.32	1.40
26	t	213	SQD	C19-C18	-2.88	1.35	1.51
20	D	354	CLA	CAA-CBA	-2.88	1.43	1.52
20	B	520	CLA	C1B-CHB	-2.87	1.32	1.40
26	t	213	SQD	C14-C13	-2.86	1.35	1.51
26	L	5213	SQD	C19-C18	-2.84	1.35	1.51
20	B	526	CLA	C1B-CHB	-2.82	1.32	1.40
20	c	5496	CLA	C1B-CHB	-2.81	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	515	CLA	C1B-CHB	-2.80	1.32	1.40
26	A	568	SQD	C17-C16	-2.79	1.35	1.51
26	t	213	SQD	C15-C14	-2.79	1.35	1.51
26	L	5213	SQD	C18-C17	-2.79	1.35	1.51
24	D	357	BCR	C19-C18	-2.78	1.39	1.45
26	L	5213	SQD	C13-C12	-2.76	1.35	1.51
20	c	5494	CLA	C1B-CHB	-2.76	1.32	1.40
20	C	494	CLA	C1B-CHB	-2.75	1.32	1.40
26	t	213	SQD	C12-C11	-2.73	1.36	1.51
26	t	213	SQD	C11-C10	-2.73	1.36	1.51
20	C	500	CLA	C1B-CHB	-2.72	1.32	1.40
20	a	5559	CLA	C1B-CHB	-2.72	1.32	1.40
20	a	5560	CLA	C1B-CHB	-2.72	1.33	1.40
20	B	525	CLA	C1B-CHB	-2.72	1.33	1.40
26	A	568	SQD	C12-C11	-2.71	1.36	1.51
26	t	213	SQD	C17-C16	-2.71	1.36	1.51
20	c	5497	CLA	C1B-CHB	-2.69	1.33	1.40
21	A	561	PHO	CAA-CBA	-2.69	1.44	1.52
20	B	517	CLA	C1B-CHB	-2.67	1.33	1.40
26	L	5213	SQD	C15-C14	-2.66	1.36	1.51
24	t	104	BCR	C23-C22	-2.66	1.40	1.45
20	b	5516	CLA	C1B-CHB	-2.66	1.33	1.40
26	t	213	SQD	C13-C12	-2.65	1.36	1.51
20	b	5522	CLA	C1B-CHB	-2.65	1.33	1.40
20	b	5526	CLA	C1B-CHB	-2.64	1.33	1.40
26	L	5213	SQD	C16-C15	-2.64	1.36	1.51
26	A	568	SQD	C16-C15	-2.64	1.36	1.51
20	B	521	CLA	C1B-CHB	-2.62	1.33	1.40
26	d	5358	SQD	C17-C16	-2.62	1.36	1.51
26	L	5213	SQD	C14-C13	-2.62	1.36	1.51
26	A	568	SQD	C15-C14	-2.61	1.36	1.51
20	c	5493	CLA	C1B-CHB	-2.59	1.33	1.40
20	C	492	CLA	C1B-CHB	-2.59	1.33	1.40
26	A	568	SQD	C11-C10	-2.59	1.36	1.51
26	t	213	SQD	C16-C15	-2.58	1.36	1.51
20	b	5517	CLA	C1B-CHB	-2.57	1.33	1.40
26	t	213	SQD	C18-C17	-2.56	1.37	1.51
20	b	5525	CLA	C1B-CHB	-2.55	1.33	1.40
20	A	558	CLA	CAA-CBA	-2.55	1.44	1.52
20	d	5355	CLA	C1B-CHB	-2.54	1.33	1.40
20	b	5513	CLA	C1B-CHB	-2.53	1.33	1.40
26	L	5213	SQD	O6-C44	-2.53	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5524	CLA	C1B-CHB	-2.52	1.33	1.40
20	C	491	CLA	C1B-CHB	-2.52	1.33	1.40
24	c	5506	BCR	C19-C18	-2.51	1.40	1.45
20	a	5558	CLA	CAA-CBA	-2.51	1.44	1.52
24	b	5527	BCR	C19-C18	-2.51	1.40	1.45
20	B	524	CLA	C1B-CHB	-2.49	1.33	1.40
26	d	5358	SQD	C32-C31	-2.47	1.37	1.51
20	A	559	CLA	C1B-CHB	-2.47	1.33	1.40
26	A	568	SQD	C13-C12	-2.46	1.37	1.51
26	d	5358	SQD	C20-C19	-2.45	1.37	1.51
26	A	568	SQD	C14-C13	-2.45	1.37	1.51
26	a	212	SQD	O6-C44	-2.44	1.39	1.43
24	T	5104	BCR	C23-C22	-2.44	1.40	1.45
20	b	5520	CLA	C1B-CHB	-2.43	1.33	1.40
32	F	51	HEM	C4D-ND	-2.42	1.33	1.36
20	c	5492	CLA	C1B-CHB	-2.42	1.33	1.40
20	c	5498	CLA	C1B-CHB	-2.41	1.33	1.40
20	B	516	CLA	C1B-CHB	-2.41	1.33	1.40
26	d	5358	SQD	C11-C10	-2.40	1.37	1.51
20	B	523	CLA	C1B-CHB	-2.39	1.33	1.40
26	d	5358	SQD	C12-C11	-2.39	1.38	1.51
26	d	5358	SQD	C33-C32	-2.39	1.38	1.51
20	C	493	CLA	C1B-CHB	-2.39	1.33	1.40
26	A	5212	SQD	O6-C44	-2.38	1.39	1.43
24	T	5104	BCR	C29-C28	-2.38	1.46	1.52
26	d	5358	SQD	C15-C14	-2.37	1.38	1.51
26	t	213	SQD	C21-C20	-2.37	1.34	1.51
26	d	5358	SQD	C19-C18	-2.36	1.38	1.51
21	a	5561	PHO	CAA-CBA	-2.36	1.45	1.52
26	A	568	SQD	C33-C32	-2.34	1.38	1.51
24	t	104	BCR	C29-C28	-2.34	1.46	1.52
26	d	5358	SQD	C16-C15	-2.34	1.38	1.51
20	c	5500	CLA	C1B-CHB	-2.31	1.34	1.40
20	B	522	CLA	C1B-CHB	-2.30	1.34	1.40
26	A	568	SQD	C32-C31	-2.30	1.38	1.51
21	a	5561	PHO	CHB-C1B	-2.29	1.34	1.38
20	C	502	CLA	C1B-CHB	-2.28	1.34	1.40
20	c	5499	CLA	C1B-CHB	-2.27	1.34	1.40
28	b	5530	MGE	O1G-C1G	-2.27	1.40	1.45
26	d	5358	SQD	C14-C13	-2.26	1.38	1.51
20	B	514	CLA	C1B-CHB	-2.26	1.34	1.40
26	A	568	SQD	C19-C18	-2.25	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	5358	SQD	C36-C35	-2.25	1.38	1.51
26	L	5213	SQD	C21-C20	-2.25	1.35	1.51
20	c	5502	CLA	C1B-CHB	-2.24	1.34	1.40
32	v	5552	HEM	C4D-ND	-2.24	1.34	1.36
26	A	568	SQD	C18-C17	-2.24	1.38	1.51
24	B	527	BCR	C19-C18	-2.23	1.41	1.45
26	A	568	SQD	C35-C34	-2.22	1.38	1.51
26	A	568	SQD	C34-C33	-2.21	1.39	1.51
20	b	5523	CLA	C1B-CHB	-2.20	1.34	1.40
20	b	5512	CLA	CAA-CBA	-2.20	1.45	1.52
20	d	5354	CLA	C3A-C4A	-2.20	1.44	1.51
26	d	5358	SQD	C13-C12	-2.19	1.39	1.51
26	A	568	SQD	C20-C19	-2.18	1.39	1.51
20	C	497	CLA	C1B-CHB	-2.18	1.34	1.40
26	d	5358	SQD	C35-C34	-2.17	1.39	1.51
20	c	5491	CLA	C1B-CHB	-2.17	1.34	1.40
20	b	5514	CLA	C1B-CHB	-2.17	1.34	1.40
20	a	5558	CLA	CBA-CGA	-2.16	1.44	1.50
20	b	5519	CLA	C1B-CHB	-2.16	1.34	1.40
21	A	561	PHO	CHB-C1B	-2.15	1.34	1.38
26	A	568	SQD	C36-C35	-2.15	1.39	1.51
20	B	521	CLA	CBA-CGA	-2.14	1.44	1.50
20	b	5515	CLA	C3A-C2A	-2.14	1.48	1.54
26	d	5358	SQD	C34-C33	-2.14	1.39	1.51
24	c	5505	BCR	C19-C18	-2.12	1.41	1.45
20	D	354	CLA	C3B-C2B	-2.11	1.37	1.40
26	d	5358	SQD	C18-C17	-2.11	1.39	1.51
21	a	5561	PHO	CBA-CGA	-2.11	1.44	1.50
20	d	5354	CLA	CBA-CGA	-2.10	1.44	1.50
20	b	5518	CLA	C1B-CHB	-2.10	1.34	1.40
26	t	213	SQD	O6-C44	-2.08	1.40	1.43
21	A	562	PHO	C1D-C2D	-2.08	1.41	1.45
24	A	566	BCR	C19-C18	-2.07	1.41	1.45
20	c	5492	CLA	C1C-NC	-2.07	1.34	1.37
21	a	5562	PHO	C1D-C2D	-2.07	1.41	1.45
24	d	5357	BCR	C19-C18	-2.07	1.41	1.45
20	b	5526	CLA	CAA-CBA	-2.06	1.46	1.52
24	C	505	BCR	C19-C18	-2.06	1.41	1.45
24	C	506	BCR	C19-C18	-2.06	1.41	1.45
24	b	5527	BCR	C23-C22	-2.05	1.41	1.45
20	C	499	CLA	C1B-CHB	-2.04	1.34	1.40
20	B	515	CLA	C3A-C2A	-2.03	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5515	CLA	CAA-CBA	-2.03	1.46	1.52
32	V	552	HEM	C3C-C2C	-2.03	1.37	1.40
20	c	5495	CLA	C1B-CHB	-2.01	1.34	1.40
20	C	496	CLA	C1B-CHB	-2.01	1.34	1.40
20	B	526	CLA	CAA-CBA	-2.00	1.46	1.52
30	c	5508	DGD	C3D-C2D	2.00	1.57	1.52
32	F	51	HEM	C2A-C3A	2.00	1.43	1.37
24	T	5104	BCR	C26-C25	2.01	1.37	1.34
20	d	5355	CLA	CMD-C2D	2.01	1.55	1.51
28	i	5201	MGE	C3G-C2G	2.01	1.56	1.50
20	B	518	CLA	OBD-CAD	2.01	1.25	1.22
20	B	520	CLA	C1C-C2C	2.01	1.48	1.44
20	d	5354	CLA	C1C-C2C	2.01	1.48	1.44
27	T	217	LMT	C3B-C2B	2.01	1.57	1.52
20	A	560	CLA	C4C-C3C	2.02	1.48	1.45
20	c	5496	CLA	C4C-NC	2.02	1.40	1.37
20	C	495	CLA	C4-C3	2.02	1.55	1.50
32	f	5051	HEM	C2A-C3A	2.02	1.43	1.37
30	c	5509	DGD	O6E-C5E	2.03	1.49	1.44
20	C	498	CLA	CAA-C2A	2.03	1.58	1.54
24	x	5130	BCR	C24-C23	2.03	1.39	1.33
32	V	552	HEM	C2A-C3A	2.03	1.43	1.37
24	X	130	BCR	C24-C23	2.03	1.39	1.33
20	A	559	CLA	CHC-C1C	2.03	1.41	1.35
24	c	5506	BCR	C14-C13	2.03	1.38	1.35
20	C	502	CLA	C4C-C3C	2.03	1.48	1.45
24	T	5104	BCR	C37-C22	2.04	1.55	1.50
20	b	5512	CLA	C4C-C3C	2.04	1.48	1.45
20	c	5502	CLA	CMB-C2B	2.04	1.55	1.51
27	T	217	LMT	C1B-C2B	2.04	1.58	1.52
20	a	5563	CLA	C4-C3	2.04	1.55	1.50
20	B	517	CLA	CMB-C2B	2.04	1.55	1.51
30	c	5509	DGD	O1G-C1A	2.04	1.39	1.33
27	T	217	LMT	O5'-C1'	2.05	1.46	1.41
28	d	5360	MGE	O2G-C1B	2.05	1.40	1.34
30	h	5208	DGD	C4E-C5E	2.05	1.57	1.53
20	b	5522	CLA	C4-C3	2.05	1.56	1.50
21	A	562	PHO	CHD-C1D	2.05	1.42	1.38
28	D	360	MGE	O2G-C1B	2.05	1.40	1.34
20	C	492	CLA	OBD-CAD	2.06	1.25	1.22
28	I	201	MGE	C3G-C2G	2.06	1.56	1.50
20	C	499	CLA	CAA-C2A	2.06	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	497	CLA	CAA-C2A	2.06	1.58	1.54
20	D	355	CLA	C4-C3	2.06	1.56	1.50
24	X	130	BCR	C10-C9	2.06	1.38	1.35
26	A	5212	SQD	C8-C7	2.06	1.56	1.49
27	M	5216	LMT	O5B-C5B	2.06	1.49	1.44
20	a	5559	CLA	CAA-C2A	2.07	1.58	1.54
26	A	568	SQD	C24-C23	2.07	1.56	1.50
20	C	503	CLA	C4-C3	2.07	1.56	1.50
20	B	513	CLA	CHC-C1C	2.07	1.41	1.35
20	B	521	CLA	C4-C3	2.07	1.56	1.50
20	B	511	CLA	CMC-C2C	2.07	1.55	1.50
20	b	5517	CLA	C1-C2	2.08	1.55	1.49
20	C	496	CLA	OBD-CAD	2.08	1.25	1.22
32	v	5552	HEM	C3C-CAC	2.08	1.51	1.47
20	c	5492	CLA	CHC-C1C	2.08	1.41	1.35
20	A	558	CLA	CAA-C2A	2.08	1.58	1.54
20	C	500	CLA	CMD-C2D	2.09	1.56	1.51
27	m	216	LMT	C1'-C2'	2.09	1.58	1.52
32	f	5051	HEM	C1B-NB	2.09	1.39	1.36
24	b	5528	BCR	C26-C25	2.09	1.38	1.34
20	B	515	CLA	C4-C3	2.09	1.56	1.50
20	c	5497	CLA	C4C-NC	2.09	1.40	1.37
28	l	5210	MGE	O6D-C5D	2.09	1.49	1.44
20	b	5521	CLA	CHC-C1C	2.10	1.41	1.35
20	C	502	CLA	C1C-C2C	2.10	1.48	1.44
20	B	526	CLA	C2-C3	2.10	1.38	1.33
20	a	5558	CLA	C1C-C2C	2.10	1.48	1.44
27	M	5216	LMT	C4B-C5B	2.10	1.57	1.53
30	C	508	DGD	O6D-C5D	2.10	1.49	1.44
28	D	358	MGE	O2G-C1B	2.10	1.40	1.34
30	H	208	DGD	C4E-C3E	2.11	1.57	1.52
20	d	5355	CLA	C4C-NC	2.11	1.41	1.37
28	i	5201	MGE	C3D-C2D	2.11	1.57	1.52
20	B	521	CLA	C1C-C2C	2.11	1.48	1.44
24	D	357	BCR	C14-C13	2.11	1.38	1.35
30	H	208	DGD	O6E-C5E	2.11	1.49	1.44
32	F	51	HEM	C1B-NB	2.11	1.39	1.36
20	B	518	CLA	C4-C3	2.11	1.56	1.50
20	B	520	CLA	CHC-C1C	2.11	1.41	1.35
20	C	492	CLA	CHC-C1C	2.12	1.41	1.35
20	b	5511	CLA	OBD-CAD	2.12	1.25	1.22
30	C	509	DGD	C3D-C2D	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	357	BCR	C38-C26	2.12	1.54	1.51
24	t	104	BCR	C35-C13	2.12	1.55	1.50
20	C	492	CLA	C5-C3	2.13	1.56	1.51
24	C	506	BCR	C35-C13	2.13	1.55	1.50
20	C	502	CLA	C4-C3	2.13	1.56	1.50
20	a	5560	CLA	C4-C3	2.13	1.56	1.50
28	d	5361	MGE	O2G-C1B	2.13	1.40	1.34
20	C	502	CLA	CMB-C2B	2.14	1.56	1.51
26	A	568	SQD	O6-C1	2.15	1.43	1.40
26	L	5213	SQD	C8-C7	2.15	1.56	1.50
28	d	5359	MGE	C4D-C5D	2.15	1.57	1.53
20	b	5523	CLA	C5-C3	2.15	1.56	1.51
20	A	563	CLA	CAA-C2A	2.15	1.58	1.54
20	a	5560	CLA	CHC-C1C	2.15	1.41	1.35
20	C	495	CLA	C4C-C3C	2.15	1.48	1.45
20	B	526	CLA	C1-C2	2.15	1.55	1.49
20	c	5495	CLA	C4-C3	2.15	1.56	1.50
27	a	5568	LMT	O5B-C5B	2.15	1.49	1.44
27	m	216	LMT	C4B-C3B	2.16	1.57	1.52
24	B	527	BCR	C38-C26	2.16	1.54	1.51
20	B	524	CLA	CAA-C2A	2.16	1.58	1.54
28	D	359	MGE	O6D-C5D	2.16	1.49	1.44
30	c	5507	DGD	C4D-C5D	2.17	1.57	1.53
20	B	519	CLA	CMD-C2D	2.17	1.56	1.51
20	c	5492	CLA	CAA-C2A	2.17	1.58	1.54
20	c	5502	CLA	CMD-C2D	2.17	1.56	1.51
24	X	130	BCR	C14-C13	2.17	1.38	1.35
30	C	509	DGD	O2G-C1B	2.17	1.40	1.34
27	m	216	LMT	O5'-C5'	2.18	1.49	1.44
22	A	564	PQ9	C11-C2	2.18	1.53	1.51
26	t	213	SQD	O6-C1	2.18	1.44	1.40
30	h	5208	DGD	C4E-C3E	2.18	1.57	1.52
22	D	356	PQ9	C3-C4	2.18	1.50	1.44
30	H	208	DGD	C1D-C2D	2.18	1.58	1.52
24	C	506	BCR	C14-C13	2.18	1.38	1.35
20	D	354	CLA	C1C-C2C	2.18	1.48	1.44
27	M	5216	LMT	O5B-C1B	2.19	1.47	1.41
20	c	5493	CLA	CMB-C2B	2.19	1.56	1.51
28	D	359	MGE	O1G-C1A	2.19	1.39	1.33
20	c	5503	CLA	CHC-C1C	2.19	1.41	1.35
30	c	5508	DGD	O6D-C5D	2.20	1.49	1.44
27	a	5568	LMT	C1B-C2B	2.20	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	523	CLA	CAA-C2A	2.20	1.58	1.54
24	C	504	BCR	C14-C13	2.20	1.38	1.35
20	B	515	CLA	CAA-C2A	2.20	1.58	1.54
20	c	5503	CLA	C1-C2	2.20	1.55	1.49
20	b	5513	CLA	C5-C3	2.21	1.56	1.51
20	c	5503	CLA	C4-C3	2.21	1.56	1.50
20	c	5499	CLA	C1C-C2C	2.21	1.48	1.44
28	B	530	MGE	C4D-C5D	2.21	1.57	1.53
20	b	5512	CLA	CHC-C1C	2.21	1.41	1.35
20	B	511	CLA	CHC-C1C	2.21	1.41	1.35
28	b	5530	MGE	O2G-C1B	2.21	1.40	1.34
28	b	5530	MGE	C1D-C2D	2.21	1.58	1.52
28	i	5201	MGE	O3G-C1D	2.21	1.44	1.40
20	c	5498	CLA	C4-C3	2.21	1.56	1.50
28	d	5360	MGE	O3G-C1D	2.22	1.44	1.40
20	b	5520	CLA	C1C-C2C	2.22	1.48	1.44
24	a	5566	BCR	C26-C25	2.23	1.38	1.34
28	L	210	MGE	C4D-C3D	2.23	1.58	1.52
20	c	5491	CLA	C4-C3	2.23	1.56	1.50
27	M	5216	LMT	C1'-C2'	2.24	1.59	1.52
20	C	496	CLA	C1C-C2C	2.24	1.48	1.44
21	A	561	PHO	C4-C3	2.24	1.56	1.50
21	a	5561	PHO	CHD-C1D	2.24	1.43	1.38
27	M	5216	LMT	C3B-C2B	2.25	1.58	1.52
32	f	5051	HEM	C4C-NC	2.25	1.39	1.36
20	c	5491	CLA	CHC-C1C	2.25	1.41	1.35
30	h	5208	DGD	C3E-C2E	2.25	1.58	1.52
20	C	492	CLA	CAA-C2A	2.25	1.58	1.54
20	c	5497	CLA	C4-C3	2.25	1.56	1.50
24	a	5566	BCR	C14-C13	2.25	1.38	1.35
28	b	5530	MGE	C4D-C3D	2.25	1.58	1.52
20	D	355	CLA	C1C-C2C	2.25	1.48	1.44
20	c	5498	CLA	C1C-C2C	2.26	1.48	1.44
24	h	5107	BCR	C5-C6	2.26	1.38	1.34
20	b	5520	CLA	C4C-C3C	2.26	1.49	1.45
30	C	507	DGD	O6E-C5E	2.26	1.49	1.44
21	a	5562	PHO	C4-C3	2.27	1.56	1.50
27	M	5216	LMT	C1B-C2B	2.27	1.59	1.52
20	b	5511	CLA	CHC-C1C	2.27	1.41	1.35
20	C	491	CLA	CHC-C1C	2.27	1.41	1.35
20	c	5499	CLA	C4C-C3C	2.27	1.49	1.45
32	V	552	HEM	C4C-NC	2.27	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	212	SQD	C44-C45	2.27	1.57	1.50
32	v	5552	HEM	CMA-C3A	2.27	1.56	1.51
26	A	5212	SQD	C44-C45	2.27	1.57	1.50
28	l	5210	MGE	C4D-C3D	2.28	1.58	1.52
20	c	5499	CLA	CHC-C1C	2.28	1.41	1.35
30	h	5208	DGD	C1D-C2D	2.28	1.59	1.52
26	a	212	SQD	O48-C23	2.28	1.44	1.33
20	A	560	CLA	CHC-C1C	2.29	1.42	1.35
30	h	5208	DGD	O6D-C1D	2.30	1.47	1.41
24	B	527	BCR	C1-C6	2.30	1.56	1.53
24	T	5104	BCR	C30-C25	2.30	1.56	1.53
28	D	360	MGE	O6D-C5D	2.31	1.50	1.44
32	v	5552	HEM	C2A-C3A	2.31	1.44	1.37
20	b	5515	CLA	CHC-C1C	2.31	1.42	1.35
30	c	5507	DGD	O6E-C5E	2.32	1.50	1.44
20	B	512	CLA	CHC-C1C	2.32	1.42	1.35
28	b	5530	MGE	C4D-C5D	2.32	1.58	1.53
30	c	5508	DGD	C4E-C3E	2.32	1.58	1.52
27	a	5568	LMT	O5B-C1B	2.32	1.47	1.41
20	A	563	CLA	C5-C3	2.32	1.56	1.51
30	C	509	DGD	O1G-C1A	2.32	1.40	1.33
20	d	5355	CLA	C1C-C2C	2.32	1.49	1.44
20	b	5520	CLA	CHC-C1C	2.33	1.42	1.35
26	d	5358	SQD	C24-C23	2.33	1.57	1.50
24	c	5506	BCR	C10-C9	2.33	1.38	1.35
20	c	5496	CLA	C4-C3	2.33	1.56	1.50
24	X	130	BCR	C33-C5	2.33	1.54	1.51
20	b	5511	CLA	CMD-C2D	2.33	1.56	1.51
20	b	5523	CLA	CHC-C1C	2.33	1.42	1.35
20	B	523	CLA	CHC-C1C	2.34	1.42	1.35
20	B	515	CLA	CHC-C1C	2.34	1.42	1.35
20	B	514	CLA	C4-C3	2.34	1.56	1.50
26	A	568	SQD	C8-C7	2.34	1.57	1.50
30	C	507	DGD	C4D-C5D	2.34	1.58	1.53
20	B	513	CLA	C4-C3	2.34	1.56	1.50
20	C	491	CLA	C4-C3	2.34	1.56	1.50
24	c	5504	BCR	C10-C9	2.35	1.38	1.35
20	c	5502	CLA	C4-C3	2.35	1.56	1.50
28	i	5201	MGE	C2A-C1A	2.35	1.57	1.50
30	c	5509	DGD	C4E-C5E	2.35	1.58	1.53
20	b	5516	CLA	CHC-C1C	2.35	1.42	1.35
30	c	5508	DGD	O5D-C1E	2.35	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	528	BCR	C5-C6	2.35	1.38	1.34
20	b	5519	CLA	C1C-C2C	2.35	1.49	1.44
32	V	552	HEM	CMA-C3A	2.36	1.56	1.51
20	C	492	CLA	C4-C3	2.36	1.56	1.50
28	d	5361	MGE	O6D-C5D	2.37	1.50	1.44
20	B	514	CLA	CHC-C1C	2.37	1.42	1.35
28	I	201	MGE	O3G-C1D	2.37	1.44	1.40
24	b	5527	BCR	C1-C6	2.37	1.57	1.53
20	C	499	CLA	OBD-CAD	2.38	1.25	1.22
28	I	201	MGE	C4D-C3D	2.38	1.58	1.52
32	V	552	HEM	C3B-CAB	2.38	1.52	1.47
24	h	5107	BCR	C14-C13	2.38	1.38	1.35
20	b	5515	CLA	C4-C3	2.38	1.56	1.50
20	C	500	CLA	CHC-C1C	2.38	1.42	1.35
20	c	5500	CLA	CHC-C1C	2.38	1.42	1.35
20	C	500	CLA	C4C-C3C	2.38	1.49	1.45
20	c	5496	CLA	CHC-C1C	2.39	1.42	1.35
20	C	497	CLA	C4-C3	2.39	1.56	1.50
20	b	5519	CLA	CHC-C1C	2.40	1.42	1.35
20	B	520	CLA	C4-C3	2.40	1.56	1.50
20	A	563	CLA	C4-C3	2.40	1.56	1.50
30	c	5507	DGD	O6D-C5D	2.40	1.50	1.44
20	b	5526	CLA	CHC-C1C	2.41	1.42	1.35
20	B	519	CLA	CHC-C1C	2.42	1.42	1.35
26	d	5358	SQD	C8-C7	2.42	1.57	1.50
20	C	496	CLA	CHC-C1C	2.42	1.42	1.35
20	a	5563	CLA	CHC-C1C	2.43	1.42	1.35
20	C	493	CLA	CHC-C1C	2.44	1.42	1.35
27	m	216	LMT	O5B-C1B	2.44	1.47	1.41
20	b	5511	CLA	C3C-C2C	2.44	1.41	1.36
20	B	511	CLA	CMD-C2D	2.44	1.56	1.51
20	b	5520	CLA	CAA-C2A	2.45	1.58	1.54
20	c	5498	CLA	CAA-C2A	2.45	1.58	1.54
21	a	5562	PHO	CHC-C1C	2.45	1.43	1.38
20	B	516	CLA	CHC-C1C	2.45	1.42	1.35
20	c	5495	CLA	C1C-C2C	2.45	1.49	1.44
20	C	494	CLA	CHC-C1C	2.45	1.42	1.35
20	b	5513	CLA	C4-C3	2.46	1.57	1.50
20	B	511	CLA	C3C-C2C	2.46	1.42	1.36
24	a	5566	BCR	C29-C30	2.46	1.59	1.54
20	b	5516	CLA	OBD-CAD	2.47	1.25	1.22
27	m	216	LMT	O5'-C1'	2.47	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	5568	LMT	C1'-C2'	2.48	1.59	1.52
21	A	561	PHO	CHD-C1D	2.48	1.43	1.38
32	V	552	HEM	C3C-CAC	2.48	1.52	1.47
20	A	559	CLA	CAA-C2A	2.48	1.58	1.54
24	A	566	BCR	C26-C25	2.49	1.38	1.34
27	M	5216	LMT	O5'-C1'	2.49	1.48	1.41
27	A	569	LMT	C1B-C2B	2.49	1.59	1.52
20	a	5563	CLA	C5-C3	2.49	1.56	1.51
20	B	511	CLA	C4C-NC	2.50	1.41	1.37
26	A	568	SQD	O5-C1	2.50	1.48	1.41
27	t	5217	LMT	C1B-C2B	2.50	1.59	1.52
28	B	530	MGE	O2G-C1B	2.50	1.41	1.34
20	C	503	CLA	CHC-C1C	2.50	1.42	1.35
20	B	525	CLA	CAA-C2A	2.51	1.58	1.54
20	B	525	CLA	CHC-C1C	2.51	1.42	1.35
28	I	201	MGE	O6D-C1D	2.51	1.48	1.41
32	v	5552	HEM	C4C-NC	2.51	1.39	1.36
20	c	5500	CLA	C4-C3	2.52	1.57	1.50
20	c	5497	CLA	CHC-C1C	2.52	1.42	1.35
28	B	530	MGE	O6D-C5D	2.53	1.50	1.44
26	a	212	SQD	C8-C7	2.53	1.58	1.49
20	C	501	CLA	CAA-C2A	2.54	1.59	1.54
20	c	5501	CLA	C1C-C2C	2.54	1.49	1.44
20	B	520	CLA	C4C-C3C	2.54	1.49	1.45
20	B	511	CLA	C1C-C2C	2.54	1.49	1.44
20	B	511	CLA	C3B-C2B	2.55	1.43	1.40
20	C	497	CLA	CHC-C1C	2.55	1.42	1.35
20	B	517	CLA	CHC-C1C	2.55	1.42	1.35
28	B	530	MGE	C1D-C2D	2.55	1.59	1.52
20	d	5354	CLA	CHC-C1C	2.56	1.42	1.35
20	C	496	CLA	CAA-C2A	2.56	1.59	1.54
20	a	5558	CLA	CAA-C2A	2.56	1.59	1.54
27	A	569	LMT	O5B-C1B	2.56	1.48	1.41
30	C	507	DGD	O6D-C5D	2.57	1.50	1.44
21	A	562	PHO	C4-C3	2.57	1.57	1.50
20	c	5502	CLA	CAA-C2A	2.58	1.59	1.54
24	b	5529	BCR	C10-C9	2.59	1.39	1.35
24	C	505	BCR	C38-C26	2.59	1.55	1.51
24	T	5104	BCR	C29-C30	2.59	1.60	1.54
27	A	569	LMT	O5B-C5B	2.59	1.50	1.44
28	d	5359	MGE	O6D-C5D	2.59	1.50	1.44
30	c	5508	DGD	C1E-C2E	2.59	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	355	CLA	CHC-C1C	2.59	1.42	1.35
30	H	208	DGD	O6E-C1E	2.60	1.48	1.41
27	T	217	LMT	O1B-C4'	2.60	1.50	1.43
20	B	513	CLA	C5-C3	2.60	1.57	1.51
20	C	493	CLA	CAA-C2A	2.60	1.59	1.54
28	D	360	MGE	O6D-C1D	2.61	1.48	1.41
30	h	5208	DGD	O5D-C1E	2.61	1.44	1.40
32	f	5051	HEM	CMA-C3A	2.61	1.56	1.51
24	B	529	BCR	C10-C9	2.62	1.39	1.35
28	I	201	MGE	O6D-C5D	2.62	1.50	1.44
20	B	524	CLA	CHC-C1C	2.62	1.42	1.35
20	c	5492	CLA	C4-C3	2.62	1.57	1.50
27	t	5217	LMT	O1B-C4'	2.63	1.50	1.43
30	c	5509	DGD	O6D-C5D	2.63	1.50	1.44
28	I	201	MGE	O2G-C1B	2.63	1.41	1.34
20	C	495	CLA	CAA-C2A	2.63	1.59	1.54
20	b	5524	CLA	CHC-C1C	2.63	1.42	1.35
30	C	508	DGD	C4D-C3D	2.63	1.59	1.52
26	d	5358	SQD	O5-C1	2.63	1.48	1.41
20	b	5525	CLA	CAA-C2A	2.64	1.59	1.54
20	C	496	CLA	C4C-C3C	2.64	1.49	1.45
20	C	501	CLA	CHC-C1C	2.64	1.43	1.35
30	c	5507	DGD	C1E-C2E	2.64	1.60	1.52
30	H	208	DGD	O6D-C5D	2.64	1.50	1.44
24	B	529	BCR	C5-C6	2.64	1.39	1.34
20	B	514	CLA	CAA-C2A	2.64	1.59	1.54
20	B	521	CLA	CHC-C1C	2.64	1.43	1.35
30	H	208	DGD	C1E-C2E	2.65	1.60	1.52
27	m	216	LMT	O1'-C1'	2.65	1.44	1.40
30	C	509	DGD	O6D-C5D	2.65	1.50	1.44
20	c	5496	CLA	C1C-C2C	2.66	1.49	1.44
28	D	359	MGE	C4D-C3D	2.66	1.59	1.52
24	x	5130	BCR	C14-C13	2.66	1.39	1.35
20	B	511	CLA	C4C-C3C	2.67	1.49	1.45
21	A	562	PHO	C3B-C4B	2.67	1.49	1.43
28	d	5360	MGE	O6D-C5D	2.67	1.50	1.44
20	c	5497	CLA	CAA-C2A	2.67	1.59	1.54
21	A	562	PHO	CHC-C1C	2.68	1.44	1.38
30	C	508	DGD	C3D-C2D	2.68	1.59	1.52
26	t	213	SQD	O5-C1	2.68	1.48	1.41
20	b	5517	CLA	CHC-C1C	2.68	1.43	1.35
28	i	5201	MGE	O6D-C1D	2.68	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	5529	BCR	C5-C6	2.68	1.39	1.34
20	c	5493	CLA	CHC-C1C	2.68	1.43	1.35
24	A	566	BCR	C29-C30	2.69	1.60	1.54
27	T	217	LMT	O1B-C1B	2.69	1.48	1.41
20	B	518	CLA	CHC-C1C	2.69	1.43	1.35
20	c	5501	CLA	CHC-C1C	2.69	1.43	1.35
30	C	507	DGD	C3E-C2E	2.69	1.59	1.52
20	b	5525	CLA	CHC-C1C	2.69	1.43	1.35
30	c	5508	DGD	O1G-C1A	2.70	1.41	1.33
20	A	563	CLA	CHC-C1C	2.70	1.43	1.35
27	T	217	LMT	O5B-C1B	2.70	1.48	1.41
24	b	5528	BCR	C5-C6	2.70	1.39	1.34
24	C	504	BCR	C5-C6	2.70	1.39	1.34
20	c	5494	CLA	CHC-C1C	2.70	1.43	1.35
26	a	212	SQD	O5-C1	2.71	1.48	1.41
20	c	5495	CLA	CHC-C1C	2.71	1.43	1.35
20	d	5355	CLA	CAA-C2A	2.71	1.59	1.54
24	b	5529	BCR	C26-C25	2.72	1.39	1.34
30	C	507	DGD	O3G-C1D	2.72	1.44	1.40
28	i	5201	MGE	O2G-C1B	2.73	1.42	1.34
21	a	5562	PHO	C3B-C4B	2.73	1.49	1.43
24	B	527	BCR	C2-C1	2.73	1.60	1.54
30	C	508	DGD	C1E-C2E	2.73	1.60	1.52
26	L	5213	SQD	C6-S	2.73	1.88	1.77
20	C	502	CLA	CHC-C1C	2.74	1.43	1.35
30	c	5507	DGD	O3G-C1D	2.74	1.45	1.40
20	b	5518	CLA	CHC-C1C	2.74	1.43	1.35
28	d	5360	MGE	O1G-C1A	2.74	1.41	1.33
20	D	354	CLA	CHC-C1C	2.74	1.43	1.35
20	b	5526	CLA	C1-C2	2.75	1.57	1.49
26	A	5212	SQD	O5-C1	2.75	1.48	1.41
20	A	558	CLA	CHC-C1C	2.75	1.43	1.35
20	C	495	CLA	CHC-C1C	2.75	1.43	1.35
20	C	501	CLA	C1C-C2C	2.76	1.49	1.44
24	b	5527	BCR	C26-C25	2.76	1.39	1.34
28	d	5359	MGE	C4D-C3D	2.77	1.59	1.52
20	b	5518	CLA	CAA-C2A	2.77	1.59	1.54
30	H	208	DGD	O6D-C1D	2.77	1.48	1.41
20	b	5521	CLA	CAA-C2A	2.78	1.59	1.54
20	d	5355	CLA	CHC-C1C	2.78	1.43	1.35
20	c	5503	CLA	C1C-C2C	2.78	1.49	1.44
20	c	5493	CLA	CAA-C2A	2.79	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	51	HEM	C3C-CAC	2.79	1.53	1.47
30	C	508	DGD	O3G-C1D	2.80	1.45	1.40
22	a	5564	PQ9	C11-C2	2.80	1.54	1.51
28	b	5530	MGE	O6D-C5D	2.80	1.51	1.44
20	c	5500	CLA	CAA-C2A	2.80	1.59	1.54
20	c	5502	CLA	CHC-C1C	2.81	1.43	1.35
27	t	5217	LMT	O5B-C1B	2.81	1.48	1.41
20	b	5522	CLA	CHC-C1C	2.81	1.43	1.35
20	b	5514	CLA	CHC-C1C	2.81	1.43	1.35
30	H	208	DGD	O5D-C1E	2.81	1.45	1.40
20	c	5491	CLA	CAA-C2A	2.81	1.59	1.54
24	H	107	BCR	C5-C6	2.82	1.39	1.34
24	b	5527	BCR	C5-C6	2.84	1.39	1.34
30	h	5208	DGD	O6D-C5D	2.84	1.51	1.44
24	b	5529	BCR	C14-C13	2.84	1.39	1.35
26	L	5213	SQD	O6-C1	2.84	1.45	1.40
24	t	104	BCR	C26-C25	2.84	1.39	1.34
30	h	5208	DGD	O6E-C1E	2.85	1.48	1.41
30	c	5508	DGD	C4D-C3D	2.85	1.59	1.52
26	A	5212	SQD	O6-C1	2.86	1.45	1.40
30	C	508	DGD	C4E-C3E	2.86	1.59	1.52
20	b	5523	CLA	CAA-C2A	2.87	1.59	1.54
20	c	5496	CLA	C4C-C3C	2.87	1.50	1.45
20	b	5511	CLA	C4C-NC	2.87	1.42	1.37
20	c	5498	CLA	CHC-C1C	2.87	1.43	1.35
28	i	5201	MGE	C4D-C5D	2.88	1.59	1.53
30	c	5507	DGD	C3E-C2E	2.88	1.59	1.52
20	B	521	CLA	CAA-C2A	2.88	1.59	1.54
24	x	5130	BCR	C26-C25	2.88	1.39	1.34
30	C	509	DGD	O6D-C1D	2.89	1.49	1.41
24	B	529	BCR	C14-C13	2.89	1.39	1.35
20	C	502	CLA	CAA-C2A	2.90	1.59	1.54
20	B	526	CLA	CAA-C2A	2.90	1.59	1.54
20	C	498	CLA	CHC-C1C	2.90	1.43	1.35
32	F	51	HEM	C4C-NC	2.90	1.40	1.36
20	b	5519	CLA	CAA-C2A	2.90	1.59	1.54
20	a	5560	CLA	CAA-C2A	2.90	1.59	1.54
26	d	5358	SQD	O8-S	2.91	1.57	1.47
24	C	506	BCR	C29-C30	2.91	1.60	1.54
27	A	569	LMT	C1'-C2'	2.91	1.60	1.52
24	t	104	BCR	C29-C30	2.92	1.60	1.54
28	D	358	MGE	O6D-C5D	2.92	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	5360	MGE	C4D-C3D	2.92	1.59	1.52
20	b	5511	CLA	C4C-C3C	2.93	1.50	1.45
20	b	5513	CLA	CAA-C2A	2.93	1.59	1.54
28	D	358	MGE	C4D-C3D	2.93	1.59	1.52
20	B	526	CLA	C4-C3	2.93	1.58	1.50
20	B	520	CLA	CAA-C2A	2.94	1.59	1.54
26	A	568	SQD	O8-S	2.94	1.57	1.47
20	B	517	CLA	CAA-C2A	2.95	1.59	1.54
24	b	5528	BCR	C2-C1	2.95	1.61	1.54
24	C	505	BCR	C5-C6	2.96	1.39	1.34
24	c	5505	BCR	C38-C26	2.97	1.56	1.51
24	X	130	BCR	C26-C25	2.97	1.39	1.34
21	a	5561	PHO	C4-C3	2.98	1.58	1.50
20	a	5563	CLA	CAA-C2A	2.98	1.59	1.54
30	C	508	DGD	O1G-C1A	2.98	1.42	1.33
20	C	495	CLA	C1C-C2C	2.98	1.50	1.44
27	A	569	LMT	O5'-C1'	3.00	1.49	1.41
32	F	51	HEM	C1A-NA	3.00	1.42	1.36
20	C	500	CLA	CAA-C2A	3.00	1.59	1.54
20	b	5511	CLA	C1C-C2C	3.01	1.50	1.44
24	d	5357	BCR	C38-C26	3.01	1.56	1.51
27	t	5217	LMT	O1B-C1B	3.02	1.49	1.41
28	d	5360	MGE	O6D-C1D	3.02	1.49	1.41
24	b	5527	BCR	C2-C1	3.02	1.61	1.54
24	C	504	BCR	C2-C1	3.03	1.61	1.54
24	A	566	BCR	C30-C25	3.03	1.57	1.53
20	b	5514	CLA	CAA-C2A	3.04	1.60	1.54
20	b	5515	CLA	CAA-C2A	3.04	1.60	1.54
24	a	5566	BCR	C2-C1	3.04	1.61	1.54
20	B	522	CLA	CHC-C1C	3.05	1.44	1.35
27	a	5568	LMT	O5'-C1'	3.05	1.49	1.41
24	c	5504	BCR	C26-C25	3.05	1.39	1.34
20	b	5516	CLA	CAA-C2A	3.06	1.60	1.54
28	d	5361	MGE	O3G-C1D	3.07	1.45	1.40
20	c	5495	CLA	CAA-C2A	3.09	1.60	1.54
20	B	526	CLA	C5-C3	3.09	1.58	1.51
24	B	529	BCR	C29-C30	3.10	1.61	1.54
26	L	5213	SQD	O5-C1	3.10	1.49	1.41
24	B	528	BCR	C2-C1	3.10	1.61	1.54
20	a	5558	CLA	CHC-C1C	3.10	1.44	1.35
28	d	5359	MGE	O3G-C1D	3.11	1.45	1.40
20	C	491	CLA	CAA-C2A	3.11	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	552	HEM	CAA-C2A	3.12	1.57	1.52
28	b	5530	MGE	O3G-C1D	3.12	1.45	1.40
24	a	5566	BCR	C5-C6	3.12	1.39	1.34
24	H	107	BCR	C14-C13	3.12	1.39	1.35
27	m	216	LMT	C3B-C2B	3.12	1.60	1.52
26	A	568	SQD	O5-C5	3.13	1.52	1.44
28	d	5359	MGE	O6D-C1D	3.14	1.49	1.41
28	D	360	MGE	O3G-C1D	3.14	1.45	1.40
30	C	508	DGD	O5D-C1E	3.15	1.45	1.40
30	C	507	DGD	O6D-C1D	3.15	1.49	1.41
32	f	5051	HEM	C3C-CAC	3.16	1.54	1.47
26	a	212	SQD	O6-C1	3.17	1.45	1.40
26	d	5358	SQD	O3-C3	3.18	1.50	1.43
24	t	104	BCR	C2-C1	3.19	1.61	1.54
24	c	5506	BCR	C29-C30	3.19	1.61	1.54
24	X	130	BCR	C2-C1	3.19	1.61	1.54
20	b	5526	CLA	C5-C3	3.20	1.58	1.51
28	l	5210	MGE	O6D-C1D	3.20	1.49	1.41
26	L	5213	SQD	O47-C7	3.21	1.43	1.34
20	b	5517	CLA	CAA-C2A	3.23	1.60	1.54
28	D	359	MGE	O6D-C1D	3.25	1.49	1.41
20	c	5499	CLA	CAA-C2A	3.26	1.60	1.54
20	c	5496	CLA	CAA-C2A	3.27	1.60	1.54
28	i	5201	MGE	O6D-C5D	3.27	1.52	1.44
24	c	5505	BCR	C29-C30	3.29	1.61	1.54
20	b	5522	CLA	CAA-C2A	3.30	1.60	1.54
24	b	5529	BCR	C1-C6	3.30	1.58	1.53
27	t	5217	LMT	O1'-C1'	3.31	1.46	1.40
24	B	527	BCR	C5-C6	3.32	1.40	1.34
30	C	508	DGD	O6D-C1D	3.32	1.50	1.41
20	B	522	CLA	CAA-C2A	3.33	1.60	1.54
30	c	5507	DGD	O6D-C1D	3.33	1.50	1.41
20	b	5526	CLA	CAA-C2A	3.34	1.60	1.54
24	d	5357	BCR	C2-C1	3.34	1.61	1.54
24	B	529	BCR	C2-C1	3.35	1.61	1.54
30	c	5509	DGD	O5D-C1E	3.35	1.46	1.40
25	a	5567	LHG	O7-C7	3.36	1.44	1.34
25	A	567	LHG	O7-C7	3.36	1.44	1.34
32	F	51	HEM	CMA-C3A	3.37	1.58	1.51
24	c	5505	BCR	C5-C6	3.38	1.40	1.34
24	b	5527	BCR	C29-C30	3.38	1.62	1.54
24	b	5529	BCR	C2-C1	3.39	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5503	CLA	CAA-C2A	3.39	1.60	1.54
20	B	518	CLA	CAA-C2A	3.39	1.60	1.54
24	T	5104	BCR	C1-C6	3.40	1.58	1.53
24	B	527	BCR	C29-C30	3.41	1.62	1.54
24	c	5505	BCR	C2-C1	3.41	1.62	1.54
20	b	5526	CLA	C4-C3	3.41	1.59	1.50
20	B	513	CLA	CAA-C2A	3.41	1.60	1.54
25	A	567	LHG	P-O6	3.41	1.73	1.59
24	A	566	BCR	C2-C1	3.42	1.62	1.54
26	A	5212	SQD	C1-C2	3.43	1.62	1.52
26	t	213	SQD	O3-C3	3.44	1.50	1.43
24	B	528	BCR	C26-C25	3.44	1.40	1.34
20	B	516	CLA	CAA-C2A	3.45	1.60	1.54
30	H	208	DGD	C4E-C5E	3.46	1.60	1.53
28	B	530	MGE	O6D-C1D	3.47	1.50	1.41
26	a	212	SQD	O3-C3	3.47	1.50	1.43
28	L	210	MGE	O3G-C1D	3.47	1.46	1.40
24	C	506	BCR	C26-C25	3.47	1.40	1.34
28	D	358	MGE	O3G-C1D	3.47	1.46	1.40
24	x	5130	BCR	C2-C1	3.48	1.62	1.54
24	C	505	BCR	C29-C30	3.48	1.62	1.54
30	C	509	DGD	O3G-C1D	3.49	1.46	1.40
20	C	503	CLA	CAA-C2A	3.49	1.60	1.54
24	b	5528	BCR	C29-C30	3.49	1.62	1.54
24	b	5529	BCR	C29-C30	3.49	1.62	1.54
24	C	506	BCR	C1-C6	3.50	1.58	1.53
24	t	104	BCR	C5-C6	3.50	1.40	1.34
26	L	5213	SQD	O3-C3	3.51	1.51	1.43
26	t	213	SQD	O47-C7	3.51	1.44	1.34
28	b	5530	MGE	O6D-C1D	3.52	1.50	1.41
26	d	5358	SQD	O5-C5	3.52	1.52	1.44
26	A	5212	SQD	O5-C5	3.52	1.52	1.44
25	a	5567	LHG	P-O6	3.52	1.74	1.59
26	A	5212	SQD	O3-C3	3.52	1.51	1.43
30	C	507	DGD	O5D-C1E	3.53	1.46	1.40
24	D	357	BCR	C2-C1	3.53	1.62	1.54
32	V	552	HEM	C1A-NA	3.54	1.43	1.36
25	a	5567	LHG	O8-C23	3.54	1.43	1.33
24	C	504	BCR	C26-C25	3.54	1.40	1.34
24	A	566	BCR	C5-C6	3.56	1.40	1.34
20	c	5501	CLA	CAA-C2A	3.56	1.61	1.54
20	B	519	CLA	CAA-C2A	3.57	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	BCR	C5-C6	3.59	1.40	1.34
24	D	357	BCR	C1-C6	3.59	1.58	1.53
32	F	51	HEM	CBC-CAC	3.62	1.54	1.28
20	C	494	CLA	CAA-C2A	3.63	1.61	1.54
24	C	504	BCR	C29-C30	3.64	1.62	1.54
25	A	567	LHG	P-O3	3.64	1.74	1.59
28	D	358	MGE	O6D-C1D	3.65	1.50	1.41
32	v	5552	HEM	CAA-C2A	3.66	1.58	1.52
32	f	5051	HEM	CBC-CAC	3.66	1.54	1.28
24	c	5504	BCR	C2-C1	3.67	1.62	1.54
24	H	107	BCR	C2-C1	3.67	1.62	1.54
20	D	355	CLA	CAA-C2A	3.68	1.61	1.54
30	c	5509	DGD	O6D-C1D	3.69	1.51	1.41
24	d	5357	BCR	C30-C25	3.69	1.58	1.53
24	B	528	BCR	C29-C30	3.70	1.62	1.54
27	T	217	LMT	O1'-C1'	3.70	1.46	1.40
32	V	552	HEM	CBC-CAC	3.71	1.55	1.28
30	C	507	DGD	C4D-C3D	3.72	1.61	1.52
25	A	567	LHG	O8-C23	3.72	1.44	1.33
24	X	130	BCR	C29-C30	3.72	1.62	1.54
24	t	104	BCR	C1-C6	3.73	1.58	1.53
24	d	5357	BCR	C29-C30	3.73	1.62	1.54
32	f	5051	HEM	C1A-NA	3.73	1.44	1.36
26	A	5212	SQD	O8-S	3.75	1.60	1.47
26	A	568	SQD	O3-C3	3.77	1.51	1.43
30	c	5508	DGD	O3G-C1D	3.77	1.46	1.40
24	T	5104	BCR	C5-C6	3.77	1.40	1.34
26	a	212	SQD	O5-C5	3.79	1.53	1.44
28	L	210	MGE	O6D-C1D	3.79	1.51	1.41
20	c	5494	CLA	CAA-C2A	3.79	1.61	1.54
32	v	5552	HEM	CBC-CAC	3.79	1.55	1.28
28	d	5361	MGE	O6D-C1D	3.80	1.51	1.41
26	A	568	SQD	O47-C7	3.80	1.45	1.34
32	F	51	HEM	CAA-C2A	3.81	1.58	1.52
32	v	5552	HEM	C1A-NA	3.82	1.44	1.36
26	a	212	SQD	O8-S	3.83	1.60	1.47
26	L	5213	SQD	O8-S	3.83	1.60	1.47
26	t	213	SQD	O8-S	3.84	1.60	1.47
28	D	359	MGE	O3G-C1D	3.85	1.46	1.40
24	T	5104	BCR	C2-C1	3.86	1.63	1.54
20	A	560	CLA	CAA-C2A	3.86	1.61	1.54
24	D	357	BCR	C29-C30	3.88	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	213	SQD	O48-C23	3.89	1.44	1.33
26	d	5358	SQD	O47-C7	3.90	1.45	1.34
32	f	5051	HEM	CAA-C2A	3.90	1.58	1.52
30	c	5507	DGD	O5D-C1E	3.90	1.47	1.40
24	C	505	BCR	C2-C1	3.93	1.63	1.54
24	c	5506	BCR	C2-C1	3.93	1.63	1.54
30	c	5507	DGD	C4D-C3D	3.94	1.62	1.52
24	h	5107	BCR	C2-C1	3.95	1.63	1.54
26	d	5358	SQD	O48-C23	3.97	1.45	1.33
26	A	568	SQD	O48-C23	3.97	1.45	1.33
24	x	5130	BCR	C29-C30	3.98	1.63	1.54
24	t	104	BCR	C30-C25	3.99	1.59	1.53
24	h	5107	BCR	C29-C30	3.99	1.63	1.54
26	L	5213	SQD	C1-C2	3.99	1.64	1.52
24	C	505	BCR	C1-C6	4.02	1.59	1.53
26	A	568	SQD	C1-C2	4.02	1.64	1.52
27	M	5216	LMT	O1'-C1'	4.04	1.47	1.40
27	a	5568	LMT	O1'-C1'	4.04	1.47	1.40
24	c	5504	BCR	C29-C30	4.05	1.63	1.54
26	L	5213	SQD	O5-C5	4.05	1.54	1.44
28	B	530	MGE	O3G-C1D	4.06	1.47	1.40
26	d	5358	SQD	C1-C2	4.08	1.64	1.52
24	b	5528	BCR	C1-C6	4.08	1.59	1.53
24	c	5506	BCR	C26-C25	4.12	1.41	1.34
24	d	5357	BCR	C26-C25	4.14	1.41	1.34
24	D	357	BCR	C5-C6	4.16	1.41	1.34
24	C	506	BCR	C2-C1	4.16	1.63	1.54
24	B	529	BCR	C1-C6	4.19	1.59	1.53
30	c	5509	DGD	O3G-C1D	4.20	1.47	1.40
24	c	5506	BCR	C5-C6	4.21	1.41	1.34
24	C	506	BCR	C30-C25	4.25	1.59	1.53
24	h	5107	BCR	C26-C25	4.25	1.41	1.34
24	H	107	BCR	C26-C25	4.26	1.41	1.34
24	d	5357	BCR	C5-C6	4.32	1.41	1.34
26	a	212	SQD	C1-C2	4.32	1.64	1.52
24	a	5566	BCR	C30-C25	4.33	1.59	1.53
24	B	529	BCR	C26-C25	4.34	1.41	1.34
30	c	5508	DGD	O6D-C1D	4.36	1.52	1.41
24	C	505	BCR	C26-C25	4.38	1.42	1.34
24	c	5505	BCR	C26-C25	4.42	1.42	1.34
25	a	5567	LHG	P-O3	4.45	1.78	1.59
26	L	5213	SQD	O48-C23	4.47	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	213	SQD	O5-C5	4.49	1.55	1.44
27	A	569	LMT	O1'-C1'	4.49	1.48	1.40
24	B	527	BCR	C26-C25	4.53	1.42	1.34
24	c	5506	BCR	C1-C6	4.59	1.60	1.53
24	D	357	BCR	C26-C25	4.60	1.42	1.34
26	A	568	SQD	O7-S	4.63	1.58	1.45
26	A	5212	SQD	O47-C7	4.63	1.45	1.35
24	x	5130	BCR	C5-C6	4.72	1.42	1.34
24	b	5529	BCR	C30-C25	4.75	1.60	1.53
24	X	130	BCR	C30-C25	4.76	1.60	1.53
24	c	5505	BCR	C1-C6	4.76	1.60	1.53
24	b	5527	BCR	C30-C25	4.81	1.60	1.53
30	h	5208	DGD	O3G-C1D	4.84	1.48	1.40
24	X	130	BCR	C5-C6	4.85	1.42	1.34
24	X	130	BCR	C1-C6	4.88	1.60	1.53
24	x	5130	BCR	C30-C25	4.89	1.60	1.53
24	x	5130	BCR	C1-C6	4.90	1.60	1.53
26	a	212	SQD	O7-S	4.90	1.59	1.45
24	B	529	BCR	C30-C25	4.93	1.60	1.53
24	C	504	BCR	C30-C25	4.98	1.60	1.53
24	H	107	BCR	C29-C30	5.00	1.65	1.54
24	a	5566	BCR	C1-C6	5.00	1.60	1.53
24	c	5506	BCR	C30-C25	5.01	1.60	1.53
26	t	213	SQD	C1-C2	5.04	1.67	1.52
20	A	563	CLA	CHB-C4A	5.09	1.40	1.33
24	h	5107	BCR	C1-C6	5.16	1.60	1.53
24	D	357	BCR	C30-C25	5.20	1.60	1.53
20	a	5563	CLA	CHB-C4A	5.32	1.40	1.33
26	A	5212	SQD	O7-S	5.32	1.60	1.45
24	B	527	BCR	C30-C25	5.32	1.61	1.53
20	C	500	CLA	CHB-C4A	5.33	1.40	1.33
24	H	107	BCR	C1-C6	5.42	1.61	1.53
30	H	208	DGD	O3G-C1D	5.48	1.49	1.40
26	a	212	SQD	O47-C7	5.51	1.47	1.35
20	a	5558	CLA	CHB-C4A	5.52	1.40	1.33
24	A	566	BCR	C1-C6	5.55	1.61	1.53
20	b	5521	CLA	CHB-C4A	5.59	1.40	1.33
24	B	528	BCR	C1-C6	5.60	1.61	1.53
24	b	5528	BCR	C30-C25	5.66	1.61	1.53
20	C	498	CLA	CHB-C4A	5.67	1.40	1.33
20	d	5354	CLA	CHB-C4A	5.69	1.40	1.33
20	B	512	CLA	CHB-C4A	5.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5517	CLA	CHB-C4A	5.77	1.40	1.33
20	b	5513	CLA	CHB-C4A	5.79	1.40	1.33
26	d	5358	SQD	O7-S	5.82	1.62	1.45
24	C	504	BCR	C1-C6	5.88	1.61	1.53
20	A	558	CLA	CHB-C4A	5.88	1.41	1.33
26	t	213	SQD	O7-S	5.90	1.62	1.45
20	A	560	CLA	CHB-C4A	5.92	1.41	1.33
24	c	5505	BCR	C30-C25	5.95	1.61	1.53
24	C	505	BCR	C30-C25	6.00	1.62	1.53
20	B	516	CLA	CHB-C4A	6.03	1.41	1.33
20	a	5560	CLA	CHB-C4A	6.07	1.41	1.33
20	C	492	CLA	CHB-C4A	6.10	1.41	1.33
20	C	494	CLA	CHB-C4A	6.10	1.41	1.33
20	c	5492	CLA	CHB-C4A	6.12	1.41	1.33
20	b	5512	CLA	CHB-C4A	6.14	1.41	1.33
24	d	5357	BCR	C1-C6	6.17	1.62	1.53
20	c	5498	CLA	CHB-C4A	6.19	1.41	1.33
20	B	520	CLA	CHB-C4A	6.20	1.41	1.33
20	b	5515	CLA	CHB-C4A	6.20	1.41	1.33
20	c	5496	CLA	CHB-C4A	6.21	1.41	1.33
26	L	5213	SQD	O7-S	6.23	1.63	1.45
20	a	5559	CLA	CHB-C4A	6.26	1.41	1.33
24	B	528	BCR	C30-C25	6.26	1.62	1.53
20	D	354	CLA	CHB-C4A	6.40	1.41	1.33
20	b	5524	CLA	CHB-C4A	6.43	1.41	1.33
20	c	5499	CLA	CHB-C4A	6.44	1.41	1.33
20	B	513	CLA	CHB-C4A	6.46	1.41	1.33
20	b	5516	CLA	CHB-C4A	6.48	1.41	1.33
20	C	497	CLA	CHB-C4A	6.54	1.41	1.33
20	c	5494	CLA	CHB-C4A	6.60	1.41	1.33
24	H	107	BCR	C30-C25	6.61	1.62	1.53
20	c	5493	CLA	CHB-C4A	6.65	1.42	1.33
24	h	5107	BCR	C30-C25	6.67	1.62	1.53
20	B	524	CLA	CHB-C4A	6.68	1.42	1.33
24	c	5504	BCR	C30-C25	6.68	1.62	1.53
20	c	5501	CLA	CHB-C4A	6.68	1.42	1.33
20	B	526	CLA	CHB-C4A	6.69	1.42	1.33
20	B	511	CLA	CHB-C4A	6.71	1.42	1.33
20	c	5500	CLA	CHB-C4A	6.73	1.42	1.33
20	C	502	CLA	CHB-C4A	6.78	1.42	1.33
20	c	5497	CLA	CHB-C4A	6.78	1.42	1.33
20	C	491	CLA	CHB-C4A	6.79	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5491	CLA	CHB-C4A	6.81	1.42	1.33
20	B	515	CLA	CHB-C4A	6.82	1.42	1.33
20	C	503	CLA	CHB-C4A	6.87	1.42	1.33
20	B	518	CLA	CHB-C4A	6.93	1.42	1.33
20	C	493	CLA	CHB-C4A	6.95	1.42	1.33
20	c	5495	CLA	CHB-C4A	6.95	1.42	1.33
20	b	5518	CLA	CHB-C4A	6.96	1.42	1.33
20	C	496	CLA	CHB-C4A	6.97	1.42	1.33
20	b	5522	CLA	CHB-C4A	6.97	1.42	1.33
20	b	5520	CLA	CHB-C4A	7.07	1.42	1.33
20	A	559	CLA	CHB-C4A	7.18	1.42	1.33
20	B	521	CLA	CHB-C4A	7.19	1.42	1.33
20	B	517	CLA	CHB-C4A	7.24	1.42	1.33
26	A	5212	SQD	C4-C3	7.24	1.70	1.52
20	b	5514	CLA	CHB-C4A	7.26	1.42	1.33
20	B	522	CLA	CHB-C4A	7.26	1.42	1.33
20	b	5519	CLA	CHB-C4A	7.34	1.42	1.33
20	b	5526	CLA	CHB-C4A	7.34	1.42	1.33
20	B	514	CLA	CHB-C4A	7.46	1.43	1.33
25	a	5567	LHG	P-O5	7.49	1.79	1.50
20	b	5523	CLA	CHB-C4A	7.49	1.43	1.33
20	D	355	CLA	CHB-C4A	7.51	1.43	1.33
20	B	519	CLA	CHB-C4A	7.51	1.43	1.33
25	A	567	LHG	P-O5	7.58	1.79	1.50
20	c	5502	CLA	CHB-C4A	7.59	1.43	1.33
20	B	525	CLA	CHB-C4A	7.60	1.43	1.33
20	d	5355	CLA	CHB-C4A	7.63	1.43	1.33
20	c	5503	CLA	CHB-C4A	7.64	1.43	1.33
24	c	5504	BCR	C1-C6	7.65	1.64	1.53
20	C	499	CLA	CHB-C4A	7.67	1.43	1.33
20	b	5511	CLA	CHB-C4A	7.71	1.43	1.33
26	L	5213	SQD	C4-C3	7.77	1.72	1.52
26	d	5358	SQD	C4-C3	7.83	1.72	1.52
20	C	495	CLA	CHB-C4A	7.84	1.43	1.33
20	b	5525	CLA	CHB-C4A	7.85	1.43	1.33
20	C	501	CLA	CHB-C4A	7.93	1.43	1.33
26	a	212	SQD	C4-C3	8.10	1.73	1.52
26	t	213	SQD	C4-C3	8.13	1.73	1.52
20	B	523	CLA	CHB-C4A	8.13	1.43	1.33
26	A	568	SQD	C4-C3	8.16	1.73	1.52

All (1678) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	568	SQD	O8-S-C6	-6.98	97.49	106.01
26	a	212	SQD	O8-S-C6	-6.58	97.98	106.01
26	d	5358	SQD	O8-S-C6	-6.50	98.07	106.01
32	F	51	HEM	CBD-CAD-C3D	-5.98	101.06	112.47
26	t	213	SQD	O8-S-C6	-5.88	98.83	106.01
32	f	5051	HEM	CBD-CAD-C3D	-5.69	101.61	112.47
26	A	5212	SQD	O8-S-C6	-5.56	99.22	106.01
32	v	5552	HEM	CBD-CAD-C3D	-5.43	102.11	112.47
20	B	515	CLA	CAA-C2A-C3A	-5.20	98.56	112.81
32	V	552	HEM	CBD-CAD-C3D	-5.01	102.91	112.47
26	L	5213	SQD	O8-S-C6	-4.98	99.93	106.01
20	b	5515	CLA	CAA-C2A-C3A	-4.87	99.47	112.81
20	B	511	CLA	CAA-C2A-C3A	-4.64	107.00	116.38
20	b	5511	CLA	CAA-C2A-C3A	-4.63	107.01	116.38
30	c	5508	DGD	C3G-O3G-C1D	-4.50	104.53	113.76
24	X	130	BCR	C8-C9-C10	-4.38	112.22	118.94
24	x	5130	BCR	C8-C9-C10	-4.32	112.31	118.94
21	A	562	PHO	CBD-CHA-C4D	-4.27	103.73	108.54
24	T	5104	BCR	C33-C5-C4	-4.19	105.51	113.45
28	L	210	MGE	C3G-O3G-C1D	-4.18	105.18	113.76
24	T	5104	BCR	C38-C26-C27	-4.18	105.53	113.45
28	l	5210	MGE	C3G-O3G-C1D	-4.17	105.20	113.76
24	x	5130	BCR	C33-C5-C4	-4.15	105.58	113.45
24	B	529	BCR	C38-C26-C27	-4.15	105.58	113.45
24	D	357	BCR	C38-C26-C27	-4.13	105.62	113.45
24	d	5357	BCR	C38-C26-C27	-4.12	105.63	113.45
21	a	5562	PHO	CBD-CHA-C4D	-4.12	103.90	108.54
24	D	357	BCR	C33-C5-C4	-4.07	105.72	113.45
24	X	130	BCR	C33-C5-C4	-4.07	105.73	113.45
30	C	508	DGD	C3G-O3G-C1D	-4.06	105.42	113.76
24	t	104	BCR	C33-C5-C4	-4.03	105.81	113.45
24	d	5357	BCR	C33-C5-C4	-4.01	105.85	113.45
20	b	5511	CLA	CMA-C3A-C2A	-3.98	108.33	116.38
24	C	504	BCR	C38-C26-C27	-3.97	105.91	113.45
20	c	5502	CLA	CAA-C2A-C3A	-3.96	101.96	112.81
24	C	505	BCR	C33-C5-C4	-3.95	105.95	113.45
24	C	506	BCR	C38-C26-C27	-3.93	105.99	113.45
20	C	495	CLA	CAA-C2A-C3A	-3.93	102.03	112.81
24	H	107	BCR	C38-C26-C27	-3.91	106.03	113.45
20	c	5495	CLA	CAA-C2A-C3A	-3.91	102.09	112.81
24	B	528	BCR	C38-C26-C27	-3.88	106.08	113.45
20	B	511	CLA	CMA-C3A-C2A	-3.88	108.53	116.38
27	a	5568	LMT	C1-O1'-C1'	-3.88	107.21	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	563	CLA	OBD-CAD-CBD	-3.87	120.10	125.94
20	C	494	CLA	CAA-C2A-C3A	-3.87	102.21	112.81
21	a	5561	PHO	CBD-CHA-C4D	-3.86	104.19	108.54
20	B	517	CLA	OBD-CAD-CBD	-3.86	120.12	125.94
27	A	569	LMT	C1-O1'-C1'	-3.84	107.27	113.87
24	C	504	BCR	C33-C5-C4	-3.84	106.16	113.45
20	c	5493	CLA	CAA-C2A-C3A	-3.83	102.32	112.81
20	C	497	CLA	C7-C6-C5	-3.82	102.48	113.11
20	c	5494	CLA	CAA-C2A-C3A	-3.82	102.33	112.81
24	B	528	BCR	C30-C25-C26	-3.82	117.23	122.59
21	A	561	PHO	CBD-CHA-C4D	-3.81	104.25	108.54
20	C	493	CLA	CAA-C2A-C3A	-3.81	102.37	112.81
24	C	506	BCR	C33-C5-C4	-3.79	106.25	113.45
24	c	5506	BCR	C38-C26-C27	-3.78	106.27	113.45
20	C	502	CLA	CAA-C2A-C3A	-3.77	102.47	112.81
24	c	5504	BCR	C38-C26-C27	-3.77	106.30	113.45
22	A	564	PQ9	C11-C12-C13	-3.75	120.43	126.71
24	A	566	BCR	C38-C26-C27	-3.75	106.34	113.45
24	b	5527	BCR	C38-C26-C27	-3.74	106.35	113.45
24	A	566	BCR	C33-C5-C4	-3.73	106.37	113.45
24	a	5566	BCR	C38-C26-C27	-3.73	106.37	113.45
24	h	5107	BCR	C38-C26-C27	-3.73	106.37	113.45
24	c	5505	BCR	C38-C26-C27	-3.72	106.39	113.45
24	c	5506	BCR	C33-C5-C4	-3.72	106.39	113.45
20	b	5517	CLA	OBD-CAD-CBD	-3.69	120.37	125.94
24	d	5357	BCR	C30-C25-C26	-3.68	117.42	122.59
24	T	5104	BCR	C30-C25-C26	-3.68	117.43	122.59
24	c	5505	BCR	C33-C5-C4	-3.67	106.48	113.45
24	B	527	BCR	C38-C26-C27	-3.67	106.49	113.45
24	X	130	BCR	C38-C26-C27	-3.67	106.49	113.45
24	b	5529	BCR	C38-C26-C27	-3.66	106.51	113.45
24	b	5527	BCR	C33-C5-C4	-3.66	106.52	113.45
24	d	5357	BCR	C1-C6-C5	-3.65	117.46	122.59
24	H	107	BCR	C33-C5-C4	-3.65	106.53	113.45
24	t	104	BCR	C38-C26-C27	-3.64	106.54	113.45
24	B	527	BCR	C33-C5-C4	-3.64	106.55	113.45
24	x	5130	BCR	C38-C26-C27	-3.62	106.58	113.45
20	c	5497	CLA	C7-C6-C5	-3.60	103.09	113.11
24	b	5529	BCR	C33-C5-C4	-3.59	106.63	113.45
24	c	5504	BCR	C1-C6-C5	-3.59	117.55	122.59
24	D	357	BCR	C1-C6-C5	-3.58	117.56	122.59
24	B	529	BCR	C33-C5-C4	-3.57	106.69	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	107	BCR	C30-C25-C26	-3.56	117.58	122.59
24	C	504	BCR	C1-C6-C5	-3.56	117.59	122.59
20	B	513	CLA	CAA-C2A-C3A	-3.55	103.06	112.81
24	D	357	BCR	C30-C25-C26	-3.55	117.60	122.59
24	a	5566	BCR	C33-C5-C4	-3.55	106.72	113.45
20	b	5520	CLA	C7-C6-C5	-3.55	103.25	113.11
24	b	5528	BCR	C30-C25-C26	-3.53	117.63	122.59
24	c	5504	BCR	C33-C5-C4	-3.53	106.76	113.45
28	B	530	MGE	C3G-O3G-C1D	-3.52	106.53	113.76
26	d	5358	SQD	O9-S-C6	-3.52	103.82	106.83
20	a	5560	CLA	CAA-C2A-C3A	-3.51	103.19	112.81
20	b	5526	CLA	OBD-CAD-CBD	-3.51	120.65	125.94
24	c	5506	BCR	C30-C25-C26	-3.50	117.67	122.59
21	a	5562	PHO	C7-C6-C5	-3.50	103.37	113.11
20	A	560	CLA	CAA-C2A-C3A	-3.48	103.26	112.81
30	C	508	DGD	C3G-C2G-C1G	-3.48	104.00	111.86
24	h	5107	BCR	C33-C5-C4	-3.48	106.86	113.45
26	A	568	SQD	O9-S-C6	-3.48	103.86	106.83
24	t	104	BCR	C30-C25-C26	-3.47	117.71	122.59
24	X	130	BCR	C30-C25-C26	-3.47	117.71	122.59
24	x	5130	BCR	C30-C25-C26	-3.47	117.72	122.59
24	b	5528	BCR	C38-C26-C27	-3.45	106.90	113.45
24	C	505	BCR	C38-C26-C27	-3.45	106.90	113.45
24	b	5528	BCR	C33-C5-C4	-3.45	106.91	113.45
20	b	5514	CLA	OBD-CAD-CBD	-3.42	120.77	125.94
24	a	5566	BCR	C30-C25-C26	-3.42	117.78	122.59
30	c	5508	DGD	C3G-C2G-C1G	-3.42	104.14	111.86
24	h	5107	BCR	C30-C25-C26	-3.40	117.81	122.59
20	B	513	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
20	b	5521	CLA	C7-C6-C5	-3.39	103.69	113.11
20	b	5513	CLA	CAA-C2A-C3A	-3.37	103.57	112.81
21	a	5562	PHO	CAB-C3B-C2B	-3.37	117.27	128.56
20	D	354	CLA	OBD-CAD-CBD	-3.36	120.86	125.94
20	B	522	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
20	C	503	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
20	B	521	CLA	C7-C6-C5	-3.36	103.78	113.11
24	A	566	BCR	C30-C25-C26	-3.36	117.88	122.59
20	B	526	CLA	OBD-CAD-CBD	-3.35	120.88	125.94
24	x	5130	BCR	C12-C13-C14	-3.35	113.81	118.94
20	B	520	CLA	C7-C6-C5	-3.34	103.82	113.11
20	b	5512	CLA	CAA-C2A-C3A	-3.34	103.65	112.81
20	c	5500	CLA	C7-C6-C5	-3.32	103.88	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5529	BCR	C30-C25-C26	-3.32	117.93	122.59
20	b	5526	CLA	CAA-C2A-C3A	-3.32	103.72	112.81
24	B	529	BCR	C30-C25-C26	-3.31	117.94	122.59
20	c	5501	CLA	C7-C6-C5	-3.31	103.91	113.11
20	d	5354	CLA	CAA-C2A-C3A	-3.29	103.78	112.81
21	A	562	PHO	CAB-C3B-C2B	-3.29	117.53	128.56
20	b	5522	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
20	B	521	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
20	B	512	CLA	CAA-C2A-C3A	-3.26	103.86	112.81
22	a	5564	PQ9	C11-C12-C13	-3.25	121.28	126.71
20	a	5563	CLA	OBD-CAD-CBD	-3.25	121.04	125.94
28	b	5530	MGE	C3G-O3G-C1D	-3.25	107.10	113.76
24	C	504	BCR	C30-C25-C26	-3.24	118.04	122.59
20	c	5495	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
20	b	5512	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
24	C	506	BCR	C30-C25-C26	-3.21	118.08	122.59
20	c	5503	CLA	OBD-CAD-CBD	-3.20	121.10	125.94
20	A	559	CLA	CAA-C2A-C3A	-3.20	104.04	112.81
24	H	107	BCR	C1-C6-C5	-3.19	118.11	122.59
20	D	354	CLA	CAA-C2A-C3A	-3.18	104.08	112.81
21	A	562	PHO	C7-C6-C5	-3.18	104.28	113.11
24	b	5528	BCR	C1-C6-C5	-3.17	118.13	122.59
20	a	5559	CLA	CAA-C2A-C3A	-3.17	104.11	112.81
24	h	5107	BCR	C1-C6-C5	-3.17	118.14	122.59
20	C	492	CLA	OBD-CAD-CBD	-3.15	121.18	125.94
20	B	512	CLA	OBD-CAD-CBD	-3.15	121.19	125.94
24	B	527	BCR	C30-C25-C26	-3.13	118.19	122.59
24	B	528	BCR	C33-C5-C4	-3.13	107.52	113.45
20	b	5522	CLA	C7-C6-C5	-3.12	104.42	113.11
20	c	5494	CLA	OBD-CAD-CBD	-3.12	121.23	125.94
24	b	5529	BCR	C1-C6-C5	-3.12	118.21	122.59
20	B	526	CLA	CAA-C2A-C3A	-3.11	104.27	112.81
20	B	524	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
20	A	560	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
24	H	107	BCR	C12-C13-C14	-3.11	114.17	118.94
20	b	5518	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
20	c	5496	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
24	x	5130	BCR	C1-C6-C5	-3.10	118.23	122.59
20	d	5355	CLA	OBD-CAD-CBD	-3.08	121.28	125.94
26	A	5212	SQD	C3-C4-C5	-3.08	104.79	110.22
24	X	130	BCR	C1-C6-C5	-3.08	118.27	122.59
20	C	501	CLA	C7-C6-C5	-3.08	104.56	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5527	BCR	C1-C6-C5	-3.06	118.28	122.59
26	a	212	SQD	C3-C4-C5	-3.05	104.84	110.22
20	B	511	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
21	A	561	PHO	CAB-C3B-C2B	-3.04	118.36	128.56
20	C	495	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
20	b	5513	CLA	OBD-CAD-CBD	-3.03	121.36	125.94
20	b	5521	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
24	B	529	BCR	C1-C6-C5	-3.02	118.34	122.59
20	a	5560	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
20	B	514	CLA	OBD-CAD-CBD	-3.00	121.42	125.94
22	d	5356	PQ9	C11-C2-C3	-2.99	118.97	123.23
20	D	355	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
20	B	520	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
24	c	5504	BCR	C30-C25-C26	-2.98	118.40	122.59
20	C	495	CLA	C7-C6-C5	-2.98	104.83	113.11
24	c	5505	BCR	C1-C6-C5	-2.97	118.41	122.59
20	B	518	CLA	CAA-C2A-C3A	-2.97	104.67	112.81
20	C	494	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
20	a	5558	CLA	C7-C6-C5	-2.96	104.87	113.11
20	B	525	CLA	C7-C6-C5	-2.96	104.87	113.11
21	a	5561	PHO	C7-C6-C5	-2.96	104.89	113.11
20	b	5523	CLA	OBD-CAD-CBD	-2.96	121.48	125.94
20	B	522	CLA	C7-C6-C5	-2.95	104.90	113.11
20	b	5516	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
21	a	5561	PHO	CAB-C3B-C2B	-2.94	118.69	128.56
21	a	5562	PHO	C2A-C1A-NA	-2.93	108.34	111.91
20	C	502	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
20	c	5493	CLA	C7-C6-C5	-2.92	104.99	113.11
20	c	5498	CLA	CAA-C2A-C3A	-2.92	104.80	112.81
20	A	558	CLA	C7-C6-C5	-2.92	104.99	113.11
24	h	5107	BCR	C12-C13-C14	-2.92	114.46	118.94
26	t	213	SQD	O9-S-C6	-2.92	104.33	106.83
24	C	506	BCR	C1-C6-C5	-2.92	118.49	122.59
28	I	201	MGE	O1G-C1G-C2G	-2.92	101.33	108.66
28	i	5201	MGE	O1G-C1G-C2G	-2.92	101.33	108.66
20	B	516	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
20	C	497	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
20	c	5496	CLA	CAA-C2A-C3A	-2.91	104.83	112.81
20	B	525	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
20	b	5518	CLA	CAA-C2A-C3A	-2.90	104.85	112.81
24	X	130	BCR	C12-C13-C14	-2.90	114.50	118.94
24	D	357	BCR	C12-C13-C14	-2.89	114.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5494	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
24	B	528	BCR	C1-C6-C5	-2.89	118.53	122.59
20	d	5354	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
22	D	356	PQ9	C11-C2-C3	-2.89	119.12	123.23
20	c	5495	CLA	C7-C6-C5	-2.88	105.10	113.11
20	A	563	CLA	CAA-C2A-C3A	-2.88	104.92	112.81
24	b	5527	BCR	C30-C25-C26	-2.88	118.55	122.59
20	C	499	CLA	OBD-CAD-CBD	-2.88	121.60	125.94
20	A	558	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
20	c	5499	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
20	b	5519	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
20	C	500	CLA	C7-C6-C5	-2.85	105.19	113.11
20	C	493	CLA	C7-C6-C5	-2.85	105.20	113.11
28	B	530	MGE	O1G-C1G-C2G	-2.85	101.51	108.66
27	m	216	LMT	C1-O1'-C1'	-2.84	108.99	113.87
30	c	5509	DGD	C3G-C2G-C1G	-2.82	105.49	111.86
20	c	5495	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
20	B	524	CLA	C7-C6-C5	-2.81	105.30	113.11
20	B	515	CLA	C7-C6-C5	-2.80	105.32	113.11
20	C	495	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
24	c	5505	BCR	C30-C25-C26	-2.80	118.66	122.59
24	T	5104	BCR	C23-C22-C21	-2.80	114.65	118.94
20	C	496	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
20	a	5560	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
20	c	5491	CLA	C7-C6-C5	-2.79	105.36	113.11
20	b	5517	CLA	C7-C6-C5	-2.78	105.39	113.11
24	C	505	BCR	C1-C6-C5	-2.77	118.69	122.59
20	c	5498	CLA	OBD-CAD-CBD	-2.77	121.75	125.94
20	b	5511	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
24	t	104	BCR	C1-C6-C5	-2.77	118.70	122.59
20	b	5524	CLA	C7-C6-C5	-2.76	105.43	113.11
21	A	562	PHO	CAA-C2A-C3A	-2.76	105.25	112.81
20	A	560	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
24	B	527	BCR	C1-C6-C5	-2.75	118.72	122.59
20	b	5520	CLA	OBD-CAD-CBD	-2.75	121.78	125.94
24	T	5104	BCR	C1-C6-C5	-2.75	118.73	122.59
21	a	5562	PHO	CAA-C2A-C3A	-2.74	105.30	112.81
20	a	5563	CLA	CAA-C2A-C3A	-2.74	105.30	112.81
20	C	499	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
20	C	496	CLA	C7-C6-C5	-2.73	105.51	113.11
20	b	5525	CLA	C7-C6-C5	-2.73	105.53	113.11
20	b	5525	CLA	OBD-CAD-CBD	-2.72	121.83	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	217	LMT	C1-O1'-C1'	-2.72	109.19	113.87
20	C	491	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
30	C	509	DGD	C3G-C2G-C1G	-2.72	105.72	111.86
24	C	505	BCR	C19-C18-C17	-2.72	114.77	118.94
22	A	564	PQ9	C16-C17-C18	-2.72	120.86	127.68
20	b	5513	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
20	C	498	CLA	CAA-C2A-C3A	-2.71	105.37	112.81
27	t	5217	LMT	C1-O1'-C1'	-2.70	109.23	113.87
20	C	496	CLA	CAA-C2A-C3A	-2.70	105.40	112.81
20	a	5560	CLA	C7-C6-C5	-2.70	105.60	113.11
21	A	562	PHO	C2A-C1A-NA	-2.70	108.63	111.91
20	B	512	CLA	C7-C6-C5	-2.69	105.62	113.11
20	B	515	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
20	C	498	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
20	B	519	CLA	OBD-CAD-CBD	-2.69	121.89	125.94
24	d	5357	BCR	C12-C13-C14	-2.68	114.82	118.94
22	a	5564	PQ9	C16-C17-C18	-2.68	120.94	127.68
20	b	5524	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
28	b	5530	MGE	O1G-C1G-C2G	-2.68	101.92	108.66
20	c	5496	CLA	C7-C6-C5	-2.68	105.67	113.11
20	B	518	CLA	C7-C6-C5	-2.67	105.68	113.11
28	l	5210	MGE	O1G-C1G-C2G	-2.67	101.94	108.66
24	C	506	BCR	C19-C18-C17	-2.67	114.85	118.94
20	B	516	CLA	C7-C6-C5	-2.67	105.70	113.11
20	A	558	CLA	CAA-C2A-C3A	-2.66	105.51	112.81
20	b	5519	CLA	C7-C6-C5	-2.66	105.71	113.11
20	B	519	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
24	t	104	BCR	C23-C22-C21	-2.66	114.86	118.94
24	C	506	BCR	C12-C13-C14	-2.66	114.86	118.94
20	B	517	CLA	CAA-C2A-C3A	-2.65	105.54	112.81
20	a	5563	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
24	C	504	BCR	C23-C22-C21	-2.65	114.88	118.94
20	a	5558	CLA	CAA-C2A-C3A	-2.65	105.55	112.81
24	C	505	BCR	C30-C25-C26	-2.64	118.88	122.59
20	B	520	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
20	B	514	CLA	C7-C6-C5	-2.64	105.79	113.11
20	B	519	CLA	C7-C6-C5	-2.63	105.79	113.11
20	C	498	CLA	C7-C6-C5	-2.63	105.80	113.11
20	b	5518	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
20	B	517	CLA	C7-C6-C5	-2.63	105.81	113.11
20	b	5523	CLA	CMB-C2B-C1B	-2.63	124.43	128.46
24	c	5506	BCR	C40-C30-C29	-2.62	98.46	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	210	MGE	O1G-C1G-C2G	-2.62	102.07	108.66
20	C	494	CLA	OBD-CAD-CBD	-2.62	121.98	125.94
32	F	51	HEM	C4C-C3C-C2C	-2.62	105.07	106.90
20	C	500	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
27	t	5217	LMT	C3'-C4'-C5'	-2.61	105.33	110.88
26	L	5213	SQD	C3-C4-C5	-2.61	105.62	110.22
20	C	493	CLA	OBD-CAD-CBD	-2.60	122.01	125.94
26	a	212	SQD	O9-S-C6	-2.60	104.61	106.83
20	b	5512	CLA	C7-C6-C5	-2.60	105.89	113.11
21	A	561	PHO	C7-C6-C5	-2.60	105.89	113.11
20	B	519	CLA	CAA-C2A-C3A	-2.59	105.70	112.81
24	A	566	BCR	C1-C6-C5	-2.58	118.96	122.59
20	b	5515	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
24	c	5506	BCR	C1-C6-C5	-2.57	118.98	122.59
24	C	506	BCR	C40-C30-C29	-2.57	98.68	108.80
20	b	5521	CLA	CAA-C2A-C3A	-2.56	105.78	112.81
20	b	5518	CLA	C7-C6-C5	-2.56	105.98	113.11
20	b	5517	CLA	CAA-C2A-C3A	-2.56	105.79	112.81
20	b	5520	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
20	b	5517	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
20	b	5526	CLA	C7-C6-C5	-2.56	106.01	113.11
20	C	503	CLA	CMB-C2B-C1B	-2.56	124.54	128.46
28	d	5360	MGE	C3G-O3G-C1D	-2.55	108.52	113.76
20	a	5559	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
20	b	5515	CLA	C7-C6-C5	-2.55	106.03	113.11
20	b	5516	CLA	C7-C6-C5	-2.54	106.06	113.11
20	a	5558	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
24	a	5566	BCR	C1-C6-C5	-2.53	119.03	122.59
20	B	512	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
20	A	560	CLA	C7-C6-C5	-2.51	106.13	113.11
28	d	5359	MGE	C3G-C2G-C1G	-2.51	106.20	111.86
20	b	5523	CLA	C7-C6-C5	-2.51	106.14	113.11
20	c	5493	CLA	OBD-CAD-CBD	-2.51	122.16	125.94
24	C	505	BCR	C12-C13-C14	-2.51	115.10	118.94
20	b	5519	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
20	c	5492	CLA	OBD-CAD-CBD	-2.50	122.16	125.94
20	c	5498	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
24	T	5104	BCR	C40-C30-C29	-2.50	98.95	108.80
28	B	530	MGE	C3G-C2G-C1G	-2.49	106.24	111.86
24	c	5506	BCR	C19-C18-C17	-2.49	115.12	118.94
24	t	104	BCR	C12-C13-C14	-2.49	115.12	118.94
20	b	5512	CLA	CMB-C2B-C1B	-2.49	124.64	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	523	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
20	A	559	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
20	b	5524	CLA	CAA-C2A-C3A	-2.48	106.02	112.81
20	C	491	CLA	C7-C6-C5	-2.48	106.23	113.11
22	D	356	PQ9	C16-C17-C18	-2.48	121.46	127.68
20	B	524	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
20	b	5519	CLA	CAA-C2A-C3A	-2.47	106.04	112.81
20	B	523	CLA	OBD-CAD-CBD	-2.47	122.21	125.94
28	D	360	MGE	O1G-C1G-C2G	-2.46	102.47	108.66
20	b	5525	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
20	B	523	CLA	C7-C6-C5	-2.46	106.28	113.11
20	A	563	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
26	A	568	SQD	C3-C4-C5	-2.45	105.89	110.22
24	t	104	BCR	C8-C9-C10	-2.44	115.19	118.94
20	D	355	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
26	t	213	SQD	C3-C4-C5	-2.43	105.93	110.22
26	d	5358	SQD	C3-C4-C5	-2.43	105.93	110.22
20	c	5492	CLA	CAA-C2A-C3A	-2.43	106.15	112.81
20	c	5497	CLA	OBD-CAD-CBD	-2.42	122.28	125.94
20	B	518	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
20	B	521	CLA	CAA-C2A-C3A	-2.42	106.17	112.81
20	c	5498	CLA	C7-C6-C5	-2.42	106.39	113.11
20	C	503	CLA	CAA-C2A-C3A	-2.42	106.18	112.81
20	B	518	CLA	OBD-CAD-CBD	-2.41	122.29	125.94
20	b	5516	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
24	c	5504	BCR	C23-C22-C21	-2.41	115.25	118.94
24	c	5505	BCR	C12-C13-C14	-2.41	115.25	118.94
24	C	504	BCR	C32-C1-C2	-2.40	99.33	108.80
24	B	527	BCR	C12-C13-C14	-2.40	115.26	118.94
24	c	5504	BCR	C12-C13-C14	-2.40	115.26	118.94
27	T	217	LMT	C3'-C4'-C5'	-2.39	105.80	110.88
20	c	5502	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
20	c	5491	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
20	c	5500	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
20	A	558	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
20	a	5558	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
20	B	524	CLA	CAA-C2A-C3A	-2.38	106.28	112.81
24	X	130	BCR	C32-C1-C2	-2.37	99.44	108.80
28	d	5361	MGE	O1G-C1G-C2G	-2.37	102.70	108.66
28	i	5201	MGE	C3G-O3G-C1D	-2.37	108.90	113.76
20	A	559	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
24	c	5506	BCR	C12-C13-C14	-2.37	115.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	526	CLA	C7-C6-C5	-2.37	106.53	113.11
24	b	5529	BCR	C12-C13-C14	-2.37	115.31	118.94
24	B	529	BCR	C12-C13-C14	-2.36	115.32	118.94
20	d	5354	CLA	C7-C6-C5	-2.35	106.57	113.11
20	c	5502	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
20	C	492	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
24	T	5104	BCR	C12-C13-C14	-2.35	115.33	118.94
20	B	513	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
20	c	5491	CLA	CAA-C2A-C3A	-2.34	106.40	112.81
20	B	513	CLA	C7-C6-C5	-2.34	106.62	113.11
20	C	498	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
24	A	566	BCR	C19-C18-C17	-2.33	115.37	118.94
20	c	5499	CLA	CMB-C2B-C1B	-2.32	124.89	128.46
22	D	356	PQ9	C11-C12-C13	-2.31	122.85	126.71
20	b	5515	CLA	C12-C11-C10	-2.31	102.08	113.25
20	c	5493	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
20	c	5493	CLA	C12-C11-C10	-2.31	102.09	113.25
20	a	5559	CLA	CMB-C2B-C1B	-2.31	124.92	128.46
30	H	208	DGD	C3G-C2G-C1G	-2.30	106.66	111.86
20	C	492	CLA	CAA-C2A-C3A	-2.30	106.50	112.81
24	t	104	BCR	C40-C30-C29	-2.30	99.73	108.80
24	c	5506	BCR	C23-C22-C21	-2.30	115.41	118.94
20	B	517	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
20	c	5503	CLA	CAA-C2A-C3A	-2.30	106.51	112.81
20	c	5497	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
20	c	5500	CLA	CAA-C2A-C3A	-2.29	106.54	112.81
20	D	354	CLA	C7-C6-C5	-2.29	106.76	113.11
22	d	5356	PQ9	C16-C17-C18	-2.28	121.94	127.68
24	D	357	BCR	C23-C22-C21	-2.28	115.44	118.94
30	C	508	DGD	C6E-C5E-C4E	-2.28	107.67	113.00
20	c	5492	CLA	C7-C6-C5	-2.28	106.78	113.11
26	L	5213	SQD	O9-S-C6	-2.28	104.88	106.83
20	b	5514	CLA	C7-C6-C5	-2.27	106.80	113.11
24	X	130	BCR	C19-C18-C17	-2.26	115.48	118.94
20	B	515	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
20	C	502	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
24	C	506	BCR	C23-C22-C21	-2.25	115.48	118.94
22	D	356	PQ9	C21-C22-C23	-2.25	122.03	127.68
24	a	5566	BCR	C12-C13-C14	-2.25	115.49	118.94
24	c	5504	BCR	C32-C1-C2	-2.24	99.96	108.80
20	c	5492	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
24	C	504	BCR	C12-C13-C14	-2.24	115.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	566	BCR	C12-C13-C14	-2.24	115.50	118.94
26	A	5212	SQD	O9-S-C6	-2.24	104.92	106.83
20	d	5355	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
20	B	516	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
20	B	515	CLA	C12-C11-C10	-2.23	102.46	113.25
20	c	5501	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
24	d	5357	BCR	C19-C18-C17	-2.22	115.53	118.94
30	h	5208	DGD	C3G-C2G-C1G	-2.22	106.85	111.86
28	D	358	MGE	C3G-C2G-C1G	-2.21	106.87	111.86
20	B	518	CLA	C2C-C1C-NC	-2.20	108.71	110.22
20	b	5524	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
24	x	5130	BCR	C32-C1-C2	-2.20	100.12	108.80
28	I	201	MGE	C3G-O3G-C1D	-2.20	109.25	113.76
20	c	5503	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
20	B	525	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
27	T	217	LMT	C1B-O1B-C4'	-2.19	112.65	118.00
20	b	5521	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
24	b	5527	BCR	C12-C13-C14	-2.19	115.58	118.94
20	c	5497	CLA	CAA-C2A-C3A	-2.18	106.82	112.81
20	C	496	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
24	B	527	BCR	C19-C18-C17	-2.18	115.60	118.94
24	a	5566	BCR	C8-C9-C10	-2.18	115.60	118.94
20	b	5522	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
20	B	514	CLA	CAA-C2A-C3A	-2.18	106.85	112.81
20	c	5501	CLA	C12-C11-C10	-2.17	102.75	113.25
20	C	501	CLA	OBD-CAD-CBD	-2.17	122.66	125.94
20	b	5514	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
24	d	5357	BCR	C23-C22-C21	-2.17	115.61	118.94
20	C	500	CLA	CMA-C3A-C2A	-2.17	104.98	113.77
20	B	526	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
20	C	497	CLA	CMB-C2B-C1B	-2.17	125.14	128.46
21	A	561	PHO	O1D-CGD-CBD	-2.17	120.71	124.60
28	D	359	MGE	C3G-O3G-C1D	-2.16	109.32	113.76
20	C	501	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
20	a	5560	CLA	C3C-C4C-NC	-2.15	108.03	110.21
27	M	5216	LMT	C1-O1'-C1'	-2.15	110.17	113.87
20	b	5514	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
20	A	558	CLA	C2C-C1C-NC	-2.15	108.75	110.22
28	b	5530	MGE	C3G-C2G-C1G	-2.15	107.01	111.86
22	A	564	PQ9	C21-C22-C23	-2.15	122.28	127.68
20	C	501	CLA	C12-C11-C10	-2.14	102.92	113.25
32	v	5552	HEM	C1D-C2D-C3D	-2.13	105.51	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	212	SQD	O10-C23-C24	-2.13	116.98	124.82
24	b	5528	BCR	C32-C1-C2	-2.13	100.39	108.80
20	C	493	CLA	C12-C11-C10	-2.13	102.94	113.25
20	B	520	CLA	CAA-C2A-C3A	-2.13	106.96	112.81
32	f	5051	HEM	C4C-C3C-C2C	-2.13	105.41	106.90
20	c	5498	CLA	C2C-C1C-NC	-2.12	108.77	110.22
24	T	5104	BCR	C8-C9-C10	-2.12	115.69	118.94
20	C	493	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
32	f	5051	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
20	B	514	CLA	CMB-C2B-C1B	-2.11	125.23	128.46
20	C	499	CLA	CAA-C2A-C3A	-2.10	107.04	112.81
20	c	5498	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
28	D	359	MGE	O1G-C1G-C2G	-2.10	103.38	108.66
20	A	563	CLA	CMA-C3A-C2A	-2.10	105.25	113.77
20	C	497	CLA	C12-C11-C10	-2.09	103.15	113.25
20	C	491	CLA	CAA-C2A-C3A	-2.09	107.08	112.81
21	a	5561	PHO	O1D-CGD-CBD	-2.09	120.85	124.60
24	c	5505	BCR	C19-C18-C17	-2.08	115.74	118.94
20	b	5513	CLA	C7-C6-C5	-2.08	107.32	113.11
22	a	5564	PQ9	C21-C22-C23	-2.08	122.45	127.68
28	d	5360	MGE	C3G-C2G-C1G	-2.08	107.17	111.86
20	B	521	CLA	C12-C11-C10	-2.07	103.22	113.25
20	b	5511	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
20	A	558	CLA	CMA-C3A-C2A	-2.07	105.36	113.77
20	b	5515	CLA	CMA-C3A-C2A	-2.07	105.36	113.77
20	b	5520	CLA	C12-C11-C10	-2.07	103.25	113.25
24	T	5104	BCR	C19-C18-C17	-2.07	115.77	118.94
20	c	5497	CLA	C12-C11-C10	-2.06	103.28	113.25
27	m	216	LMT	C1B-O1B-C4'	-2.06	112.97	118.00
20	b	5526	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
30	c	5508	DGD	C6E-C5E-C4E	-2.06	108.19	113.00
20	D	354	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
32	f	5051	HEM	CBA-CAA-C2A	-2.05	108.56	112.48
20	C	498	CLA	C12-C11-C10	-2.05	103.33	113.25
24	b	5527	BCR	C19-C18-C17	-2.05	115.79	118.94
27	M	5216	LMT	C6B-C5B-C4B	-2.05	108.20	113.00
24	a	5566	BCR	C19-C18-C17	-2.05	115.80	118.94
20	b	5521	CLA	C12-C11-C10	-2.04	103.38	113.25
26	t	213	SQD	O48-C23-O10	-2.04	118.49	123.55
20	C	492	CLA	C7-C6-C5	-2.03	107.46	113.11
24	h	5107	BCR	C8-C9-C10	-2.03	115.82	118.94
20	b	5513	CLA	CMA-C3A-C2A	-2.03	105.53	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5496	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
20	d	5354	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
20	C	500	CLA	CAA-C2A-C3A	-2.02	107.26	112.81
30	C	509	DGD	C3G-O3G-C1D	-2.02	109.61	113.76
20	B	522	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
26	t	213	SQD	O6-C44-C45	-2.02	106.19	110.99
24	x	5130	BCR	C19-C18-C17	-2.01	115.85	118.94
27	A	569	LMT	C1'-O5'-C5'	-2.01	109.93	113.72
20	c	5500	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
27	m	216	LMT	C4B-C3B-C2B	-2.01	107.30	110.84
32	F	51	HEM	C1D-C2D-C3D	-2.00	105.60	107.00
32	V	552	HEM	CBA-CAA-C2A	2.00	116.31	112.48
20	A	560	CLA	C6-C7-C8	2.00	122.30	115.73
20	B	520	CLA	O2D-CGD-CBD	2.00	114.88	111.30
20	b	5520	CLA	C6-C5-C3	2.00	117.20	112.66
20	B	512	CLA	C1-O2A-CGA	2.00	121.58	116.77
20	C	503	CLA	C2A-C3A-C4A	2.00	105.11	101.87
20	b	5519	CLA	C2A-C3A-C4A	2.01	105.11	101.87
20	C	503	CLA	O2D-CGD-CBD	2.01	114.89	111.30
20	c	5497	CLA	CMB-C2B-C3B	2.01	128.62	124.89
24	B	528	BCR	C30-C25-C24	2.01	121.38	115.73
20	c	5491	CLA	C6-C5-C3	2.01	117.21	112.66
20	C	496	CLA	CBA-CAA-C2A	2.01	119.81	113.80
20	b	5525	CLA	CMB-C2B-C3B	2.01	128.62	124.89
20	C	496	CLA	C2A-C1A-CHA	2.01	127.48	123.92
26	a	212	SQD	O5-C5-C4	2.01	113.37	109.66
20	a	5559	CLA	CAA-CBA-CGA	2.01	119.41	113.35
20	b	5518	CLA	CMB-C2B-C3B	2.02	128.63	124.89
32	f	5051	HEM	C4A-C3A-C2A	2.02	108.40	107.00
20	B	523	CLA	CBA-CAA-C2A	2.02	119.83	113.80
20	B	520	CLA	C2A-C1A-CHA	2.02	127.50	123.92
20	c	5501	CLA	C2A-C3A-C4A	2.02	105.13	101.87
20	c	5501	CLA	C2A-C1A-CHA	2.02	127.50	123.92
24	b	5529	BCR	C30-C25-C24	2.02	121.41	115.73
30	c	5508	DGD	O3G-C3G-C2G	2.02	115.80	110.99
20	B	519	CLA	CMB-C2B-C3B	2.02	128.65	124.89
20	b	5523	CLA	CBA-CAA-C2A	2.02	119.85	113.80
20	c	5500	CLA	O2D-CGD-CBD	2.03	114.92	111.30
20	B	517	CLA	C2A-C3A-C4A	2.03	105.14	101.87
22	a	5564	PQ9	C11-C2-C1	2.03	118.52	116.88
20	B	514	CLA	C6-C5-C3	2.03	117.26	112.66
20	b	5517	CLA	CMB-C2B-C3B	2.03	128.66	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	201	MGE	O1G-C1A-C2A	2.03	117.81	111.90
24	A	566	BCR	C34-C9-C8	2.03	121.34	118.10
20	a	5559	CLA	C1-C2-C3	2.03	129.70	125.96
20	C	496	CLA	C1C-NC-C4C	2.03	108.22	107.06
20	B	514	CLA	C1-C2-C3	2.04	129.71	125.96
20	c	5491	CLA	C2A-C1A-CHA	2.04	127.53	123.92
20	C	499	CLA	OBD-CAD-C3D	2.04	131.78	128.03
20	b	5525	CLA	C2A-C1A-CHA	2.04	127.53	123.92
20	c	5500	CLA	CMB-C2B-C3B	2.04	128.67	124.89
20	B	516	CLA	C1C-NC-C4C	2.04	108.23	107.06
24	c	5505	BCR	C40-C30-C25	2.04	113.61	110.31
24	H	107	BCR	C34-C9-C8	2.04	121.35	118.10
24	B	529	BCR	C1-C6-C7	2.04	121.46	115.73
24	h	5107	BCR	C11-C12-C13	2.04	132.15	126.42
24	D	357	BCR	C36-C18-C19	2.04	121.35	118.10
20	b	5521	CLA	OBD-CAD-C3D	2.04	131.79	128.03
25	A	567	LHG	O8-C6-C5	2.04	113.79	108.66
20	A	558	CLA	C1C-NC-C4C	2.04	108.23	107.06
20	A	560	CLA	O2D-CGD-CBD	2.04	114.95	111.30
20	c	5499	CLA	C1-O2A-CGA	2.04	122.73	116.72
20	b	5518	CLA	C16-C15-C13	2.04	122.45	115.73
24	X	130	BCR	C28-C27-C26	2.05	117.30	113.78
24	D	357	BCR	C34-C9-C8	2.05	121.36	118.10
21	A	561	PHO	CMD-C2D-C1D	2.05	128.23	125.04
20	B	521	CLA	C1C-NC-C4C	2.05	108.24	107.06
20	B	517	CLA	O2D-CGD-CBD	2.06	114.98	111.30
20	b	5515	CLA	O2D-CGD-CBD	2.06	114.98	111.30
20	c	5492	CLA	C1-C2-C3	2.06	129.75	125.96
24	c	5504	BCR	C34-C9-C8	2.06	121.38	118.10
20	b	5511	CLA	C2A-C1A-CHA	2.06	127.56	123.91
24	A	566	BCR	C30-C25-C24	2.06	121.53	115.73
21	a	5561	PHO	C6-C5-C3	2.07	117.34	112.66
20	c	5493	CLA	C6-C5-C3	2.07	117.34	112.66
20	b	5513	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	C	497	CLA	C2A-C3A-C4A	2.07	105.21	101.87
21	a	5562	PHO	O2D-CGD-CBD	2.07	114.99	111.30
20	B	525	CLA	C6-C5-C3	2.07	117.34	112.66
20	c	5494	CLA	C2A-C1A-CHA	2.07	127.58	123.92
20	c	5495	CLA	OBD-CAD-C3D	2.07	131.84	128.03
20	C	493	CLA	CBA-CAA-C2A	2.07	119.99	113.80
20	C	499	CLA	CMB-C2B-C3B	2.07	128.73	124.89
20	B	515	CLA	CBA-CAA-C2A	2.07	119.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	568	SQD	C17-C16-C15	2.07	125.13	114.45
20	D	355	CLA	C2A-C3A-C4A	2.08	105.22	101.87
24	x	5130	BCR	C24-C23-C22	2.08	129.33	126.21
26	a	212	SQD	O47-C45-C44	2.08	115.99	108.44
22	a	5564	PQ9	C6-C5-C4	2.08	119.26	114.84
24	d	5357	BCR	C34-C9-C8	2.08	121.41	118.10
28	D	359	MGE	O1G-C1A-C2A	2.08	117.95	111.90
20	C	491	CLA	CBA-CAA-C2A	2.08	120.03	113.80
20	c	5496	CLA	C6-C5-C3	2.08	117.38	112.66
24	d	5357	BCR	C32-C1-C6	2.09	113.69	110.31
20	B	511	CLA	C2A-C1A-CHA	2.09	127.60	123.91
24	B	529	BCR	C11-C10-C9	2.09	130.29	127.31
24	B	529	BCR	C36-C18-C19	2.09	121.43	118.10
20	B	524	CLA	C2A-C3A-C4A	2.09	105.24	101.87
20	b	5514	CLA	C1-O2A-CGA	2.09	121.79	116.77
24	A	566	BCR	C1-C6-C7	2.09	121.61	115.73
21	a	5562	PHO	C1-C2-C3	2.09	129.81	125.96
20	b	5516	CLA	O2D-CGD-CBD	2.09	115.04	111.30
20	C	496	CLA	C6-C5-C3	2.09	117.40	112.66
20	B	518	CLA	C2A-C3A-C4A	2.09	105.25	101.87
30	c	5509	DGD	O1G-C1A-C2A	2.09	117.99	111.90
20	B	525	CLA	C2A-C1A-CHA	2.09	127.63	123.92
28	l	5210	MGE	O1G-C1A-C2A	2.09	117.99	111.90
24	x	5130	BCR	C8-C7-C6	2.09	133.12	127.25
24	b	5528	BCR	C35-C13-C12	2.10	121.44	118.10
20	D	355	CLA	CBA-CAA-C2A	2.10	120.07	113.80
20	C	496	CLA	C2A-C3A-C4A	2.10	105.26	101.87
20	b	5518	CLA	OBD-CAD-C3D	2.10	131.89	128.03
20	C	492	CLA	OBD-CAD-C3D	2.10	131.89	128.03
20	B	511	CLA	C2A-C3A-C4A	2.10	104.47	101.82
20	c	5495	CLA	C1-O2A-CGA	2.10	121.81	116.77
20	b	5518	CLA	C2A-C3A-C4A	2.10	105.26	101.87
20	A	563	CLA	OBD-CAD-C3D	2.10	131.90	128.03
20	C	503	CLA	CMB-C2B-C3B	2.10	128.79	124.89
20	B	515	CLA	C2A-C1A-CHA	2.10	127.64	123.92
24	h	5107	BCR	C36-C18-C19	2.10	121.45	118.10
24	c	5505	BCR	C34-C9-C8	2.10	121.45	118.10
20	C	502	CLA	CBA-CAA-C2A	2.10	120.09	113.80
24	b	5529	BCR	C15-C14-C13	2.10	130.31	127.31
20	d	5355	CLA	C1-O2A-CGA	2.10	121.82	116.77
20	C	493	CLA	C6-C5-C3	2.11	117.43	112.66
20	c	5493	CLA	CBA-CAA-C2A	2.11	120.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	5558	CLA	CMB-C2B-C3B	2.11	128.80	124.89
24	B	528	BCR	C40-C30-C25	2.11	113.73	110.31
20	b	5516	CLA	OBD-CAD-C3D	2.11	131.91	128.03
24	H	107	BCR	C30-C25-C24	2.11	121.66	115.73
20	c	5495	CLA	C2A-C3A-C4A	2.11	105.28	101.87
20	c	5503	CLA	C1-O2A-CGA	2.11	121.84	116.77
24	b	5528	BCR	C30-C25-C24	2.11	121.67	115.73
24	C	506	BCR	C32-C1-C6	2.11	113.74	110.31
20	b	5524	CLA	C6-C5-C3	2.12	117.45	112.66
24	T	5104	BCR	C34-C9-C8	2.12	121.47	118.10
21	a	5562	PHO	C6-C5-C3	2.12	117.46	112.66
28	b	5530	MGE	O1G-C1A-C2A	2.12	118.06	111.90
24	t	104	BCR	C16-C17-C18	2.12	130.34	127.31
24	X	130	BCR	C8-C7-C6	2.12	133.19	127.25
28	L	210	MGE	O1G-C1A-C2A	2.12	118.08	111.90
32	v	5552	HEM	C4A-C3A-C2A	2.12	108.47	107.00
20	A	559	CLA	CAA-CBA-CGA	2.12	119.75	113.35
20	b	5519	CLA	C2A-C1A-CHA	2.13	127.69	123.92
24	h	5107	BCR	C30-C25-C24	2.13	121.71	115.73
20	c	5493	CLA	C2A-C1A-CHA	2.13	127.69	123.92
20	c	5491	CLA	O2D-CGD-CBD	2.13	115.10	111.30
20	b	5517	CLA	C2A-C3A-C4A	2.13	105.31	101.87
20	c	5493	CLA	O2D-CGD-CBD	2.13	115.10	111.30
22	D	356	PQ9	C14-C13-C15	2.13	118.98	115.29
24	C	504	BCR	C16-C17-C18	2.13	130.35	127.31
20	B	524	CLA	C6-C5-C3	2.13	117.49	112.66
20	a	5563	CLA	CMB-C2B-C3B	2.13	128.85	124.89
20	C	496	CLA	C1-O2A-CGA	2.13	121.89	116.77
20	B	526	CLA	OBD-CAD-C3D	2.13	131.96	128.03
26	L	5213	SQD	O8-S-O7	2.13	116.26	111.37
20	A	563	CLA	O2D-CGD-CBD	2.14	115.11	111.30
32	v	5552	HEM	CBA-CAA-C2A	2.14	116.57	112.48
20	B	520	CLA	C2A-C3A-C4A	2.14	105.32	101.87
20	C	499	CLA	C1C-NC-C4C	2.14	108.28	107.06
20	c	5492	CLA	O2D-CGD-CBD	2.14	115.12	111.30
20	b	5523	CLA	O2D-CGD-CBD	2.14	115.12	111.30
20	C	497	CLA	C1C-NC-C4C	2.14	108.29	107.06
30	C	508	DGD	O3G-C3G-C2G	2.14	116.08	110.99
24	H	107	BCR	C37-C22-C23	2.14	121.51	118.10
20	B	512	CLA	CMB-C2B-C3B	2.14	128.87	124.89
20	b	5511	CLA	CMB-C2B-C3B	2.14	128.87	124.89
20	B	514	CLA	C2A-C1A-CHA	2.14	127.72	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	5212	SQD	O47-C45-C44	2.15	116.23	108.44
20	B	521	CLA	C1-C2-C3	2.15	129.91	125.96
20	b	5521	CLA	C1-C2-C3	2.15	129.91	125.96
24	b	5529	BCR	C1-C6-C7	2.15	121.77	115.73
21	A	562	PHO	CMD-C2D-C1D	2.15	128.39	125.04
20	b	5517	CLA	C2A-C1A-CHA	2.15	127.73	123.92
20	b	5514	CLA	C2A-C1A-CHA	2.15	127.73	123.92
24	C	505	BCR	C7-C8-C9	2.15	129.44	126.21
21	A	561	PHO	C3D-C4D-CHA	2.15	115.54	109.97
20	B	518	CLA	CBA-CAA-C2A	2.15	120.24	113.80
20	C	502	CLA	O2D-CGD-CBD	2.15	115.14	111.30
20	B	517	CLA	CBA-CAA-C2A	2.15	120.24	113.80
24	a	5566	BCR	C7-C8-C9	2.16	129.45	126.21
20	b	5520	CLA	O2D-CGD-CBD	2.16	115.15	111.30
20	b	5515	CLA	CBA-CAA-C2A	2.16	120.25	113.80
20	d	5355	CLA	C2A-C3A-C4A	2.16	105.36	101.87
24	a	5566	BCR	C34-C9-C8	2.16	121.54	118.10
20	B	514	CLA	C1-O2A-CGA	2.16	121.96	116.77
26	A	568	SQD	C34-C33-C32	2.16	125.59	114.45
21	a	5562	PHO	C3D-C4D-CHA	2.16	115.57	109.97
24	C	504	BCR	C30-C25-C24	2.16	121.81	115.73
22	A	564	PQ9	C6-C5-C4	2.16	119.44	114.84
20	b	5518	CLA	C6-C7-C8	2.17	122.85	115.73
20	B	515	CLA	O2D-CGD-CBD	2.17	115.17	111.30
20	C	498	CLA	C2A-C3A-C4A	2.17	105.37	101.87
20	d	5355	CLA	O2D-CGD-CBD	2.17	115.18	111.30
30	C	507	DGD	O6D-C1D-C2D	2.17	114.48	110.30
20	B	516	CLA	C2A-C3A-C4A	2.17	105.38	101.87
20	c	5502	CLA	CBA-CAA-C2A	2.17	120.30	113.80
21	A	561	PHO	C1-O2A-CGA	2.17	121.98	116.77
20	b	5512	CLA	O2D-CGD-CBD	2.17	115.18	111.30
30	C	508	DGD	O1G-C1A-C2A	2.17	118.22	111.90
20	b	5515	CLA	C1-C2-C3	2.17	129.96	125.96
24	x	5130	BCR	C28-C27-C26	2.17	117.52	113.78
20	c	5500	CLA	CBA-CAA-C2A	2.18	120.31	113.80
20	b	5520	CLA	C2A-C3A-C4A	2.18	105.39	101.87
20	C	500	CLA	O2D-CGD-CBD	2.18	115.19	111.30
20	b	5518	CLA	CBA-CAA-C2A	2.18	120.32	113.80
20	c	5501	CLA	C1-C2-C3	2.18	129.97	125.96
20	C	500	CLA	C6-C5-C3	2.18	117.60	112.66
20	B	512	CLA	O2D-CGD-CBD	2.18	115.20	111.30
20	c	5496	CLA	CBA-CAA-C2A	2.18	120.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	V	552	HEM	CMB-C2B-C3B	2.18	128.94	124.89
20	C	491	CLA	C6-C5-C3	2.18	117.61	112.66
24	x	5130	BCR	C36-C18-C19	2.18	121.58	118.10
20	b	5511	CLA	C2A-C3A-C4A	2.18	104.57	101.82
24	b	5528	BCR	C7-C8-C9	2.19	129.50	126.21
30	c	5508	DGD	O2D-C2D-C1D	2.19	114.60	110.03
20	B	513	CLA	C2A-C3A-C4A	2.19	105.40	101.87
20	b	5511	CLA	CED-O2D-CGD	2.19	121.09	115.97
20	c	5503	CLA	C1C-NC-C4C	2.19	108.31	107.06
26	t	213	SQD	C15-C14-C13	2.19	125.74	114.45
24	x	5130	BCR	C37-C22-C23	2.19	121.59	118.10
20	b	5512	CLA	C2A-C3A-C4A	2.19	105.41	101.87
20	B	523	CLA	CMB-C2B-C3B	2.19	128.96	124.89
26	d	5358	SQD	C17-C16-C15	2.19	125.75	114.45
20	C	500	CLA	CED-O2D-CGD	2.20	121.12	115.97
22	A	564	PQ9	C11-C2-C1	2.20	118.66	116.88
30	C	509	DGD	O5D-C6D-C5D	2.20	112.62	108.94
20	b	5525	CLA	C2A-C3A-C4A	2.20	105.42	101.87
20	C	495	CLA	C2A-C1A-CHA	2.20	127.82	123.92
24	X	130	BCR	C36-C18-C19	2.20	121.61	118.10
20	a	5560	CLA	CMB-C2B-C3B	2.20	128.98	124.89
20	c	5498	CLA	C2A-C3A-C4A	2.21	105.43	101.87
30	c	5508	DGD	O1G-C1A-C2A	2.21	118.33	111.90
21	a	5562	PHO	C2A-C3A-C4A	2.21	105.75	101.33
20	C	493	CLA	C2A-C1A-CHA	2.21	127.84	123.92
26	d	5358	SQD	C34-C33-C32	2.21	125.85	114.45
24	c	5504	BCR	C11-C10-C9	2.21	130.47	127.31
20	B	511	CLA	CED-O2D-CGD	2.21	121.16	115.97
20	b	5512	CLA	CMB-C2B-C3B	2.21	129.00	124.89
20	b	5524	CLA	O2D-CGD-CBD	2.22	115.26	111.30
21	a	5561	PHO	C3D-C4D-CHA	2.22	115.71	109.97
24	c	5504	BCR	C7-C8-C9	2.22	129.54	126.21
20	b	5526	CLA	C2A-C3A-C4A	2.22	105.45	101.87
20	B	519	CLA	C2A-C1A-CHA	2.22	127.86	123.92
24	c	5505	BCR	C7-C8-C9	2.22	129.55	126.21
24	h	5107	BCR	C34-C9-C8	2.22	121.64	118.10
28	d	5360	MGE	O1G-C1A-C2A	2.22	118.37	111.90
20	C	501	CLA	C2A-C1A-CHA	2.22	127.86	123.92
20	b	5521	CLA	O2D-CGD-CBD	2.23	115.27	111.30
24	D	357	BCR	C40-C30-C25	2.23	113.92	110.31
24	D	357	BCR	C7-C8-C9	2.23	129.56	126.21
20	B	519	CLA	C6-C5-C3	2.23	117.71	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	213	SQD	O8-S-O7	2.23	116.48	111.37
20	a	5560	CLA	C6-C5-C3	2.23	117.72	112.66
20	b	5520	CLA	CMB-C2B-C3B	2.23	129.03	124.89
20	B	518	CLA	C6-C7-C8	2.23	123.07	115.73
24	t	104	BCR	C34-C9-C8	2.24	121.66	118.10
20	A	563	CLA	C6-C5-C3	2.24	117.74	112.66
20	B	525	CLA	C1C-NC-C4C	2.24	108.34	107.06
24	H	107	BCR	C7-C8-C9	2.24	129.58	126.21
30	h	5208	DGD	O5D-C1E-C2E	2.25	111.90	108.23
20	b	5524	CLA	C1C-NC-C4C	2.25	108.35	107.06
20	B	523	CLA	CED-O2D-CGD	2.25	121.24	115.97
20	C	492	CLA	O2D-CGD-CBD	2.25	115.31	111.30
20	b	5512	CLA	C6-C5-C3	2.25	117.75	112.66
20	C	499	CLA	C1-O2A-CGA	2.25	123.32	116.72
20	C	494	CLA	O2A-CGA-CBA	2.25	121.61	112.33
26	L	5213	SQD	C15-C14-C13	2.25	126.05	114.45
20	B	513	CLA	O2D-CGD-CBD	2.25	115.32	111.30
20	D	354	CLA	C1C-NC-C4C	2.25	108.35	107.06
20	b	5514	CLA	CED-O2D-CGD	2.25	121.25	115.97
20	a	5563	CLA	O2D-CGD-CBD	2.26	115.33	111.30
24	a	5566	BCR	C35-C13-C12	2.26	121.69	118.10
20	a	5560	CLA	C1C-NC-C4C	2.26	108.35	107.06
24	H	107	BCR	C36-C18-C19	2.26	121.70	118.10
20	C	492	CLA	C1-C2-C3	2.26	130.12	125.96
20	b	5526	CLA	O2D-CGD-CBD	2.26	115.34	111.30
24	c	5505	BCR	C36-C18-C19	2.26	121.70	118.10
20	B	514	CLA	CED-O2D-CGD	2.26	121.28	115.97
24	C	504	BCR	C11-C10-C9	2.26	130.54	127.31
24	C	506	BCR	C24-C23-C22	2.26	129.62	126.21
20	c	5494	CLA	O2A-CGA-CBA	2.27	121.67	112.33
20	c	5500	CLA	CED-O2D-CGD	2.27	121.29	115.97
28	D	360	MGE	O1G-C1A-C2A	2.27	118.50	111.90
21	A	562	PHO	C2A-C3A-C4A	2.27	105.87	101.33
21	A	561	PHO	C2A-C3A-C4A	2.27	105.87	101.33
20	c	5494	CLA	C2A-C3A-C4A	2.27	105.54	101.87
24	B	529	BCR	C15-C14-C13	2.27	130.55	127.31
22	d	5356	PQ9	C19-C18-C20	2.28	119.23	115.29
20	B	524	CLA	C1-C2-C3	2.28	130.15	125.96
20	c	5495	CLA	CMB-C2B-C3B	2.28	129.12	124.89
20	c	5494	CLA	CMB-C2B-C3B	2.28	129.12	124.89
21	A	562	PHO	C3D-C4D-CHA	2.28	115.87	109.97
24	T	5104	BCR	C36-C18-C19	2.28	121.73	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	512	CLA	C2A-C3A-C4A	2.28	105.55	101.87
20	c	5495	CLA	CED-O2D-CGD	2.28	121.32	115.97
24	c	5506	BCR	C36-C18-C19	2.28	121.74	118.10
20	A	560	CLA	O2A-CGA-CBA	2.29	118.55	111.90
20	b	5521	CLA	C1C-NC-C4C	2.29	108.37	107.06
20	a	5563	CLA	C2A-C3A-C4A	2.29	105.56	101.87
20	b	5518	CLA	O2D-CGD-CBD	2.29	115.39	111.30
24	h	5107	BCR	C37-C22-C23	2.29	121.75	118.10
24	t	104	BCR	C23-C24-C25	2.29	133.67	127.25
20	B	513	CLA	C1C-NC-C4C	2.29	108.37	107.06
20	A	563	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	c	5491	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	C	495	CLA	C2A-C3A-C4A	2.30	105.58	101.87
20	B	520	CLA	CMB-C2B-C3B	2.30	129.15	124.89
21	a	5561	PHO	O2D-CGD-CBD	2.30	115.40	111.30
20	c	5498	CLA	C6-C5-C3	2.30	117.87	112.66
20	c	5497	CLA	C2A-C3A-C4A	2.30	105.59	101.87
24	t	104	BCR	C37-C22-C23	2.30	121.77	118.10
24	T	5104	BCR	C23-C24-C25	2.30	133.69	127.25
20	C	493	CLA	O2D-CGD-CBD	2.30	115.41	111.30
20	B	525	CLA	C2A-C3A-C4A	2.30	105.59	101.87
24	t	104	BCR	C36-C18-C19	2.30	121.77	118.10
20	B	519	CLA	C1-O2A-CGA	2.31	122.30	116.77
20	c	5499	CLA	C2A-C1A-CHA	2.31	128.01	123.92
24	b	5528	BCR	C32-C1-C6	2.31	114.05	110.31
20	B	511	CLA	CMB-C2B-C3B	2.31	129.18	124.89
24	B	529	BCR	C32-C1-C6	2.31	114.05	110.31
20	c	5502	CLA	C1C-NC-C4C	2.31	108.39	107.06
20	C	491	CLA	O2D-CGD-CBD	2.31	115.43	111.30
20	D	354	CLA	O2D-CGD-CBD	2.32	115.44	111.30
24	H	107	BCR	C35-C13-C12	2.32	121.79	118.10
20	d	5354	CLA	C2A-C3A-C4A	2.32	105.61	101.87
20	C	494	CLA	CMB-C2B-C3B	2.32	129.20	124.89
20	D	354	CLA	CED-O2D-CGD	2.32	121.42	115.97
20	b	5526	CLA	OBD-CAD-C3D	2.33	132.31	128.03
20	D	355	CLA	C1-O2A-CGA	2.33	122.35	116.77
20	C	498	CLA	C6-C5-C3	2.33	117.93	112.66
24	a	5566	BCR	C32-C1-C6	2.33	114.08	110.31
20	B	522	CLA	C2A-C3A-C4A	2.33	105.63	101.87
20	b	5525	CLA	C1C-NC-C4C	2.33	108.39	107.06
24	B	529	BCR	C40-C30-C25	2.33	114.09	110.31
20	C	492	CLA	C2A-C3A-C4A	2.33	105.64	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	5566	BCR	C30-C25-C24	2.33	122.29	115.73
20	c	5500	CLA	C2A-C3A-C4A	2.34	105.64	101.87
26	a	212	SQD	O8-S-O7	2.34	116.73	111.37
21	A	561	PHO	C6-C5-C3	2.34	117.96	112.66
24	x	5130	BCR	C30-C25-C24	2.34	122.30	115.73
24	C	504	BCR	C40-C30-C25	2.34	114.10	110.31
24	H	107	BCR	C1-C6-C7	2.34	122.31	115.73
20	C	501	CLA	C1-O2A-CGA	2.34	122.39	116.77
20	C	502	CLA	C1-C2-C3	2.34	130.27	125.96
20	b	5513	CLA	CMB-C2B-C3B	2.34	129.24	124.89
20	b	5523	CLA	CMB-C2B-C3B	2.34	129.24	124.89
20	B	519	CLA	C2A-C3A-C4A	2.34	105.66	101.87
20	c	5500	CLA	C6-C5-C3	2.34	117.97	112.66
24	d	5357	BCR	C35-C13-C12	2.35	121.83	118.10
21	a	5561	PHO	O2A-CGA-CBA	2.35	118.73	111.90
20	B	524	CLA	C1C-NC-C4C	2.35	108.41	107.06
20	C	503	CLA	C1-C2-C3	2.35	130.40	126.68
24	C	506	BCR	C37-C22-C23	2.35	121.85	118.10
20	B	518	CLA	C6-C5-C3	2.36	118.00	112.66
20	b	5517	CLA	C6-C5-C3	2.36	118.01	112.66
20	C	493	CLA	C2A-C3A-C4A	2.36	105.68	101.87
20	B	517	CLA	OBD-CAD-C3D	2.36	132.38	128.03
20	c	5502	CLA	C2A-C1A-CHA	2.36	128.11	123.92
20	C	503	CLA	C1C-NC-C4C	2.36	108.42	107.06
24	b	5528	BCR	C1-C6-C7	2.37	122.38	115.73
20	c	5496	CLA	C2A-C3A-C4A	2.37	105.69	101.87
20	C	495	CLA	CMB-C2B-C3B	2.37	129.29	124.89
20	B	526	CLA	C2A-C3A-C4A	2.37	105.70	101.87
20	C	502	CLA	C2A-C1A-CHA	2.37	128.13	123.92
20	b	5515	CLA	C2A-C3A-C4A	2.38	105.71	101.87
21	a	5561	PHO	CAB-C3B-C4B	2.38	135.26	126.11
20	A	560	CLA	CMB-C2B-C3B	2.38	129.30	124.89
20	C	494	CLA	C2A-C1A-CHA	2.38	128.13	123.92
20	b	5512	CLA	C1-C2-C3	2.38	130.34	125.96
24	C	506	BCR	C36-C18-C19	2.38	121.89	118.10
22	A	564	PQ9	C14-C13-C15	2.38	119.42	115.29
20	a	5560	CLA	O2A-CGA-CBA	2.38	118.83	111.90
22	a	5564	PQ9	C14-C13-C15	2.38	119.42	115.29
20	B	519	CLA	O2A-CGA-CBA	2.38	118.84	111.90
24	T	5104	BCR	C37-C22-C23	2.38	121.90	118.10
24	c	5504	BCR	C30-C25-C24	2.39	122.44	115.73
26	A	568	SQD	C15-C14-C13	2.39	126.76	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	528	BCR	C1-C6-C7	2.39	122.45	115.73
24	h	5107	BCR	C28-C27-C26	2.39	117.89	113.78
24	C	505	BCR	C36-C18-C19	2.39	121.91	118.10
24	A	566	BCR	C2-C1-C6	2.40	114.22	110.48
20	A	560	CLA	C1-C2-C3	2.40	130.37	125.96
24	A	566	BCR	C37-C22-C23	2.40	121.92	118.10
20	b	5521	CLA	O2A-CGA-CBA	2.40	118.88	111.90
24	X	130	BCR	C37-C22-C23	2.40	121.92	118.10
20	a	5559	CLA	C2A-C3A-C4A	2.40	105.75	101.87
24	A	566	BCR	C8-C7-C6	2.41	133.99	127.25
20	b	5522	CLA	C2A-C3A-C4A	2.41	105.76	101.87
21	A	562	PHO	O2D-CGD-CBD	2.41	115.60	111.30
20	A	563	CLA	C1C-NC-C4C	2.41	108.44	107.06
20	c	5495	CLA	C2A-C1A-CHA	2.41	128.19	123.92
26	d	5358	SQD	C44-O6-C1	2.41	118.70	113.76
24	C	505	BCR	C8-C7-C6	2.41	134.00	127.25
20	C	495	CLA	CED-O2D-CGD	2.41	121.63	115.97
24	X	130	BCR	C35-C13-C12	2.41	121.94	118.10
20	a	5560	CLA	C2A-C3A-C4A	2.42	105.77	101.87
20	C	502	CLA	C1C-NC-C4C	2.42	108.45	107.06
32	v	5552	HEM	CMB-C2B-C3B	2.42	129.38	124.89
24	B	528	BCR	C32-C1-C6	2.42	114.24	110.31
20	B	521	CLA	O2A-CGA-CBA	2.43	118.96	111.90
20	a	5558	CLA	CBA-CAA-C2A	2.43	121.06	113.80
24	B	527	BCR	C36-C18-C19	2.43	121.97	118.10
20	B	517	CLA	C2A-C1A-CHA	2.43	128.23	123.92
20	B	521	CLA	O2D-CGD-CBD	2.43	115.64	111.30
20	B	523	CLA	C2A-C3A-C4A	2.43	105.80	101.87
24	C	506	BCR	C30-C25-C24	2.43	122.57	115.73
26	A	5212	SQD	O8-S-O7	2.43	116.95	111.37
24	a	5566	BCR	C2-C1-C6	2.44	114.29	110.48
20	b	5517	CLA	OBD-CAD-C3D	2.44	132.52	128.03
20	c	5494	CLA	CBA-CAA-C2A	2.44	121.10	113.80
24	D	357	BCR	C16-C17-C18	2.44	130.79	127.31
20	c	5493	CLA	C2A-C3A-C4A	2.44	105.81	101.87
20	b	5525	CLA	O2D-CGD-CBD	2.44	115.66	111.30
24	d	5357	BCR	C16-C17-C18	2.44	130.79	127.31
32	V	552	HEM	C4A-C3A-C2A	2.44	108.69	107.00
20	B	517	CLA	C6-C5-C3	2.44	118.19	112.66
20	B	512	CLA	C6-C5-C3	2.45	118.20	112.66
24	X	130	BCR	C30-C25-C24	2.45	122.61	115.73
20	a	5558	CLA	C2A-C3A-C4A	2.45	105.83	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5513	CLA	C1-C2-C3	2.45	130.47	125.96
24	a	5566	BCR	C16-C17-C18	2.45	130.81	127.31
24	H	107	BCR	C28-C27-C26	2.45	118.00	113.78
20	A	559	CLA	C2A-C3A-C4A	2.46	105.83	101.87
26	L	5213	SQD	C31-C30-C29	2.46	132.59	113.42
24	b	5527	BCR	C35-C13-C12	2.46	122.01	118.10
24	D	357	BCR	C37-C22-C23	2.46	122.02	118.10
24	h	5107	BCR	C16-C17-C18	2.46	130.83	127.31
20	B	520	CLA	C1-C2-C3	2.47	130.50	125.96
20	D	354	CLA	C2A-C3A-C4A	2.47	105.86	101.87
20	b	5520	CLA	C1-C2-C3	2.47	130.51	125.96
20	d	5354	CLA	CED-O2D-CGD	2.47	121.76	115.97
27	T	217	LMT	O1B-C1B-C2B	2.47	113.68	108.11
20	A	563	CLA	CED-O2D-CGD	2.47	121.77	115.97
30	H	208	DGD	O5D-C1E-C2E	2.48	112.27	108.23
24	T	5104	BCR	C7-C8-C9	2.48	129.93	126.21
24	C	504	BCR	C7-C8-C9	2.48	129.94	126.21
22	d	5356	PQ9	C14-C13-C15	2.48	119.59	115.29
20	B	513	CLA	C1-C2-C3	2.48	130.53	125.96
20	A	558	CLA	CBA-CAA-C2A	2.48	121.22	113.80
21	A	561	PHO	CAB-C3B-C4B	2.48	135.67	126.11
26	A	568	SQD	C44-O6-C1	2.49	118.86	113.76
20	b	5522	CLA	C1C-NC-C4C	2.49	108.49	107.06
20	B	521	CLA	C2A-C3A-C4A	2.49	105.89	101.87
20	b	5519	CLA	C1-C2-C3	2.49	130.54	125.96
20	d	5354	CLA	C1C-NC-C4C	2.49	108.49	107.06
20	b	5516	CLA	C1C-NC-C4C	2.49	108.49	107.06
24	a	5566	BCR	C36-C18-C19	2.49	122.07	118.10
24	b	5529	BCR	C32-C1-C6	2.49	114.35	110.31
20	B	514	CLA	C2A-C3A-C4A	2.50	105.90	101.87
20	B	526	CLA	C1-O2A-CGA	2.50	122.76	116.77
28	B	530	MGE	O6D-C5D-C6D	2.50	112.39	106.41
20	A	560	CLA	C6-C5-C3	2.50	118.32	112.66
21	A	562	PHO	C6-C5-C3	2.50	118.33	112.66
20	c	5503	CLA	O2A-CGA-CBA	2.50	119.18	111.90
20	b	5523	CLA	C1C-NC-C4C	2.50	108.50	107.06
24	h	5107	BCR	C1-C6-C7	2.50	122.77	115.73
20	b	5519	CLA	O2A-CGA-CBA	2.51	119.19	111.90
26	a	212	SQD	O48-C23-C24	2.52	123.76	112.44
30	C	508	DGD	O6D-C5D-C6D	2.52	111.66	106.64
20	B	523	CLA	C1-C2-C3	2.52	130.59	125.96
20	a	5560	CLA	CED-O2D-CGD	2.52	121.87	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5504	BCR	C37-C22-C23	2.52	122.11	118.10
27	t	5217	LMT	O1B-C1B-C2B	2.52	113.79	108.11
20	A	558	CLA	C2A-C3A-C4A	2.52	105.94	101.87
20	D	355	CLA	O2D-CGD-CBD	2.52	115.81	111.30
20	D	355	CLA	C1C-NC-C4C	2.52	108.51	107.06
24	H	107	BCR	C16-C17-C18	2.53	130.92	127.31
20	C	494	CLA	C2A-C3A-C4A	2.53	105.95	101.87
24	b	5529	BCR	C7-C8-C9	2.53	130.01	126.21
20	B	522	CLA	C1C-NC-C4C	2.53	108.51	107.06
24	C	504	BCR	C37-C22-C23	2.54	122.14	118.10
20	b	5519	CLA	C6-C5-C3	2.54	118.42	112.66
21	A	561	PHO	CBD-CHA-C1A	2.54	132.34	126.36
20	b	5513	CLA	O2D-CGD-CBD	2.54	115.84	111.30
21	A	561	PHO	O2D-CGD-CBD	2.54	115.84	111.30
24	b	5527	BCR	C8-C7-C6	2.55	134.38	127.25
21	A	561	PHO	O2A-CGA-CBA	2.55	119.31	111.90
20	c	5498	CLA	C1C-NC-C4C	2.55	108.52	107.06
20	B	517	CLA	C1C-NC-C4C	2.55	108.52	107.06
20	B	512	CLA	C1-C2-C3	2.55	130.66	125.96
20	c	5498	CLA	O2D-CGD-CBD	2.55	115.86	111.30
24	B	529	BCR	C35-C13-C12	2.55	122.17	118.10
20	B	519	CLA	C1-C2-C3	2.56	130.67	125.96
20	C	499	CLA	CED-O2D-CGD	2.56	121.97	115.97
21	a	5562	PHO	CAB-C3B-C4B	2.56	135.97	126.11
24	c	5505	BCR	C8-C7-C6	2.56	134.42	127.25
20	C	494	CLA	CBA-CAA-C2A	2.56	121.47	113.80
26	A	5212	SQD	O48-C23-C24	2.56	123.98	112.44
26	d	5358	SQD	O8-S-O7	2.56	117.25	111.37
20	C	499	CLA	C2A-C3A-C4A	2.57	106.01	101.87
20	b	5521	CLA	CED-O2D-CGD	2.57	121.99	115.97
21	A	562	PHO	CAB-C3B-C4B	2.57	136.00	126.11
26	d	5358	SQD	C15-C14-C13	2.57	127.69	114.45
20	c	5501	CLA	O2A-CGA-CBA	2.57	119.38	111.90
24	a	5566	BCR	C37-C22-C23	2.57	122.19	118.10
20	a	5563	CLA	C1C-NC-C4C	2.57	108.53	107.06
28	B	530	MGE	O3G-C1D-C2D	2.57	112.43	108.23
24	A	566	BCR	C7-C8-C9	2.57	130.08	126.21
26	t	213	SQD	C31-C30-C29	2.57	133.50	113.42
24	h	5107	BCR	C35-C13-C12	2.58	122.21	118.10
24	c	5504	BCR	C35-C13-C12	2.58	122.21	118.10
20	B	525	CLA	O2D-CGD-CBD	2.58	115.91	111.30
24	A	566	BCR	C35-C13-C12	2.58	122.21	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5506	BCR	C37-C22-C23	2.59	122.22	118.10
24	A	566	BCR	C36-C18-C19	2.59	122.23	118.10
24	c	5506	BCR	C16-C17-C18	2.59	131.01	127.31
20	c	5502	CLA	C1-C2-C3	2.60	130.74	125.96
24	X	130	BCR	C24-C23-C22	2.60	130.11	126.21
24	B	527	BCR	C16-C17-C18	2.60	131.03	127.31
20	c	5492	CLA	O2A-CGA-CBA	2.61	119.48	111.90
21	a	5561	PHO	CBD-CHA-C1A	2.61	132.50	126.36
20	B	526	CLA	C1-C2-C3	2.61	130.76	125.96
24	x	5130	BCR	C35-C13-C12	2.61	122.26	118.10
20	c	5502	CLA	C2A-C3A-C4A	2.61	106.09	101.87
20	C	498	CLA	C1C-NC-C4C	2.61	108.56	107.06
24	c	5506	BCR	C24-C23-C22	2.62	130.14	126.21
20	c	5497	CLA	O2D-CGD-CBD	2.62	115.98	111.30
24	A	566	BCR	C16-C17-C18	2.62	131.05	127.31
24	D	357	BCR	C35-C13-C12	2.63	122.28	118.10
20	A	560	CLA	CAA-CBA-CGA	2.63	121.26	113.35
24	d	5357	BCR	C7-C8-C9	2.63	130.16	126.21
20	b	5526	CLA	C6-C5-C3	2.63	118.63	112.66
20	b	5518	CLA	C1C-NC-C4C	2.64	108.58	107.06
20	A	560	CLA	C2A-C3A-C4A	2.64	106.14	101.87
20	B	526	CLA	C6-C5-C3	2.64	118.65	112.66
24	c	5506	BCR	C30-C25-C24	2.65	123.17	115.73
24	b	5529	BCR	C35-C13-C12	2.65	122.32	118.10
20	b	5514	CLA	C2A-C3A-C4A	2.65	106.15	101.87
20	b	5519	CLA	C1-O2A-CGA	2.65	123.13	116.77
20	C	498	CLA	CED-O2D-CGD	2.65	122.19	115.97
20	b	5526	CLA	C1-C2-C3	2.65	130.84	125.96
20	c	5500	CLA	O2A-CGA-CBA	2.66	119.63	111.90
20	b	5514	CLA	C1-C2-C3	2.66	130.86	125.96
24	t	104	BCR	C7-C8-C9	2.66	130.21	126.21
20	c	5499	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	b	5521	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	C	498	CLA	O2A-CGA-CBA	2.66	119.65	111.90
20	b	5524	CLA	O2A-CGA-CBA	2.67	119.66	111.90
20	C	500	CLA	C2A-C3A-C4A	2.67	106.19	101.87
24	B	527	BCR	C8-C7-C6	2.67	134.74	127.25
24	c	5506	BCR	C35-C13-C12	2.68	122.36	118.10
28	d	5359	MGE	O6D-C5D-C6D	2.68	112.83	106.41
20	b	5513	CLA	C6-C5-C3	2.68	118.73	112.66
21	A	562	PHO	CED-O2D-CGD	2.68	122.25	115.97
24	C	504	BCR	C1-C6-C7	2.68	123.26	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5518	CLA	C6-C5-C3	2.68	118.73	112.66
20	B	515	CLA	CED-O2D-CGD	2.68	122.25	115.97
20	C	501	CLA	CED-O2D-CGD	2.68	122.26	115.97
20	d	5355	CLA	C1C-NC-C4C	2.68	108.60	107.06
30	c	5508	DGD	O6D-C5D-C6D	2.69	112.00	106.64
20	b	5516	CLA	CBA-CAA-C2A	2.69	121.86	113.80
20	d	5354	CLA	O2D-CGD-CBD	2.69	116.11	111.30
20	C	499	CLA	C2A-C1A-CHA	2.70	128.70	123.92
24	X	130	BCR	C16-C17-C18	2.70	131.16	127.31
24	a	5566	BCR	C8-C7-C6	2.70	134.81	127.25
30	H	208	DGD	O6D-C5D-C4D	2.70	114.63	109.66
20	C	502	CLA	C2A-C3A-C4A	2.70	106.24	101.87
24	d	5357	BCR	C36-C18-C19	2.70	122.41	118.10
22	A	564	PQ9	C24-C23-C25	2.71	119.98	115.29
30	h	5208	DGD	O6D-C5D-C4D	2.71	114.64	109.66
22	A	564	PQ9	C19-C18-C20	2.71	119.98	115.29
24	b	5528	BCR	C24-C23-C22	2.71	130.28	126.21
22	D	356	PQ9	C19-C18-C20	2.71	119.99	115.29
20	C	500	CLA	C1-C2-C3	2.71	130.95	125.96
24	C	505	BCR	C35-C13-C12	2.72	122.43	118.10
26	A	568	SQD	C36-C35-C34	2.72	128.47	114.45
20	b	5520	CLA	CED-O2D-CGD	2.72	122.35	115.97
20	A	560	CLA	CED-O2D-CGD	2.72	122.36	115.97
20	C	493	CLA	C1-C2-C3	2.73	130.98	125.96
20	B	513	CLA	CED-O2D-CGD	2.73	122.37	115.97
20	b	5523	CLA	C2A-C3A-C4A	2.74	106.29	101.87
26	d	5358	SQD	C36-C35-C34	2.74	128.58	114.45
20	a	5560	CLA	CAA-CBA-CGA	2.74	121.60	113.35
21	A	562	PHO	CBD-CHA-C1A	2.74	132.82	126.36
24	B	527	BCR	C24-C23-C22	2.74	130.33	126.21
24	T	5104	BCR	C11-C10-C9	2.74	131.22	127.31
20	C	499	CLA	O2D-CGD-CBD	2.74	116.20	111.30
24	D	357	BCR	C24-C23-C22	2.75	130.34	126.21
24	h	5107	BCR	C15-C14-C13	2.75	131.23	127.31
20	d	5355	CLA	O2A-CGA-CBA	2.75	119.89	111.90
20	c	5501	CLA	CED-O2D-CGD	2.75	122.41	115.97
20	B	516	CLA	CBA-CAA-C2A	2.75	122.02	113.80
21	a	5562	PHO	CBD-CHA-C1A	2.75	132.83	126.36
24	T	5104	BCR	C2-C1-C6	2.75	114.78	110.48
20	b	5523	CLA	C1-C2-C3	2.75	131.02	125.96
20	c	5497	CLA	CED-O2D-CGD	2.75	122.42	115.97
20	c	5498	CLA	O2A-CGA-CBA	2.76	119.92	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5527	BCR	C16-C17-C18	2.76	131.24	127.31
20	A	559	CLA	CED-O2D-CGD	2.76	122.44	115.97
20	C	497	CLA	CED-O2D-CGD	2.76	122.44	115.97
20	a	5558	CLA	C1-C2-C3	2.76	131.04	125.96
20	b	5513	CLA	CED-O2D-CGD	2.77	122.45	115.97
28	b	5530	MGE	O6D-C5D-C6D	2.77	113.03	106.41
20	c	5496	CLA	O2A-CGA-CBA	2.77	119.96	111.90
26	a	212	SQD	O47-C7-C8	2.77	116.30	111.10
22	a	5564	PQ9	C19-C18-C20	2.77	120.10	115.29
22	a	5564	PQ9	C24-C23-C25	2.77	120.10	115.29
24	c	5505	BCR	C16-C17-C18	2.78	131.27	127.31
20	A	558	CLA	CED-O2D-CGD	2.78	122.48	115.97
20	C	501	CLA	O2A-CGA-CBA	2.78	119.98	111.90
20	c	5499	CLA	O2D-CGD-CBD	2.78	116.27	111.30
20	c	5495	CLA	C1-C2-C3	2.78	131.08	125.96
24	d	5357	BCR	C37-C22-C23	2.79	122.54	118.10
20	C	500	CLA	O2A-CGA-CBA	2.79	120.01	111.90
20	B	525	CLA	CED-O2D-CGD	2.79	122.51	115.97
24	C	504	BCR	C32-C1-C6	2.79	114.83	110.31
20	C	501	CLA	C1-C2-C3	2.79	131.10	125.96
20	b	5525	CLA	CED-O2D-CGD	2.79	122.52	115.97
20	C	497	CLA	C6-C5-C3	2.80	119.00	112.66
20	B	515	CLA	C2A-C3A-C4A	2.80	106.39	101.87
20	C	495	CLA	C1-C2-C3	2.80	131.11	125.96
26	A	5212	SQD	O47-C7-C8	2.80	116.36	111.10
24	B	529	BCR	C8-C7-C6	2.80	135.09	127.25
20	C	497	CLA	O2D-CGD-CBD	2.80	116.30	111.30
24	H	107	BCR	C32-C1-C6	2.81	114.86	110.31
20	B	516	CLA	C1D-CHD-C4C	2.81	126.32	122.48
20	D	355	CLA	CED-O2D-CGD	2.81	122.55	115.97
20	B	513	CLA	C6-C5-C3	2.81	119.03	112.66
24	C	504	BCR	C35-C13-C12	2.82	122.58	118.10
26	A	568	SQD	O8-S-O7	2.82	117.83	111.37
20	A	559	CLA	O2A-CGA-CBA	2.82	120.11	111.90
26	d	5358	SQD	C32-C31-C30	2.82	129.01	114.45
20	b	5518	CLA	CED-O2D-CGD	2.82	122.59	115.97
20	c	5497	CLA	C6-C5-C3	2.82	119.06	112.66
28	l	5210	MGE	O2G-C1B-C2B	2.82	117.42	111.55
24	T	5104	BCR	C35-C13-C12	2.83	122.61	118.10
20	B	523	CLA	O2A-CGA-CBA	2.84	120.15	111.90
20	B	523	CLA	C1C-NC-C4C	2.84	108.69	107.06
20	c	5496	CLA	C1-C2-C3	2.84	131.19	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	5507	DGD	O5D-C1E-C2E	2.85	112.88	108.23
24	b	5528	BCR	C8-C7-C6	2.85	135.22	127.25
20	B	524	CLA	O2A-CGA-CBA	2.85	120.20	111.90
20	c	5499	CLA	CED-O2D-CGD	2.85	122.66	115.97
24	c	5504	BCR	C40-C30-C25	2.86	114.94	110.31
20	c	5498	CLA	CED-O2D-CGD	2.86	122.68	115.97
20	c	5500	CLA	C1-C2-C3	2.86	131.23	125.96
20	c	5493	CLA	C1-C2-C3	2.86	131.23	125.96
24	c	5504	BCR	C29-C30-C25	2.87	114.96	110.48
24	b	5529	BCR	C24-C23-C22	2.87	130.53	126.21
28	L	210	MGE	O2G-C1B-C2B	2.88	117.53	111.55
20	C	498	CLA	O2D-CGD-CBD	2.89	116.47	111.30
20	b	5526	CLA	O2A-CGA-CBA	2.89	120.31	111.90
24	c	5504	BCR	C1-C6-C7	2.89	123.86	115.73
24	B	529	BCR	C7-C8-C9	2.90	130.57	126.21
20	b	5516	CLA	C1D-CHD-C4C	2.91	126.46	122.48
20	a	5563	CLA	CED-O2D-CGD	2.91	122.79	115.97
24	C	504	BCR	C23-C24-C25	2.91	135.40	127.25
20	a	5563	CLA	C1-C2-C3	2.91	131.32	125.96
30	C	507	DGD	O5D-C1E-C2E	2.92	112.99	108.23
24	B	528	BCR	C8-C7-C6	2.92	135.42	127.25
24	t	104	BCR	C2-C1-C6	2.92	115.04	110.48
24	c	5504	BCR	C23-C24-C25	2.92	135.44	127.25
20	d	5355	CLA	CED-O2D-CGD	2.93	122.83	115.97
24	t	104	BCR	C35-C13-C12	2.93	122.77	118.10
26	A	568	SQD	C45-O47-C7	2.93	124.81	117.88
20	C	502	CLA	CED-O2D-CGD	2.93	122.85	115.97
20	C	491	CLA	O2A-CGA-CBA	2.93	120.44	111.90
21	a	5562	PHO	CED-O2D-CGD	2.94	122.85	115.97
21	a	5561	PHO	CED-O2D-CGD	2.94	122.86	115.97
20	b	5523	CLA	C6-C5-C3	2.94	119.33	112.66
26	L	5213	SQD	C44-O6-C1	2.94	119.80	113.76
24	a	5566	BCR	C23-C24-C25	2.95	135.51	127.25
24	B	528	BCR	C24-C23-C22	2.95	130.64	126.21
20	a	5558	CLA	O2A-CGA-CBA	2.95	120.49	111.90
24	B	527	BCR	C35-C13-C12	2.95	122.80	118.10
20	b	5524	CLA	CED-O2D-CGD	2.95	122.90	115.97
28	D	358	MGE	O6D-C5D-C6D	2.96	113.49	106.41
24	X	130	BCR	C34-C9-C8	2.96	122.81	118.10
20	c	5499	CLA	C1D-CHD-C4C	2.97	126.54	122.48
20	B	521	CLA	CED-O2D-CGD	2.97	122.93	115.97
20	D	355	CLA	O2A-CGA-CBA	2.97	120.54	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	515	CLA	C6-C5-C3	2.97	119.39	112.66
20	C	493	CLA	CED-O2D-CGD	2.97	122.94	115.97
24	B	527	BCR	C29-C30-C25	2.98	115.13	110.48
20	B	520	CLA	CED-O2D-CGD	2.98	122.95	115.97
20	b	5526	CLA	C1-O2A-CGA	2.98	123.92	116.77
20	b	5515	CLA	C1D-CHD-C4C	2.98	126.56	122.48
24	d	5357	BCR	C8-C7-C6	2.98	135.60	127.25
20	B	512	CLA	CED-O2D-CGD	2.99	122.97	115.97
20	A	558	CLA	O2A-CGA-CBA	2.99	120.61	111.90
20	B	516	CLA	CED-O2D-CGD	2.99	122.99	115.97
20	b	5522	CLA	CED-O2D-CGD	3.00	123.00	115.97
20	B	518	CLA	C1C-NC-C4C	3.00	108.78	107.06
20	b	5516	CLA	C1-C2-C3	3.00	131.48	125.96
20	B	522	CLA	CED-O2D-CGD	3.00	123.00	115.97
20	B	515	CLA	C1D-CHD-C4C	3.00	126.58	122.48
24	A	566	BCR	C23-C24-C25	3.00	135.65	127.25
24	b	5529	BCR	C8-C7-C6	3.00	135.65	127.25
24	t	104	BCR	C11-C10-C9	3.00	131.59	127.31
20	c	5495	CLA	C6-C5-C3	3.00	119.46	112.66
25	a	5567	LHG	O7-C7-C8	3.00	117.79	111.55
20	c	5497	CLA	C1-C2-C3	3.01	131.49	125.96
26	A	568	SQD	C32-C31-C30	3.01	129.96	114.45
24	b	5527	BCR	C29-C30-C25	3.01	115.18	110.48
24	h	5107	BCR	C32-C1-C6	3.01	115.20	110.31
20	a	5563	CLA	C1D-CHD-C4C	3.02	126.61	122.48
24	x	5130	BCR	C34-C9-C8	3.02	122.91	118.10
20	C	496	CLA	C1-C2-C3	3.02	131.52	125.96
20	B	526	CLA	O2A-CGA-CBA	3.02	120.70	111.90
20	c	5492	CLA	C6-C5-C3	3.03	119.52	112.66
20	A	563	CLA	O2A-CGA-CBA	3.03	120.71	111.90
20	b	5523	CLA	O2A-CGA-CBA	3.03	120.71	111.90
20	B	518	CLA	CED-O2D-CGD	3.03	123.07	115.97
20	B	525	CLA	O2A-CGA-CBA	3.03	120.73	111.90
24	B	527	BCR	C23-C24-C25	3.03	135.75	127.25
20	b	5511	CLA	C1D-CHD-C4C	3.04	126.64	122.48
20	A	563	CLA	C1-C2-C3	3.04	131.55	125.96
20	C	503	CLA	O2A-CGA-CBA	3.04	120.74	111.90
20	a	5559	CLA	O2A-CGA-CBA	3.04	120.74	111.90
24	H	107	BCR	C8-C7-C6	3.04	135.76	127.25
20	a	5563	CLA	O2A-CGA-CBA	3.04	120.75	111.90
24	h	5107	BCR	C24-C23-C22	3.05	130.79	126.21
24	c	5504	BCR	C32-C1-C6	3.05	115.25	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	558	CLA	C1D-CHD-C4C	3.05	126.65	122.48
20	B	512	CLA	O2A-CGA-CBA	3.05	120.77	111.90
24	c	5505	BCR	C35-C13-C12	3.05	122.96	118.10
20	C	495	CLA	CBA-CAA-C2A	3.05	122.93	113.80
20	C	491	CLA	CED-O2D-CGD	3.06	123.13	115.97
20	B	521	CLA	C6-C5-C3	3.06	119.58	112.66
24	C	506	BCR	C35-C13-C12	3.06	122.98	118.10
24	d	5357	BCR	C23-C24-C25	3.06	135.83	127.25
20	B	512	CLA	C1D-CHD-C4C	3.07	126.68	122.48
20	c	5495	CLA	CBA-CAA-C2A	3.07	123.00	113.80
20	c	5497	CLA	C1D-CHD-C4C	3.07	126.69	122.48
20	b	5515	CLA	CED-O2D-CGD	3.08	123.18	115.97
24	B	527	BCR	C2-C1-C6	3.08	115.29	110.48
24	C	506	BCR	C16-C17-C18	3.08	131.71	127.31
20	B	514	CLA	O2A-CGA-CBA	3.08	120.87	111.90
28	i	5201	MGE	O6D-C5D-C6D	3.08	113.80	106.41
20	a	5558	CLA	C1D-CHD-C4C	3.08	126.70	122.48
24	B	529	BCR	C24-C23-C22	3.09	130.85	126.21
20	B	524	CLA	CED-O2D-CGD	3.09	123.20	115.97
30	H	208	DGD	O6D-C5D-C6D	3.09	112.81	106.64
20	c	5502	CLA	CED-O2D-CGD	3.09	123.22	115.97
20	c	5495	CLA	O2A-CGA-CBA	3.10	120.91	111.90
24	D	357	BCR	C8-C7-C6	3.10	135.93	127.25
20	B	515	CLA	O2A-CGA-CBA	3.10	120.92	111.90
20	b	5517	CLA	C1-C2-C3	3.10	131.67	125.96
20	C	492	CLA	O2A-CGA-CBA	3.10	120.93	111.90
24	h	5107	BCR	C2-C1-C6	3.11	115.34	110.48
20	b	5515	CLA	C6-C5-C3	3.11	119.71	112.66
24	C	504	BCR	C29-C30-C25	3.11	115.34	110.48
20	d	5354	CLA	C1-C2-C3	3.11	131.69	125.96
25	A	567	LHG	O7-C7-C8	3.12	118.02	111.55
20	c	5499	CLA	O2A-CGA-CBA	3.12	120.97	111.90
20	d	5354	CLA	C1D-CHD-C4C	3.12	126.75	122.48
20	C	499	CLA	O2A-CGA-CBA	3.12	120.97	111.90
20	B	520	CLA	O2A-CGA-CBA	3.12	120.98	111.90
20	c	5492	CLA	C1D-CHD-C4C	3.12	126.75	122.48
30	H	208	DGD	C1E-O6E-C5E	3.13	119.60	113.72
24	C	505	BCR	C16-C17-C18	3.13	131.78	127.31
20	C	496	CLA	O2A-CGA-CBA	3.14	121.03	111.90
20	B	511	CLA	C1D-CHD-C4C	3.14	126.77	122.48
24	H	107	BCR	C24-C23-C22	3.14	130.93	126.21
20	b	5525	CLA	O2A-CGA-CBA	3.14	121.04	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	354	CLA	O2A-CGA-CBA	3.14	121.05	111.90
24	H	107	BCR	C15-C14-C13	3.15	131.80	127.31
24	b	5529	BCR	C23-C24-C25	3.15	136.07	127.25
20	b	5512	CLA	C1D-CHD-C4C	3.15	126.79	122.48
24	c	5506	BCR	C2-C1-C6	3.15	115.41	110.48
30	C	509	DGD	O2G-C1B-C2B	3.15	118.10	111.55
26	t	213	SQD	C44-O6-C1	3.15	120.23	113.76
30	C	508	DGD	C1E-O6E-C5E	3.17	119.68	113.72
20	a	5560	CLA	C1D-CHD-C4C	3.17	126.81	122.48
20	b	5512	CLA	O2A-CGA-CBA	3.17	121.13	111.90
20	B	523	CLA	C6-C5-C3	3.17	119.85	112.66
20	b	5520	CLA	C1D-CHD-C4C	3.18	126.83	122.48
20	B	519	CLA	C1D-CHD-C4C	3.18	126.83	122.48
28	d	5360	MGE	O2G-C1B-C2B	3.18	118.16	111.55
20	b	5512	CLA	CED-O2D-CGD	3.18	123.43	115.97
30	c	5509	DGD	O2G-C1B-C2B	3.19	118.18	111.55
20	B	526	CLA	C1D-CHD-C4C	3.19	126.85	122.48
24	c	5506	BCR	C23-C24-C25	3.20	136.21	127.25
20	C	494	CLA	C1D-CHD-C4C	3.20	126.86	122.48
24	H	107	BCR	C2-C1-C6	3.20	115.48	110.48
20	A	559	CLA	C1D-CHD-C4C	3.20	126.86	122.48
20	C	493	CLA	C1D-CHD-C4C	3.20	126.86	122.48
20	C	492	CLA	C1D-CHD-C4C	3.21	126.87	122.48
20	C	498	CLA	C1D-CHD-C4C	3.21	126.87	122.48
20	C	495	CLA	O2A-CGA-CBA	3.21	121.23	111.90
24	B	529	BCR	C23-C24-C25	3.21	136.24	127.25
32	F	51	HEM	CAD-CBD-CGD	3.21	118.15	112.66
24	C	504	BCR	C2-C1-C6	3.22	115.51	110.48
21	A	561	PHO	CED-O2D-CGD	3.22	123.51	115.97
24	B	528	BCR	C23-C24-C25	3.22	136.26	127.25
24	b	5528	BCR	C23-C24-C25	3.23	136.29	127.25
20	c	5493	CLA	C1D-CHD-C4C	3.23	126.90	122.48
20	c	5494	CLA	C1D-CHD-C4C	3.24	126.91	122.48
24	B	528	BCR	C29-C30-C25	3.24	115.55	110.48
28	L	210	MGE	O6D-C5D-C6D	3.25	114.19	106.41
30	c	5508	DGD	O5D-C1E-C2E	3.25	113.53	108.23
20	a	5559	CLA	CED-O2D-CGD	3.25	123.59	115.97
28	I	201	MGE	O6D-C5D-C6D	3.25	114.19	106.41
24	A	566	BCR	C24-C23-C22	3.25	131.10	126.21
20	B	520	CLA	C1D-CHD-C4C	3.25	126.93	122.48
20	C	495	CLA	C6-C5-C3	3.26	120.04	112.66
24	h	5107	BCR	C8-C7-C6	3.26	136.37	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	492	CLA	C6-C5-C3	3.26	120.04	112.66
26	d	5358	SQD	C45-O47-C7	3.26	125.58	117.88
20	c	5496	CLA	C1D-CHD-C4C	3.26	126.94	122.48
20	D	354	CLA	C1D-CHD-C4C	3.26	126.94	122.48
20	b	5525	CLA	C1D-CHD-C4C	3.26	126.94	122.48
26	a	212	SQD	C45-O47-C7	3.26	124.24	117.94
30	c	5507	DGD	C1E-O6E-C5E	3.27	119.87	113.72
20	A	558	CLA	C1-C2-C3	3.27	131.97	125.96
24	B	528	BCR	C2-C1-C6	3.27	115.59	110.48
20	c	5491	CLA	O2A-CGA-CBA	3.27	121.41	111.90
20	b	5526	CLA	C1D-CHD-C4C	3.27	126.95	122.48
30	h	5208	DGD	O2G-C1B-C2B	3.27	118.34	111.55
20	b	5514	CLA	O2A-CGA-CBA	3.27	121.42	111.90
30	c	5507	DGD	O2G-C1B-C2B	3.27	118.35	111.55
20	B	516	CLA	C1-C2-C3	3.28	131.99	125.96
20	d	5354	CLA	O2A-CGA-CBA	3.28	121.45	111.90
20	b	5520	CLA	O2A-CGA-CBA	3.28	121.45	111.90
30	c	5508	DGD	C1E-O6E-C5E	3.28	119.90	113.72
20	C	497	CLA	C1D-CHD-C4C	3.28	126.97	122.48
24	b	5527	BCR	C23-C24-C25	3.29	136.46	127.25
24	t	104	BCR	C24-C23-C22	3.29	131.16	126.21
24	d	5357	BCR	C24-C23-C22	3.30	131.16	126.21
24	D	357	BCR	C29-C30-C25	3.30	115.64	110.48
20	b	5521	CLA	C6-C5-C3	3.31	120.15	112.66
24	D	357	BCR	C23-C24-C25	3.31	136.51	127.25
20	C	491	CLA	C1D-CHD-C4C	3.31	127.01	122.48
24	c	5504	BCR	C2-C1-C6	3.31	115.65	110.48
20	c	5498	CLA	C1D-CHD-C4C	3.31	127.01	122.48
24	H	107	BCR	C23-C24-C25	3.31	136.52	127.25
20	C	497	CLA	O2A-CGA-CBA	3.31	121.53	111.90
20	d	5355	CLA	C1D-CHD-C4C	3.31	127.01	122.48
20	a	5558	CLA	CED-O2D-CGD	3.31	123.74	115.97
21	a	5561	PHO	C1-C2-C3	3.32	132.06	125.96
20	b	5516	CLA	CED-O2D-CGD	3.32	123.75	115.97
20	D	355	CLA	C1-C2-C3	3.32	131.93	126.68
20	B	526	CLA	CED-O2D-CGD	3.32	123.76	115.97
20	B	524	CLA	C1D-CHD-C4C	3.33	127.03	122.48
20	B	519	CLA	CED-O2D-CGD	3.33	123.77	115.97
20	C	503	CLA	CED-O2D-CGD	3.33	123.78	115.97
24	a	5566	BCR	C24-C23-C22	3.34	131.22	126.21
30	C	507	DGD	O2G-C1B-C2B	3.34	118.48	111.55
20	a	5559	CLA	C1D-CHD-C4C	3.34	127.05	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	5530	MGE	O2G-C1B-C2B	3.34	118.48	111.55
20	C	503	CLA	C1D-CHD-C4C	3.34	127.05	122.48
20	b	5514	CLA	C1D-CHD-C4C	3.35	127.06	122.48
30	h	5208	DGD	O6D-C5D-C6D	3.35	113.33	106.64
20	b	5524	CLA	C1D-CHD-C4C	3.35	127.07	122.48
20	c	5502	CLA	C1D-CHD-C4C	3.35	127.07	122.48
20	c	5493	CLA	CED-O2D-CGD	3.36	123.85	115.97
20	b	5519	CLA	C1D-CHD-C4C	3.36	127.08	122.48
20	B	517	CLA	C1-C2-C3	3.37	132.16	125.96
20	c	5496	CLA	CED-O2D-CGD	3.37	123.87	115.97
20	C	497	CLA	C1-C2-C3	3.37	132.17	125.96
24	b	5527	BCR	C2-C1-C6	3.38	115.76	110.48
28	D	358	MGE	O2G-C1B-C2B	3.38	118.58	111.55
24	C	506	BCR	C29-C30-C25	3.39	115.77	110.48
28	l	5210	MGE	O6D-C5D-C6D	3.39	114.52	106.41
28	D	359	MGE	O2G-C1B-C2B	3.39	118.59	111.55
28	B	530	MGE	O2G-C1B-C2B	3.39	118.60	111.55
20	b	5522	CLA	O2A-CGA-CBA	3.39	121.77	111.90
20	c	5503	CLA	C1D-CHD-C4C	3.39	127.12	122.48
20	b	5518	CLA	C1D-CHD-C4C	3.40	127.13	122.48
26	A	5212	SQD	C45-O47-C7	3.40	124.50	117.94
20	B	514	CLA	C1D-CHD-C4C	3.40	127.13	122.48
24	c	5505	BCR	C2-C1-C6	3.40	115.80	110.48
20	C	499	CLA	C1D-CHD-C4C	3.40	127.14	122.48
20	b	5515	CLA	O2A-CGA-CBA	3.41	121.81	111.90
20	c	5501	CLA	C1D-CHD-C4C	3.41	127.15	122.48
20	c	5491	CLA	C1D-CHD-C4C	3.42	127.16	122.48
24	h	5107	BCR	C23-C24-C25	3.42	136.82	127.25
20	B	521	CLA	C1D-CHD-C4C	3.42	127.17	122.48
28	D	359	MGE	O6D-C5D-C6D	3.43	114.62	106.41
20	b	5521	CLA	C1D-CHD-C4C	3.43	127.17	122.48
30	c	5507	DGD	O6D-C5D-C6D	3.43	113.49	106.64
21	A	562	PHO	O2A-CGA-CBA	3.43	121.89	111.90
30	C	507	DGD	O6D-C5D-C6D	3.44	113.50	106.64
24	d	5357	BCR	C2-C1-C6	3.44	115.85	110.48
26	L	5213	SQD	C11-C10-C9	3.44	132.18	114.45
24	C	506	BCR	C2-C1-C6	3.44	115.86	110.48
20	B	518	CLA	C1D-CHD-C4C	3.44	127.19	122.48
22	D	356	PQ9	C24-C23-C25	3.44	121.26	115.29
28	I	201	MGE	O2G-C1B-C2B	3.44	118.70	111.55
28	i	5201	MGE	O2G-C1B-C2B	3.44	118.70	111.55
30	H	208	DGD	O2G-C1B-C2B	3.45	118.71	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5513	CLA	C1D-CHD-C4C	3.45	127.20	122.48
20	b	5517	CLA	C1D-CHD-C4C	3.45	127.20	122.48
20	C	492	CLA	CED-O2D-CGD	3.45	124.07	115.97
20	C	495	CLA	C1D-CHD-C4C	3.46	127.21	122.48
20	A	560	CLA	C1D-CHD-C4C	3.46	127.22	122.48
21	a	5562	PHO	O2A-CGA-CBA	3.46	121.98	111.90
20	A	563	CLA	C1D-CHD-C4C	3.47	127.22	122.48
20	c	5497	CLA	O2A-CGA-CBA	3.47	122.00	111.90
32	f	5051	HEM	CAD-CBD-CGD	3.47	118.60	112.66
20	b	5513	CLA	O2A-CGA-CBA	3.48	122.01	111.90
24	C	506	BCR	C23-C24-C25	3.48	136.99	127.25
30	C	509	DGD	C1E-O6E-C5E	3.48	120.27	113.72
20	C	496	CLA	C1D-CHD-C4C	3.48	127.24	122.48
30	C	508	DGD	O5D-C1E-C2E	3.49	113.92	108.23
30	C	508	DGD	O2G-C1B-C2B	3.49	118.80	111.55
20	C	493	CLA	O2A-CGA-CBA	3.49	122.06	111.90
20	c	5493	CLA	O2A-CGA-CBA	3.49	122.06	111.90
20	c	5495	CLA	C1D-CHD-C4C	3.49	127.26	122.48
20	B	525	CLA	C1D-CHD-C4C	3.49	127.26	122.48
20	c	5502	CLA	O2A-CGA-CBA	3.49	122.07	111.90
20	b	5522	CLA	C1D-CHD-C4C	3.51	127.28	122.48
24	c	5506	BCR	C29-C30-C25	3.52	115.97	110.48
20	B	513	CLA	O2A-CGA-CBA	3.52	122.13	111.90
20	a	5558	CLA	C4A-NA-C1A	3.52	110.82	106.45
24	B	529	BCR	C2-C1-C6	3.52	115.98	110.48
20	D	355	CLA	C1D-CHD-C4C	3.53	127.31	122.48
24	B	529	BCR	C29-C30-C25	3.53	116.00	110.48
22	d	5356	PQ9	C24-C23-C25	3.54	121.42	115.29
20	B	522	CLA	O2A-CGA-CBA	3.54	122.19	111.90
30	c	5507	DGD	O5D-C6D-C5D	3.54	114.86	108.94
24	x	5130	BCR	C16-C17-C18	3.54	132.36	127.31
20	C	500	CLA	C1D-CHD-C4C	3.55	127.34	122.48
24	H	107	BCR	C29-C30-C25	3.55	116.03	110.48
24	D	357	BCR	C2-C1-C6	3.55	116.04	110.48
20	C	502	CLA	O2A-CGA-CBA	3.55	122.24	111.90
30	c	5509	DGD	C1E-O6E-C5E	3.56	120.42	113.72
20	C	502	CLA	C1D-CHD-C4C	3.56	127.36	122.48
20	D	354	CLA	C4A-NA-C1A	3.56	110.88	106.45
20	d	5355	CLA	C1-C2-C3	3.57	132.32	126.68
20	C	501	CLA	C1D-CHD-C4C	3.57	127.36	122.48
20	c	5503	CLA	CED-O2D-CGD	3.57	124.34	115.97
20	b	5517	CLA	O2A-CGA-CBA	3.58	122.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5492	CLA	CED-O2D-CGD	3.58	124.37	115.97
26	d	5358	SQD	C11-C10-C9	3.59	132.98	114.45
24	A	566	BCR	C29-C30-C25	3.59	116.10	110.48
26	t	213	SQD	C11-C10-C9	3.60	133.00	114.45
20	C	496	CLA	CED-O2D-CGD	3.61	124.42	115.97
24	b	5528	BCR	C2-C1-C6	3.61	116.12	110.48
20	B	516	CLA	O2A-CGA-CBA	3.63	122.46	111.90
24	T	5104	BCR	C8-C7-C6	3.63	137.42	127.25
30	C	507	DGD	O5D-C6D-C5D	3.63	115.02	108.94
24	H	107	BCR	C11-C10-C9	3.64	132.50	127.31
30	c	5508	DGD	O2G-C1B-C2B	3.64	119.11	111.55
20	c	5491	CLA	CED-O2D-CGD	3.64	124.50	115.97
24	b	5529	BCR	C2-C1-C6	3.64	116.17	110.48
20	B	522	CLA	C1D-CHD-C4C	3.64	127.46	122.48
20	b	5512	CLA	C4A-NA-C1A	3.64	110.98	106.45
20	B	513	CLA	C1D-CHD-C4C	3.64	127.47	122.48
24	h	5107	BCR	C11-C10-C9	3.64	132.51	127.31
30	H	208	DGD	O3G-C1D-C2D	3.66	114.21	108.23
20	D	354	CLA	C1-C2-C3	3.66	132.70	125.96
24	x	5130	BCR	C2-C1-C6	3.67	116.21	110.48
26	A	568	SQD	O48-C23-C24	3.67	122.58	111.90
24	a	5566	BCR	C29-C30-C25	3.67	116.22	110.48
26	A	568	SQD	C11-C10-C9	3.67	133.38	114.45
25	a	5567	LHG	O8-C23-C24	3.68	122.60	111.90
28	d	5359	MGE	O2G-C1B-C2B	3.68	119.19	111.55
24	b	5528	BCR	C29-C30-C25	3.69	116.24	110.48
20	A	558	CLA	C4A-NA-C1A	3.69	111.03	106.45
30	C	507	DGD	C1E-O6E-C5E	3.69	120.66	113.72
24	c	5505	BCR	C29-C30-C25	3.69	116.25	110.48
24	C	505	BCR	C29-C30-C25	3.69	116.25	110.48
20	b	5519	CLA	CED-O2D-CGD	3.69	124.63	115.97
24	C	505	BCR	C2-C1-C6	3.70	116.26	110.48
24	X	130	BCR	C29-C30-C25	3.70	116.27	110.48
20	c	5500	CLA	C1D-CHD-C4C	3.71	127.56	122.48
20	b	5513	CLA	C4A-NA-C1A	3.71	111.06	106.45
24	c	5504	BCR	C24-C23-C22	3.74	131.83	126.21
20	a	5563	CLA	C4A-NA-C1A	3.74	111.09	106.45
20	B	517	CLA	O2A-CGA-CBA	3.75	122.80	111.90
26	A	568	SQD	C31-C30-C29	3.75	133.77	114.45
24	T	5104	BCR	C24-C23-C22	3.76	131.85	126.21
28	d	5360	MGE	O6D-C5D-C6D	3.76	115.42	106.41
30	h	5208	DGD	C1E-O6E-C5E	3.77	120.81	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5515	CLA	C4A-NA-C1A	3.77	111.13	106.45
24	t	104	BCR	C8-C7-C6	3.78	137.84	127.25
24	X	130	BCR	C2-C1-C6	3.79	116.40	110.48
20	B	517	CLA	C1D-CHD-C4C	3.79	127.67	122.48
24	h	5107	BCR	C29-C30-C25	3.79	116.41	110.48
32	f	5051	HEM	CAA-CBA-CGA	3.81	119.16	112.66
24	c	5506	BCR	C8-C7-C6	3.82	137.95	127.25
20	b	5516	CLA	O2A-CGA-CBA	3.83	123.03	111.90
20	B	512	CLA	C4A-NA-C1A	3.83	111.20	106.45
26	d	5358	SQD	C31-C30-C29	3.83	134.21	114.45
24	x	5130	BCR	C29-C30-C25	3.85	116.50	110.48
26	d	5358	SQD	O48-C23-C24	3.85	123.12	111.90
30	h	5208	DGD	O3G-C1D-C2D	3.86	114.53	108.23
20	b	5518	CLA	O2A-CGA-CBA	3.87	123.15	111.90
20	B	523	CLA	C1D-CHD-C4C	3.87	127.77	122.48
24	X	130	BCR	C23-C24-C25	3.87	138.10	127.25
24	d	5357	BCR	C29-C30-C25	3.89	116.56	110.48
24	x	5130	BCR	C23-C24-C25	3.89	138.13	127.25
30	C	508	DGD	O5D-C6D-C5D	3.89	115.45	108.94
20	B	518	CLA	O2A-CGA-CBA	3.89	123.22	111.90
24	C	504	BCR	C24-C23-C22	3.90	132.07	126.21
32	F	51	HEM	CAA-CBA-CGA	3.90	119.33	112.66
20	d	5354	CLA	C4A-NA-C1A	3.91	111.30	106.45
20	B	515	CLA	C4A-NA-C1A	3.92	111.31	106.45
25	A	567	LHG	O8-C23-C24	3.93	123.35	111.90
20	B	513	CLA	C4A-NA-C1A	3.94	111.34	106.45
20	A	563	CLA	C4A-NA-C1A	3.95	111.36	106.45
20	b	5526	CLA	CED-O2D-CGD	3.96	125.26	115.97
20	A	559	CLA	C4A-NA-C1A	3.99	111.40	106.45
20	b	5520	CLA	C4A-NA-C1A	3.99	111.41	106.45
20	c	5494	CLA	CED-O2D-CGD	3.99	125.33	115.97
30	c	5509	DGD	O6D-C5D-C6D	4.00	114.62	106.64
20	C	491	CLA	C4A-NA-C1A	4.01	111.43	106.45
21	A	561	PHO	C1-C2-C3	4.02	133.36	125.96
28	d	5361	MGE	O2G-C1B-C2B	4.02	119.90	111.55
30	c	5508	DGD	O5D-C6D-C5D	4.03	115.68	108.94
20	a	5559	CLA	C4A-NA-C1A	4.03	111.45	106.45
24	t	104	BCR	C29-C30-C25	4.03	116.79	110.48
28	d	5361	MGE	O6D-C5D-C6D	4.05	116.12	106.41
24	C	506	BCR	C8-C7-C6	4.05	138.60	127.25
20	B	520	CLA	C4A-NA-C1A	4.07	111.50	106.45
20	c	5494	CLA	C4A-NA-C1A	4.08	111.52	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	560	CLA	C4A-NA-C1A	4.08	111.52	106.45
26	t	213	SQD	O48-C23-C24	4.08	123.78	111.90
24	C	505	BCR	C23-C24-C25	4.09	138.71	127.25
26	A	5212	SQD	C44-O6-C1	4.10	122.17	113.76
30	C	509	DGD	O6D-C5D-C6D	4.11	114.84	106.64
20	B	522	CLA	C4A-NA-C1A	4.13	111.57	106.45
24	b	5529	BCR	C29-C30-C25	4.13	116.94	110.48
26	L	5213	SQD	O48-C23-C24	4.14	123.94	111.90
28	D	360	MGE	O2G-C1B-C2B	4.15	120.16	111.55
20	c	5500	CLA	C4A-NA-C1A	4.16	111.61	106.45
24	c	5505	BCR	C23-C24-C25	4.17	138.93	127.25
20	b	5526	CLA	C4A-NA-C1A	4.18	111.64	106.45
20	C	500	CLA	C4A-NA-C1A	4.18	111.64	106.45
20	B	511	CLA	C4A-NA-C1A	4.19	111.66	106.45
20	c	5497	CLA	C4A-NA-C1A	4.22	111.68	106.45
20	a	5560	CLA	C4A-NA-C1A	4.24	111.71	106.45
20	b	5519	CLA	C4A-NA-C1A	4.25	111.72	106.45
20	b	5522	CLA	C4A-NA-C1A	4.27	111.75	106.45
20	B	519	CLA	C4A-NA-C1A	4.27	111.75	106.45
20	c	5496	CLA	C4A-NA-C1A	4.29	111.77	106.45
20	c	5499	CLA	C4A-NA-C1A	4.30	111.79	106.45
20	B	526	CLA	C4A-NA-C1A	4.33	111.82	106.45
21	a	5562	PHO	C4A-NA-C1A	4.35	111.68	108.16
20	C	495	CLA	C4A-NA-C1A	4.36	111.87	106.45
20	c	5493	CLA	C4A-NA-C1A	4.36	111.87	106.45
21	A	562	PHO	C4A-NA-C1A	4.37	111.69	108.16
20	b	5523	CLA	C1D-CHD-C4C	4.37	128.46	122.48
20	b	5517	CLA	C4A-NA-C1A	4.38	111.89	106.45
20	b	5521	CLA	C4A-NA-C1A	4.39	111.89	106.45
20	C	494	CLA	CED-O2D-CGD	4.39	126.25	115.97
20	C	499	CLA	C4A-NA-C1A	4.41	111.92	106.45
21	a	5561	PHO	C4A-NA-C1A	4.41	111.73	108.16
20	B	525	CLA	C4A-NA-C1A	4.42	111.94	106.45
20	b	5524	CLA	C4A-NA-C1A	4.42	111.94	106.45
24	T	5104	BCR	C29-C30-C25	4.42	117.39	110.48
20	C	496	CLA	C4A-NA-C1A	4.43	111.94	106.45
20	C	498	CLA	C4A-NA-C1A	4.43	111.95	106.45
20	C	492	CLA	C4A-NA-C1A	4.44	111.96	106.45
20	b	5511	CLA	C4A-NA-C1A	4.45	111.97	106.45
28	D	360	MGE	O6D-C5D-C6D	4.46	117.08	106.41
21	A	561	PHO	C4A-NA-C1A	4.46	111.77	108.16
20	C	493	CLA	C4A-NA-C1A	4.47	112.00	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	502	CLA	C4A-NA-C1A	4.48	112.02	106.45
20	D	355	CLA	C4A-NA-C1A	4.49	112.03	106.45
32	v	5552	HEM	CAD-C3D-C2D	4.51	141.87	129.00
20	b	5518	CLA	C4A-NA-C1A	4.52	112.07	106.45
26	a	212	SQD	C44-O6-C1	4.54	123.07	113.76
20	d	5355	CLA	C4A-NA-C1A	4.55	112.10	106.45
24	B	528	BCR	C33-C5-C6	4.55	129.60	124.51
20	C	494	CLA	C4A-NA-C1A	4.56	112.11	106.45
20	B	516	CLA	C4A-NA-C1A	4.58	112.13	106.45
24	c	5504	BCR	C33-C5-C6	4.58	129.64	124.51
20	c	5495	CLA	C4A-NA-C1A	4.58	112.14	106.45
20	b	5523	CLA	C4A-NA-C1A	4.59	112.15	106.45
32	V	552	HEM	CAD-C3D-C2D	4.59	142.12	129.00
20	c	5498	CLA	C4A-NA-C1A	4.59	112.15	106.45
20	B	523	CLA	C4A-NA-C1A	4.61	112.17	106.45
20	c	5492	CLA	C4A-NA-C1A	4.62	112.19	106.45
20	B	517	CLA	C4A-NA-C1A	4.62	112.19	106.45
20	c	5502	CLA	C4A-NA-C1A	4.63	112.20	106.45
20	b	5525	CLA	C4A-NA-C1A	4.63	112.20	106.45
20	B	521	CLA	C4A-NA-C1A	4.64	112.21	106.45
32	F	51	HEM	CAD-C3D-C2D	4.64	142.26	129.00
20	B	518	CLA	C4A-NA-C1A	4.65	112.22	106.45
20	C	503	CLA	C4A-NA-C1A	4.65	112.23	106.45
20	b	5516	CLA	C4A-NA-C1A	4.67	112.25	106.45
20	C	497	CLA	C4A-NA-C1A	4.67	112.25	106.45
20	c	5503	CLA	C4A-NA-C1A	4.72	112.31	106.45
20	c	5491	CLA	C4A-NA-C1A	4.75	112.35	106.45
32	f	5051	HEM	CAD-C3D-C2D	4.78	142.66	129.00
20	B	524	CLA	C4A-NA-C1A	4.79	112.39	106.45
24	b	5528	BCR	C33-C5-C6	4.80	129.88	124.51
24	x	5130	BCR	C11-C10-C9	4.82	134.19	127.31
24	C	504	BCR	C33-C5-C6	4.83	129.92	124.51
20	B	514	CLA	C4A-NA-C1A	4.87	112.49	106.45
24	h	5107	BCR	C33-C5-C6	4.90	129.99	124.51
20	C	501	CLA	C4A-NA-C1A	4.90	112.54	106.45
20	b	5514	CLA	C4A-NA-C1A	4.92	112.56	106.45
24	b	5529	BCR	C33-C5-C6	4.93	130.03	124.51
20	c	5501	CLA	C4A-NA-C1A	4.94	112.59	106.45
24	c	5505	BCR	C33-C5-C6	4.96	130.06	124.51
24	H	107	BCR	C33-C5-C6	5.02	130.13	124.51
22	D	356	PQ9	C11-C2-C1	5.05	120.98	116.88
26	L	5213	SQD	O7-S-C6	5.09	111.17	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	130	BCR	C38-C26-C25	5.16	130.29	124.51
24	c	5506	BCR	C33-C5-C6	5.22	130.35	124.51
24	x	5130	BCR	C38-C26-C25	5.23	130.36	124.51
24	C	505	BCR	C33-C5-C6	5.27	130.41	124.51
24	X	130	BCR	C11-C10-C9	5.28	134.85	127.31
24	C	506	BCR	C33-C5-C6	5.34	130.48	124.51
24	b	5527	BCR	C38-C26-C25	5.34	130.49	124.51
24	c	5504	BCR	C38-C26-C25	5.36	130.51	124.51
24	H	107	BCR	C38-C26-C25	5.40	130.56	124.51
24	a	5566	BCR	C33-C5-C6	5.41	130.57	124.51
24	B	529	BCR	C33-C5-C6	5.44	130.59	124.51
24	x	5130	BCR	C7-C8-C9	5.45	134.40	126.21
24	A	566	BCR	C38-C26-C25	5.46	130.62	124.51
22	d	5356	PQ9	C11-C2-C1	5.47	121.32	116.88
24	b	5529	BCR	C38-C26-C25	5.47	130.63	124.51
24	a	5566	BCR	C38-C26-C25	5.47	130.63	124.51
24	T	5104	BCR	C33-C5-C6	5.52	130.69	124.51
24	b	5528	BCR	C38-C26-C25	5.53	130.70	124.51
24	t	104	BCR	C33-C5-C6	5.53	130.70	124.51
24	b	5527	BCR	C33-C5-C6	5.54	130.71	124.51
24	C	504	BCR	C38-C26-C25	5.56	130.73	124.51
24	A	566	BCR	C33-C5-C6	5.56	130.73	124.51
24	B	527	BCR	C33-C5-C6	5.60	130.77	124.51
24	c	5506	BCR	C38-C26-C25	5.60	130.77	124.51
24	X	130	BCR	C7-C8-C9	5.60	134.63	126.21
24	h	5107	BCR	C38-C26-C25	5.68	130.87	124.51
24	C	506	BCR	C38-C26-C25	5.71	130.90	124.51
26	A	568	SQD	C25-C24-C23	5.80	134.74	113.58
24	C	505	BCR	C38-C26-C25	5.80	131.00	124.51
24	B	528	BCR	C38-C26-C25	5.80	131.00	124.51
26	L	5213	SQD	C25-C24-C23	5.80	134.76	113.58
24	B	527	BCR	C38-C26-C25	5.88	131.09	124.51
26	t	213	SQD	C25-C24-C23	5.88	135.06	113.58
26	L	5213	SQD	C10-C9-C8	5.93	134.96	113.24
26	d	5358	SQD	C10-C9-C8	5.94	135.02	113.24
26	t	213	SQD	C10-C9-C8	5.96	135.07	113.24
24	D	357	BCR	C33-C5-C6	6.00	131.22	124.51
26	A	568	SQD	C10-C9-C8	6.01	135.25	113.24
25	a	5567	LHG	C25-C24-C23	6.07	135.74	113.58
24	t	104	BCR	C38-C26-C25	6.15	131.39	124.51
26	d	5358	SQD	C25-C24-C23	6.17	136.09	113.58
25	A	567	LHG	C25-C24-C23	6.17	136.10	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	5212	SQD	O6-C1-C2	6.21	118.36	108.23
24	x	5130	BCR	C33-C5-C6	6.23	131.48	124.51
24	B	529	BCR	C38-C26-C25	6.26	131.51	124.51
24	d	5357	BCR	C38-C26-C25	6.28	131.54	124.51
24	c	5505	BCR	C38-C26-C25	6.29	131.55	124.51
24	d	5357	BCR	C33-C5-C6	6.32	131.58	124.51
26	a	212	SQD	O6-C1-C2	6.42	118.71	108.23
24	T	5104	BCR	C38-C26-C25	6.48	131.77	124.51
24	X	130	BCR	C33-C5-C6	6.51	131.79	124.51
24	D	357	BCR	C38-C26-C25	6.52	131.80	124.51
26	A	568	SQD	O6-C1-C2	6.77	119.27	108.23
26	A	5212	SQD	O7-S-C6	6.82	112.66	106.83
26	d	5358	SQD	O7-S-C6	6.82	112.66	106.83
26	d	5358	SQD	O6-C1-C2	6.92	119.53	108.23
26	t	213	SQD	O7-S-C6	6.96	112.78	106.83
26	L	5213	SQD	O6-C1-C2	7.00	119.65	108.23
30	h	5208	DGD	O6E-C5E-C4E	7.05	122.65	109.66
30	c	5509	DGD	O6E-C5E-C4E	7.06	122.66	109.66
30	C	509	DGD	O6E-C5E-C4E	7.08	122.70	109.66
30	C	508	DGD	O6E-C5E-C4E	7.17	122.87	109.66
30	C	507	DGD	O6E-C5E-C4E	7.17	122.88	109.66
30	c	5508	DGD	O6E-C5E-C4E	7.33	123.17	109.66
26	t	213	SQD	O6-C1-C2	7.35	120.22	108.23
30	H	208	DGD	O6E-C5E-C4E	7.40	123.29	109.66
30	c	5507	DGD	O6E-C5E-C4E	7.57	123.60	109.66
26	t	213	SQD	O5-C1-O6	7.69	128.28	110.02
26	A	5212	SQD	C5-C6-S	7.78	125.17	114.34
26	a	212	SQD	C5-C6-S	7.87	125.30	114.34
26	a	212	SQD	O7-S-C6	8.00	113.66	106.83
26	L	5213	SQD	O5-C1-O6	8.03	129.09	110.02
26	d	5358	SQD	O5-C1-O6	8.06	129.16	110.02
26	A	568	SQD	O5-C1-O6	8.33	129.81	110.02
26	a	212	SQD	O5-C1-O6	8.36	129.88	110.02
26	A	568	SQD	O7-S-C6	8.44	114.04	106.83
26	A	5212	SQD	O5-C1-O6	8.73	130.76	110.02
26	d	5358	SQD	C5-C6-S	8.78	126.56	114.34
26	t	213	SQD	C5-C6-S	9.68	127.82	114.34
26	A	568	SQD	C5-C6-S	9.69	127.83	114.34
26	L	5213	SQD	C5-C6-S	10.02	128.29	114.34

All (234) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	b	5526	CLA	NC
20	b	5526	CLA	ND
20	b	5526	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	ND
20	C	503	CLA	NA
20	b	5517	CLA	NC
20	b	5517	CLA	ND
20	b	5517	CLA	NA
20	B	512	CLA	NC
20	B	512	CLA	ND
20	B	512	CLA	NA
20	c	5495	CLA	NC
20	c	5495	CLA	ND
20	c	5495	CLA	NA
20	B	526	CLA	NC
20	B	526	CLA	ND
20	B	526	CLA	NA
20	C	495	CLA	NC
20	C	495	CLA	ND
20	C	495	CLA	NA
20	d	5354	CLA	NC
20	d	5354	CLA	ND
20	d	5354	CLA	NA
20	c	5492	CLA	NC
20	c	5492	CLA	ND
20	c	5492	CLA	NA
20	B	518	CLA	NC
20	B	518	CLA	ND
20	B	518	CLA	NA
20	c	5497	CLA	NC
20	c	5497	CLA	ND
20	c	5497	CLA	NA
20	c	5496	CLA	NC
20	c	5496	CLA	ND
20	c	5496	CLA	NA
20	a	5559	CLA	NC
20	a	5559	CLA	ND
20	a	5559	CLA	NA
20	c	5503	CLA	NC
20	c	5503	CLA	ND
20	c	5503	CLA	NA
20	C	496	CLA	NC

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Mol	Chain	Res	Type	Atom
20	C	496	CLA	ND
20	C	496	CLA	NA
20	B	520	CLA	NC
20	B	520	CLA	ND
20	B	520	CLA	NA
20	C	494	CLA	NC
20	C	494	CLA	ND
20	C	494	CLA	NA
20	C	491	CLA	NC
20	C	491	CLA	ND
20	C	491	CLA	NA
20	b	5520	CLA	NC
20	b	5520	CLA	ND
20	b	5520	CLA	NA
20	C	500	CLA	NC
20	C	500	CLA	ND
20	C	500	CLA	NA
20	C	493	CLA	NC
20	C	493	CLA	ND
20	C	493	CLA	NA
20	b	5514	CLA	NC
20	b	5514	CLA	ND
20	b	5514	CLA	NA
20	B	519	CLA	NC
20	B	519	CLA	ND
20	B	519	CLA	NA
20	D	354	CLA	NC
20	D	354	CLA	ND
20	D	354	CLA	NA
20	B	516	CLA	NC
20	B	516	CLA	ND
20	B	516	CLA	NA
20	b	5512	CLA	NC
20	b	5512	CLA	ND
20	b	5512	CLA	NA
20	B	513	CLA	NC
20	B	513	CLA	ND
20	B	513	CLA	NA
20	c	5499	CLA	NC
20	c	5499	CLA	ND
20	c	5499	CLA	NA
30	h	5208	DGD	C2D

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Mol	Chain	Res	Type	Atom
30	h	5208	DGD	C5D
30	h	5208	DGD	C5E
20	A	560	CLA	NC
20	A	560	CLA	ND
20	A	560	CLA	NA
20	d	5355	CLA	NC
20	d	5355	CLA	ND
20	d	5355	CLA	NA
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D
30	c	5507	DGD	C5E
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
20	B	525	CLA	NC
20	B	525	CLA	ND
20	B	525	CLA	NA
20	c	5500	CLA	NC
20	c	5500	CLA	ND
20	c	5500	CLA	NA
20	b	5518	CLA	NC
20	b	5518	CLA	ND
20	b	5518	CLA	NA
20	B	524	CLA	NC
20	B	524	CLA	ND
20	B	524	CLA	NA
20	B	515	CLA	NC
20	B	515	CLA	ND
20	B	515	CLA	NA
20	b	5525	CLA	NC
20	b	5525	CLA	ND
20	b	5525	CLA	NA
30	C	508	DGD	C2D
30	C	508	DGD	C5D
30	C	508	DGD	C5E
20	C	502	CLA	NC
20	C	502	CLA	ND
20	C	502	CLA	NA
20	a	5558	CLA	NC
20	a	5558	CLA	ND
20	a	5558	CLA	NA
20	B	511	CLA	NC

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Mol	Chain	Res	Type	Atom
20	B	511	CLA	ND
20	B	511	CLA	NA
20	b	5522	CLA	NC
20	b	5522	CLA	ND
20	b	5522	CLA	NA
20	b	5519	CLA	NC
20	b	5519	CLA	ND
20	b	5519	CLA	NA
20	B	522	CLA	NC
20	B	522	CLA	ND
20	B	522	CLA	NA
20	b	5516	CLA	NC
20	b	5516	CLA	ND
20	b	5516	CLA	NA
20	b	5513	CLA	NC
20	b	5513	CLA	ND
20	b	5513	CLA	NA
30	C	507	DGD	C2D
30	C	507	DGD	C5D
30	C	507	DGD	C5E
20	c	5502	CLA	NC
20	c	5502	CLA	ND
20	c	5502	CLA	NA
20	b	5523	CLA	NC
20	b	5523	CLA	ND
20	b	5523	CLA	NA
20	a	5563	CLA	NC
20	a	5563	CLA	ND
20	a	5563	CLA	NA
30	c	5509	DGD	C2D
30	c	5509	DGD	C5D
30	c	5509	DGD	C5E
30	c	5508	DGD	C2D
30	c	5508	DGD	C5D
30	c	5508	DGD	C5E
20	b	5515	CLA	NC
20	b	5515	CLA	ND
20	b	5515	CLA	NA
20	c	5494	CLA	NC
20	c	5494	CLA	ND
20	c	5494	CLA	NA
20	c	5493	CLA	NC

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Mol	Chain	Res	Type	Atom
20	c	5493	CLA	ND
20	c	5493	CLA	NA
20	B	523	CLA	NC
20	B	523	CLA	ND
20	B	523	CLA	NA
20	b	5511	CLA	NC
20	b	5511	CLA	ND
20	b	5511	CLA	NA
20	C	498	CLA	NC
20	C	498	CLA	ND
20	C	498	CLA	NA
30	C	509	DGD	C2D
30	C	509	DGD	C5D
30	C	509	DGD	C5E
20	A	563	CLA	NC
20	A	563	CLA	ND
20	A	563	CLA	NA
20	b	5521	CLA	NC
20	b	5521	CLA	ND
20	b	5521	CLA	NA
20	A	559	CLA	NC
20	A	559	CLA	ND
20	A	559	CLA	NA
20	A	558	CLA	NC
20	A	558	CLA	ND
20	A	558	CLA	NA
20	B	517	CLA	NC
20	B	517	CLA	ND
20	B	517	CLA	NA
20	a	5560	CLA	NC
20	a	5560	CLA	ND
20	a	5560	CLA	NA
20	C	501	CLA	NC
20	C	501	CLA	ND
20	C	501	CLA	NA
20	D	355	CLA	NC
20	D	355	CLA	ND
20	D	355	CLA	NA
20	C	499	CLA	NC
20	C	499	CLA	ND
20	C	499	CLA	NA
20	b	5524	CLA	NC

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Mol	Chain	Res	Type	Atom
20	b	5524	CLA	ND
20	b	5524	CLA	NA
20	c	5498	CLA	NC
20	c	5498	CLA	ND
20	c	5498	CLA	NA
20	c	5491	CLA	NC
20	c	5491	CLA	ND
20	c	5491	CLA	NA
20	B	521	CLA	NC
20	B	521	CLA	ND
20	B	521	CLA	NA
20	C	492	CLA	NC
20	C	492	CLA	ND
20	C	492	CLA	NA
20	c	5501	CLA	NC
20	c	5501	CLA	ND
20	c	5501	CLA	NA
20	C	497	CLA	NC
20	C	497	CLA	ND
20	C	497	CLA	NA
20	B	514	CLA	NC
20	B	514	CLA	ND
20	B	514	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	d	5354	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C4

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	558	CLA	10	0
20	A	559	CLA	5	0
20	A	560	CLA	1	0
21	A	561	PHO	7	0
21	A	562	PHO	5	0
22	A	564	PQ9	2	0
24	A	566	BCR	1	0
25	A	567	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	511	CLA	1	0
20	B	512	CLA	2	0
20	B	513	CLA	8	0
20	B	514	CLA	5	0
20	B	515	CLA	12	0
20	B	516	CLA	6	0
20	B	517	CLA	9	0
20	B	518	CLA	11	0
20	B	519	CLA	5	0
20	B	520	CLA	6	0
20	B	521	CLA	2	0
20	B	522	CLA	4	0
20	B	523	CLA	2	0
20	B	524	CLA	4	0
20	B	525	CLA	4	0
20	B	526	CLA	2	0
24	B	527	BCR	2	0
24	B	528	BCR	2	0
24	B	529	BCR	2	0
28	B	530	MGE	1	0
20	C	491	CLA	4	0
20	C	492	CLA	2	0
20	C	493	CLA	7	0
20	C	494	CLA	2	0
20	C	495	CLA	9	0
20	C	496	CLA	2	0
20	C	497	CLA	5	0
20	C	498	CLA	6	0
20	C	499	CLA	2	0
20	C	500	CLA	3	0
20	C	501	CLA	13	0
20	C	502	CLA	2	0
20	C	503	CLA	1	0
24	C	504	BCR	7	0
24	C	505	BCR	6	0
24	C	506	BCR	7	0
30	C	507	DGD	6	0
30	C	508	DGD	2	0
30	C	509	DGD	10	0
20	D	354	CLA	5	0
20	D	355	CLA	3	0
22	D	356	PQ9	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	357	BCR	4	0
28	D	358	MGE	2	0
28	D	359	MGE	1	0
28	D	360	MGE	7	0
32	F	51	HEM	3	0
24	H	107	BCR	3	0
30	H	208	DGD	3	0
28	I	201	MGE	1	0
28	L	210	MGE	2	0
27	T	217	LMT	3	0
24	T	5104	BCR	5	0
32	V	552	HEM	2	0
24	X	130	BCR	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	-0.59	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.54	4 (1%) 79 53	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.53	2 (0%) 92 77	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.50	1 (0%) 94 85	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.52	3 (0%) 87 67	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.35	4 (0%) 84 61	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 93 82	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.57	1 (0%) 93 82	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.19	1 (1%) 79 53	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.01	3 (3%) 42 18	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.22	1 (2%) 52 24	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	3 (8%) 11 4	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.38	1 (1%) 72 44	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.21	3 (4%) 32 13	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	1 (2%) 52 24	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.34	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.60	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.50	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.54	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.41	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.14	1 (2%) 55 26	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.35	3 (8%) 13 5	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.42	1 (2%) 53 25	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.36	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/247 (97%)	-0.39	3 (1%) 79 53	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.30	9 (3%) 42 18	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.48	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.73	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.39	1 (1%) 82 58	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.41	3 (3%) 49 22	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.47	2 (1%) 74 47	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.23	5 (3%) 43 18	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.26	4 (6%) 20 7	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.19	2 (3%) 48 21	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.45	63 (1%) 79 53	35, 66, 85, 101	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	5010	SER	4.6
3	c	5473	ASP	4.4
13	o	5049	ASP	4.3
4	D	13	GLY	4.1
11	l	5001	MET	4.0
13	O	114	ASN	4.0
6	f	5013	TYR	3.7
11	L	5	PRO	3.5
7	h	5065	LEU	3.5
15	U	37	GLU	3.4
1	a	5011	ALA	3.4
1	a	5015	GLU	3.3
5	e	5003	GLY	3.3
6	f	5011	VAL	3.3
5	e	5060	GLN	3.2
5	E	84	LYS	3.1
18	Z	30	PRO	3.0
13	o	5050	ASP	2.9
5	e	5017	VAL	2.8
3	C	192	GLY	2.8
16	V	27	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
18	z	5062	VAL	2.7
3	c	5029	GLU	2.7
13	O	87	GLN	2.7
7	h	5064	ALA	2.7
6	f	5012	SER	2.7
13	o	5060	SER	2.6
6	F	12	SER	2.6
12	M	36	SER	2.6
13	O	59	ASP	2.6
18	z	5003	ILE	2.6
18	Z	60	PHE	2.6
3	C	182	PHE	2.6
16	v	5111	GLU	2.5
16	v	5041	GLU	2.5
7	h	5006	TRP	2.4
15	u	5053	GLU	2.4
13	o	5030	THR	2.4
13	o	5061	SER	2.4
3	C	460	ASP	2.4
3	c	5472	LEU	2.3
11	l	5003	PRO	2.3
16	V	81	ARG	2.3
1	a	5227	THR	2.3
13	o	5048	LEU	2.3
2	B	130	GLU	2.2
2	b	5294	SER	2.2
18	Z	29	SER	2.2
2	B	129	GLY	2.2
7	H	26	GLY	2.2
18	Z	34	ASP	2.2
3	c	5033	PHE	2.2
4	d	5226	GLY	2.1
15	u	5052	GLY	2.1
13	o	5089	ALA	2.1
8	I	35	LYS	2.1
13	o	5082	PRO	2.1
15	u	5086	GLU	2.1
11	l	5002	GLU	2.0
16	v	5027	ALA	2.0
16	v	5043	LYS	2.0
13	o	5088	GLU	2.0
16	v	5039	ASN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
27	LMT	A	569	35/35	0.72	0.47	7.86	80,89,92,93	0
29	UNK	c	5484	5/-	0.84	0.53	6.31	69,69,70,72	0
20	CLA	B	511	41/65	0.73	0.41	6.16	88,90,92,98	0
27	LMT	a	5568	35/35	0.81	0.43	6.11	79,92,94,96	0
27	LMT	t	5217	35/35	0.68	0.46	6.11	76,95,104,105	0
24	BCR	H	107	40/40	0.82	0.29	5.91	77,83,88,89	0
29	UNK	C	489	7/-	0.78	0.44	5.91	75,76,77,78	0
29	UNK	c	5489	7/-	0.78	0.41	5.88	73,73,74,74	0
29	UNK	c	5485	5/-	0.85	0.39	5.12	68,69,69,70	0
20	CLA	c	5503	50/65	0.85	0.28	4.62	88,91,92,93	0
22	PQ9	a	5564	30/45	0.87	0.32	4.56	51,55,62,62	30
29	UNK	c	5477	7/-	0.90	0.33	4.56	67,68,70,70	0
20	CLA	b	5511	41/65	0.64	0.40	4.31	88,92,95,96	0
22	PQ9	A	564	30/45	0.77	0.37	4.06	54,57,63,64	30
29	UNK	C	481	13/-	0.73	0.36	4.05	61,64,68,69	0
24	BCR	C	505	40/40	0.81	0.43	4.04	75,81,91,92	0
27	LMT	T	217	35/35	0.75	0.31	3.66	83,93,96,97	0
24	BCR	x	5130	40/40	0.79	0.42	3.65	77,81,85,86	0
29	UNK	c	5474	15/-	0.89	0.24	3.37	39,50,56,56	0
20	CLA	a	5560	65/65	0.90	0.22	3.30	62,68,100,101	0
24	BCR	X	130	40/40	0.84	0.32	3.05	68,71,80,81	0
24	BCR	h	5107	40/40	0.86	0.28	3.04	74,79,82,83	0
24	BCR	d	5357	40/40	0.83	0.37	2.98	61,72,86,88	0
28	MGE	d	5359	47/48	0.76	0.30	2.84	72,81,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	B	528	40/40	0.84	0.25	2.73	54,68,74,75	0
20	CLA	a	5563	55/65	0.84	0.31	2.72	59,65,102,103	0
24	BCR	c	5504	40/40	0.86	0.29	2.72	73,80,88,89	0
24	BCR	b	5529	40/40	0.86	0.34	2.67	69,72,74,74	0
24	BCR	C	504	40/40	0.91	0.27	2.50	57,64,70,70	0
24	BCR	D	357	40/40	0.89	0.26	2.27	61,66,78,80	0
29	UNK	C	482	13/-	0.84	0.25	2.08	64,66,67,67	0
27	LMT	M	5216	35/35	0.77	0.31	2.02	58,83,90,90	0
20	CLA	A	563	55/65	0.88	0.26	1.96	43,49,75,78	0
20	CLA	B	519	65/65	0.88	0.26	1.93	73,82,85,87	0
24	BCR	T	5104	40/40	0.88	0.25	1.90	67,71,78,79	0
20	CLA	c	5498	65/65	0.85	0.25	1.86	81,90,93,93	0
28	MGE	D	358	47/48	0.82	0.24	1.85	65,72,79,81	0
20	CLA	B	526	65/65	0.79	0.28	1.82	71,82,97,98	0
30	DGD	C	507	53/66	0.89	0.25	1.81	55,66,86,88	0
24	BCR	c	5505	40/40	0.88	0.31	1.80	84,87,91,92	0
28	MGE	d	5361	48/48	0.89	0.22	1.78	61,68,78,83	0
20	CLA	c	5501	65/65	0.88	0.26	1.77	82,91,94,95	0
20	CLA	b	5516	65/65	0.82	0.28	1.76	62,66,84,86	0
29	UNK	c	5476	9/-	0.79	0.33	1.68	58,60,62,62	0
27	LMT	m	216	35/35	0.80	0.28	1.68	62,87,89,91	0
20	CLA	D	355	50/65	0.91	0.22	1.60	63,65,68,70	0
20	CLA	b	5519	65/65	0.89	0.24	1.59	70,75,80,81	0
20	CLA	B	515	65/65	0.93	0.21	1.59	55,66,71,72	0
26	SQD	A	568	54/54	0.84	0.32	1.58	76,82,90,90	0
21	PHO	a	5562	64/64	0.91	0.22	1.57	70,75,81,82	0
20	CLA	C	495	65/65	0.92	0.21	1.55	58,68,74,76	0
20	CLA	B	520	65/65	0.90	0.23	1.53	62,67,76,79	0
20	CLA	b	5520	65/65	0.90	0.24	1.49	63,72,74,76	0
24	BCR	c	5506	40/40	0.76	0.32	1.44	75,81,86,86	0
24	BCR	t	104	40/40	0.91	0.20	1.44	65,72,84,85	0
24	BCR	A	566	40/40	0.92	0.24	1.43	50,57,64,66	0
25	LHG	A	567	39/49	0.92	0.23	1.41	57,73,79,81	0
20	CLA	C	501	65/65	0.89	0.25	1.39	70,78,83,85	0
20	CLA	C	498	65/65	0.88	0.22	1.39	64,74,98,101	0
20	CLA	c	5497	65/65	0.89	0.23	1.38	66,82,84,87	0
22	PQ9	D	356	30/45	0.91	0.21	1.31	49,67,80,83	0
20	CLA	B	512	65/65	0.91	0.24	1.29	68,75,78,79	0
28	MGE	b	5530	48/48	0.89	0.18	1.27	59,64,71,73	0
24	BCR	a	5566	40/40	0.90	0.25	1.27	59,75,78,79	0
20	CLA	B	522	65/65	0.94	0.21	1.25	54,65,75,77	0
32	HEM	f	5051	43/43	0.94	0.28	1.25	80,84,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNK	C	485	5/-	0.90	0.23	1.24	57,59,61,61	0
20	CLA	c	5495	65/65	0.91	0.21	1.22	74,81,86,88	0
20	CLA	b	5515	65/65	0.94	0.21	1.21	46,51,74,76	0
20	CLA	A	560	65/65	0.91	0.20	1.20	49,57,86,88	0
20	CLA	C	503	50/65	0.86	0.26	1.16	83,86,88,94	0
20	CLA	b	5512	65/65	0.92	0.23	1.14	68,72,75,76	0
30	DGD	c	5509	57/66	0.86	0.28	1.10	67,72,77,78	0
20	CLA	C	497	65/65	0.88	0.24	1.07	74,78,80,82	0
28	MGE	D	359	41/48	0.88	0.23	1.04	60,67,76,79	0
22	PQ9	d	5356	30/45	0.93	0.20	1.02	51,57,66,66	0
24	BCR	B	529	40/40	0.89	0.24	1.00	62,69,80,80	0
20	CLA	B	516	65/65	0.82	0.27	0.98	61,76,92,97	0
20	CLA	d	5354	65/65	0.95	0.17	0.98	39,47,64,65	0
30	DGD	c	5507	53/66	0.89	0.23	0.98	66,74,90,91	0
29	UNK	c	5481	13/-	0.87	0.23	0.96	60,62,66,66	0
28	MGE	l	5210	48/48	0.90	0.21	0.95	59,69,78,81	0
20	CLA	b	5513	65/65	0.94	0.20	0.95	54,61,84,90	0
20	CLA	c	5496	65/65	0.82	0.27	0.95	79,83,95,97	0
32	HEM	F	51	43/43	0.95	0.26	0.93	78,84,92,95	0
28	MGE	d	5360	41/48	0.90	0.21	0.93	68,72,78,80	0
28	MGE	L	210	48/48	0.88	0.24	0.88	59,68,73,75	0
29	UNK	C	474	15/-	0.89	0.18	0.88	26,37,40,40	0
26	SQD	a	212	26/54	0.79	0.26	0.87	82,94,101,103	0
25	LHG	a	5567	39/49	0.90	0.26	0.87	65,68,74,80	0
24	BCR	b	5527	40/40	0.92	0.20	0.85	58,63,72,72	0
28	MGE	D	360	48/48	0.91	0.20	0.85	52,60,63,68	0
32	HEM	v	5552	43/43	0.96	0.22	0.85	65,67,70,70	0
20	CLA	B	514	65/65	0.93	0.21	0.83	59,64,82,83	0
30	DGD	C	508	47/66	0.91	0.19	0.79	61,71,80,83	0
30	DGD	H	208	54/66	0.90	0.20	0.75	61,69,75,76	0
28	MGE	i	5201	48/48	0.84	0.27	0.74	67,83,88,90	0
26	SQD	d	5358	54/54	0.80	0.29	0.72	74,85,106,107	0
26	SQD	A	5212	26/54	0.81	0.24	0.72	75,100,107,107	0
29	UNK	C	476	9/-	0.81	0.29	0.72	61,62,63,64	0
28	MGE	I	201	48/48	0.87	0.23	0.71	73,81,89,90	0
20	CLA	C	496	65/65	0.84	0.26	0.70	71,78,88,89	0
20	CLA	B	513	65/65	0.94	0.18	0.68	56,61,67,67	0
20	CLA	C	502	51/65	0.88	0.21	0.67	74,80,83,84	0
21	PHO	a	5561	64/64	0.94	0.18	0.67	51,55,66,68	0
32	HEM	V	552	43/43	0.97	0.18	0.63	37,54,58,59	0
20	CLA	B	525	65/65	0.93	0.20	0.62	67,84,91,92	0
26	SQD	t	213	47/54	0.85	0.26	0.61	61,95,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNK	C	477	7/-	0.96	0.16	0.60	47,49,51,51	0
26	SQD	L	5213	47/54	0.80	0.27	0.60	52,85,106,108	0
20	CLA	b	5522	65/65	0.94	0.20	0.59	60,66,75,76	0
28	MGE	B	530	48/48	0.88	0.19	0.58	55,64,70,72	0
30	DGD	C	509	57/66	0.91	0.20	0.55	52,60,69,70	0
20	CLA	c	5502	51/65	0.87	0.24	0.51	93,96,97,98	0
29	UNK	c	5482	13/-	0.90	0.19	0.51	60,61,71,72	0
31	BCT	D	353	4/4	0.96	0.19	0.51	72,73,73,74	0
21	PHO	A	562	64/64	0.94	0.17	0.49	47,53,63,66	0
20	CLA	d	5355	50/65	0.87	0.23	0.48	74,77,80,81	0
24	BCR	b	5528	40/40	0.93	0.18	0.48	61,64,72,73	0
20	CLA	c	5500	65/65	0.92	0.20	0.42	64,69,82,83	0
20	CLA	C	500	65/65	0.94	0.16	0.41	59,63,73,74	0
20	CLA	b	5526	65/65	0.79	0.28	0.37	66,71,92,95	0
20	CLA	D	354	65/65	0.95	0.17	0.36	35,43,63,66	0
20	CLA	b	5514	65/65	0.94	0.18	0.32	41,51,74,75	0
20	CLA	C	499	47/65	0.95	0.17	0.31	57,60,66,69	0
24	BCR	C	506	40/40	0.88	0.22	0.30	68,72,79,80	0
24	BCR	B	527	40/40	0.91	0.18	0.30	58,65,68,69	0
20	CLA	C	491	65/65	0.95	0.18	0.27	63,70,77,79	0
20	CLA	B	518	65/65	0.93	0.19	0.27	53,64,79,79	0
29	UNK	C	484	5/-	0.86	0.21	0.26	47,51,52,53	0
20	CLA	C	492	60/65	0.95	0.17	0.23	53,58,76,77	0
20	CLA	B	521	65/65	0.95	0.17	0.21	58,63,66,68	0
21	PHO	A	561	64/64	0.95	0.16	0.18	32,52,55,59	0
20	CLA	C	493	65/65	0.94	0.18	0.17	67,71,77,79	0
20	CLA	c	5491	65/65	0.92	0.20	0.16	70,78,81,86	0
20	CLA	b	5525	65/65	0.93	0.19	0.13	71,77,80,82	0
20	CLA	c	5493	65/65	0.90	0.21	0.05	67,81,86,86	0
20	CLA	a	5559	65/65	0.95	0.16	-0.02	42,49,60,60	0
20	CLA	c	5499	47/65	0.92	0.20	-0.04	60,69,76,78	0
30	DGD	c	5508	47/66	0.91	0.18	-0.04	66,76,82,84	0
20	CLA	b	5517	65/65	0.95	0.15	-0.05	54,58,66,71	0
20	CLA	B	523	65/65	0.95	0.16	-0.06	47,56,73,74	0
20	CLA	B	524	56/65	0.93	0.19	-0.09	67,72,77,80	0
30	DGD	h	5208	54/66	0.93	0.17	-0.10	57,68,73,75	0
20	CLA	b	5523	65/65	0.95	0.15	-0.13	45,52,74,75	0
20	CLA	C	494	46/65	0.95	0.15	-0.18	59,66,68,72	0
20	CLA	a	5558	65/65	0.95	0.16	-0.22	41,50,55,61	0
20	CLA	b	5524	56/65	0.93	0.18	-0.23	63,68,89,91	0
20	CLA	A	559	65/65	0.96	0.14	-0.31	39,43,49,52	0
20	CLA	B	517	65/65	0.96	0.14	-0.35	37,44,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	c	5492	60/65	0.93	0.17	-0.38	57,61,83,84	0
20	CLA	b	5518	65/65	0.95	0.16	-0.38	60,64,69,75	0
20	CLA	c	5494	46/65	0.93	0.16	-0.47	72,77,86,88	0
23	OEC	a	5565	5/9	0.96	0.13	-0.50	63,64,71,87	0
20	CLA	b	5521	65/65	0.94	0.15	-0.63	48,57,63,64	0
20	CLA	A	558	65/65	0.97	0.14	-0.73	41,46,50,51	0
23	OEC	A	565	5/9	0.96	0.13	-0.75	62,63,65,66	0
31	BCT	d	5353	4/4	0.98	0.15	-1.06	75,75,76,77	0
19	FE2	a	5557	1/1	1.00	0.11	-2.30	75,75,75,75	0
19	FE2	A	557	1/1	0.95	0.05	-3.60	60,60,60,60	0
29	UNK	C	480	7/-	0.92	0.21	-	35,36,38,38	0
29	UNK	C	490	4/-	0.96	0.15	-	67,67,68,68	0
29	UNK	C	488	5/-	0.87	0.16	-	41,45,47,47	0
29	UNK	c	5475	12/-	0.75	0.34	-	74,78,84,84	0
29	UNK	C	479	11/-	0.85	0.26	-	58,64,67,67	0
29	UNK	c	5487	7/-	0.88	0.20	-	57,57,58,58	0
33	CA	k	5056	1/1	0.94	0.19	-	119,119,119,119	0
29	UNK	C	475	12/-	0.73	0.32	-	68,69,72,73	0
29	UNK	c	5488	5/-	0.92	0.21	-	59,59,59,60	0
29	UNK	C	483	13/-	0.89	0.22	-	61,68,78,78	0
29	UNK	c	5486	8/-	0.89	0.30	-	63,64,65,66	0
29	UNK	c	5480	7/-	0.89	0.27	-	65,66,66,67	0
29	UNK	C	486	8/-	0.80	0.36	-	55,56,59,60	0
29	UNK	c	5483	13/-	0.88	0.25	-	71,75,80,82	0
33	CA	K	56	1/1	0.96	0.09	-	119,119,119,119	0
29	UNK	C	478	11/-	0.85	0.23	-	58,65,66,66	0
29	UNK	C	487	7/-	0.86	0.23	-	49,52,52,53	0
29	UNK	c	5479	11/-	0.85	0.23	-	76,77,77,77	0
29	UNK	c	5478	11/-	0.70	0.39	-	76,79,81,81	0
29	UNK	c	5490	4/-	0.71	0.34	-	91,92,92,92	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.