



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

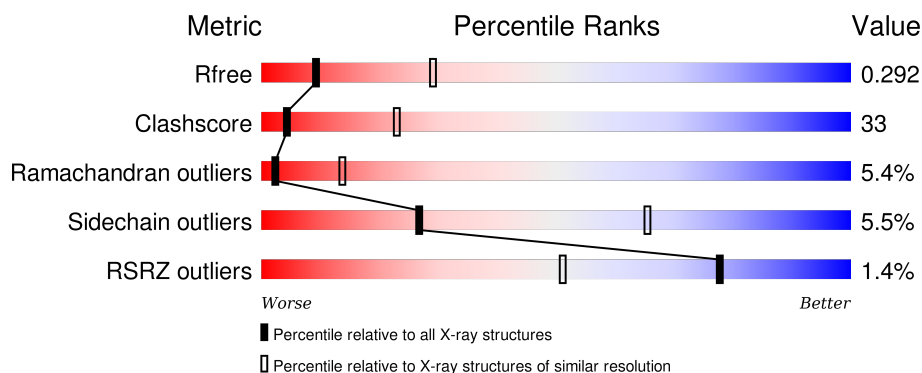
1 Overall quality at a glance

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.




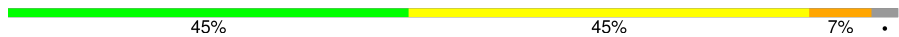


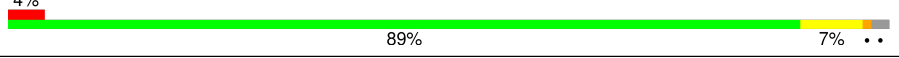
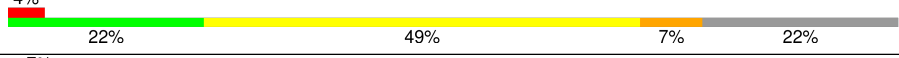

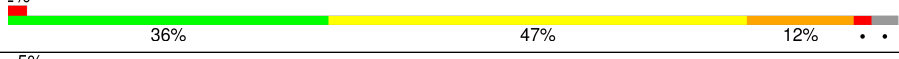
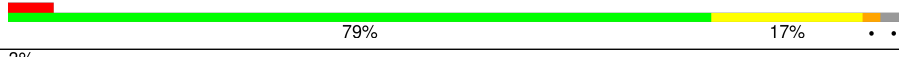
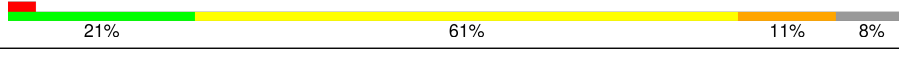
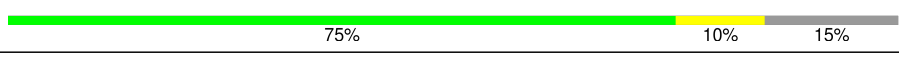


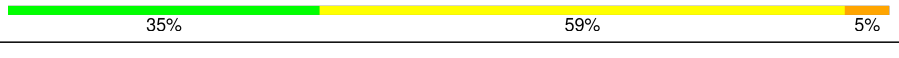




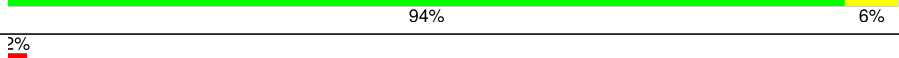

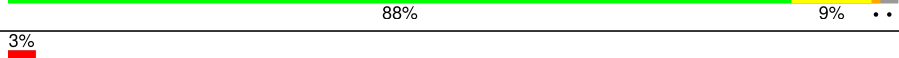


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>42%48%6% . .</div> </div>
1	a	344	<div> <div>%</div> <div>88%9% . .</div> </div>
2	B	510	<div> <div></div> <div>55%36%5% . .</div> </div>
2	b	510	<div> <div></div> <div>89%6% . .</div> </div>
3	C	473	<div> <div>%</div> <div>40%48%6% 5%</div> </div>

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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
22	UNK	C	481	-	-	-	X
22	UNK	C	482	-	-	-	X
22	UNK	C	489	-	-	-	X
22	UNK	c	5474	-	-	-	X
22	UNK	c	5477	-	-	-	X
22	UNK	c	5484	-	-	-	X
22	UNK	c	5485	-	-	-	X
22	UNK	c	5489	-	-	-	X
23	CLA	A	558	X	-	-	-
23	CLA	A	559	X	-	-	-
23	CLA	A	560	X	-	-	-
23	CLA	A	563	X	-	-	-
23	CLA	B	511	X	-	-	X
23	CLA	B	512	X	-	-	-
23	CLA	B	513	X	-	-	-
23	CLA	B	514	X	-	-	-
23	CLA	B	515	X	-	-	-
23	CLA	B	516	X	-	-	-
23	CLA	B	517	X	-	-	-
23	CLA	B	518	X	-	-	-
23	CLA	B	519	X	-	-	-
23	CLA	B	520	X	-	-	-
23	CLA	B	521	X	-	-	-
23	CLA	B	522	X	-	-	-
23	CLA	B	523	X	-	-	-
23	CLA	B	524	X	-	-	-
23	CLA	B	525	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	526	X	-	-	-
23	CLA	C	491	X	-	-	-
23	CLA	C	492	X	-	-	-
23	CLA	C	493	X	-	-	-
23	CLA	C	494	X	-	-	-
23	CLA	C	495	X	-	-	-
23	CLA	C	496	X	-	-	-
23	CLA	C	497	X	-	-	-
23	CLA	C	498	X	-	-	-
23	CLA	C	499	X	-	-	-
23	CLA	C	500	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	D	354	X	-	-	-
23	CLA	D	355	X	-	-	-
23	CLA	a	5558	X	-	-	-
23	CLA	a	5559	X	-	-	-
23	CLA	a	5560	X	-	-	X
23	CLA	a	5563	X	-	-	X
23	CLA	b	5511	X	-	-	X
23	CLA	b	5512	X	-	-	-
23	CLA	b	5513	X	-	-	-
23	CLA	b	5514	X	-	-	-
23	CLA	b	5515	X	-	-	-
23	CLA	b	5516	X	-	-	-
23	CLA	b	5517	X	-	-	-
23	CLA	b	5518	X	-	-	-
23	CLA	b	5519	X	-	-	-
23	CLA	b	5520	X	-	-	-
23	CLA	b	5521	X	-	-	-
23	CLA	b	5522	X	-	-	-
23	CLA	b	5523	X	-	-	-
23	CLA	b	5524	X	-	-	-
23	CLA	b	5525	X	-	-	-
23	CLA	b	5526	X	-	-	-
23	CLA	c	5491	X	-	-	-
23	CLA	c	5492	X	-	-	-
23	CLA	c	5493	X	-	-	-
23	CLA	c	5494	X	-	-	-
23	CLA	c	5495	X	-	-	-
23	CLA	c	5496	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	5497	X	-	-	-
23	CLA	c	5498	X	-	-	-
23	CLA	c	5499	X	-	-	-
23	CLA	c	5500	X	-	-	-
23	CLA	c	5501	X	-	-	-
23	CLA	c	5502	X	-	-	-
23	CLA	c	5503	X	-	-	X
23	CLA	d	5354	X	-	-	-
23	CLA	d	5355	X	-	-	-
26	PQ9	A	564	-	-	-	X
26	PQ9	a	5564	-	-	-	X
28	BCR	B	528	-	-	-	X
28	BCR	C	504	-	-	-	X
28	BCR	C	505	-	-	-	X
28	BCR	D	357	-	-	-	X
28	BCR	H	107	-	-	-	X
28	BCR	X	130	-	-	-	X
28	BCR	b	5529	-	-	-	X
28	BCR	c	5504	-	-	-	X
28	BCR	d	5357	-	-	-	X
28	BCR	h	5107	-	-	-	X
28	BCR	x	5130	-	-	-	X
29	MGE	d	5359	-	-	-	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	-	-	-
33	LMT	A	569	-	-	-	X
33	LMT	M	5216	-	-	-	X
33	LMT	T	217	-	-	-	X
33	LMT	a	5568	-	-	-	X
33	LMT	t	5217	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 atoms, of which 0 are 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	110	3	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	110	3	131	1			

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

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

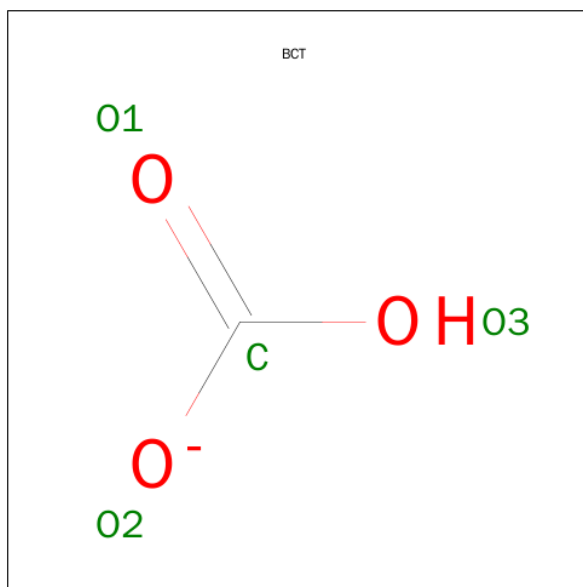
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).

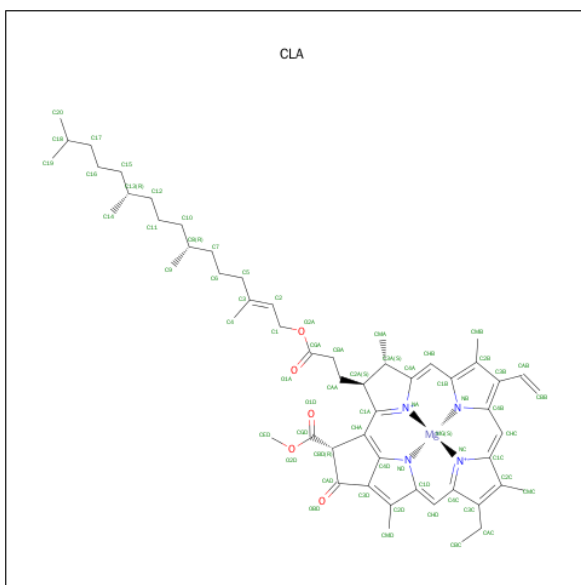


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

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

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

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

[illegible]

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

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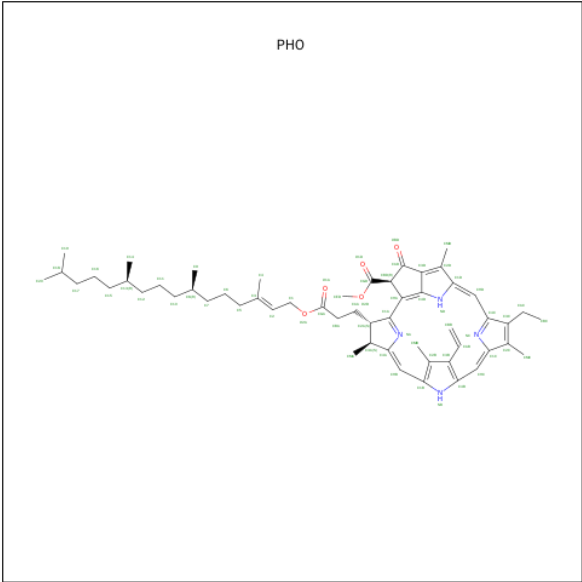
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
23	d	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
23	b	1	Total 41	C 33	Mg 1	N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

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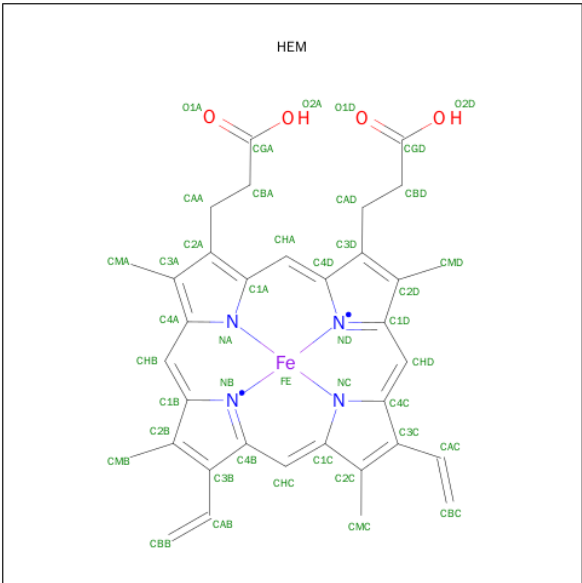
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



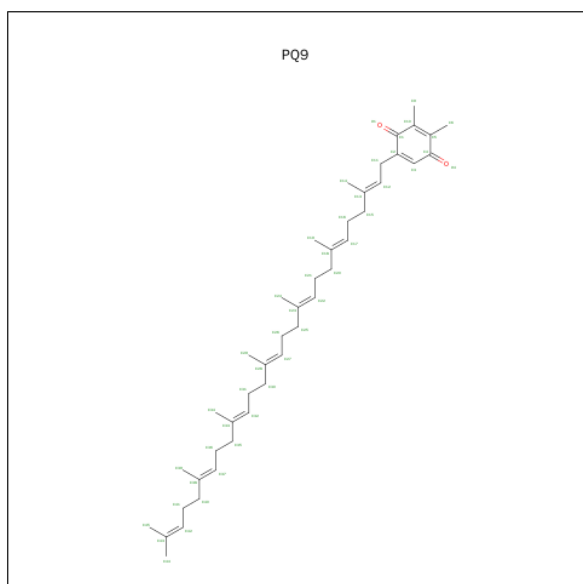
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



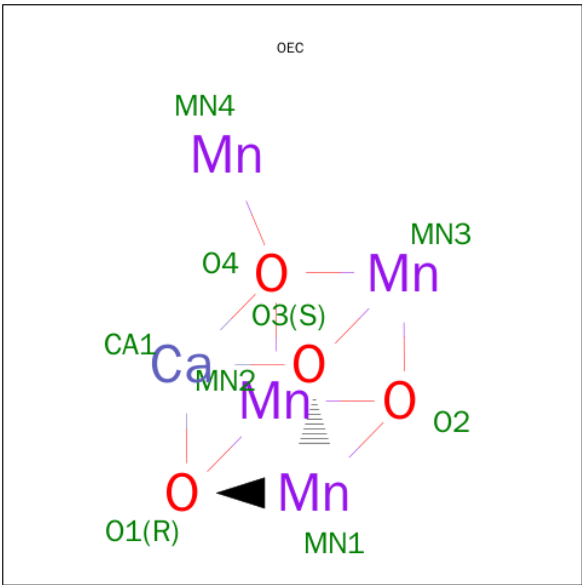
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
25	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 26 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).



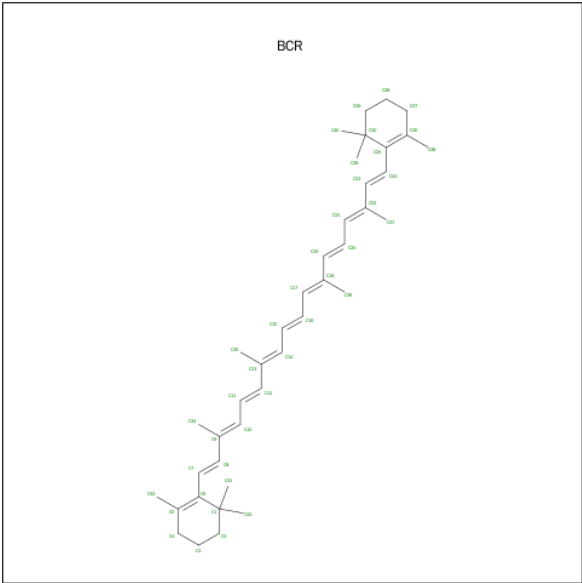
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O		
			30	28	2		
26	A	1	Total	C	O		
			30	28	2		
26	d	1	Total	C	O		
			30	28	2		
26	a	1	Total	C	O		
			30	28	2		

- Molecule 27 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



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

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



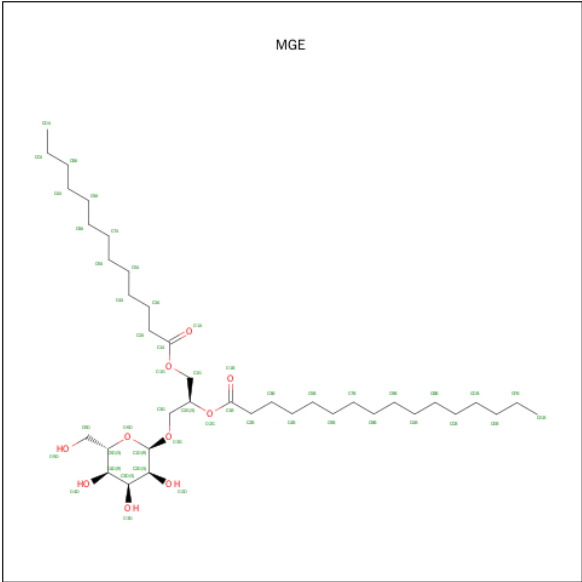
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		

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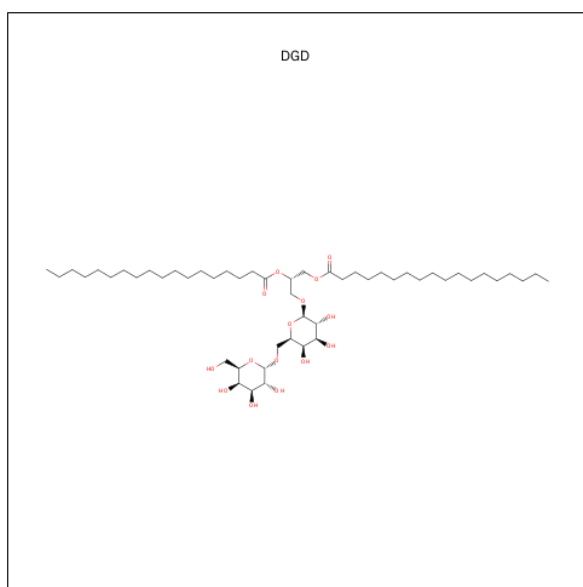
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	t	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	H	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	X	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	a	1	Total C 40 40	0	0
28	b	1	Total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

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



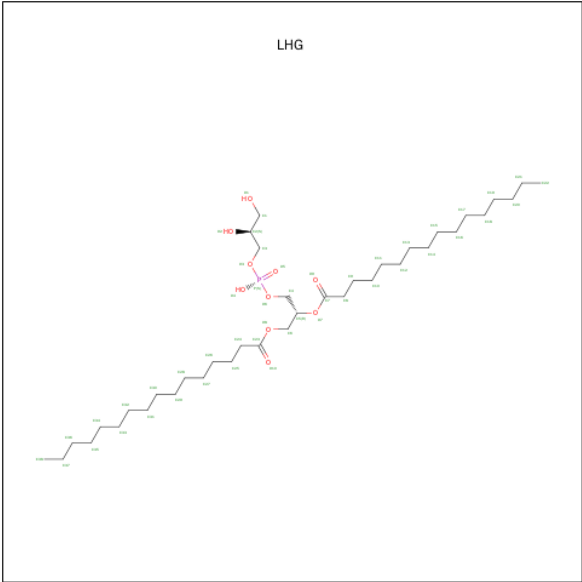
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	I	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			47	37	10		
29	D	1	Total	C	O	0	0
			41	31	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			48	38	10		
29	i	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total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

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



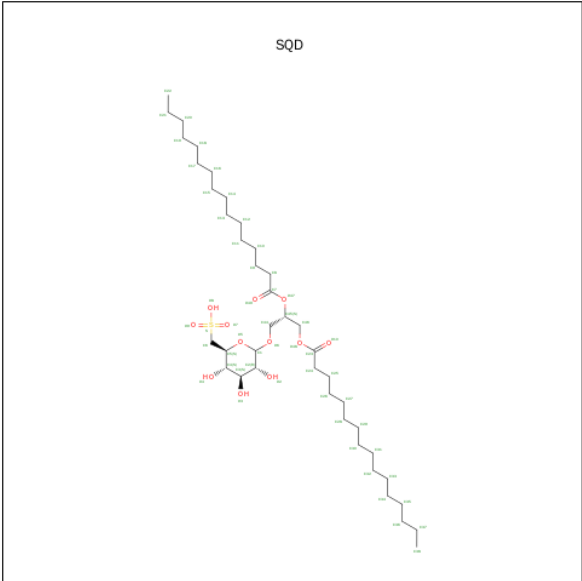
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total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

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



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

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



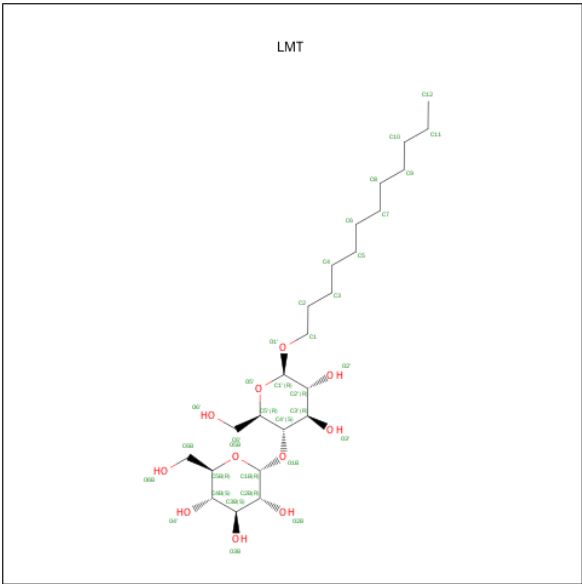
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			54	41	12	1		

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

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

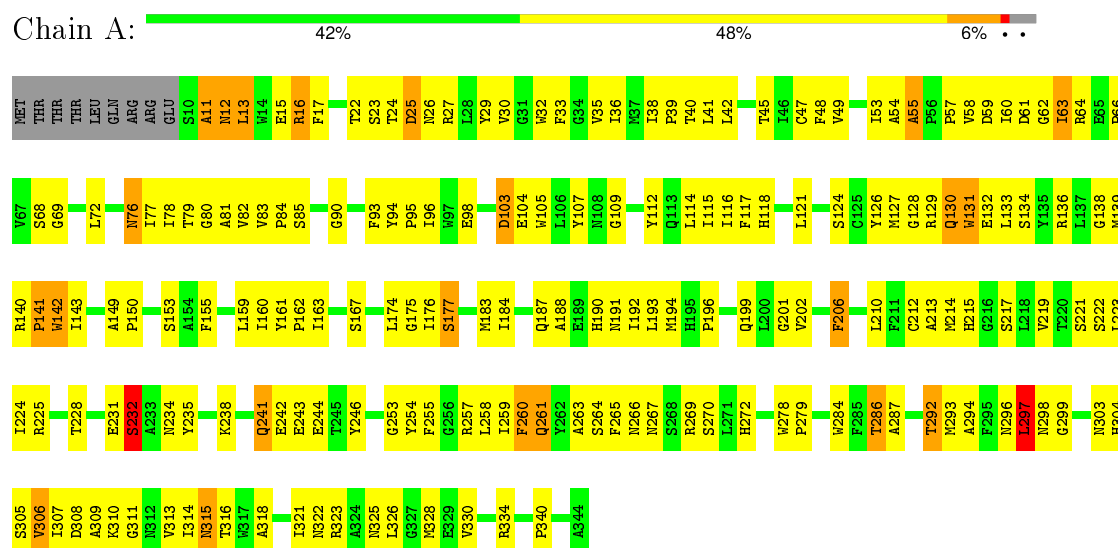


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O		0	0
			35	24	11			
33	m	1	Total	C	O		0	0
			35	24	11			
33	T	1	Total	C	O		0	0
			35	24	11			
33	a	1	Total	C	O		0	0
			35	24	11			
33	M	1	Total	C	O		0	0
			35	24	11			
33	t	1	Total	C	O		0	0
			35	24	11			

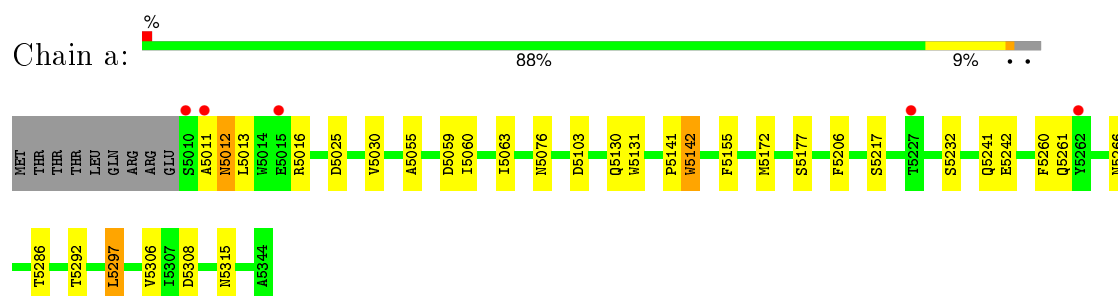
3 Residue-property plots

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

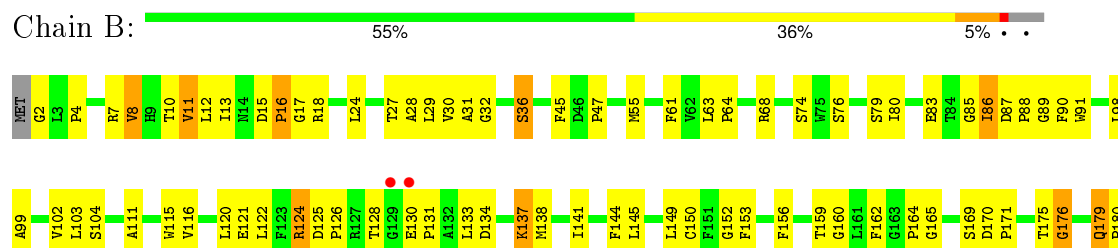
• Molecule 1: Photosystem Q(B) protein

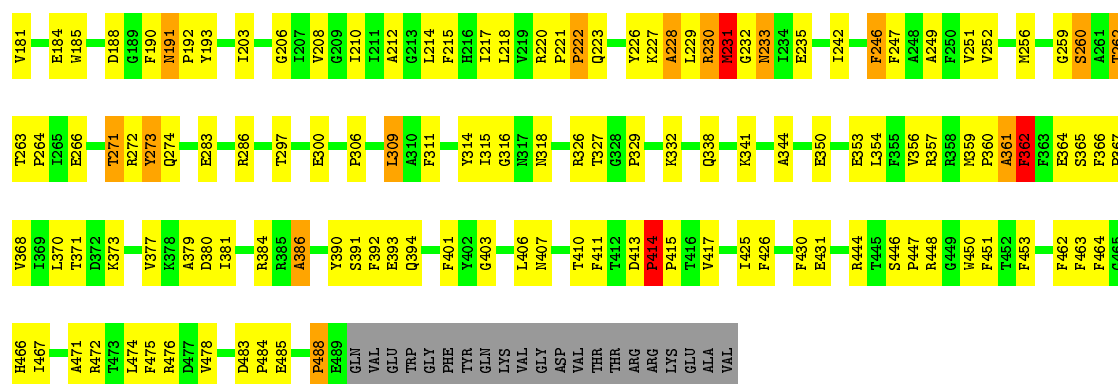


• Molecule 1: Photosystem Q(B) protein

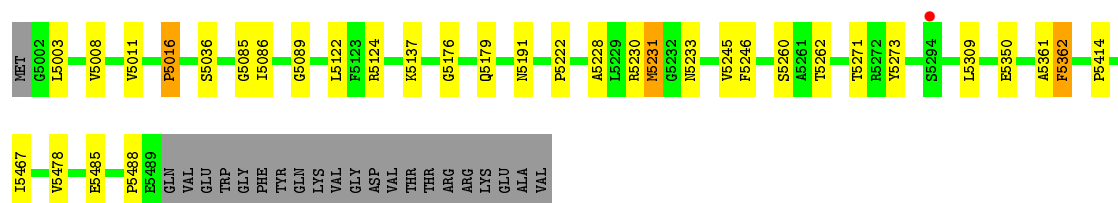


• Molecule 2: CP47 protein

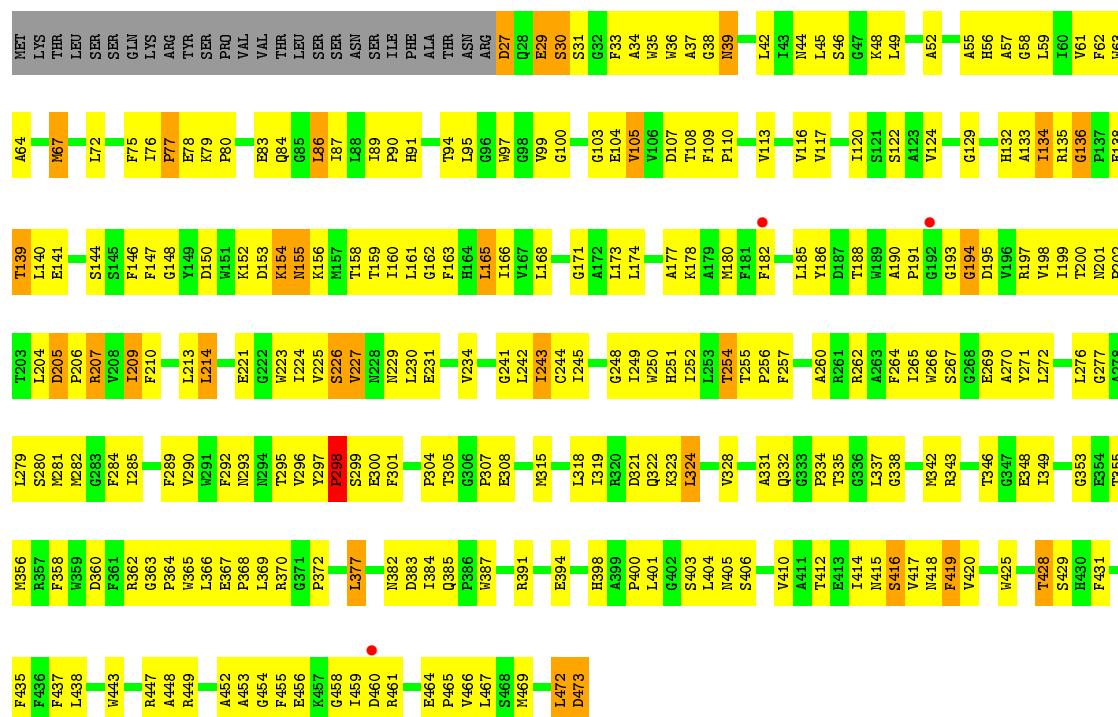




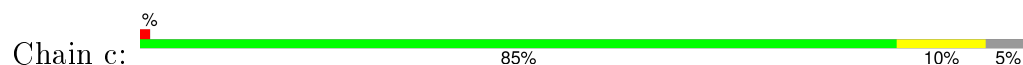
- Molecule 2: CP47 protein

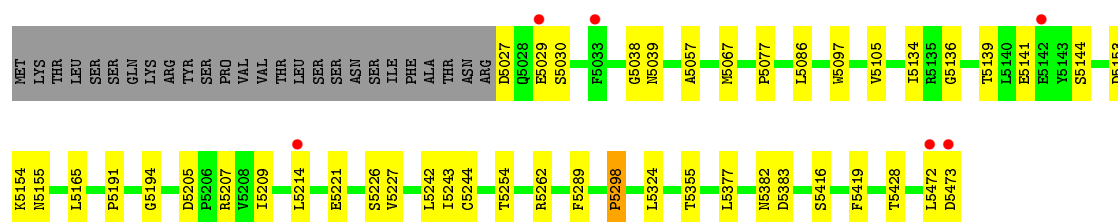


- Molecule 3: photosystem II CP43 protein



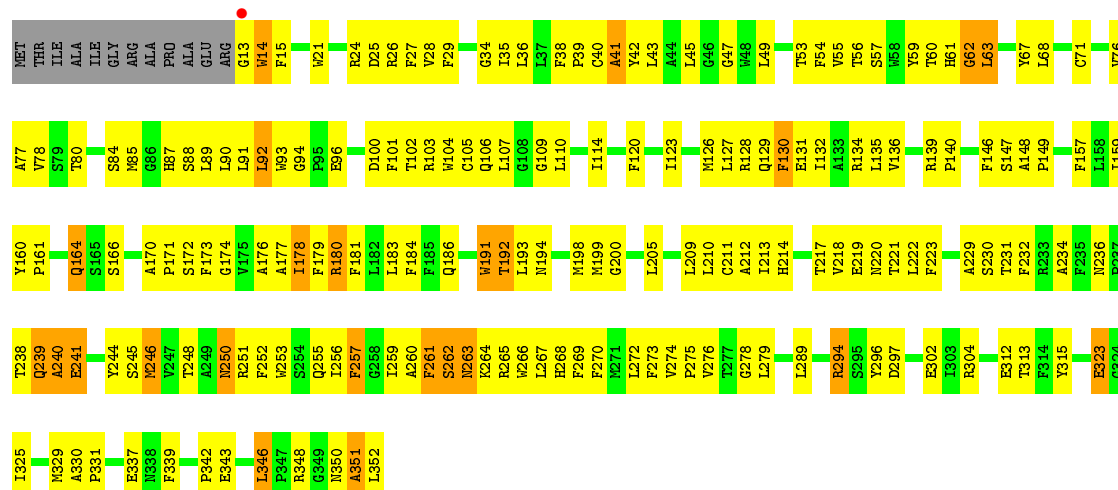
- Molecule 3: photosystem II CP43 protein





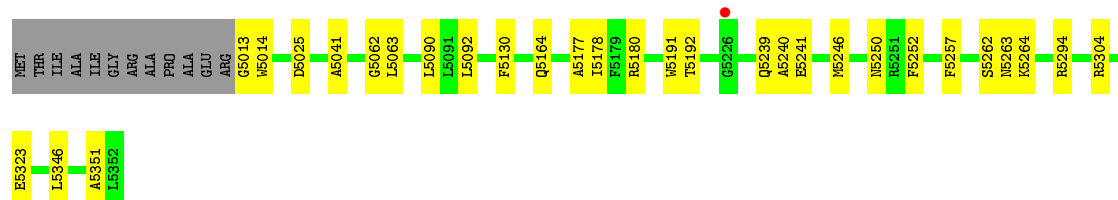
• Molecule 4: photosystem II reaction center D2 protein

Chain D: 45% 45% 7% .



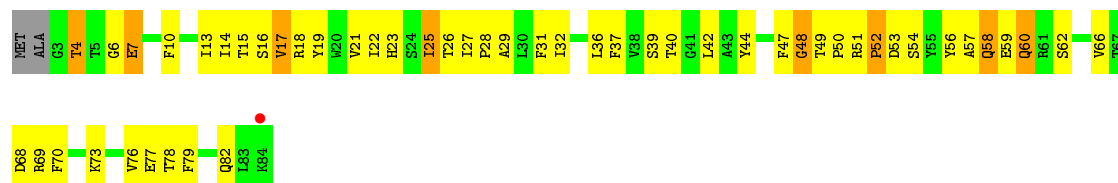
• Molecule 4: photosystem II reaction center D2 protein

Chain d: 88% 9% 9% .



• Molecule 5: Cytochrome b559 alpha subunit

Chain E: 37% 51% 10% .



• Molecule 5: Cytochrome b559 alpha subunit

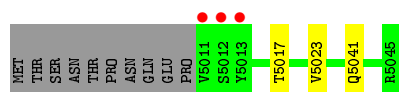
Chain e: 4% 89% 7% .



- Molecule 6: Cytochrome b559 beta subunit



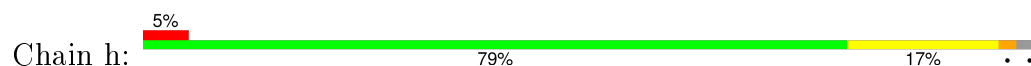
- Molecule 6: Cytochrome b559 beta subunit



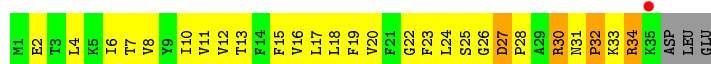
- Molecule 7: Photosystem II reaction center H protein



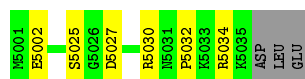
- Molecule 7: Photosystem II reaction center H protein



- Molecule 8: Photosystem II reaction center I protein



- Molecule 8: Photosystem II reaction center I protein



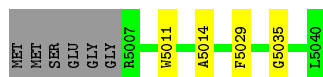
- Molecule 9: Photosystem II reaction center J protein





- 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%



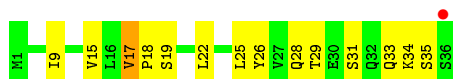
- Molecule 11: Photosystem II reaction center L protein

Chain l: 8% 84% 16%



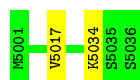
- Molecule 12: Photosystem II reaction center M protein

Chain M: 3% 61% 36%

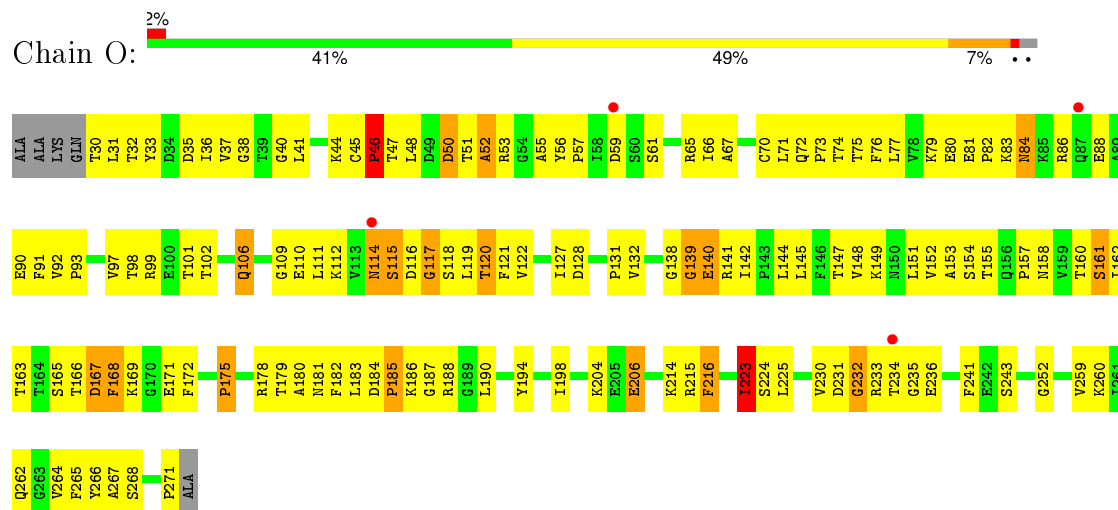


- Molecule 12: Photosystem II reaction center M protein

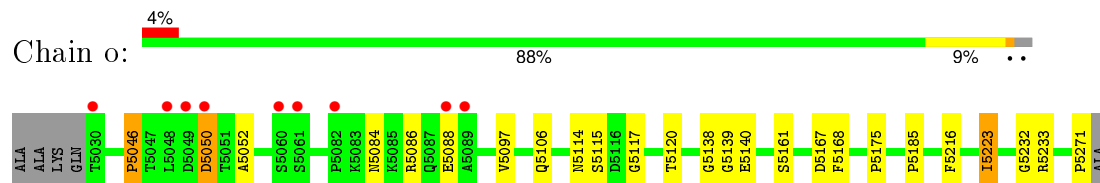
Chain m: 94% 6%



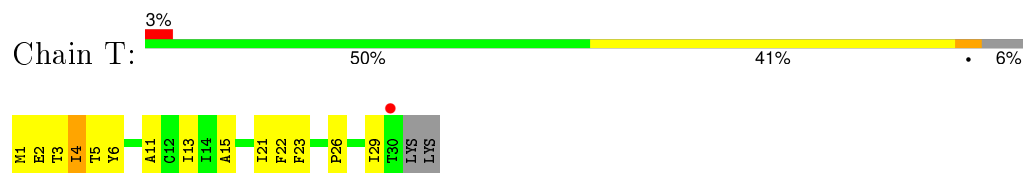
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



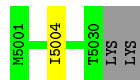
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



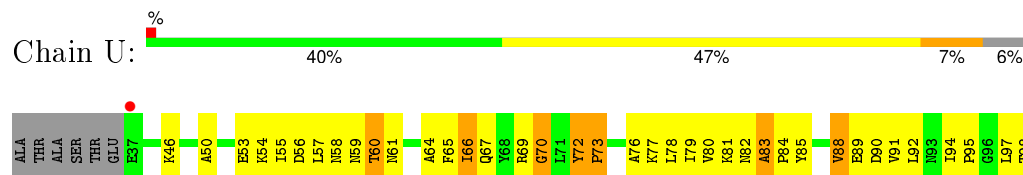
- Molecule 14: Photosystem II reaction center T protein

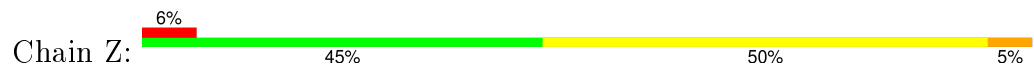


- Molecule 14: Photosystem II reaction center T protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein







● Molecule 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, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.242 , 0.292	Depositor DCC
R_{free} test set	1860 reflections (1.35%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 155340 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	63	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	k	1	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	D	4	0	0	0	0
21	d	4	0	0	0	0
22	C	152	0	17	2	0
22	c	152	0	17	0	0
23	A	250	0	265	15	0
23	B	1007	0	1088	74	0
23	C	774	0	783	51	0
23	D	115	0	111	8	0
23	a	250	0	265	0	0
23	b	1007	0	1088	0	0
23	c	774	0	783	0	0
23	d	115	0	111	0	0
24	A	128	0	148	12	0
24	a	128	0	148	0	0
25	F	43	0	30	3	0
25	V	43	0	30	2	0
25	f	43	0	30	0	0
25	v	43	0	30	0	0
26	A	30	0	37	2	0
26	D	30	0	37	7	0
26	a	30	0	37	0	0
26	d	30	0	37	0	0
27	A	5	0	0	0	0
27	a	5	0	0	0	0
28	A	40	0	56	1	0
28	B	120	0	168	6	0
28	C	120	0	168	20	0
28	D	40	0	56	4	0
28	H	40	0	56	3	0
28	T	40	0	56	5	0
28	X	40	0	56	9	0
28	a	40	0	56	0	0
28	b	120	0	168	0	0
28	c	120	0	168	0	0
28	d	40	0	56	0	0
28	h	40	0	56	0	0
28	t	40	0	56	0	0
28	x	40	0	56	0	0
29	B	48	0	72	1	0

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

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 (1544) 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:126:UNK:NE	17:X:126:UNK:CD	1.46	1.53
17:X:126:UNK:CZ	17:X:126:UNK:NE	1.33	1.43
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:NE2	17:X:26:UNK:CD	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07
3:C:473:ASP:HB3	14:T:26:PRO:HB3	1.33	1.05
1:A:322:ASN:HD21	3:C:412:THR:HA	1.24	1.01

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.04	0.86
2:B:327:THR:HG22	23:B:517:CLA:H12	1.58	0.86
13:O:145:LEU:HD23	13:O:175:PRO:HG2	1.57	0.86
16:V:159:GLY:O	16:V:161:VAL:N	2.08	0.86
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.05	0.86
13:O:145:LEU:CD2	13:O:175:PRO:HG2	2.06	0.86
17:X:26:UNK:NE2	17:X:26:UNK:CG	2.44	0.86
10:K:45:PHE:O	10:K:46:ARG:OXT	1.95	0.85
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.42	0.85
16:V:38:LEU:HD13	16:V:45:ILE:HD11	1.57	0.84
1:A:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
1:A:306:VAL:O	1:A:306:VAL:HG23	1.77	0.84
14:T:29:ILE:HD12	14:T:29:ILE:H	1.43	0.84
23:C:493:CLA:HBA1	23:C:493:CLA:HBD	1.59	0.83
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.60	0.83
18:Z:5:PHE:HA	18:Z:57:LEU:HD13	1.59	0.83
7:H:38:PHE:HB2	28:H:107:BCR:H10C	1.61	0.83
1:A:279:PRO:HB2	24:A:561:PHO:HBC1	1.58	0.83
3:C:209:ILE:HG23	28:C:506:BCR:H382	1.61	0.83
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.58	0.83
8:I:34:ARG:HE	8:I:34:ARG:N	1.76	0.83
23:B:518:CLA:H42	4:D:127:LEU:HD11	1.60	0.83
2:B:263:THR:HG22	2:B:448:ARG:HH22	1.44	0.83
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.60	0.82
3:C:293:ASN:ND2	3:C:296:VAL:HG22	1.94	0.82
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.62	0.82
17:X:126:UNK:NE	17:X:126:UNK:CG	2.47	0.82
13:O:151:LEU:HD13	13:O:223:ILE:HD11	1.59	0.82
13:O:45:CYS:H	13:O:72:GLN:NE2	1.77	0.82
3:C:406:SER:O	3:C:418:ASN:HB2	1.78	0.81
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
4:D:192:THR:HG23	23:D:354:CLA:HBC2	1.60	0.81
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.62	0.81
5:E:18:ARG:HG2	5:E:22:ILE:HD11	1.62	0.81
28:C:504:BCR:H353	28:X:130:BCR:H321	1.62	0.81
3:C:116:VAL:HG11	28:C:505:BCR:H323	1.62	0.80
6:F:21:VAL:O	6:F:25:THR:HG23	1.80	0.80
4:D:351:ALA:O	4:D:352:LEU:OXT	1.99	0.80
3:C:464:GLU:HB2	3:C:467:LEU:HD12	1.61	0.80
23:C:491:CLA:HMB3	28:C:506:BCR:H403	1.62	0.80

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:298:PRO:O	3:C:299:SER:HB3	1.85	0.75
3:C:276:LEU:HD21	23:C:498:CLA:HBB1	1.69	0.75
6:F:34:LEU:HD22	9:J:24:ILE:HD13	1.69	0.75
4:D:266:TRP:CD1	29:D:360:MGE:H3D	2.22	0.75
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.69	0.75
4:D:337:GLU:HG2	4:D:339:PHE:CZ	2.22	0.75
1:A:202:VAL:O	1:A:206:PHE:HB2	1.87	0.74
13:O:52:ALA:HB1	13:O:230:VAL:H	1.52	0.74
3:C:103:GLY:HA3	3:C:301:PHE:HE1	1.51	0.74
3:C:419:PHE:HA	30:C:508:DGD:HE5	1.70	0.74
2:B:150:CYS:HB2	23:B:513:CLA:HMC3	1.69	0.74
23:A:558:CLA:HBB1	23:D:354:CLA:NB	2.02	0.74
3:C:204:LEU:O	3:C:205:ASP:HB3	1.85	0.74
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	0.73
3:C:449:ARG:HH22	8:I:27:ASP:HB3	1.51	0.73
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.70	0.73
15:U:50:ALA:HB3	15:U:113:THR:HG21	1.70	0.73
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.53	0.73
1:A:309:ALA:HB3	16:V:28:GLU:HG3	1.68	0.73
2:B:27:THR:O	23:B:515:CLA:HBC1	1.89	0.73
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.19	0.72
13:O:144:LEU:HD23	13:O:144:LEU:H	1.54	0.72
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.71	0.72
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.71	0.72
3:C:204:LEU:CD2	3:C:204:LEU:H	2.02	0.72
24:A:562:PHO:HBC1	4:D:275:PRO:HB2	1.71	0.72
5:E:17:VAL:O	5:E:21:VAL:HG23	1.89	0.72
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	0.72
23:B:518:CLA:HMD1	23:B:520:CLA:HAB	1.70	0.72
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.54	0.72
3:C:337:LEU:HD23	13:O:131:PRO:HG3	1.71	0.72
3:C:464:GLU:CB	3:C:467:LEU:HD12	2.20	0.72
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.20	0.72
3:C:29:GLU:HB3	10:K:46:ARG:O	1.89	0.72
28:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	0.72
3:C:334:PRO:HA	13:O:179:THR:HB	1.72	0.71
3:C:293:ASN:ND2	3:C:296:VAL:H	1.87	0.71
15:U:66:ILE:HG12	15:U:72:TYR:CG	2.25	0.71
2:B:271:THR:HG23	2:B:273:TYR:H	1.56	0.71
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG22	2:B:484:PRO:HG3	1.71	0.71
10:K:17:ILE:HD11	18:Z:6:GLN:HE21	1.56	0.71
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.26	0.71
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.55	0.71
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.25	0.71
4:D:36:LEU:O	4:D:39:PRO:HD2	1.89	0.70
2:B:263:THR:CG2	2:B:448:ARG:HH12	2.02	0.70
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.19	0.70
1:A:306:VAL:HG21	1:A:316:THR:HG23	1.74	0.70
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.26	0.70
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.56	0.69
12:M:25:LEU:O	12:M:28:GLN:HG3	1.92	0.69
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.07	0.69
24:A:562:PHO:H42	4:D:41:ALA:HB1	1.74	0.69
2:B:271:THR:CG2	2:B:273:TYR:H	2.04	0.69
2:B:371:THR:HG22	2:B:377:VAL:HA	1.73	0.69
3:C:42:LEU:HD13	23:C:501:CLA:HMA3	1.74	0.69
10:K:17:ILE:CD1	18:Z:6:GLN:HE21	2.05	0.69
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.74	0.69
18:Z:21:ILE:O	18:Z:25:VAL:HG23	1.91	0.69
3:C:241:GLY:C	3:C:243:ILE:H	1.96	0.69
13:O:73:PRO:CG	13:O:102:THR:HB	2.22	0.69
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.75	0.69
23:C:495:CLA:HBD	23:C:495:CLA:HBA1	1.75	0.69
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
7:H:11:LEU:C	7:H:13:PRO:HD2	2.14	0.69
11:L:14:ARG:HG2	12:M:26:TYR:HE1	1.58	0.69
3:C:214:LEU:H	3:C:214:LEU:HD23	1.58	0.69
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.68
18:Z:15:LEU:HD23	18:Z:50:LEU:HD12	1.75	0.68
23:A:559:CLA:HED2	4:D:198:MET:SD	2.33	0.68
2:B:126:PRO:HG3	7:H:12:ARG:NH2	2.09	0.68
3:C:84:GLN:HB2	3:C:86:LEU:HD22	1.75	0.68
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	0.68
1:A:22:THR:HG23	1:A:136:ARG:HH11	1.59	0.68
3:C:363:GLY:O	3:C:367:GLU:HG2	1.93	0.68
5:E:58:GLN:HE22	16:V:28:GLU:HA	1.58	0.68
2:B:344:ALA:HB2	2:B:401:PHE:CE1	2.29	0.68
4:D:84:SER:HB2	5:E:68:ASP:HA	1.74	0.68
28:C:505:BCR:H312	18:Z:55:GLY:HA2	1.75	0.68
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:SER:HA	4:D:232:PHE:CE2	2.29	0.68
13:O:36:ILE:HG23	13:O:41:LEU:HB2	1.76	0.68
1:A:47:CYS:SG	1:A:114:LEU:HD23	2.34	0.67
5:E:4:THR:HG23	17:X:90:UNK:CD2	2.24	0.67
2:B:231:MET:HG3	23:B:520:CLA:HAC2	1.75	0.67
23:B:515:CLA:HMB3	23:B:516:CLA:H11	1.76	0.67
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	0.67
2:B:222:PRO:HG3	7:H:27:THR:H	1.60	0.67
3:C:124:VAL:HB	28:C:505:BCR:H362	1.77	0.67
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.24	0.67
4:D:261:PHE:O	4:D:262:SER:HB3	1.94	0.67
2:B:191:ASN:HD22	2:B:192:PRO:CD	2.07	0.67
4:D:89:LEU:HG	7:H:50:ASN:OD1	1.95	0.67
13:O:234:THR:OG1	13:O:236:GLU:HG2	1.95	0.67
13:O:163:THR:H	13:O:166:THR:HG23	1.60	0.67
3:C:150:ASP:O	3:C:153:ASP:HB3	1.96	0.67
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.75	0.67
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	0.67
17:X:54:UNK:HB1	17:X:57:UNK:CG2	2.25	0.67
5:E:40:THR:HG21	17:X:102:UNK:CB	2.25	0.67
3:C:153:ASP:O	3:C:155:ASN:N	2.28	0.66
3:C:210:PHE:O	3:C:213:LEU:HB2	1.95	0.66
2:B:353:GLU:HB3	2:B:373:LYS:NZ	2.10	0.66
1:A:60:ILE:HG23	1:A:61:ASP:N	2.09	0.66
10:K:35:LEU:HD22	17:X:17:UNK:CB	2.26	0.66
13:O:32:THR:H	13:O:35:ASP:HB2	1.61	0.66
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.78	0.66
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.78	0.66
14:T:4:ILE:HD13	14:T:4:ILE:C	2.16	0.66
3:C:56:HIS:C	3:C:58:GLY:H	1.99	0.66
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.11	0.66
2:B:463:PHE:HZ	23:B:518:CLA:HBB1	1.61	0.65
28:X:130:BCR:H331	28:X:130:BCR:HC8	1.78	0.65
4:D:267:LEU:HD23	4:D:267:LEU:C	2.17	0.65
2:B:297:THR:CB	2:B:300:GLU:HG3	2.26	0.65
13:O:77:LEU:N	13:O:77:LEU:HD12	2.10	0.65
5:E:10:PHE:O	5:E:13:ILE:HG22	1.95	0.65
10:K:23:ASP:OD2	17:X:6:UNK:NE2	2.34	0.65
5:E:22:ILE:HG23	17:X:116:UNK:HA	1.78	0.65
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.25	0.65
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:SER:HA	4:D:232:PHE:HE2	1.61	0.65
10:K:28:ILE:O	10:K:31:LEU:HB2	1.97	0.65
3:C:466:VAL:HA	3:C:469:MET:HE3	1.79	0.65
1:A:76:ASN:ND2	1:A:79:THR:H	1.95	0.65
17:X:51:UNK:O	17:X:52:UNK:C	2.44	0.65
2:B:176:GLY:HA3	2:B:266:GLU:OE1	1.96	0.65
23:A:558:CLA:H143	24:A:561:PHO:H62	1.78	0.65
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.62	0.65
2:B:392:PHE:O	2:B:393:GLU:HB2	1.96	0.65
5:E:78:THR:O	5:E:82:GLN:HG2	1.97	0.65
1:A:94:TYR:OH	1:A:104:GLU:HG2	1.97	0.65
23:C:501:CLA:H151	18:Z:20:VAL:HG13	1.78	0.64
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.80	0.64
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.80	0.64
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.33	0.64
3:C:265:ILE:HD13	23:C:495:CLA:HED1	1.78	0.64
3:C:449:ARG:NH2	8:I:27:ASP:HB3	2.12	0.64
1:A:305:SER:O	1:A:306:VAL:C	2.35	0.64
2:B:223:GLN:HE22	2:B:227:LYS:HD3	1.62	0.64
3:C:279:LEU:HA	3:C:282:MET:HE3	1.80	0.64
4:D:210:LEU:HD21	26:D:356:PQ9:H17	1.80	0.64
6:F:37:ILE:HG22	9:J:28:PHE:CE1	2.33	0.64
23:C:495:CLA:CMD	23:C:497:CLA:HAB	2.27	0.64
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.33	0.64
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.80	0.64
2:B:223:GLN:HE22	2:B:227:LYS:CD	2.10	0.64
1:A:134:SER:HB2	1:A:139:MET:HG3	1.79	0.63
16:V:95:ILE:O	16:V:99:VAL:HG23	1.97	0.63
1:A:187:GLN:HG3	1:A:325:ASN:OD1	1.98	0.63
28:C:504:BCR:H311	28:C:504:BCR:H343	1.81	0.63
28:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
7:H:12:ARG:N	7:H:13:PRO:HD2	2.13	0.63
13:O:184:ASP:HB2	13:O:185:PRO:HD2	1.80	0.63
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	0.63
23:B:519:CLA:HMC2	28:H:107:BCR:H343	1.81	0.63
16:V:49:GLU:O	16:V:53:LEU:HG	1.98	0.63
2:B:120:LEU:HD13	23:B:526:CLA:HMD2	1.79	0.63
4:D:229:ALA:O	4:D:231:THR:HG23	1.97	0.63
1:A:243:GLU:HA	4:D:241:GLU:HA	1.80	0.63
4:D:36:LEU:C	4:D:39:PRO:HD2	2.19	0.63
3:C:248:GLY:O	3:C:252:ILE:HG13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	0.63
3:C:343:ARG:HB2	13:O:101:THR:HG23	1.80	0.63
16:V:38:LEU:HD13	16:V:45:ILE:CD1	2.29	0.63
4:D:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63
7:H:43:LEU:HD23	17:X:60:UNK:CZ	2.29	0.63
2:B:208:VAL:HG21	23:B:512:CLA:HMC1	1.81	0.63
3:C:52:ALA:HA	23:C:501:CLA:HMB3	1.80	0.63
3:C:417:VAL:O	3:C:417:VAL:HG22	1.99	0.63
1:A:16:ARG:HD3	1:A:17:PHE:N	2.14	0.63
13:O:45:CYS:HB2	13:O:46:PRO:CD	2.27	0.63
15:U:82:ASN:HB2	15:U:85:TYR:OH	1.99	0.63
7:H:6:TRP:O	7:H:10:ILE:HG13	1.99	0.63
3:C:158:THR:HG22	3:C:251:HIS:O	1.99	0.63
5:E:23:HIS:C	5:E:25:ILE:H	2.02	0.62
15:U:89:GLU:CD	15:U:89:GLU:H	2.02	0.62
2:B:246:PHE:C	2:B:246:PHE:CD1	2.72	0.62
5:E:57:ALA:O	5:E:59:GLU:N	2.32	0.62
16:V:135:GLU:O	16:V:139:VAL:HG23	1.98	0.62
13:O:110:GLU:O	13:O:110:GLU:HG3	1.99	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.81	0.62
1:A:40:THR:HG21	1:A:121:LEU:HB3	1.81	0.62
13:O:45:CYS:H	13:O:72:GLN:HE22	1.48	0.62
23:C:501:CLA:H171	18:Z:20:VAL:HA	1.79	0.62
1:A:72:LEU:HD23	14:T:3:THR:HG21	1.82	0.62
13:O:183:LEU:HD22	13:O:187:GLY:O	1.99	0.62
2:B:2:GLY:HA3	11:L:11:GLU:OE1	2.00	0.62
4:D:103:ARG:NH1	5:E:77:GLU:HG3	2.15	0.62
13:O:46:PRO:HB2	13:O:266:TYR:CG	2.35	0.62
3:C:55:ALA:HB1	28:C:504:BCR:H373	1.82	0.62
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.30	0.62
4:D:90:LEU:HD23	4:D:109:GLY:HA2	1.81	0.62
1:A:253:GLY:O	1:A:257:ARG:HD2	2.00	0.61
2:B:357:ARG:NH2	4:D:337:GLU:HG3	2.14	0.61
17:X:28:UNK:CG2	18:Z:29:SER:HA	2.30	0.61
1:A:49:VAL:O	1:A:53:ILE:HG13	2.00	0.61
6:F:41:GLN:HE21	6:F:41:GLN:HA	1.64	0.61
17:X:26:UNK:HG2	17:X:26:UNK:NE2	2.20	0.61
2:B:329:PRO:CB	23:B:517:CLA:HED1	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:TRP:NE1	3:C:36:TRP:HD1	1.99	0.61
1:A:25:ASP:HB3	4:D:251:ARG:HH22	1.65	0.61
6:F:41:GLN:NE2	6:F:41:GLN:HA	2.15	0.61
3:C:90:PRO:O	3:C:94:THR:HG23	2.01	0.61
6:F:31:ILE:HG13	25:F:51:HEM:HMC2	1.82	0.61
16:V:39:ASN:HD21	16:V:41:GLU:HB2	1.64	0.61
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.01	0.61
7:H:21:VAL:HG22	7:H:22:ALA:O	2.01	0.61
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
3:C:298:PRO:O	3:C:299:SER:CB	2.48	0.61
5:E:10:PHE:HA	5:E:13:ILE:HG22	1.83	0.61
2:B:247:PHE:O	2:B:251:VAL:HG23	2.00	0.61
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.82	0.61
2:B:31:ALA:HB2	23:B:515:CLA:HBC3	1.83	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	0.61
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
22:C:474:UNK:C15	26:D:356:PQ9:H293	2.31	0.61
1:A:64:ARG:C	1:A:66:PRO:HD3	2.21	0.61
2:B:185:TRP:HH2	2:B:203:ILE:HG21	1.66	0.61
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.31	0.60
13:O:128:ASP:OD2	13:O:149:LYS:HG2	2.01	0.60
2:B:271:THR:HG22	2:B:274:GLN:H	1.64	0.60
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.16	0.60
5:E:56:TYR:HB3	5:E:60:GLN:HG3	1.83	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	0.60
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.83	0.60
15:U:66:ILE:HG22	15:U:66:ILE:O	2.01	0.60
5:E:36:LEU:HA	5:E:39:SER:HB3	1.82	0.60
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.15	0.60
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.16	0.60
2:B:137:LYS:O	2:B:141:ILE:HG13	2.02	0.60
14:T:21:ILE:HD12	28:T:5104:BCR:H332	1.83	0.60
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	0.60
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
9:J:8:ILE:H	9:J:8:ILE:HD12	1.66	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	0.60
7:H:49:TYR:CD2	30:H:208:DGD:HB22	2.37	0.60
2:B:10:THR:O	2:B:13:ILE:HG13	2.02	0.60
1:A:315:ASN:O	4:D:63:LEU:HB3	2.02	0.60
15:U:117:VAL:HG13	15:U:122:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:LEU:O	2:B:231:MET:N	2.35	0.60
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
3:C:230:LEU:O	3:C:234:VAL:HG23	2.01	0.59
4:D:337:GLU:HG2	4:D:339:PHE:CE2	2.36	0.59
5:E:60:GLN:HG3	5:E:60:GLN:O	2.01	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59
13:O:55:ALA:O	13:O:57:PRO:HD3	2.02	0.59
13:O:179:THR:CG2	13:O:180:ALA:N	2.65	0.59
3:C:458:GLY:HA2	4:D:222:LEU:O	2.02	0.59
3:C:428:THR:HG22	3:C:429:SER:N	2.17	0.59
13:O:112:LYS:HE2	13:O:114:ASN:HB3	1.84	0.59
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.32	0.59
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.84	0.59
16:V:147:VAL:O	16:V:150:LYS:HB2	2.02	0.59
4:D:60:THR:HG23	4:D:61:HIS:N	2.18	0.59
18:Z:14:ILE:O	18:Z:18:VAL:HG23	2.02	0.59
1:A:326:LEU:CD2	3:C:412:THR:HB	2.33	0.59
18:Z:16:SER:O	18:Z:20:VAL:HG23	2.03	0.59
7:H:62:TRP:CD1	30:H:208:DGD:HE5	2.37	0.59
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.84	0.59
13:O:230:VAL:HG12	13:O:231:ASP:N	2.17	0.59
2:B:384:ARG:NH1	15:U:132:LEU:HD22	2.18	0.59
7:H:29:PRO:O	7:H:33:VAL:HG23	2.02	0.59
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.38	0.59
4:D:279:LEU:HD22	23:D:354:CLA:HBA2	1.85	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
1:A:307:ILE:HD11	1:A:311:GLY:O	2.00	0.58
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.84	0.58
4:D:39:PRO:O	4:D:43:LEU:HB2	2.03	0.58
13:O:204:LYS:HB3	13:O:206:GLU:HG2	1.85	0.58
3:C:265:ILE:HG22	3:C:270:ALA:CB	2.33	0.58
3:C:465:PRO:C	3:C:469:MET:HE2	2.23	0.58
3:C:315:MET:O	3:C:319:ILE:HG13	2.04	0.58
1:A:131:TRP:CE3	1:A:132:GLU:N	2.72	0.58
13:O:76:PHE:C	13:O:77:LEU:HD12	2.23	0.58
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.85	0.58
3:C:456:GLU:N	3:C:456:GLU:OE1	2.35	0.58
18:Z:5:PHE:CA	18:Z:57:LEU:HD13	2.32	0.58
4:D:102:THR:O	4:D:105:CYS:HB2	2.04	0.58
4:D:120:PHE:HA	4:D:123:ILE:HD12	1.85	0.58
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:7:UNK:O	17:X:11:UNK:HG2	2.04	0.58
2:B:471:ALA:O	2:B:475:PHE:HB2	2.04	0.58
24:A:562:PHO:CMC	4:D:279:LEU:HD11	2.34	0.58
2:B:24:LEU:HD21	23:B:526:CLA:HAB	1.86	0.58
13:O:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58
2:B:149:LEU:HG	23:B:513:CLA:CB	2.28	0.58
4:D:103:ARG:HD3	4:D:106:GLN:OE1	2.04	0.58
4:D:110:LEU:O	4:D:114:ILE:HG13	2.04	0.58
13:O:152:VAL:HG13	13:O:152:VAL:O	2.04	0.58
1:A:54:ALA:O	1:A:55:ALA:HB2	2.03	0.57
3:C:452:ALA:C	3:C:454:GLY:N	2.56	0.57
13:O:65:ARG:HA	13:O:111:LEU:H	1.68	0.57
1:A:62:GLY:HA3	3:C:356:MET:SD	2.44	0.57
3:C:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	0.57
5:E:60:GLN:C	5:E:62:SER:H	2.07	0.57
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.69	0.57
6:F:34:LEU:HD22	9:J:24:ILE:CD1	2.32	0.57
4:D:343:GLU:HG2	16:V:161:VAL:HG11	1.86	0.57
1:A:217:SER:HA	4:D:272:LEU:HD12	1.86	0.57
13:O:142:ILE:HD12	13:O:142:ILE:N	2.19	0.57
8:I:27:ASP:N	8:I:28:PRO:CD	2.67	0.57
9:J:14:ALA:HB1	28:X:130:BCR:H393	1.85	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	1.85	0.57
2:B:150:CYS:HA	23:B:513:CLA:HBC2	1.87	0.57
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.57
18:Z:39:LEU:O	18:Z:42:LEU:HB3	2.05	0.57
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.04	0.57
3:C:428:THR:CG2	30:C:508:DGD:HA91	2.35	0.57
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	0.57
4:D:261:PHE:HB2	26:D:356:PQ9:H92	1.84	0.57
4:D:239:GLN:O	4:D:240:ALA:HB3	2.05	0.57
4:D:273:PHE:CZ	29:L:210:MGE:H3B2	2.40	0.57
3:C:44:ASN:O	3:C:45:LEU:HG	2.04	0.57
10:K:18:PHE:O	10:K:19:ASP:C	2.43	0.57
14:T:4:ILE:O	14:T:4:ILE:HD13	2.04	0.57
5:E:15:THR:HG23	9:J:8:ILE:O	2.04	0.57
4:D:239:GLN:O	4:D:240:ALA:CB	2.53	0.57
13:O:168:PHE:CD1	13:O:168:PHE:N	2.71	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:172:PHE:CE2	13:O:223:ILE:HG12	2.39	0.57
23:B:518:CLA:HMA1	4:D:130:PHE:CE1	2.40	0.57
4:D:14:TRP:HD1	4:D:15:PHE:N	2.03	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57
9:J:15:THR:HG22	10:K:38:VAL:HG22	1.85	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
6:F:40:MET:HA	6:F:43:ILE:HG13	1.84	0.57
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
4:D:348:ARG:NH2	4:D:352:LEU:OXT	2.37	0.57
13:O:73:PRO:HG2	13:O:102:THR:OG1	2.05	0.57
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.35	0.57
13:O:145:LEU:O	13:O:147:THR:HG22	2.05	0.56
2:B:391:SER:OG	2:B:394:GLN:HB2	2.05	0.56
2:B:138:MET:SD	23:B:525:CLA:HAC1	2.45	0.56
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	0.56
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.26	0.56
4:D:221:THR:HG22	4:D:245:SER:H	1.69	0.56
13:O:163:THR:H	13:O:166:THR:CG2	2.18	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
16:V:39:ASN:ND2	16:V:41:GLU:HB2	2.20	0.56
1:A:213:ALA:O	1:A:217:SER:HB2	2.06	0.56
8:I:19:PHE:CE1	8:I:23:PHE:HE2	2.24	0.56
3:C:27:ASP:O	10:K:46:ARG:HD3	2.06	0.56
3:C:72:LEU:HD11	3:C:108:THR:OG1	2.05	0.56
3:C:198:VAL:HG12	3:C:200:THR:HG23	1.87	0.56
3:C:56:HIS:C	3:C:58:GLY:N	2.59	0.56
16:V:81:ARG:HH11	16:V:81:ARG:HG3	1.71	0.56
3:C:315:MET:CE	3:C:319:ILE:HD11	2.35	0.56
1:A:29:TYR:HD1	1:A:133:LEU:HB2	1.69	0.56
15:U:77:LYS:O	15:U:81:LYS:HB2	2.06	0.56
8:I:11:VAL:O	8:I:15:PHE:HD1	1.89	0.56
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.41	0.56
2:B:55:MET:HE3	2:B:80:ILE:HG12	1.87	0.56
2:B:353:GLU:HB3	2:B:373:LYS:HZ3	1.71	0.56
4:D:103:ARG:HH12	5:E:77:GLU:HG3	1.70	0.56
9:J:33:TYR:O	9:J:34:ALA:HB3	2.04	0.56
4:D:178:ILE:HG22	4:D:179:PHE:N	2.21	0.56
3:C:293:ASN:HD21	3:C:296:VAL:H	1.51	0.56
1:A:13:LEU:N	1:A:13:LEU:HD23	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ILE:HD13	4:D:126:MET:SD	2.46	0.56
1:A:221:SER:HA	4:D:139:ARG:HB2	1.86	0.56
2:B:63:LEU:N	2:B:64:PRO:HD2	2.21	0.56
16:V:107:THR:HG22	16:V:108:TYR:H	1.69	0.55
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.41	0.55
3:C:194:GLY:O	3:C:195:ASP:HB2	2.06	0.55
3:C:332:GLN:HA	3:C:338:GLY:HA2	1.88	0.55
10:K:39:TRP:O	10:K:43:VAL:HG23	2.05	0.55
3:C:348:GLU:OE2	13:O:37:VAL:HA	2.06	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.89	0.55
16:V:103:LYS:O	16:V:122:ARG:HG3	2.07	0.55
3:C:400:PRO:C	3:C:401:LEU:HD23	2.26	0.55
3:C:260:ALA:O	3:C:264:PHE:HD2	1.89	0.55
3:C:284:PHE:HB3	30:C:507:DGD:HA51	1.87	0.55
13:O:163:THR:HG23	13:O:165:SER:H	1.71	0.55
16:V:124:ALA:HB1	16:V:131:ARG:HG3	1.87	0.55
4:D:176:ALA:C	4:D:178:ILE:H	2.10	0.55
15:U:72:TYR:CB	15:U:73:PRO:CD	2.84	0.55
1:A:38:ILE:O	1:A:42:LEU:HG	2.07	0.55
6:F:18:VAL:HG13	6:F:19:ARG:N	2.22	0.55
5:E:13:ILE:HD13	25:F:51:HEM:O1D	2.07	0.55
2:B:283:GLU:OE1	2:B:286:ARG:HD2	2.07	0.55
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.34	0.55
1:A:224:ILE:CG2	2:B:484:PRO:HG3	2.35	0.55
2:B:233:ASN:HD22	2:B:233:ASN:C	2.10	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
2:B:229:LEU:O	2:B:230:ARG:C	2.44	0.55
3:C:42:LEU:CD1	23:C:501:CLA:HMA3	2.36	0.55
3:C:209:ILE:CG2	28:C:506:BCR:H382	2.35	0.55
1:A:264:SER:OG	1:A:265:PHE:N	2.40	0.55
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.89	0.55
23:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
10:K:39:TRP:NE1	17:X:31:UNK:HG3	2.12	0.55
18:Z:23:VAL:HB	18:Z:24:PRO:HD3	1.89	0.55
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.55
16:V:159:GLY:O	16:V:160:LYS:C	2.45	0.55
2:B:18:ARG:HG3	2:B:18:ARG:HH11	1.70	0.55
13:O:47:THR:HG22	13:O:48:LEU:N	2.22	0.55
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.70	0.55
3:C:37:ALA:HA	23:C:498:CLA:O1A	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:145:LEU:HD23	13:O:175:PRO:CG	2.34	0.55
3:C:466:VAL:HA	3:C:469:MET:CE	2.36	0.55
9:J:14:ALA:CB	28:X:130:BCR:H393	2.38	0.54
3:C:416:SER:O	3:C:417:VAL:CG1	2.55	0.54
2:B:10:THR:C	2:B:12:LEU:H	2.10	0.54
4:D:346:LEU:O	4:D:348:ARG:HG3	2.07	0.54
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.82	0.54
13:O:75:THR:HG22	13:O:77:LEU:HD11	1.88	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.71	0.54
30:C:509:DGD:HD2	9:J:32:ALA:O	2.06	0.54
3:C:91:HIS:HB3	23:C:493:CLA:HBA2	1.88	0.54
10:K:43:VAL:HG12	10:K:46:ARG:HG3	1.90	0.54
28:B:527:BCR:H322	29:B:530:MGE:H2G	1.89	0.54
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.37	0.54
3:C:405:ASN:HD22	30:C:509:DGD:C5D	2.19	0.54
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.89	0.54
3:C:55:ALA:HB1	28:C:504:BCR:C37	2.37	0.54
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.35	0.54
5:E:25:ILE:O	5:E:29:ALA:HB2	2.08	0.54
4:D:325:ILE:O	4:D:329:MET:HB3	2.08	0.54
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	0.54
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	0.54
3:C:418:ASN:HB3	30:C:509:DGD:HE2	1.89	0.54
3:C:52:ALA:HB1	23:C:499:CLA:HAB	1.89	0.54
2:B:221:PRO:O	7:H:21:VAL:HG23	2.08	0.54
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.43	0.54
3:C:75:PHE:CE2	3:C:77:PRO:HA	2.43	0.54
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.33	0.54
2:B:392:PHE:O	2:B:393:GLU:CB	2.54	0.54
15:U:57:LEU:HD22	15:U:79:ILE:CG2	2.37	0.54
10:K:45:PHE:O	10:K:46:ARG:C	2.46	0.54
1:A:174:LEU:HD22	24:A:561:PHO:H152	1.89	0.54
5:E:76:VAL:O	5:E:79:PHE:HB2	2.07	0.54
4:D:100:ASP:OD1	4:D:102:THR:HG22	2.07	0.54
3:C:201:ASN:N	3:C:202:PRO:HD3	2.22	0.54
3:C:276:LEU:CD2	23:C:498:CLA:HBB1	2.37	0.54
4:D:67:TYR:CD2	4:D:76:VAL:HG11	2.43	0.54
12:M:26:TYR:O	12:M:29:THR:HB	2.08	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	0.54
4:D:45:LEU:HD13	4:D:49:LEU:HD12	1.90	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.89	0.53
3:C:99:VAL:HG23	3:C:100:GLY:H	1.72	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.53
1:A:159:LEU:O	1:A:163:ILE:HG13	2.08	0.53
1:A:76:ASN:HD22	1:A:76:ASN:C	2.11	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	0.53
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.44	0.53
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
17:X:72:UNK:O	17:X:73:UNK:C	2.57	0.53
2:B:124:ARG:O	7:H:12:ARG:NH2	2.42	0.53
14:T:29:ILE:CD1	14:T:29:ILE:H	2.18	0.53
11:L:11:GLU:HG2	11:L:12:LEU:N	2.24	0.53
11:L:14:ARG:HG3	11:L:14:ARG:NH1	2.22	0.53
3:C:84:GLN:HB2	3:C:86:LEU:CD2	2.37	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.90	0.53
3:C:158:THR:O	3:C:251:HIS:HB3	2.07	0.53
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.37	0.53
10:K:14:ALA:HB2	18:Z:61:VAL:HG11	1.90	0.53
4:D:14:TRP:HD1	4:D:15:PHE:H	1.55	0.53
5:E:51:ARG:O	5:E:53:ASP:N	2.41	0.53
3:C:318:LEU:C	3:C:318:LEU:HD23	2.28	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
2:B:12:LEU:HB2	23:B:522:CLA:HMC2	1.90	0.53
3:C:48:LYS:HE2	3:C:133:ALA:HA	1.90	0.53
1:A:286:THR:HB	23:A:558:CLA:O1D	2.09	0.53
13:O:162:ILE:HA	13:O:166:THR:HG21	1.90	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CD2	2.44	0.53
17:X:122:UNK:C	17:X:124:UNK:N	2.70	0.53
1:A:314:ILE:CG2	1:A:314:ILE:O	2.55	0.53
1:A:40:THR:HG22	1:A:118:HIS:O	2.09	0.53
3:C:193:GLY:O	3:C:194:GLY:C	2.47	0.53
4:D:172:SER:O	4:D:173:PHE:HB2	2.08	0.53
16:V:74:THR:O	16:V:75:ASN:HB2	2.07	0.53
3:C:29:GLU:HG3	3:C:30:SER:N	2.22	0.53
15:U:72:TYR:O	15:U:73:PRO:C	2.46	0.53
4:D:221:THR:O	4:D:221:THR:HG22	2.08	0.53
1:A:238:LYS:O	1:A:241:GLN:HB3	2.09	0.53
1:A:124:SER:O	1:A:127:MET:HB3	2.09	0.53
1:A:183:MET:HA	23:A:558:CLA:HMD2	1.90	0.53
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:LEU:HB2	13:O:106:GLN:HG2	1.91	0.53
1:A:176:ILE:HD13	23:A:559:CLA:HED3	1.91	0.53
24:A:561:PHO:NC	4:D:209:LEU:HD12	2.24	0.53
1:A:141:PRO:O	1:A:143:ILE:N	2.38	0.53
2:B:102:VAL:HA	28:B:528:BCR:C40	2.39	0.52
2:B:152:GLY:C	23:B:516:CLA:HMC3	2.30	0.52
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
23:C:492:CLA:H111	23:C:493:CLA:HMB2	1.90	0.52
29:D:360:MGE:H241	14:T:13:ILE:HG21	1.90	0.52
10:K:31:LEU:HB3	28:X:130:BCR:C15	2.39	0.52
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.52
13:O:33:TYR:C	13:O:35:ASP:H	2.12	0.52
5:E:32:ILE:O	5:E:36:LEU:HG	2.10	0.52
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.75	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.09	0.52
3:C:362:ARG:HG3	3:C:362:ARG:HH11	1.71	0.52
2:B:476:ARG:HG3	2:B:476:ARG:HH11	1.74	0.52
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
3:C:318:LEU:HD23	3:C:318:LEU:O	2.10	0.52
3:C:63:TRP:O	3:C:64:ALA:C	2.47	0.52
2:B:263:THR:O	2:B:263:THR:HG22	2.08	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	0.52
3:C:103:GLY:HA3	3:C:301:PHE:CE1	2.37	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
2:B:391:SER:OG	2:B:394:GLN:NE2	2.43	0.52
3:C:56:HIS:O	3:C:58:GLY:N	2.42	0.52
17:X:12:UNK:CG	18:Z:17:PHE:CE1	2.90	0.52
5:E:69:ARG:O	5:E:70:PHE:HB2	2.09	0.52
4:D:93:TRP:HZ2	23:D:355:CLA:O1A	1.93	0.52
1:A:103:ASP:OD1	1:A:103:ASP:N	2.40	0.52
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.45	0.52
4:D:348:ARG:HH21	4:D:352:LEU:C	2.12	0.52
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.24	0.52
14:T:1:MET:C	14:T:4:ILE:HG22	2.30	0.52
3:C:29:GLU:C	3:C:31:SER:H	2.13	0.52
2:B:220:ARG:HD2	7:H:20:LYS:O	2.10	0.52
13:O:206:GLU:CD	13:O:206:GLU:H	2.13	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	0.52
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.52
2:B:214:LEU:O	2:B:218:LEU:HG	2.09	0.52
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:134:THR:HG23	16:V:137:ASP:OD2	2.10	0.52
8:I:13:THR:O	8:I:17:LEU:HG	2.09	0.52
2:B:262:THR:C	2:B:264:PRO:HD3	2.30	0.52
2:B:362:PHE:HE2	4:D:164:GLN:NE2	2.08	0.52
1:A:63:ILE:CG2	3:C:335:THR:HG21	2.40	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.45	0.52
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.91	0.52
3:C:116:VAL:HG21	28:C:505:BCR:C32	2.40	0.52
23:C:503:CLA:HMC2	28:C:505:BCR:H372	1.91	0.52
1:A:64:ARG:O	1:A:66:PRO:HD3	2.10	0.52
2:B:137:LYS:HD2	7:H:14:LEU:O	2.10	0.52
1:A:27:ARG:NH1	1:A:27:ARG:O	2.43	0.52
13:O:118:SER:HB3	13:O:157:PRO:HA	1.90	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
11:L:2:GLU:HB3	11:L:3:PRO:HD2	1.92	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
16:V:33:VAL:HG12	16:V:33:VAL:O	2.10	0.52
9:J:24:ILE:HG23	9:J:25:VAL:N	2.24	0.51
18:Z:57:LEU:O	18:Z:61:VAL:HG23	2.10	0.51
1:A:257:ARG:HH12	1:A:261:GLN:CD	2.13	0.51
13:O:110:GLU:OE2	13:O:112:LYS:HB2	2.10	0.51
4:D:14:TRP:CD1	4:D:15:PHE:N	2.78	0.51
2:B:413:ASP:OD1	2:B:415:PRO:HD2	2.09	0.51
4:D:223:PHE:CZ	4:D:245:SER:HB3	2.44	0.51
13:O:144:LEU:N	13:O:144:LEU:HD23	2.23	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
13:O:172:PHE:HE2	13:O:223:ILE:HG12	1.75	0.51
2:B:463:PHE:CZ	23:B:518:CLA:HBB1	2.43	0.51
16:V:59:PHE:HA	16:V:63:CYS:SG	2.50	0.51
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
2:B:212:ALA:HB2	23:B:519:CLA:HMC3	1.91	0.51
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.91	0.51
1:A:192:ILE:HG23	1:A:193:LEU:N	2.25	0.51
23:C:493:CLA:HBA1	23:C:493:CLA:CB D	2.37	0.51
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
17:X:76:UNK:O	17:X:77:UNK:C	2.57	0.51
14:T:4:ILE:HB	33:T:217:LMT:O6'	2.11	0.51
1:A:326:LEU:HD21	3:C:412:THR:HB	1.93	0.51
2:B:229:LEU:HD11	23:B:519:CLA:O1A	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	0.51
15:U:69:ARG:O	15:U:70:GLY:C	2.47	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
2:B:380:ASP:OD2	2:B:380:ASP:C	2.47	0.51
14:T:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
2:B:233:ASN:ND2	2:B:235:GLU:H	2.08	0.51
10:K:39:TRP:HE1	17:X:31:UNK:CG	2.14	0.51
14:T:29:ILE:HD12	14:T:29:ILE:N	2.18	0.51
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.92	0.51
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.45	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
3:C:438:LEU:HD11	23:C:495:CLA:HBB1	1.92	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.51
23:C:495:CLA:HMD3	23:C:497:CLA:HAB	1.92	0.51
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
2:B:31:ALA:O	2:B:32:GLY:C	2.49	0.51
3:C:226:SER:HA	30:C:507:DGD:HE62	1.93	0.51
3:C:438:LEU:CD2	30:C:507:DGD:HAH2	2.41	0.51
3:C:449:ARG:HG3	3:C:449:ARG:O	2.10	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.93	0.51
6:F:11:VAL:HG12	6:F:12:SER:N	2.26	0.51
3:C:48:LYS:HE2	3:C:132:HIS:O	2.11	0.51
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.51
2:B:175:THR:HG22	2:B:175:THR:O	2.11	0.51
8:I:4:LEU:O	8:I:8:VAL:HG23	2.11	0.51
23:B:517:CLA:H202	11:L:27:LEU:HD11	1.93	0.50
2:B:233:ASN:C	2:B:233:ASN:ND2	2.64	0.50
17:X:85:UNK:C	17:X:86:UNK:OD1	2.59	0.50
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.09	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HH11	1.75	0.50
4:D:63:LEU:N	4:D:63:LEU:HD12	2.26	0.50
3:C:372:PRO:O	13:O:36:ILE:HD12	2.11	0.50
23:B:525:CLA:H162	23:B:525:CLA:H112	1.93	0.50
3:C:146:PHE:HD2	3:C:147:PHE:CE1	2.29	0.50
3:C:140:LEU:HB2	3:C:148:GLY:HA2	1.93	0.50
6:F:45:ARG:HG2	6:F:45:ARG:OXT	2.11	0.50
3:C:150:ASP:HB3	3:C:153:ASP:CB	2.32	0.50
23:A:560:CLA:HAB	23:D:354:CLA:H72	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
3:C:241:GLY:C	3:C:243:ILE:N	2.64	0.50
15:U:64:ALA:O	15:U:67:GLN:HG2	2.10	0.50
14:T:15:ALA:HB2	28:T:5104:BCR:H14C	1.92	0.50
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.32	0.50
13:O:145:LEU:CD2	13:O:175:PRO:CG	2.86	0.50
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.36	0.50
22:C:484:UNK:HG1	22:C:485:UNK:C	2.40	0.50
10:K:19:ASP:N	10:K:20:PRO:HD2	2.26	0.50
1:A:22:THR:HG23	1:A:136:ARG:NH1	2.26	0.50
10:K:37:PHE:HB3	28:X:130:BCR:C40	2.42	0.50
2:B:368:VAL:HG11	2:B:381:ILE:CD1	2.37	0.50
3:C:245:ILE:O	3:C:249:ILE:HD13	2.12	0.50
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.93	0.50
1:A:62:GLY:O	1:A:63:ILE:O	2.29	0.50
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.93	0.50
2:B:231:MET:C	2:B:233:ASN:H	2.15	0.50
10:K:43:VAL:HG21	17:X:31:UNK:HG3	1.93	0.50
18:Z:36:SER:CA	18:Z:39:LEU:HD12	2.35	0.50
12:M:15:VAL:O	12:M:19:SER:HB2	2.12	0.50
1:A:72:LEU:HD22	33:T:217:LMT:O3'	2.12	0.50
13:O:147:THR:HG21	13:O:175:PRO:HD2	1.93	0.50
4:D:60:THR:HG23	4:D:61:HIS:H	1.77	0.50
2:B:341:LYS:O	2:B:406:LEU:HB2	2.11	0.50
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.50
2:B:15:ASP:O	2:B:17:GLY:N	2.45	0.50
3:C:178:LYS:HD2	3:C:182:PHE:O	2.11	0.50
2:B:463:PHE:CZ	2:B:467:ILE:HD12	2.46	0.50
1:A:299:GLY:O	3:C:403:SER:HB2	2.11	0.50
16:V:128:PRO:O	16:V:130:MET:N	2.45	0.50
13:O:216:PHE:C	13:O:216:PHE:CD2	2.85	0.50
2:B:31:ALA:HB2	23:B:515:CLA:CBC	2.42	0.49
4:D:176:ALA:C	4:D:178:ILE:N	2.66	0.49
4:D:35:ILE:O	4:D:35:ILE:HG22	2.12	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.11	0.49
7:H:59:ASN:OD1	7:H:59:ASN:O	2.29	0.49
13:O:73:PRO:CG	13:O:102:THR:CB	2.90	0.49
3:C:416:SER:O	3:C:417:VAL:HG12	2.11	0.49
2:B:246:PHE:C	2:B:246:PHE:HD1	2.15	0.49
2:B:286:ARG:HD3	2:B:286:ARG:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:144:HIS:CE1	16:V:148:GLU:OE2	2.65	0.49
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.46	0.49
2:B:474:LEU:HD11	23:B:518:CLA:HAA1	1.94	0.49
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	0.49
5:E:47:PHE:O	5:E:49:THR:N	2.45	0.49
3:C:67:MET:HE1	23:C:494:CLA:NC	2.26	0.49
16:V:104:ASN:HD21	16:V:113:GLU:CD	2.14	0.49
4:D:55:VAL:HG12	4:D:56:THR:N	2.26	0.49
3:C:46:SER:HA	3:C:49:LEU:HB3	1.93	0.49
9:J:12:ILE:O	9:J:16:VAL:HG23	2.12	0.49
3:C:277:GLY:C	23:C:495:CLA:HBC2	2.33	0.49
13:O:51:THR:O	13:O:52:ALA:O	2.30	0.49
3:C:188:THR:HG23	3:C:300:GLU:OE2	2.13	0.49
4:D:102:THR:CG2	4:D:103:ARG:N	2.74	0.49
13:O:216:PHE:C	13:O:216:PHE:HD2	2.15	0.49
2:B:13:ILE:HG22	2:B:13:ILE:O	2.11	0.49
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.28	0.49
2:B:124:ARG:HD3	2:B:131:PRO:N	2.28	0.49
2:B:222:PRO:HG3	7:H:27:THR:N	2.26	0.49
13:O:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
2:B:145:LEU:CD1	23:B:525:CLA:HMB2	2.43	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.92	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	0.49
2:B:165:GLY:HA3	2:B:179:GLN:O	2.11	0.49
3:C:199:ILE:N	3:C:199:ILE:HD12	2.27	0.49
2:B:271:THR:HB	2:B:274:GLN:HG3	1.95	0.49
13:O:65:ARG:HG2	13:O:66:ILE:N	2.27	0.49
1:A:78:ILE:O	1:A:177:SER:HB2	2.12	0.49
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.95	0.49
3:C:78:GLU:OE2	3:C:78:GLU:HA	2.12	0.49
10:K:43:VAL:HG12	10:K:43:VAL:O	2.13	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
13:O:101:THR:O	13:O:101:THR:HG22	2.13	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
3:C:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
1:A:232:SER:OG	1:A:235:TYR:CD1	2.65	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.32	0.49
3:C:281:MET:HG3	29:I:201:MGE:H231	1.94	0.49
3:C:250:TRP:HE1	23:C:496:CLA:HED1	1.78	0.49
18:Z:28:ALA:O	18:Z:30:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:24:LEU:C	8:I:26:GLY:H	2.16	0.49
28:T:5104:BCR:H23C	28:T:5104:BCR:H403	1.95	0.49
15:U:73:PRO:HD2	16:V:109:ASP:HB3	1.94	0.49
6:F:40:MET:O	6:F:42:PHE:N	2.46	0.49
2:B:28:ALA:O	2:B:104:SER:HB2	2.13	0.49
2:B:153:PHE:N	23:B:516:CLA:HMC3	2.27	0.49
3:C:269:GLU:CG	3:C:448:ALA:HB2	2.34	0.49
3:C:162:GLY:O	3:C:166:ILE:HG13	2.12	0.49
1:A:58:VAL:O	1:A:60:ILE:N	2.46	0.49
16:V:128:PRO:O	16:V:129:LYS:C	2.51	0.49
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
1:A:153:SER:CB	23:A:558:CLA:H43	2.43	0.48
4:D:57:SER:O	4:D:63:LEU:O	2.31	0.48
13:O:259:VAL:HG12	13:O:260:LYS:N	2.28	0.48
13:O:33:TYR:O	13:O:37:VAL:HG23	2.13	0.48
13:O:75:THR:HG22	13:O:77:LEU:CD1	2.43	0.48
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.48
13:O:154:SER:O	13:O:168:PHE:HA	2.13	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.30	0.48
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	0.48
3:C:342:MET:HE3	3:C:353:GLY:H	1.78	0.48
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.48
3:C:369:LEU:HD21	3:C:384:ILE:HG12	1.95	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
15:U:72:TYR:CG	15:U:73:PRO:N	2.79	0.48
1:A:140:ARG:NH2	31:A:567:LHG:O5	2.46	0.48
3:C:315:MET:HE3	3:C:319:ILE:HD11	1.94	0.48
12:M:33:GLN:C	12:M:35:SER:H	2.16	0.48
11:L:14:ARG:HG2	12:M:26:TYR:CE1	2.44	0.48
23:B:520:CLA:OBD	23:B:520:CLA:H151	2.13	0.48
2:B:18:ARG:NH1	2:B:18:ARG:HG3	2.28	0.48
10:K:15:TYR:C	10:K:17:ILE:H	2.17	0.48
1:A:228:THR:OG1	1:A:231:GLU:HG2	2.13	0.48
13:O:264:VAL:HG12	13:O:265:PHE:N	2.29	0.48
13:O:83:LYS:O	13:O:84:ASN:CB	2.60	0.48
23:B:513:CLA:H2	23:B:515:CLA:H91	1.95	0.48
3:C:48:LYS:HB3	23:C:501:CLA:HMA2	1.95	0.48
4:D:312:GLU:HB2	13:O:185:PRO:HB3	1.96	0.48
18:Z:15:LEU:O	18:Z:19:MET:HG2	2.13	0.48
16:V:39:ASN:OD1	16:V:43:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:246:MET:HE3	4:D:263:ASN:H	1.78	0.48
2:B:124:ARG:HD3	2:B:130:GLU:C	2.33	0.48
29:L:210:MGE:H5A2	12:M:22:LEU:HD21	1.94	0.48
4:D:180:ARG:HD3	4:D:180:ARG:C	2.33	0.48
4:D:67:TYR:CE2	4:D:76:VAL:HG11	2.48	0.48
10:K:17:ILE:HG22	10:K:17:ILE:O	2.14	0.48
2:B:353:GLU:HB3	2:B:373:LYS:HZ1	1.78	0.48
2:B:86:ILE:C	2:B:86:ILE:HD12	2.33	0.48
4:D:126:MET:HE1	4:D:147:SER:HA	1.95	0.48
29:D:358:MGE:O3D	9:J:37:GLY:HA3	2.14	0.48
17:X:86:UNK:N	17:X:86:UNK:OD1	2.45	0.48
16:V:160:LYS:O	16:V:161:VAL:C	2.52	0.48
3:C:116:VAL:HG13	3:C:117:VAL:N	2.29	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.49	0.48
3:C:435:PHE:O	3:C:438:LEU:N	2.47	0.48
1:A:153:SER:HB3	23:A:558:CLA:H43	1.96	0.48
3:C:254:THR:HG22	3:C:255:THR:N	2.19	0.48
13:O:33:TYR:C	13:O:35:ASP:N	2.66	0.48
3:C:229:ASN:HD22	3:C:231:GLU:HG2	1.79	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.13	0.48
2:B:61:PHE:CZ	23:B:517:CLA:HBB1	2.49	0.48
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.14	0.48
18:Z:20:VAL:O	18:Z:24:PRO:HG2	2.14	0.48
18:Z:5:PHE:HE1	18:Z:54:VAL:HG13	1.79	0.48
15:U:73:PRO:HG2	16:V:109:ASP:N	2.29	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
7:H:45:ILE:O	7:H:46:LEU:C	2.51	0.48
1:A:191:ASN:ND2	1:A:194:MET:HB2	2.28	0.48
1:A:77:ILE:HD13	11:L:29:LEU:HG	1.96	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
17:X:3:UNK:C	17:X:5:UNK:N	2.76	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.47
13:O:67:ALA:HB3	13:O:268:SER:OG	2.14	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.47	0.47
3:C:59:LEU:HD13	23:C:500:CLA:HMD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	0.47
13:O:73:PRO:HG2	13:O:102:THR:CB	2.45	0.47
11:L:14:ARG:HH11	11:L:14:ARG:HG3	1.78	0.47
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.48	0.47
9:J:18:GLY:O	9:J:22:ILE:HG12	2.14	0.47
2:B:12:LEU:HD12	23:B:522:CLA:HBB1	1.96	0.47
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47
31:A:567:LHG:HC61	3:C:443:TRP:HH2	1.77	0.47
1:A:303:ASN:O	3:C:415:ASN:OD1	2.32	0.47
1:A:78:ILE:HD13	11:L:33:SER:HB2	1.96	0.47
2:B:262:THR:O	2:B:262:THR:CG2	2.61	0.47
3:C:449:ARG:HD3	23:C:495:CLA:HED1	1.95	0.47
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.36	0.47
3:C:62:PHE:CE2	10:K:28:ILE:HB	2.50	0.47
3:C:293:ASN:HD21	3:C:295:THR:HB	1.79	0.47
3:C:459:ILE:HD12	4:D:245:SER:OG	2.13	0.47
2:B:191:ASN:HD22	2:B:192:PRO:N	2.12	0.47
4:D:213:ILE:HG23	4:D:214:HIS:N	2.28	0.47
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.28	0.47
11:L:12:LEU:HD12	12:M:25:LEU:HD12	1.95	0.47
6:F:11:VAL:HG12	6:F:12:SER:H	1.79	0.47
3:C:152:LYS:O	3:C:154:LYS:N	2.47	0.47
14:T:4:ILE:HB	33:T:217:LMT:C6'	2.44	0.47
2:B:228:ALA:O	2:B:230:ARG:NH1	2.47	0.47
4:D:49:LEU:HD13	28:D:357:BCR:C15	2.45	0.47
13:O:147:THR:OG1	13:O:148:VAL:N	2.47	0.47
7:H:12:ARG:HG3	7:H:12:ARG:NH1	2.30	0.47
1:A:314:ILE:HG22	1:A:314:ILE:O	2.14	0.47
11:L:14:ARG:HD3	12:M:26:TYR:OH	2.15	0.47
1:A:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
1:A:213:ALA:O	1:A:217:SER:CB	2.63	0.47
13:O:169:LYS:HG2	13:O:224:SER:HB2	1.96	0.47
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
16:V:134:THR:N	16:V:137:ASP:OD2	2.45	0.47
16:V:144:HIS:HE1	16:V:148:GLU:OE2	1.97	0.47
15:U:105:LEU:O	15:U:109:LEU:HG	2.15	0.47
23:B:518:CLA:HMB1	4:D:126:MET:HB3	1.97	0.47
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.95	0.47
2:B:179:GLN:HE21	2:B:179:GLN:HA	1.78	0.47
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.91	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:7:ARG:NH2	29:D:359:MGE:O3D	2.47	0.47
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.47
23:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47
23:A:558:CLA:H201	29:D:360:MGE:H232	1.96	0.47
7:H:12:ARG:HG3	7:H:12:ARG:HH11	1.80	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HE3	1.96	0.47
4:D:251:ARG:HE	4:D:255:GLN:NE2	2.12	0.47
9:J:33:TYR:CD2	9:J:33:TYR:N	2.83	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	0.47
1:A:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
17:X:111:UNK:C	17:X:113:UNK:N	2.76	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47
13:O:79:LYS:HA	13:O:90:GLU:O	2.15	0.47
17:X:75:UNK:O	17:X:79:UNK:HG2	2.15	0.47
4:D:102:THR:HG23	4:D:103:ARG:N	2.29	0.47
6:F:41:GLN:HE21	6:F:41:GLN:CA	2.26	0.47
2:B:145:LEU:HD11	23:B:525:CLA:HMB2	1.96	0.47
1:A:29:TYR:CD1	1:A:133:LEU:HB2	2.49	0.47
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.30	0.47
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.15	0.47
16:V:162:TYR:O	16:V:163:TYR:OXT	2.33	0.47
4:D:40:CYS:O	4:D:41:ALA:C	2.53	0.47
3:C:55:ALA:C	28:C:504:BCR:H373	2.35	0.47
1:A:306:VAL:O	1:A:306:VAL:CG2	2.49	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	0.47
1:A:140:ARG:HH22	31:A:567:LHG:P	2.38	0.47
2:B:29:LEU:HD12	23:B:524:CLA:HBB2	1.95	0.47
4:D:68:LEU:HD21	5:E:44:TYR:CD1	2.50	0.47
14:T:1:MET:O	14:T:1:MET:HG2	2.14	0.47
15:U:73:PRO:HG2	16:V:109:ASP:H	1.80	0.47
4:D:214:HIS:HA	26:D:356:PQ9:O4	2.15	0.47
1:A:296:ASN:HB2	3:C:400:PRO:O	2.15	0.47
3:C:201:ASN:OD1	3:C:201:ASN:O	2.33	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
17:X:114:UNK:O	17:X:117:UNK:HB1	2.15	0.47
16:V:133:LEU:H	16:V:133:LEU:HD23	1.80	0.47
3:C:255:THR:HG23	3:C:256:PRO:CD	2.41	0.46
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.46
2:B:169:SER:HA	2:B:176:GLY:HA2	1.97	0.46
13:O:225:LEU:HD12	13:O:225:LEU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:6:ILE:O	8:I:10:ILE:HG12	2.15	0.46
23:B:513:CLA:H162	7:H:38:PHE:HE2	1.80	0.46
13:O:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
3:C:453:ALA:CB	8:I:31:ASN:ND2	2.76	0.46
3:C:415:ASN:O	3:C:416:SER:CB	2.64	0.46
3:C:180:MET:CE	3:C:202:PRO:HG2	2.45	0.46
3:C:460:ASP:O	3:C:461:ARG:C	2.52	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
2:B:390:TYR:CD1	2:B:390:TYR:N	2.83	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.50	0.46
8:I:32:PRO:O	8:I:33:LYS:HG3	2.14	0.46
9:J:21:VAL:HA	9:J:24:ILE:HG22	1.97	0.46
4:D:222:LEU:HA	4:D:244:TYR:HA	1.97	0.46
3:C:290:VAL:HG23	3:C:297:TYR:CE1	2.50	0.46
3:C:89:ILE:N	3:C:90:PRO:CD	2.79	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	1.97	0.46
17:X:126:UNK:N	17:X:126:UNK:CD	2.77	0.46
6:F:25:THR:O	6:F:29:PRO:HG2	2.15	0.46
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.51	0.46
1:A:60:ILE:CG2	1:A:61:ASP:H	2.23	0.46
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
13:O:47:THR:HG22	13:O:48:LEU:H	1.80	0.46
13:O:80:GLU:O	13:O:81:GLU:C	2.53	0.46
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	0.46
15:U:98:THR:C	15:U:100:ARG:H	2.16	0.46
15:U:113:THR:O	15:U:114:VAL:HG23	2.16	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
1:A:183:MET:HB3	23:A:558:CLA:HBC2	1.98	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
18:Z:5:PHE:HA	18:Z:57:LEU:CD1	2.40	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
14:T:11:ALA:HB3	28:T:5104:BCR:H363	1.96	0.46
2:B:263:THR:CG2	2:B:448:ARG:NH1	2.70	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
3:C:39:ASN:OD1	23:C:499:CLA:HBB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:9:ILE:N	12:M:9:ILE:HD12	2.30	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
6:F:45:ARG:CG	6:F:45:ARG:OXT	2.64	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.46
23:C:497:CLA:H142	28:C:506:BCR:H362	1.96	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
5:E:23:HIS:C	5:E:25:ILE:N	2.69	0.46
5:E:59:GLU:O	5:E:60:GLN:C	2.53	0.46
4:D:106:GLN:NE2	5:E:48:GLY:HA3	2.31	0.46
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.46
17:X:112:UNK:C	17:X:114:UNK:N	2.79	0.46
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	0.46
15:U:59:ASN:O	15:U:60:THR:C	2.54	0.46
2:B:10:THR:O	2:B:12:LEU:N	2.49	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
1:A:210:LEU:O	1:A:210:LEU:HD12	2.16	0.46
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
1:A:63:ILE:HG21	3:C:335:THR:HG21	1.97	0.46
1:A:57:PRO:HA	1:A:68:SER:HA	1.97	0.46
17:X:117:UNK:HB1	17:X:117:UNK:NZ	2.31	0.46
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.46	0.46
2:B:462:PHE:CE1	23:B:523:CLA:HMB3	2.50	0.46
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.97	0.46
2:B:149:LEU:HB2	23:B:514:CLA:H203	1.97	0.46
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.46
2:B:249:ALA:O	2:B:252:VAL:HG22	2.16	0.46
23:B:518:CLA:H51	23:B:519:CLA:H101	1.97	0.46
1:A:60:ILE:CG2	1:A:61:ASP:N	2.79	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.46
4:D:229:ALA:O	4:D:231:THR:N	2.49	0.46
1:A:26:ASN:O	1:A:27:ARG:C	2.54	0.46
13:O:116:ASP:O	13:O:158:ASN:N	2.35	0.46
13:O:151:LEU:HD12	13:O:171:GLU:O	2.17	0.45
3:C:410:VAL:HG12	3:C:412:THR:H	1.80	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
1:A:126:TYR:O	1:A:130:GLN:HG3	2.16	0.45
1:A:163:ILE:HD13	30:C:507:DGD:HB22	1.97	0.45
2:B:356:VAL:HA	2:B:370:LEU:HD23	1.96	0.45
13:O:114:ASN:O	13:O:115:SER:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.45
3:C:400:PRO:O	3:C:401:LEU:HD23	2.15	0.45
23:D:355:CLA:H3A	23:D:355:CLA:HBA2	1.53	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
7:H:44:ILE:O	7:H:48:ILE:HG13	2.16	0.45
2:B:329:PRO:HD3	23:B:517:CLA:HED2	1.98	0.45
13:O:98:THR:CG2	13:O:99:ARG:H	2.04	0.45
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.97	0.45
6:F:30:THR:HG22	6:F:34:LEU:HD12	1.98	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45
13:O:70:CYS:SG	13:O:71:LEU:N	2.89	0.45
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
2:B:156:PHE:HB2	23:B:516:CLA:HAC1	1.99	0.45
23:B:511:CLA:CAA	28:H:107:BCR:H19C	2.47	0.45
3:C:453:ALA:HB1	8:I:31:ASN:HD22	1.81	0.45
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.45
1:A:306:VAL:HG21	1:A:316:THR:CG2	2.42	0.45
11:L:14:ARG:HH11	11:L:14:ARG:CG	2.29	0.45
3:C:331:ALA:O	3:C:338:GLY:HA2	2.17	0.45
15:U:115:THR:HG22	15:U:116:GLU:N	2.32	0.45
26:A:564:PQ9:H91	26:A:564:PQ9:H61	1.69	0.45
2:B:215:PHE:C	2:B:215:PHE:CD2	2.89	0.45
2:B:235:GLU:O	2:B:235:GLU:HG2	2.16	0.45
3:C:334:PRO:HG2	4:D:350:ASN:ND2	2.32	0.45
1:A:22:THR:O	1:A:22:THR:HG22	2.16	0.45
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.52	0.45
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.45
13:O:265:PHE:C	13:O:265:PHE:CD1	2.90	0.45
1:A:131:TRP:CZ2	23:C:495:CLA:HAA1	2.51	0.45
3:C:299:SER:OG	3:C:304:PRO:HA	2.17	0.45
9:J:8:ILE:N	9:J:8:ILE:HD12	2.30	0.45
4:D:213:ILE:CG2	4:D:214:HIS:N	2.79	0.45
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.45
2:B:193:TYR:CE1	2:B:260:SER:N	2.84	0.45
3:C:139:THR:HG23	3:C:139:THR:O	2.16	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	0.45
4:D:179:PHE:O	4:D:183:LEU:HG	2.17	0.45
1:A:210:LEU:HD13	24:A:562:PHO:ND	2.31	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	0.45
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.97	0.45
3:C:250:TRP:HE1	23:C:496:CLA:CED	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:70:CYS:O	13:O:265:PHE:HB2	2.16	0.45
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.45
15:U:50:ALA:O	15:U:53:GLU:HB2	2.17	0.45
10:K:46:ARG:HH22	17:X:31:UNK:CG2	2.30	0.45
2:B:271:THR:HG22	2:B:274:GLN:N	2.31	0.45
4:D:96:GLU:H	4:D:96:GLU:CD	2.20	0.45
15:U:92:LEU:HD11	15:U:109:LEU:HD11	1.98	0.45
18:Z:2:THR:O	18:Z:3:ILE:C	2.55	0.45
2:B:124:ARG:HE	2:B:131:PRO:HG3	1.82	0.45
2:B:124:ARG:NH1	2:B:124:ARG:CG	2.77	0.45
13:O:160:THR:O	13:O:161:SER:O	2.34	0.45
13:O:166:THR:O	13:O:167:ASP:HB3	2.16	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	0.45
2:B:98:LEU:O	2:B:99:ALA:C	2.55	0.45
3:C:264:PHE:CD2	3:C:264:PHE:N	2.85	0.45
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.78	0.45
7:H:55:LEU:HB2	7:H:58:VAL:HG21	1.98	0.45
3:C:349:ILE:HD13	13:O:127:ILE:CD1	2.47	0.45
13:O:139:GLY:O	13:O:140:GLU:O	2.34	0.45
23:B:514:CLA:O1A	23:B:515:CLA:HBA1	2.16	0.45
3:C:305:THR:CG2	3:C:307:PRO:HD2	2.31	0.45
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.99	0.45
23:A:559:CLA:H61	24:A:561:PHO:HMB3	1.99	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	0.45
1:A:40:THR:CG2	1:A:118:HIS:O	2.65	0.45
4:D:68:LEU:HB2	6:F:40:MET:HE1	1.99	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.82	0.45
13:O:59:ASP:C	13:O:61:SER:H	2.21	0.45
2:B:10:THR:HG23	2:B:13:ILE:HD11	1.99	0.45
23:B:519:CLA:HBA2	7:H:31:MET:SD	2.57	0.45
2:B:7:ARG:O	2:B:8:VAL:C	2.55	0.45
4:D:130:PHE:HE2	4:D:140:PRO:HB2	1.81	0.45
4:D:244:TYR:OH	4:D:264:LYS:HD3	2.17	0.45
6:F:18:VAL:CG1	6:F:19:ARG:N	2.80	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.45
2:B:297:THR:H	2:B:300:GLU:CD	2.20	0.45
2:B:171:PRO:HD3	7:H:65:LEU:C	2.37	0.45
23:B:517:CLA:H3A	23:B:517:CLA:HBA2	1.71	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
25:F:51:HEM:HAD2	25:F:51:HEM:HHA	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.52	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
4:D:100:ASP:C	4:D:100:ASP:OD1	2.55	0.44
8:I:17:LEU:O	8:I:18:LEU:C	2.55	0.44
12:M:31:SER:C	12:M:33:GLN:H	2.21	0.44
4:D:302:GLU:OE1	13:O:186:LYS:CE	2.65	0.44
12:M:33:GLN:O	12:M:35:SER:N	2.50	0.44
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.51	0.44
3:C:265:ILE:HB	23:C:495:CLA:HED3	1.98	0.44
28:C:504:BCR:H11C	28:X:130:BCR:H322	1.99	0.44
2:B:124:ARG:HA	2:B:131:PRO:HA	1.99	0.44
5:E:60:GLN:C	5:E:62:SER:N	2.71	0.44
15:U:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.52	0.44
13:O:81:GLU:O	13:O:82:PRO:C	2.56	0.44
1:A:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	0.44
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.64	0.44
17:X:126:UNK:HB2	17:X:127:UNK:H	1.41	0.44
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.19	0.44
3:C:116:VAL:O	3:C:117:VAL:C	2.56	0.44
16:V:63:CYS:SG	25:V:552:HEM:HAB	2.57	0.44
16:V:64:ALA:O	16:V:66:CYS:N	2.51	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
5:E:28:PRO:O	5:E:32:ILE:HG13	2.18	0.44
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.00	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.82	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
4:D:85:MET:HE3	4:D:107:LEU:HB3	1.99	0.44
3:C:257:PHE:CD1	3:C:257:PHE:N	2.85	0.44
17:X:128:UNK:O	17:X:129:UNK:C	2.66	0.44
3:C:42:LEU:HD11	23:C:501:CLA:C1A	2.48	0.44
3:C:292:PHE:HB3	30:C:507:DGD:HD62	1.99	0.44
23:A:558:CLA:HBD	23:A:559:CLA:HAC2	1.99	0.44
10:K:21:LEU:HD11	28:X:130:BCR:HC42	1.99	0.44
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.00	0.44
10:K:17:ILE:CD1	18:Z:6:GLN:NE2	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:THR:CG2	4:D:61:HIS:H	2.31	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:452:ALA:C	3:C:454:GLY:H	2.21	0.44
24:A:561:PHO:HED2	4:D:257:PHE:CE2	2.52	0.44
5:E:17:VAL:HA	9:J:8:ILE:HD11	2.00	0.44
5:E:26:THR:O	5:E:29:ALA:HB3	2.18	0.44
1:A:13:LEU:H	1:A:13:LEU:HD23	1.83	0.44
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.33	0.44
10:K:13:GLU:O	10:K:16:ALA:HB3	2.18	0.44
13:O:241:PHE:CD1	13:O:241:PHE:C	2.90	0.44
2:B:450:TRP:O	2:B:451:PHE:C	2.55	0.44
5:E:51:ARG:O	5:E:54:SER:N	2.48	0.44
2:B:476:ARG:HG3	2:B:476:ARG:NH1	2.33	0.44
15:U:98:THR:C	15:U:100:ARG:N	2.71	0.44
3:C:135:ARG:O	3:C:136:GLY:O	2.35	0.44
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.44	0.44
3:C:405:ASN:HB2	30:C:509:DGD:HG32	2.00	0.44
23:C:501:CLA:HMD2	10:K:40:GLN:CD	2.37	0.44
13:O:52:ALA:HA	13:O:230:VAL:O	2.18	0.44
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.99	0.44
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.48	0.44
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	0.43
2:B:450:TRP:O	2:B:453:PHE:N	2.51	0.43
10:K:15:TYR:OH	18:Z:58:ASN:HB2	2.17	0.43
11:L:7:ARG:HD2	11:L:7:ARG:HA	1.69	0.43
2:B:341:LYS:HB3	2:B:406:LEU:HD12	2.00	0.43
4:D:21:TRP:CE2	4:D:26:ARG:NH2	2.78	0.43
3:C:321:ASP:OD2	15:U:129:ASN:HB2	2.18	0.43
3:C:225:VAL:HG12	3:C:225:VAL:O	2.18	0.43
2:B:36:SER:OG	28:B:528:BCR:H362	2.18	0.43
23:C:498:CLA:H122	23:C:500:CLA:HED1	2.00	0.43
3:C:134:ILE:HD11	23:C:501:CLA:H92	2.00	0.43
4:D:256:ILE:O	4:D:256:ILE:HG12	2.19	0.43
4:D:263:ASN:HB3	29:D:360:MGE:O3D	2.19	0.43
7:H:19:GLY:O	7:H:21:VAL:HG12	2.17	0.43
2:B:193:TYR:HE1	2:B:260:SER:N	2.17	0.43
4:D:93:TRP:CZ2	23:D:355:CLA:O1A	2.71	0.43
2:B:217:ILE:HG22	2:B:218:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:HA	1:A:115:ILE:CD1	2.48	0.43
16:V:117:VAL:O	16:V:117:VAL:HG12	2.17	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.91	0.43
2:B:31:ALA:N	23:B:515:CLA:HBC3	2.33	0.43
3:C:305:THR:HB	3:C:308:GLU:HB2	1.99	0.43
28:D:357:BCR:H383	29:D:358:MGE:H6B1	2.00	0.43
15:U:78:LEU:HD13	15:U:97:LEU:HD21	2.01	0.43
13:O:231:ASP:O	13:O:232:GLY:C	2.56	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.54	0.43
18:Z:12:LEU:HA	18:Z:50:LEU:HD13	1.99	0.43
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43
23:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43
1:A:76:ASN:HD21	1:A:79:THR:H	1.66	0.43
23:B:520:CLA:H122	23:B:522:CLA:H43	2.00	0.43
4:D:120:PHE:CD1	4:D:123:ILE:HD12	2.53	0.43
4:D:157:PHE:CE2	4:D:171:PRO:HB2	2.53	0.43
23:C:491:CLA:H42	23:C:492:CLA:HMD1	2.00	0.43
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.43
26:D:356:PQ9:H61	26:D:356:PQ9:H91	1.75	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
2:B:332:LYS:HG3	2:B:444:ARG:HH21	1.84	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
2:B:318:ASN:ND2	2:B:361:ALA:HB2	2.34	0.43
28:X:130:BCR:HC31	18:Z:13:VAL:HG13	2.00	0.43
17:X:102:UNK:O	17:X:103:UNK:C	2.66	0.43
3:C:33:PHE:HE1	4:D:229:ALA:HB2	1.82	0.43
13:O:153:ALA:HB1	13:O:168:PHE:HB3	2.00	0.43
5:E:6:GLY:O	5:E:7:GLU:HG2	2.18	0.43
1:A:32:TRP:CE2	8:I:22:GLY:HA3	2.53	0.43
23:C:498:CLA:H191	30:C:509:DGD:HA91	2.00	0.43
4:D:148:ALA:CB	4:D:149:PRO:HD3	2.35	0.43
4:D:246:MET:HE3	4:D:263:ASN:N	2.34	0.43
1:A:225:ARG:NH1	2:B:484:PRO:HD3	2.34	0.43
2:B:271:THR:HG22	2:B:273:TYR:N	2.34	0.43
2:B:188:ASP:C	2:B:190:PHE:H	2.22	0.43
2:B:191:ASN:HD22	2:B:191:ASN:C	2.20	0.43
1:A:25:ASP:HA	4:D:251:ARG:NH2	2.32	0.43
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.54	0.43
6:F:22:ALA:O	6:F:24:HIS:N	2.52	0.43
1:A:284:TRP:O	1:A:287:ALA:HB3	2.18	0.43

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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
3:C:206:PRO:O	3:C:207:ARG:C	2.57	0.43
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.43
4:D:53:THR:HG22	4:D:67:TYR:CE1	2.53	0.43
2:B:208:VAL:HG21	23:B:512:CLA:CMC	2.48	0.43
2:B:403:GLY:O	2:B:407:ASN:HB2	2.18	0.43
1:A:35:VAL:HG22	28:A:566:BCR:HC42	2.00	0.43
14:T:4:ILE:CD1	14:T:4:ILE:C	2.85	0.43
4:D:178:ILE:CG2	4:D:179:PHE:N	2.81	0.43
3:C:205:ASP:C	3:C:205:ASP:OD2	2.57	0.43
23:C:491:CLA:CAD	23:C:493:CLA:H12	2.49	0.43
2:B:368:VAL:O	2:B:368:VAL:HG13	2.19	0.43
13:O:231:ASP:OD1	13:O:231:ASP:O	2.37	0.43
3:C:214:LEU:N	3:C:214:LEU:HD23	2.31	0.43
2:B:360:PRO:O	2:B:362:PHE:N	2.51	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	0.43
3:C:168:LEU:HD13	23:C:497:CLA:H2	2.01	0.43
28:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	0.43
3:C:180:MET:SD	3:C:202:PRO:HG2	2.57	0.43
4:D:134:ARG:HA	4:D:134:ARG:NE	2.34	0.43
3:C:385:GLN:HB2	3:C:387:TRP:CD1	2.54	0.43
23:B:515:CLA:CHA	23:B:515:CLA:HBA1	2.48	0.43
3:C:404:LEU:C	3:C:406:SER:H	2.23	0.43
4:D:35:ILE:O	4:D:39:PRO:HG2	2.18	0.43
15:U:66:ILE:HD11	15:U:72:TYR:CZ	2.54	0.43
2:B:221:PRO:O	2:B:222:PRO:C	2.56	0.43
13:O:32:THR:H	13:O:35:ASP:CB	2.28	0.43
2:B:464:PHE:HD2	23:B:521:CLA:HAC2	1.83	0.43
3:C:394:GLU:O	3:C:398:HIS:HD2	2.02	0.43
3:C:323:LYS:O	3:C:324:LEU:HB2	2.19	0.43
14:T:22:PHE:O	14:T:23:PHE:CD2	2.71	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.00	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
3:C:87:ILE:C	3:C:90:PRO:HD2	2.39	0.42
3:C:417:VAL:O	3:C:417:VAL:HG13	2.18	0.42
3:C:201:ASN:O	3:C:202:PRO:C	2.58	0.42
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.54	0.42
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.79	0.42
2:B:31:ALA:CA	23:B:515:CLA:HBC3	2.49	0.42
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:GLU:O	3:C:31:SER:N	2.52	0.42
3:C:452:ALA:O	3:C:454:GLY:N	2.52	0.42
1:A:206:PHE:CD1	24:A:562:PHO:HBB2	2.54	0.42
2:B:271:THR:CG2	2:B:273:TYR:N	2.79	0.42
2:B:271:THR:HG22	2:B:273:TYR:H	1.82	0.42
13:O:120:THR:OG1	13:O:154:SER:HB3	2.19	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.42
3:C:104:GLU:O	3:C:105:VAL:C	2.57	0.42
17:X:118:UNK:C	17:X:120:UNK:N	2.80	0.42
4:D:313:THR:C	4:D:315:TYR:N	2.72	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42
23:B:518:CLA:HBA1	23:B:518:CLA:HBD	2.00	0.42
4:D:246:MET:CE	4:D:264:LYS:HG3	2.49	0.42
4:D:40:CYS:O	4:D:43:LEU:N	2.52	0.42
11:L:12:LEU:CD1	12:M:25:LEU:HD12	2.49	0.42
2:B:90:PHE:CZ	2:B:98:LEU:HD23	2.55	0.42
3:C:201:ASN:N	3:C:202:PRO:CD	2.82	0.42
2:B:314:TYR:CZ	2:B:316:GLY:HA3	2.55	0.42
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.85	0.42
13:O:30:THR:HG22	13:O:31:LEU:N	2.33	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
1:A:225:ARG:HH12	2:B:483:ASP:CA	2.19	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
1:A:261:GLN:O	1:A:264:SER:HB3	2.19	0.42
4:D:103:ARG:HA	4:D:103:ARG:HD3	1.81	0.42
23:B:524:CLA:H102	28:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:N	3:C:147:PHE:CD1	2.85	0.42
1:A:69:GLY:O	1:A:80:GLY:HA2	2.19	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	0.42
4:D:47:GLY:HA2	28:D:357:BCR:H332	2.01	0.42
2:B:271:THR:HG22	2:B:274:GLN:HG3	2.02	0.42
2:B:214:LEU:O	2:B:217:ILE:HB	2.18	0.42
2:B:125:ASP:O	2:B:128:THR:O	2.38	0.42
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.79	0.42
23:B:516:CLA:H72	28:B:529:BCR:H311	2.02	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.25	0.42
3:C:113:VAL:O	3:C:117:VAL:HG23	2.20	0.42
16:V:64:ALA:O	16:V:65:SER:C	2.57	0.42
17:X:23:UNK:CG2	18:Z:25:VAL:HG11	2.50	0.42
17:X:54:UNK:O	17:X:55:UNK:C	2.66	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.42
3:C:171:GLY:HA3	23:C:502:CLA:H41	2.01	0.42
3:C:472:LEU:HD12	3:C:472:LEU:H	1.84	0.42
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.42
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.42
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.49	0.42
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	0.42
1:A:33:PHE:CE1	1:A:128:GLY:HA3	2.55	0.42
14:T:2:GLU:O	14:T:3:THR:C	2.57	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:103:LEU:HD21	23:B:515:CLA:HMC3	2.01	0.42
3:C:168:LEU:CD1	23:C:497:CLA:H2	2.49	0.42
1:A:184:ILE:HA	23:A:558:CLA:HBC1	2.02	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
25:V:552:HEM:HAD2	25:V:552:HEM:HHA	1.56	0.42
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
12:M:15:VAL:O	12:M:19:SER:CB	2.68	0.42
7:H:54:ILE:O	7:H:55:LEU:HD23	2.20	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
23:B:515:CLA:H152	23:B:520:CLA:HED1	2.02	0.42
7:H:12:ARG:N	7:H:13:PRO:CD	2.82	0.42
1:A:257:ARG:HH12	1:A:261:GLN:NE2	2.18	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.83	0.42
11:L:12:LEU:HD13	12:M:25:LEU:HB2	2.02	0.42
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.82	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:B:30:VAL:O	2:B:30:VAL:HG12	2.19	0.42
16:V:29:LEU:HG	16:V:29:LEU:O	2.18	0.42
13:O:98:THR:CG2	13:O:99:ARG:N	2.70	0.42
13:O:44:LYS:HA	13:O:72:GLN:CD	2.40	0.42
3:C:405:ASN:ND2	30:C:509:DGD:HD5	2.26	0.42
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	0.42
4:D:274:VAL:HG13	26:D:356:PQ9:H251	2.02	0.42
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	0.42
3:C:138:GLU:O	3:C:139:THR:HB	2.20	0.42
5:E:37:PHE:CD1	5:E:42:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:GLU:O	4:D:135:LEU:HG	2.20	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42
13:O:266:TYR:CG	13:O:267:ALA:N	2.88	0.41
13:O:45:CYS:CB	13:O:46:PRO:HD2	2.31	0.41
23:C:493:CLA:H171	23:C:500:CLA:HBB2	2.01	0.41
23:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	0.41
1:A:314:ILE:O	1:A:315:ASN:O	2.38	0.41
4:D:270:PHE:HZ	26:D:356:PQ9:H243	1.85	0.41
2:B:462:PHE:CZ	23:B:523:CLA:HMB3	2.55	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
3:C:61:VAL:O	3:C:62:PHE:C	2.57	0.41
31:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
4:D:267:LEU:C	4:D:267:LEU:CD2	2.88	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	0.41
3:C:322:GLN:O	3:C:324:LEU:N	2.49	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
2:B:10:THR:C	2:B:12:LEU:N	2.73	0.41
8:I:33:LYS:HA	8:I:34:ARG:NH2	2.16	0.41
6:F:40:MET:C	6:F:42:PHE:N	2.74	0.41
16:V:75:ASN:N	16:V:76:PRO:HD3	2.35	0.41
13:O:106:GLN:N	13:O:106:GLN:HE21	2.18	0.41
15:U:69:ARG:HG3	15:U:70:GLY:N	2.33	0.41
3:C:120:ILE:C	3:C:122:SER:H	2.23	0.41
3:C:120:ILE:C	3:C:122:SER:N	2.73	0.41
1:A:76:ASN:ND2	1:A:76:ASN:C	2.73	0.41
3:C:334:PRO:O	13:O:182:PHE:HB2	2.19	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.52	0.41
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.55	0.41
17:X:52:UNK:O	17:X:54:UNK:N	2.54	0.41
23:B:513:CLA:CGA	23:B:513:CLA:H3A	2.50	0.41
4:D:178:ILE:O	4:D:181:PHE:N	2.54	0.41
8:I:27:ASP:O	8:I:28:PRO:C	2.58	0.41
3:C:166:ILE:HG23	3:C:245:ILE:CG2	2.42	0.41
3:C:419:PHE:CD1	3:C:419:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.41
2:B:208:VAL:HG12	2:B:208:VAL:O	2.20	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.20	0.41
3:C:190:ALA:HB3	3:C:193:GLY:C	2.41	0.41
17:X:120:UNK:C	17:X:122:UNK:N	2.82	0.41
1:A:292:THR:C	1:A:294:ALA:H	2.23	0.41
4:D:259:ILE:HG22	4:D:260:ALA:N	2.34	0.41
1:A:54:ALA:O	1:A:55:ALA:CB	2.69	0.41
28:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
13:O:77:LEU:N	13:O:77:LEU:CD1	2.81	0.41
23:B:521:CLA:C4	23:B:524:CLA:HBC3	2.50	0.41
3:C:75:PHE:CE2	3:C:105:VAL:HG11	2.56	0.41
3:C:95:LEU:O	3:C:185:LEU:HD23	2.21	0.41
2:B:359:MET:HB2	2:B:425:ILE:HG23	2.02	0.41
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.01	0.41
16:V:59:PHE:CD1	16:V:63:CYS:HB2	2.56	0.41
16:V:64:ALA:HB1	16:V:68:VAL:HG12	2.03	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.21	0.41
7:H:46:LEU:HD11	30:H:208:DGD:HA22	2.02	0.41
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.41
2:B:61:PHE:HZ	23:B:517:CLA:HBB1	1.85	0.41
4:D:159:ILE:O	4:D:160:TYR:C	2.58	0.41
3:C:418:ASN:HB3	30:C:509:DGD:C2E	2.51	0.41
3:C:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
17:X:4:UNK:O	17:X:5:UNK:C	2.69	0.41
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.20	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	0.41
1:A:321:ILE:HG22	1:A:322:ASN:N	2.35	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
3:C:56:HIS:O	3:C:59:LEU:N	2.53	0.41
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	0.41
3:C:42:LEU:HG	23:C:501:CLA:O1D	2.20	0.41
10:K:43:VAL:HG21	17:X:31:UNK:CG	2.51	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	0.41
10:K:17:ILE:HD11	18:Z:6:GLN:NE2	2.31	0.41
2:B:272:ARG:HH12	4:D:164:GLN:HG3	1.86	0.41
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
3:C:416:SER:C	3:C:417:VAL:HG12	2.41	0.41
3:C:229:ASN:HD22	3:C:231:GLU:CG	2.34	0.41
23:C:502:CLA:HBA2	23:C:502:CLA:O2D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:18:PHE:CD1	10:K:18:PHE:N	2.89	0.41
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.28	0.41
3:C:438:LEU:HD21	30:C:507:DGD:HAH2	2.02	0.41
3:C:109:PHE:O	3:C:110:PRO:C	2.59	0.41
1:A:13:LEU:H	1:A:13:LEU:CD2	2.33	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
3:C:146:PHE:CD2	3:C:147:PHE:CE1	3.09	0.41
1:A:78:ILE:HD12	1:A:78:ILE:N	2.36	0.41
2:B:410:THR:HG22	2:B:411:PHE:N	2.36	0.41
5:E:16:SER:OG	5:E:19:TYR:HB2	2.21	0.41
2:B:68:ARG:HH12	23:B:514:CLA:CED	2.33	0.40
23:B:518:CLA:HBA1	23:B:518:CLA:CHA	2.51	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	0.40
4:D:38:PHE:HZ	4:D:128:ARG:NH2	2.18	0.40
1:A:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
23:C:494:CLA:HBA1	23:C:494:CLA:CHA	2.52	0.40
2:B:87:ASP:O	2:B:88:PRO:C	2.58	0.40
12:M:17:VAL:HG12	12:M:18:PRO:N	2.35	0.40
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.40
3:C:173:LEU:HD23	3:C:173:LEU:HA	1.86	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
2:B:12:LEU:CD1	23:B:522:CLA:HBB1	2.51	0.40
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.89	0.40
10:K:45:PHE:C	10:K:46:ARG:OXT	2.58	0.40
8:I:31:ASN:HB2	8:I:32:PRO:HD2	2.03	0.40
24:A:561:PHO:HND	4:D:209:LEU:HD12	1.87	0.40
13:O:142:ILE:N	13:O:142:ILE:CD1	2.84	0.40
2:B:74:SER:C	2:B:76:SER:N	2.74	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
15:U:69:ARG:HB2	15:U:69:ARG:HE	1.69	0.40
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.40
8:I:30:ARG:H	8:I:30:ARG:HG2	1.60	0.40
2:B:450:TRP:HB3	23:B:517:CLA:HMB2	2.04	0.40
2:B:164:PRO:HD3	23:B:516:CLA:O1D	2.22	0.40
2:B:230:ARG:NH1	2:B:474:LEU:HD22	2.36	0.40
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.79	0.40
23:C:491:CLA:HMA1	28:C:506:BCR:H401	2.02	0.40
17:X:85:UNK:N	17:X:85:UNK:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:HA	1:A:206:PHE:HD2	1.75	0.40
29:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.40
4:D:103:ARG:O	4:D:106:GLN:N	2.55	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40
17:X:62:UNK:O	17:X:66:UNK:N	2.55	0.40
14:T:22:PHE:O	14:T:23:PHE:CG	2.75	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
1:A:131:TRP:CD2	1:A:132:GLU:N	2.89	0.40
4:D:34:GLY:C	4:D:36:LEU:H	2.25	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
3:C:252:ILE:HG22	3:C:252:ILE:O	2.21	0.40
8:I:24:LEU:O	8:I:26:GLY:N	2.48	0.40
1:A:255:PHE:CE2	26:A:564:PQ9:H151	2.57	0.40
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.40
15:U:54:LYS:HB3	15:U:111:HIS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	18
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	15
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	4	21
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	4	24
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	13
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	3	17
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	20
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
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	11
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	11
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	29
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	5	29
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	1	4
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	1	4
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	7
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	7
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	15
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2	15
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	8
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	8
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	2	14

All (269) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN
2	B	230	ARG
2	B	260	SER
2	B	362	PHE
2	B	488	PRO
3	C	154	LYS
3	C	324	LEU
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	257	PHE
4	D	262	SER
5	E	7	GLU
5	E	58	GLN
5	E	60	GLN
7	H	18	TYR
7	H	64	ALA
13	O	46	PRO
13	O	52	ALA
13	O	86	ARG
13	O	115	SER
13	O	140	GLU
13	O	175	PRO
15	U	72	TYR
15	U	73	PRO
15	U	83	ALA
16	V	133	LEU
16	V	160	LYS
1	a	5011	ALA
1	a	5012	ASN
1	a	5063	ILE
1	a	5141	PRO
1	a	5142	TRP
1	a	5315	ASN
2	b	5230	ARG
2	b	5260	SER
2	b	5362	PHE
2	b	5488	PRO
3	c	5154	LYS

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Mol	Chain	Res	Type
3	c	5226	SER
3	c	5324	LEU
3	c	5416	SER
4	d	5239	GLN
4	d	5240	ALA
4	d	5262	SER
5	e	5007	GLU
5	e	5058	GLN
5	e	5060	GLN
7	h	5018	TYR
7	h	5064	ALA
13	o	5046	PRO
13	o	5052	ALA
13	o	5086	ARG
13	o	5115	SER
13	o	5140	GLU
13	o	5175	PRO
15	u	5072	TYR
15	u	5073	PRO
15	u	5083	ALA
16	v	5133	LEU
16	v	5160	LYS
1	A	12	ASN
1	A	130	GLN
1	A	261	GLN
1	A	266	ASN
2	B	11	VAL
2	B	85	GLY
2	B	176	GLY
2	B	231	MET
3	C	57	ALA
3	C	136	GLY
3	C	139	THR
3	C	141	GLU
3	C	144	SER
3	C	207	ARG
3	C	209	ILE
3	C	226	SER
3	C	242	LEU
4	D	92	LEU
4	D	263	ASN
5	E	48	GLY

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Mol	Chain	Res	Type
7	H	26	GLY
8	I	25	SER
9	J	35	GLY
10	K	13	GLU
10	K	16	ALA
12	M	34	LYS
13	O	50	ASP
13	O	84	ASN
13	O	88	GLU
13	O	138	GLY
13	O	161	SER
15	U	70	GLY
18	Z	31	GLN
18	Z	32	ASP
1	a	5055	ALA
1	a	5130	GLN
1	a	5242	GLU
1	a	5266	ASN
2	b	5011	VAL
2	b	5085	GLY
3	c	5136	GLY
3	c	5141	GLU
3	c	5144	SER
3	c	5207	ARG
3	c	5209	ILE
4	d	5092	LEU
4	d	5192	THR
4	d	5252	PHE
4	d	5257	PHE
4	d	5263	ASN
5	e	5048	GLY
6	f	5041	GLN
7	h	5026	GLY
8	i	5025	SER
9	j	5035	GLY
10	k	5013	GLU
10	k	5016	ALA
12	m	5034	LYS
13	o	5050	ASP
13	o	5084	ASN
13	o	5088	GLU
13	o	5138	GLY

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

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Mol	Chain	Res	Type
9	j	5011	TRP
11	l	5005	PRO
11	l	5007	ARG
13	o	5167	ASP
13	o	5232	GLY
15	u	5088	VAL
16	v	5064	ALA
1	A	232	SER
1	A	260	PHE
2	B	91	TRP
2	B	485	GLU
3	C	30	SER
3	C	38	GLY
3	C	77	PRO
3	C	205	ASP
3	C	298	PRO
4	D	41	ALA
4	D	177	ALA
4	D	261	PHE
9	J	11	TRP
13	O	167	ASP
13	O	232	GLY
15	U	60	THR
16	V	65	SER
1	a	5260	PHE
2	b	5231	MET
2	b	5485	GLU
3	c	5194	GLY
3	c	5205	ASP
4	d	5062	GLY
7	h	5003	ARG
9	j	5014	ALA
16	v	5129	LYS
2	B	16	PRO
2	B	89	GLY
2	B	386	ALA
3	C	227	VAL
3	C	382	ASN
4	D	29	PHE
4	D	62	GLY
12	M	17	VAL
13	O	139	GLY

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Mol	Chain	Res	Type
16	V	129	LYS
1	a	5172	MET
1	a	5217	SER
2	b	5089	GLY
2	b	5122	LEU
2	b	5361	ALA
3	c	5030	SER
3	c	5077	PRO
3	c	5153	ASP
3	c	5227	VAL
3	c	5298	PRO
3	c	5382	ASN
4	d	5177	ALA
16	v	5075	ASN
2	B	361	ALA
3	C	243	ILE
13	O	185	PRO
3	c	5038	GLY
3	c	5134	ILE
4	d	5264	LYS
12	m	5017	VAL
13	o	5139	GLY
16	v	5065	SER
2	B	8	VAL
6	F	23	VAL
18	Z	24	PRO
2	b	5016	PRO
3	c	5243	ILE
13	o	5185	PRO
15	u	5066	ILE
2	B	414	PRO
3	C	105	VAL
3	C	134	ILE
13	O	117	GLY
2	b	5008	VAL
2	b	5414	PRO
18	z	5003	ILE
4	D	80	THR
18	Z	3	ILE
1	a	5060	ILE
3	c	5105	VAL
6	f	5023	VAL

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	251 (93%)	18 (7%)	20	57
1	a	269/280 (96%)	252 (94%)	17 (6%)	22	60
2	B	378/407 (93%)	361 (96%)	17 (4%)	34	74
2	b	378/407 (93%)	360 (95%)	18 (5%)	31	71
3	C	341/374 (91%)	320 (94%)	21 (6%)	23	60
3	c	341/374 (91%)	320 (94%)	21 (6%)	23	60
4	D	273/283 (96%)	259 (95%)	14 (5%)	29	69
4	d	273/283 (96%)	258 (94%)	15 (6%)	27	65
5	E	68/73 (93%)	65 (96%)	3 (4%)	35	74
5	e	68/73 (93%)	66 (97%)	2 (3%)	50	84
6	F	27/39 (69%)	26 (96%)	1 (4%)	41	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	27/39 (69%)	26 (96%)	1 (4%)	41	79
7	H	50/55 (91%)	42 (84%)	8 (16%)	3	15
7	h	50/55 (91%)	43 (86%)	7 (14%)	4	19
8	I	32/35 (91%)	27 (84%)	5 (16%)	3	16
8	i	32/35 (91%)	27 (84%)	5 (16%)	3	16
9	J	22/28 (79%)	21 (96%)	1 (4%)	34	74
9	j	22/28 (79%)	21 (96%)	1 (4%)	34	74
10	K	29/30 (97%)	28 (97%)	1 (3%)	44	81
10	k	29/30 (97%)	28 (97%)	1 (3%)	44	81
11	L	34/35 (97%)	31 (91%)	3 (9%)	12	42
11	l	34/35 (97%)	31 (91%)	3 (9%)	12	42
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%)	27	65
13	o	181/208 (87%)	172 (95%)	9 (5%)	30	70
14	T	26/29 (90%)	25 (96%)	1 (4%)	40	78
14	t	26/29 (90%)	25 (96%)	1 (4%)	40	78
15	U	83/89 (93%)	80 (96%)	3 (4%)	42	79
15	u	83/89 (93%)	80 (96%)	3 (4%)	42	79
16	V	117/117 (100%)	113 (97%)	4 (3%)	44	81
16	v	117/117 (100%)	111 (95%)	6 (5%)	29	69
18	Z	43/52 (83%)	42 (98%)	1 (2%)	58	87
18	z	43/52 (83%)	42 (98%)	1 (2%)	58	87
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	27	65

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

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Mol	Chain	Res	Type
1	A	76	ASN
1	A	103	ASP
1	A	131	TRP
1	A	155	PHE
1	A	177	SER
1	A	206	PHE
1	A	232	SER
1	A	241	GLN
1	A	286	THR
1	A	292	THR
1	A	297	LEU
1	A	308	ASP
2	B	36	SER
2	B	124	ARG
2	B	137	LYS
2	B	179	GLN
2	B	191	ASN
2	B	222	PRO
2	B	231	MET
2	B	233	ASN
2	B	246	PHE
2	B	262	THR
2	B	271	THR
2	B	309	LEU
2	B	350	GLU
2	B	354	LEU
2	B	362	PHE
2	B	414	PRO
2	B	478	VAL
3	C	27	ASP
3	C	29	GLU
3	C	67	MET
3	C	86	LEU
3	C	97	TRP
3	C	155	ASN
3	C	165	LEU
3	C	191	PRO
3	C	214	LEU
3	C	244	CYS
3	C	254	THR
3	C	262	ARG
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	298	PRO
3	C	355	THR
3	C	377	LEU
3	C	383	ASP
3	C	419	PHE
3	C	428	THR
3	C	472	LEU
3	C	473	ASP
4	D	14	TRP
4	D	63	LEU
4	D	130	PHE
4	D	164	GLN
4	D	178	ILE
4	D	180	ARG
4	D	191	TRP
4	D	241	GLU
4	D	246	MET
4	D	250	ASN
4	D	294	ARG
4	D	304	ARG
4	D	323	GLU
4	D	346	LEU
5	E	4	THR
5	E	17	VAL
5	E	52	PRO
6	F	17	THR
7	H	12	ARG
7	H	21	VAL
7	H	27	THR
7	H	41	PHE
7	H	49	TYR
7	H	50	ASN
7	H	53	LEU
7	H	59	ASN
8	I	2	GLU
8	I	27	ASP
8	I	30	ARG
8	I	32	PRO
8	I	34	ARG
9	J	29	PHE
10	K	11	LEU
11	L	3	PRO

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

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Mol	Chain	Res	Type
2	b	5179	GLN
2	b	5191	ASN
2	b	5222	PRO
2	b	5231	MET
2	b	5233	ASN
2	b	5245	VAL
2	b	5246	PHE
2	b	5262	THR
2	b	5271	THR
2	b	5309	LEU
2	b	5350	GLU
2	b	5362	PHE
2	b	5467	ILE
2	b	5478	VAL
3	c	5027	ASP
3	c	5029	GLU
3	c	5067	MET
3	c	5086	LEU
3	c	5097	TRP
3	c	5155	ASN
3	c	5165	LEU
3	c	5191	PRO
3	c	5214	LEU
3	c	5244	CYS
3	c	5254	THR
3	c	5262	ARG
3	c	5289	PHE
3	c	5298	PRO
3	c	5355	THR
3	c	5377	LEU
3	c	5383	ASP
3	c	5419	PHE
3	c	5428	THR
3	c	5472	LEU
3	c	5473	ASP
4	d	5014	TRP
4	d	5063	LEU
4	d	5090	LEU
4	d	5130	PHE
4	d	5164	GLN
4	d	5178	ILE
4	d	5180	ARG

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Mol	Chain	Res	Type
4	d	5191	TRP
4	d	5241	GLU
4	d	5246	MET
4	d	5250	ASN
4	d	5294	ARG
4	d	5304	ARG
4	d	5323	GLU
4	d	5346	LEU
5	e	5017	VAL
5	e	5052	PRO
6	f	5017	THR
7	h	5012	ARG
7	h	5021	VAL
7	h	5027	THR
7	h	5041	PHE
7	h	5049	TYR
7	h	5050	ASN
7	h	5059	ASN
8	i	5002	GLU
8	i	5027	ASP
8	i	5030	ARG
8	i	5032	PRO
8	i	5034	ARG
9	j	5029	PHE
10	k	5011	LEU
11	l	5010	VAL
11	l	5014	ARG
11	l	5016	SER
13	o	5046	PRO
13	o	5050	ASP
13	o	5097	VAL
13	o	5106	GLN
13	o	5114	ASN
13	o	5120	THR
13	o	5168	PHE
13	o	5216	PHE
13	o	5223	ILE
14	t	5004	ILE
15	u	5046	LYS
15	u	5061	ASN
15	u	5090	ASP
16	v	5035	THR

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Mol	Chain	Res	Type
16	v	5037	PRO
16	v	5081	ARG
16	v	5111	GLU
16	v	5122	ARG
16	v	5128	PRO
18	z	5058	ASN

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

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

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Mol	Chain	Res	Type
4	D	98	GLN
4	D	224	GLN
4	D	250	ASN
4	D	255	GLN
5	E	58	GLN
6	F	41	GLN
7	H	15	ASN
12	M	5	GLN
13	O	72	GLN
13	O	106	GLN
13	O	114	ASN
13	O	130	GLN
13	O	262	GLN
15	U	108	ASN
16	V	104	ASN
16	V	144	HIS
18	Z	6	GLN
1	a	5012	ASN
1	a	5019	ASN
1	a	5075	ASN
1	a	5076	ASN
1	a	5118	HIS
1	a	5165	GLN
1	a	5241	GLN
1	a	5272	HIS
1	a	5296	ASN
1	a	5298	ASN
1	a	5304	HIS
1	a	5322	ASN
2	b	5157	HIS
2	b	5179	GLN
2	b	5191	ASN
2	b	5223	GLN
2	b	5233	ASN
2	b	5274	GLN
2	b	5289	GLN
2	b	5394	GLN
2	b	5438	ASN
3	c	5155	ASN
3	c	5201	ASN
3	c	5229	ASN
3	c	5293	ASN

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Mol	Chain	Res	Type
3	c	5332	GLN
3	c	5398	HIS
3	c	5415	ASN
4	d	5061	HIS
4	d	5098	GLN
4	d	5164	GLN
4	d	5224	GLN
4	d	5250	ASN
4	d	5255	GLN
5	e	5058	GLN
6	f	5041	GLN
7	h	5015	ASN
7	h	5059	ASN
12	m	5005	GLN
13	o	5072	GLN
13	o	5106	GLN
13	o	5114	ASN
13	o	5130	GLN
13	o	5262	GLN
15	u	5108	ASN
16	v	5104	ASN
16	v	5144	HIS
18	z	5006	GLN

5.3.3 RNA ⓘ

There are no RNA 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$
32	SQD	A	5212	-	25,26,54	2.86	13 (52%)	33,37,65	2.91	11 (33%)
23	CLA	A	558	1	55,73,73	1.03	4 (7%)	61,113,113	1.44	14 (22%)
23	CLA	A	559	-	55,73,73	0.94	2 (3%)	61,113,113	1.37	9 (14%)
23	CLA	A	560	-	55,73,73	1.08	4 (7%)	61,113,113	1.49	13 (21%)
24	PHO	A	561	-	67,69,69	1.01	4 (5%)	84,99,99	1.32	12 (14%)
24	PHO	A	562	-	67,69,69	1.03	6 (8%)	84,99,99	1.43	15 (17%)
23	CLA	A	563	-	45,63,73	1.20	5 (11%)	49,101,113	1.54	10 (20%)
26	PQ9	A	564	-	30,30,45	0.90	1 (3%)	38,39,57	1.62	7 (18%)
27	OEC	A	565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	A	566	-	41,41,41	1.57	7 (17%)	56,56,56	2.14	21 (37%)
31	LHG	A	567	-	38,38,48	1.86	5 (13%)	39,44,54	1.41	3 (7%)
32	SQD	A	568	-	53,54,54	2.45	29 (54%)	61,65,65	2.73	18 (29%)
33	LMT	A	569	-	36,36,36	1.48	6 (16%)	47,47,47	1.08	2 (4%)
23	CLA	B	511	-	30,49,73	1.45	8 (26%)	34,84,113	1.65	9 (26%)
23	CLA	B	512	2	55,73,73	1.03	2 (3%)	61,113,113	1.45	11 (18%)
23	CLA	B	513	2	55,73,73	1.12	5 (9%)	61,113,113	1.52	11 (18%)
23	CLA	B	514	2	55,73,73	1.02	4 (7%)	61,113,113	1.39	9 (14%)
23	CLA	B	515	-	55,73,73	1.01	4 (7%)	61,113,113	1.59	13 (21%)
23	CLA	B	516	-	55,73,73	1.01	3 (5%)	61,113,113	1.45	9 (14%)
23	CLA	B	517	-	55,73,73	1.02	5 (9%)	61,113,113	1.58	11 (18%)
23	CLA	B	518	2	55,73,73	1.03	4 (7%)	61,113,113	1.56	14 (22%)
23	CLA	B	519	-	55,73,73	1.07	4 (7%)	61,113,113	1.42	12 (19%)
23	CLA	B	520	-	55,73,73	1.08	4 (7%)	61,113,113	1.43	10 (16%)
23	CLA	B	521	2	55,73,73	1.06	6 (10%)	61,113,113	1.52	10 (16%)
23	CLA	B	522	-	55,73,73	0.93	3 (5%)	61,113,113	1.42	8 (13%)
23	CLA	B	523	-	55,73,73	1.00	3 (5%)	61,113,113	1.43	10 (16%)
23	CLA	B	524	2	46,64,73	1.05	3 (6%)	50,102,113	1.55	10 (20%)
23	CLA	B	525	-	55,73,73	0.92	3 (5%)	61,113,113	1.50	10 (16%)
23	CLA	B	526	-	55,73,73	1.24	6 (10%)	61,113,113	1.47	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	B	527	-	41,41,41	1.72	8 (19%)	56,56,56	2.09	16 (28%)
28	BCR	B	528	-	41,41,41	1.85	7 (17%)	56,56,56	2.02	16 (28%)
28	BCR	B	529	-	41,41,41	1.80	8 (19%)	56,56,56	2.23	21 (37%)
29	MGE	B	530	-	48,48,48	1.18	6 (12%)	56,56,56	1.22	6 (10%)
23	CLA	C	491	3	55,73,73	1.03	4 (7%)	61,113,113	1.38	10 (16%)
23	CLA	C	492	3	50,68,73	1.04	4 (8%)	55,107,113	1.57	9 (16%)
23	CLA	C	493	3	55,73,73	0.97	4 (7%)	61,113,113	1.52	13 (21%)
23	CLA	C	494	-	36,54,73	1.23	3 (8%)	41,90,113	1.75	10 (24%)
23	CLA	C	495	-	55,73,73	1.08	5 (9%)	61,113,113	1.59	13 (21%)
23	CLA	C	496	3	55,73,73	1.12	5 (9%)	61,113,113	1.46	10 (16%)
23	CLA	C	497	-	55,73,73	1.00	2 (3%)	61,113,113	1.56	9 (14%)
23	CLA	C	498	3	55,73,73	1.02	3 (5%)	61,113,113	1.46	11 (18%)
23	CLA	C	499	-	37,55,73	1.04	1 (2%)	42,91,113	1.68	11 (26%)
23	CLA	C	500	-	55,73,73	1.05	6 (10%)	61,113,113	1.38	11 (18%)
23	CLA	C	501	3	55,73,73	1.03	4 (7%)	61,113,113	1.40	9 (14%)
23	CLA	C	502	-	41,59,73	1.27	5 (12%)	44,96,113	1.72	11 (25%)
23	CLA	C	503	3	40,58,73	1.19	3 (7%)	44,95,113	1.65	10 (22%)
28	BCR	C	504	-	41,41,41	1.82	7 (17%)	56,56,56	2.21	22 (39%)
28	BCR	C	505	-	41,41,41	1.91	8 (19%)	56,56,56	2.13	18 (32%)
28	BCR	C	506	-	41,41,41	1.72	9 (21%)	56,56,56	2.22	21 (37%)
30	DGD	C	507	-	54,54,67	1.32	8 (14%)	68,68,81	1.51	7 (10%)
30	DGD	C	508	-	48,48,67	1.39	9 (18%)	62,62,81	1.73	12 (19%)
30	DGD	C	509	-	58,58,67	1.09	6 (10%)	72,72,81	1.40	6 (8%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	55,73,73	1.03	5 (9%)	61,113,113	1.43	8 (13%)
23	CLA	D	355	-	40,58,73	1.21	3 (7%)	44,95,113	1.68	10 (22%)
26	PQ9	D	356	-	30,30,45	0.86	1 (3%)	38,39,57	1.74	9 (23%)
28	BCR	D	357	-	41,41,41	1.92	9 (21%)	56,56,56	2.29	18 (32%)
29	MGE	D	358	-	47,47,48	1.19	5 (10%)	55,55,56	0.98	3 (5%)
29	MGE	D	359	-	41,41,48	1.22	5 (12%)	49,49,56	1.04	3 (6%)
29	MGE	D	360	-	48,48,48	0.91	3 (6%)	56,56,56	1.13	4 (7%)
25	HEM	F	51	5,6	30,50,50	2.44	13 (43%)	24,82,82	3.23	11 (45%)
28	BCR	H	107	-	41,41,41	2.06	7 (17%)	56,56,56	2.28	23 (41%)
30	DGD	H	208	-	55,55,67	1.44	10 (18%)	69,69,81	1.59	8 (11%)
29	MGE	I	201	-	48,48,48	1.08	6 (12%)	56,56,56	1.10	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MGE	L	210	-	48,48,48	0.95	3 (6%)	56,56,56	1.17	5 (8%)
32	SQD	L	5213	-	46,47,54	2.84	24 (52%)	54,58,65	2.55	13 (24%)
33	LMT	M	5216	-	36,36,36	1.41	7 (19%)	47,47,47	0.91	1 (2%)
33	LMT	T	217	-	36,36,36	1.37	4 (11%)	47,47,47	1.02	4 (8%)
28	BCR	T	5104	-	41,41,41	1.52	9 (21%)	56,56,56	2.31	22 (39%)
25	HEM	V	552	16	30,50,50	2.49	11 (36%)	24,82,82	3.32	8 (33%)
28	BCR	X	130	-	41,41,41	1.90	10 (24%)	56,56,56	2.53	24 (42%)
32	SQD	a	212	-	25,26,54	3.20	14 (56%)	33,37,65	3.03	12 (36%)
23	CLA	a	5558	1	55,73,73	1.07	5 (9%)	61,113,113	1.39	9 (14%)
23	CLA	a	5559	-	55,73,73	0.94	1 (1%)	61,113,113	1.38	8 (13%)
23	CLA	a	5560	-	55,73,73	1.02	3 (5%)	61,113,113	1.48	11 (18%)
24	PHO	a	5561	-	67,69,69	1.04	6 (8%)	84,99,99	1.27	10 (11%)
24	PHO	a	5562	-	67,69,69	1.03	5 (7%)	84,99,99	1.41	12 (14%)
23	CLA	a	5563	-	45,63,73	1.21	5 (11%)	49,101,113	1.50	9 (18%)
26	PQ9	a	5564	-	30,30,45	0.97	1 (3%)	38,39,57	1.61	7 (18%)
27	OEC	a	5565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	a	5566	-	41,41,41	1.63	7 (17%)	56,56,56	2.13	21 (37%)
31	LHG	a	5567	-	38,38,48	1.88	5 (13%)	39,44,54	1.37	3 (7%)
33	LMT	a	5568	-	36,36,36	1.41	6 (16%)	47,47,47	1.11	2 (4%)
23	CLA	b	5511	-	30,49,73	1.46	6 (20%)	34,84,113	1.66	8 (23%)
23	CLA	b	5512	2	55,73,73	1.00	3 (5%)	61,113,113	1.47	11 (18%)
23	CLA	b	5513	2	55,73,73	1.09	4 (7%)	61,113,113	1.53	12 (19%)
23	CLA	b	5514	2	55,73,73	0.99	3 (5%)	61,113,113	1.41	8 (13%)
23	CLA	b	5515	-	55,73,73	1.07	5 (9%)	61,113,113	1.59	12 (19%)
23	CLA	b	5516	-	55,73,73	1.08	4 (7%)	61,113,113	1.53	11 (18%)
23	CLA	b	5517	-	55,73,73	1.09	4 (7%)	61,113,113	1.50	12 (19%)
23	CLA	b	5518	2	55,73,73	0.96	2 (3%)	61,113,113	1.58	14 (22%)
23	CLA	b	5519	-	55,73,73	1.03	3 (5%)	61,113,113	1.45	12 (19%)
23	CLA	b	5520	-	55,73,73	1.04	6 (10%)	61,113,113	1.42	10 (16%)
23	CLA	b	5521	2	55,73,73	0.97	2 (3%)	61,113,113	1.49	10 (16%)
23	CLA	b	5522	-	55,73,73	1.00	4 (7%)	61,113,113	1.40	6 (9%)
23	CLA	b	5523	-	55,73,73	1.02	4 (7%)	61,113,113	1.50	10 (16%)
23	CLA	b	5524	2	46,64,73	1.04	2 (4%)	50,102,113	1.52	9 (18%)
23	CLA	b	5525	-	55,73,73	0.95	3 (5%)	61,113,113	1.47	10 (16%)
23	CLA	b	5526	-	55,73,73	1.30	7 (12%)	61,113,113	1.54	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	b	5527	-	41,41,41	1.52	8 (19%)	56,56,56	2.00	13 (23%)
28	BCR	b	5528	-	41,41,41	1.67	7 (17%)	56,56,56	2.05	17 (30%)
28	BCR	b	5529	-	41,41,41	1.67	8 (19%)	56,56,56	2.14	20 (35%)
29	MGE	b	5530	-	48,48,48	1.16	8 (16%)	56,56,56	1.15	7 (12%)
23	CLA	c	5491	3	55,73,73	0.97	3 (5%)	61,113,113	1.46	10 (16%)
23	CLA	c	5492	3	50,68,73	1.06	4 (8%)	55,107,113	1.52	10 (18%)
23	CLA	c	5493	3	55,73,73	1.01	4 (7%)	61,113,113	1.52	14 (22%)
23	CLA	c	5494	-	36,54,73	1.17	3 (8%)	41,90,113	1.67	10 (24%)
23	CLA	c	5495	-	55,73,73	1.09	4 (7%)	61,113,113	1.59	13 (21%)
23	CLA	c	5496	-	55,73,73	1.20	6 (10%)	61,113,113	1.43	10 (16%)
23	CLA	c	5497	-	55,73,73	1.08	4 (7%)	61,113,113	1.52	11 (18%)
23	CLA	c	5498	3	55,73,73	1.06	5 (9%)	61,113,113	1.48	11 (18%)
23	CLA	c	5499	-	37,55,73	1.18	5 (13%)	42,91,113	1.62	8 (19%)
23	CLA	c	5500	-	55,73,73	1.01	4 (7%)	61,113,113	1.42	11 (18%)
23	CLA	c	5501	3	55,73,73	1.03	3 (5%)	61,113,113	1.38	8 (13%)
23	CLA	c	5502	-	41,59,73	1.27	7 (17%)	44,96,113	1.68	10 (22%)
23	CLA	c	5503	3	40,58,73	1.28	5 (12%)	44,95,113	1.59	7 (15%)
28	BCR	c	5504	-	41,41,41	2.07	7 (17%)	56,56,56	2.17	22 (39%)
28	BCR	c	5505	-	41,41,41	1.94	8 (19%)	56,56,56	2.14	19 (33%)
28	BCR	c	5506	-	41,41,41	1.93	9 (21%)	56,56,56	2.14	20 (35%)
30	DGD	c	5507	-	54,54,67	1.43	9 (16%)	68,68,81	1.50	6 (8%)
30	DGD	c	5508	-	48,48,67	1.44	8 (16%)	62,62,81	1.77	12 (19%)
30	DGD	c	5509	-	58,58,67	1.31	6 (10%)	72,72,81	1.39	5 (6%)
21	BCT	d	5353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	5354	4	55,73,73	1.06	5 (9%)	61,113,113	1.45	8 (13%)
23	CLA	d	5355	-	40,58,73	1.32	4 (10%)	44,95,113	1.62	8 (18%)
26	PQ9	d	5356	-	30,30,45	0.79	0	38,39,57	1.71	7 (18%)
28	BCR	d	5357	-	41,41,41	1.97	9 (21%)	56,56,56	2.34	20 (35%)
32	SQD	d	5358	-	53,54,54	2.40	27 (50%)	61,65,65	2.67	18 (29%)
29	MGE	d	5359	-	47,47,48	1.11	5 (10%)	55,55,56	0.99	3 (5%)
29	MGE	d	5360	-	41,41,48	1.17	5 (12%)	49,49,56	1.06	5 (10%)
29	MGE	d	5361	-	48,48,48	1.02	4 (8%)	56,56,56	1.07	4 (7%)
25	HEM	f	5051	5,6	30,50,50	2.44	15 (50%)	24,82,82	3.20	10 (41%)
28	BCR	h	5107	-	41,41,41	1.96	7 (17%)	56,56,56	2.28	24 (42%)
30	DGD	h	5208	-	55,55,67	1.35	9 (16%)	69,69,81	1.60	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	MGE	i	5201	-	48,48,48	1.22	8 (16%)	56,56,56	1.12	5 (8%)
29	MGE	l	5210	-	48,48,48	0.87	3 (6%)	56,56,56	1.14	5 (8%)
33	LMT	m	216	-	36,36,36	1.42	7 (19%)	47,47,47	0.97	1 (2%)
28	BCR	t	104	-	41,41,41	1.63	9 (21%)	56,56,56	2.27	22 (39%)
32	SQD	t	213	-	46,47,54	2.75	22 (47%)	54,58,65	2.67	14 (25%)
33	LMT	t	5217	-	36,36,36	1.42	5 (13%)	47,47,47	0.99	3 (6%)
25	HEM	v	5552	16	30,50,50	2.53	11 (36%)	24,82,82	3.43	8 (33%)
28	BCR	x	5130	-	41,41,41	1.94	8 (19%)	56,56,56	2.51	23 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	A	5212	-	-	0/19/39/69	0/1/1/1
23	CLA	A	558	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	559	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	560	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	561	-	-	0/53/103/103	0/1/6/6
24	PHO	A	562	-	-	0/53/103/103	0/1/6/6
23	CLA	A	563	-	3/3/18/25	0/25/123/135	0/0/9/9
26	PQ9	A	564	-	-	0/23/43/61	0/1/1/1
27	OEC	A	565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	A	566	-	-	0/29/63/63	0/2/2/2
31	LHG	A	567	-	-	0/43/43/53	0/0/0/0
32	SQD	A	568	-	-	0/49/69/69	0/1/1/1
33	LMT	A	569	-	-	0/21/61/61	0/2/2/2
23	CLA	B	511	-	3/3/15/25	0/8/106/135	0/0/9/9
23	CLA	B	512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	514	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	515	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	516	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	517	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	518	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	519	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	520	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	522	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	523	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	524	2	3/3/18/25	0/27/125/135	0/0/9/9
23	CLA	B	525	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	526	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	B	527	-	-	0/29/63/63	0/2/2/2
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
29	MGE	B	530	-	-	0/43/63/63	0/1/1/1
23	CLA	C	491	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	492	3	3/3/19/25	0/31/129/135	0/0/9/9
23	CLA	C	493	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	494	-	3/3/16/25	0/15/113/135	0/0/9/9
23	CLA	C	495	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	496	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	497	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	498	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	499	-	3/3/16/25	0/16/114/135	0/0/9/9
23	CLA	C	500	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	501	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	3/3/17/25	0/21/119/135	0/0/9/9
23	CLA	C	503	3	3/3/17/25	0/19/117/135	0/0/9/9
28	BCR	C	504	-	-	0/29/63/63	0/2/2/2
28	BCR	C	505	-	-	0/29/63/63	0/2/2/2
28	BCR	C	506	-	-	0/29/63/63	0/2/2/2
30	DGD	C	507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	C	509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	D	355	-	3/3/17/25	0/19/117/135	0/0/9/9
26	PQ9	D	356	-	-	0/23/43/61	0/1/1/1
28	BCR	D	357	-	-	0/29/63/63	0/2/2/2
29	MGE	D	358	-	-	0/42/62/63	0/1/1/1
29	MGE	D	359	-	-	0/36/56/63	0/1/1/1
29	MGE	D	360	-	-	0/43/63/63	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	HEM	F	51	5,6	-	0/10/54/54	0/0/8/8
28	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	I	201	-	-	0/43/63/63	0/1/1/1
29	MGE	L	210	-	-	0/43/63/63	0/1/1/1
32	SQD	L	5213	-	-	0/42/62/69	0/1/1/1
33	LMT	M	5216	-	-	0/21/61/61	0/2/2/2
33	LMT	T	217	-	-	0/21/61/61	0/2/2/2
28	BCR	T	5104	-	-	0/29/63/63	0/2/2/2
25	HEM	V	552	16	-	0/10/54/54	0/0/8/8
28	BCR	X	130	-	-	0/29/63/63	0/2/2/2
32	SQD	a	212	-	-	0/19/39/69	0/1/1/1
23	CLA	a	5558	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	5559	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	5560	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	5561	-	-	0/53/103/103	0/1/6/6
24	PHO	a	5562	-	-	0/53/103/103	0/1/6/6
23	CLA	a	5563	-	3/3/18/25	0/25/123/135	0/0/9/9
26	PQ9	a	5564	-	-	0/23/43/61	0/1/1/1
27	OEC	a	5565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	a	5566	-	-	0/29/63/63	0/2/2/2
31	LHG	a	5567	-	-	0/43/43/53	0/0/0/0
33	LMT	a	5568	-	-	0/21/61/61	0/2/2/2
23	CLA	b	5511	-	3/3/15/25	0/8/106/135	0/0/9/9
23	CLA	b	5512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5514	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5515	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5516	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5517	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5518	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5519	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5520	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5522	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5523	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	5524	2	3/3/18/25	0/27/125/135	0/0/9/9
23	CLA	b	5525	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	5526	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	b	5527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5528	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5529	-	-	0/29/63/63	0/2/2/2
29	MGE	b	5530	-	-	0/43/63/63	0/1/1/1
23	CLA	c	5491	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5492	3	3/3/19/25	0/31/129/135	0/0/9/9
23	CLA	c	5493	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5494	-	3/3/16/25	0/15/113/135	0/0/9/9
23	CLA	c	5495	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5496	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5497	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5498	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5499	-	3/3/16/25	0/16/114/135	0/0/9/9
23	CLA	c	5500	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5501	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	5502	-	3/3/17/25	0/21/119/135	0/0/9/9
23	CLA	c	5503	3	3/3/17/25	0/19/117/135	0/0/9/9
28	BCR	c	5504	-	-	0/29/63/63	0/2/2/2
28	BCR	c	5505	-	-	0/29/63/63	0/2/2/2
28	BCR	c	5506	-	-	0/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	c	5509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	d	5353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	5354	4	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	d	5355	-	3/3/17/25	0/19/117/135	0/0/9/9
26	PQ9	d	5356	-	-	0/23/43/61	0/1/1/1
28	BCR	d	5357	-	-	0/29/63/63	0/2/2/2
32	SQD	d	5358	-	-	0/49/69/69	0/1/1/1
29	MGE	d	5359	-	-	0/42/62/63	0/1/1/1
29	MGE	d	5360	-	-	0/36/56/63	0/1/1/1
29	MGE	d	5361	-	-	0/43/63/63	0/1/1/1
25	HEM	f	5051	5,6	-	0/10/54/54	0/0/8/8
28	BCR	h	5107	-	-	0/29/63/63	0/2/2/2
30	DGD	h	5208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	i	5201	-	-	0/43/63/63	0/1/1/1
29	MGE	l	5210	-	-	0/43/63/63	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	m	216	-	-	0/21/61/61	0/2/2/2
28	BCR	t	104	-	-	0/29/63/63	0/2/2/2
32	SQD	t	213	-	-	0/42/62/69	0/1/1/1
33	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
25	HEM	v	5552	16	-	0/10/54/54	0/0/8/8
28	BCR	x	5130	-	-	0/29/63/63	0/2/2/2

All (831) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	552	HEM	C3B-C4B	-6.53	1.46	1.51
25	v	5552	HEM	C3B-C4B	-6.00	1.46	1.51
25	f	5051	HEM	C2D-C3D	-5.15	1.39	1.54
25	F	51	HEM	C2D-C3D	-4.90	1.39	1.54
25	v	5552	HEM	CAD-C3D	-4.68	1.44	1.54
25	v	5552	HEM	C2D-C3D	-4.66	1.40	1.54
25	V	552	HEM	C2D-C3D	-4.42	1.41	1.54
25	V	552	HEM	CAD-C3D	-4.19	1.45	1.54
25	f	5051	HEM	C3D-C4D	-4.01	1.46	1.51
25	F	51	HEM	C3D-C4D	-4.00	1.46	1.51
25	f	5051	HEM	CAD-C3D	-3.95	1.46	1.54
25	F	51	HEM	CAD-C3D	-3.95	1.46	1.54
25	v	5552	HEM	C3D-C4D	-3.89	1.46	1.51
25	V	552	HEM	C3D-C4D	-3.85	1.46	1.51
25	f	5051	HEM	C3B-C4B	-3.57	1.48	1.51
25	V	552	HEM	C2D-C1D	-3.55	1.40	1.51
25	v	5552	HEM	C2D-C1D	-3.51	1.40	1.51
25	F	51	HEM	C3B-C4B	-3.51	1.48	1.51
25	F	51	HEM	C2D-C1D	-3.31	1.41	1.51
24	A	562	PHO	CHB-C1B	-3.27	1.32	1.38
25	f	5051	HEM	C2D-C1D	-3.24	1.41	1.51
23	A	563	CLA	C1B-CHB	-3.21	1.31	1.39
23	D	354	CLA	C1B-CHB	-3.18	1.31	1.39
24	a	5562	PHO	CHB-C1B	-3.12	1.33	1.38
32	A	568	SQD	O6-C44	-3.12	1.38	1.43
32	t	213	SQD	C20-C19	-3.01	1.34	1.51
23	a	5563	CLA	C1B-CHB	-3.01	1.31	1.39
23	d	5354	CLA	C1B-CHB	-2.97	1.31	1.39
32	L	5213	SQD	C12-C11	-2.94	1.34	1.51
32	L	5213	SQD	C17-C16	-2.92	1.34	1.51
32	L	5213	SQD	C11-C10	-2.91	1.34	1.51
32	L	5213	SQD	C20-C19	-2.89	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	512	CLA	C1B-CHB	-2.88	1.31	1.39
23	a	5558	CLA	C1B-CHB	-2.86	1.32	1.39
32	d	5358	SQD	O6-C44	-2.85	1.38	1.43
32	t	213	SQD	C19-C18	-2.84	1.35	1.51
32	t	213	SQD	C14-C13	-2.81	1.35	1.51
32	L	5213	SQD	C19-C18	-2.80	1.35	1.51
23	A	560	CLA	C1B-CHB	-2.79	1.32	1.39
23	d	5354	CLA	CAA-CBA	-2.79	1.43	1.52
23	D	354	CLA	CAA-CBA	-2.77	1.43	1.52
32	A	568	SQD	C17-C16	-2.75	1.35	1.51
32	t	213	SQD	C15-C14	-2.74	1.35	1.51
32	L	5213	SQD	C18-C17	-2.74	1.35	1.51
23	C	498	CLA	C1B-CHB	-2.74	1.32	1.39
23	A	558	CLA	C1B-CHB	-2.73	1.32	1.39
23	b	5521	CLA	C1B-CHB	-2.73	1.32	1.39
28	D	357	BCR	C19-C18	-2.72	1.39	1.45
32	L	5213	SQD	C13-C12	-2.72	1.35	1.51
23	B	513	CLA	C1B-CHB	-2.69	1.32	1.39
32	t	213	SQD	C12-C11	-2.69	1.36	1.51
32	t	213	SQD	C11-C10	-2.69	1.36	1.51
23	b	5515	CLA	C1B-CHB	-2.67	1.32	1.39
23	b	5512	CLA	C1B-CHB	-2.67	1.32	1.39
32	A	568	SQD	C12-C11	-2.66	1.36	1.51
32	t	213	SQD	C17-C16	-2.66	1.36	1.51
23	B	520	CLA	C1B-CHB	-2.65	1.32	1.39
32	L	5213	SQD	C15-C14	-2.62	1.36	1.51
28	t	104	BCR	C23-C22	-2.61	1.40	1.45
32	t	213	SQD	C13-C12	-2.60	1.36	1.51
23	B	526	CLA	C1B-CHB	-2.60	1.32	1.39
32	L	5213	SQD	C16-C15	-2.60	1.36	1.51
32	A	568	SQD	C16-C15	-2.60	1.36	1.51
23	c	5496	CLA	C1B-CHB	-2.59	1.32	1.39
23	B	515	CLA	C1B-CHB	-2.58	1.32	1.39
32	d	5358	SQD	C17-C16	-2.58	1.36	1.51
24	A	561	PHO	CAA-CBA	-2.58	1.44	1.52
32	L	5213	SQD	C14-C13	-2.58	1.36	1.51
32	A	568	SQD	C15-C14	-2.57	1.36	1.51
32	A	568	SQD	C11-C10	-2.55	1.36	1.51
23	c	5494	CLA	C1B-CHB	-2.54	1.32	1.39
32	t	213	SQD	C16-C15	-2.53	1.36	1.51
23	C	494	CLA	C1B-CHB	-2.53	1.32	1.39
32	t	213	SQD	C18-C17	-2.51	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	500	CLA	C1B-CHB	-2.51	1.32	1.39
23	a	5559	CLA	C1B-CHB	-2.50	1.32	1.39
23	a	5560	CLA	C1B-CHB	-2.50	1.33	1.39
23	B	525	CLA	C1B-CHB	-2.50	1.33	1.39
25	f	5051	HEM	C2C-C1C	-2.48	1.47	1.52
23	c	5497	CLA	C1B-CHB	-2.47	1.33	1.39
28	c	5506	BCR	C19-C18	-2.46	1.40	1.45
28	b	5527	BCR	C19-C18	-2.46	1.40	1.45
23	B	517	CLA	C1B-CHB	-2.45	1.33	1.39
23	A	558	CLA	CAA-CBA	-2.45	1.44	1.52
23	b	5516	CLA	C1B-CHB	-2.45	1.33	1.39
23	b	5522	CLA	C1B-CHB	-2.43	1.33	1.39
23	b	5526	CLA	C1B-CHB	-2.43	1.33	1.39
32	d	5358	SQD	C32-C31	-2.43	1.37	1.51
32	A	568	SQD	C13-C12	-2.42	1.37	1.51
32	L	5213	SQD	O6-C44	-2.42	1.39	1.43
23	B	521	CLA	C1B-CHB	-2.41	1.33	1.39
32	d	5358	SQD	C20-C19	-2.41	1.37	1.51
32	A	568	SQD	C14-C13	-2.41	1.37	1.51
23	a	5558	CLA	CAA-CBA	-2.41	1.44	1.52
28	T	5104	BCR	C23-C22	-2.39	1.40	1.45
24	a	5561	PHO	CHB-C1B	-2.39	1.34	1.38
23	c	5493	CLA	C1B-CHB	-2.38	1.33	1.39
23	C	492	CLA	C1B-CHB	-2.38	1.33	1.39
23	b	5517	CLA	C1B-CHB	-2.36	1.33	1.39
32	d	5358	SQD	C11-C10	-2.36	1.37	1.51
32	d	5358	SQD	C12-C11	-2.35	1.38	1.51
32	d	5358	SQD	C33-C32	-2.35	1.38	1.51
23	b	5525	CLA	C1B-CHB	-2.34	1.33	1.39
32	a	212	SQD	O6-C44	-2.34	1.39	1.43
32	d	5358	SQD	C15-C14	-2.33	1.38	1.51
23	d	5355	CLA	C1B-CHB	-2.33	1.33	1.39
23	b	5513	CLA	C1B-CHB	-2.33	1.33	1.39
32	d	5358	SQD	C19-C18	-2.32	1.38	1.51
23	b	5524	CLA	C1B-CHB	-2.31	1.33	1.39
23	C	491	CLA	C1B-CHB	-2.31	1.33	1.39
32	A	568	SQD	C33-C32	-2.30	1.38	1.51
32	d	5358	SQD	C16-C15	-2.30	1.38	1.51
28	T	5104	BCR	C29-C28	-2.28	1.46	1.52
23	B	524	CLA	C1B-CHB	-2.28	1.33	1.39
32	A	5212	SQD	O6-C44	-2.28	1.39	1.43
23	A	559	CLA	C1B-CHB	-2.26	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	568	SQD	C32-C31	-2.26	1.38	1.51
24	a	5561	PHO	CAA-CBA	-2.26	1.45	1.52
32	t	213	SQD	C21-C20	-2.26	1.34	1.51
28	t	104	BCR	C29-C28	-2.25	1.46	1.52
24	A	561	PHO	CHB-C1B	-2.25	1.34	1.38
29	b	5530	MGE	O1G-C1G	-2.24	1.40	1.45
32	d	5358	SQD	C14-C13	-2.22	1.38	1.51
23	b	5520	CLA	C1B-CHB	-2.22	1.33	1.39
32	A	568	SQD	C19-C18	-2.22	1.38	1.51
32	d	5358	SQD	C36-C35	-2.21	1.38	1.51
23	c	5492	CLA	C1B-CHB	-2.21	1.33	1.39
23	c	5498	CLA	C1B-CHB	-2.21	1.33	1.39
23	B	516	CLA	C1B-CHB	-2.20	1.33	1.39
23	d	5354	CLA	C3A-C4A	-2.20	1.44	1.51
32	A	568	SQD	C18-C17	-2.20	1.38	1.51
23	B	523	CLA	C1B-CHB	-2.19	1.33	1.39
23	C	493	CLA	C1B-CHB	-2.18	1.33	1.39
28	B	527	BCR	C19-C18	-2.18	1.41	1.45
32	A	568	SQD	C35-C34	-2.18	1.38	1.51
32	A	568	SQD	C34-C33	-2.17	1.39	1.51
32	d	5358	SQD	C13-C12	-2.16	1.39	1.51
32	L	5213	SQD	C21-C20	-2.14	1.35	1.51
32	A	568	SQD	C20-C19	-2.14	1.39	1.51
32	d	5358	SQD	C35-C34	-2.14	1.39	1.51
32	A	568	SQD	C36-C35	-2.11	1.39	1.51
23	c	5500	CLA	C1B-CHB	-2.11	1.34	1.39
23	b	5512	CLA	CAA-CBA	-2.11	1.45	1.52
23	B	522	CLA	C1B-CHB	-2.10	1.34	1.39
32	d	5358	SQD	C34-C33	-2.10	1.39	1.51
23	D	354	CLA	C3B-C2B	-2.09	1.37	1.40
23	a	5558	CLA	CBA-CGA	-2.09	1.44	1.50
28	c	5505	BCR	C19-C18	-2.08	1.41	1.45
23	C	502	CLA	C1B-CHB	-2.08	1.34	1.39
32	d	5358	SQD	C18-C17	-2.07	1.39	1.51
23	c	5499	CLA	C1B-CHB	-2.07	1.34	1.39
23	B	521	CLA	CBA-CGA	-2.07	1.44	1.50
23	b	5515	CLA	C3A-C2A	-2.07	1.48	1.54
23	B	514	CLA	C1B-CHB	-2.06	1.34	1.39
23	c	5502	CLA	C1B-CHB	-2.04	1.34	1.39
28	A	566	BCR	C19-C18	-2.03	1.41	1.45
24	a	5561	PHO	CBA-CGA	-2.03	1.44	1.50
23	d	5354	CLA	CBA-CGA	-2.03	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	5492	CLA	C1C-NC	-2.02	1.34	1.37
28	d	5357	BCR	C19-C18	-2.02	1.41	1.45
28	C	505	BCR	C19-C18	-2.02	1.41	1.45
28	C	506	BCR	C19-C18	-2.01	1.41	1.45
28	b	5527	BCR	C23-C22	-2.01	1.41	1.45
23	b	5523	CLA	C1B-CHB	-2.01	1.34	1.39
24	A	562	PHO	C1D-C2D	-2.00	1.41	1.45
30	c	5509	DGD	O1G-C1A	2.00	1.39	1.33
25	F	51	HEM	C2A-C3A	2.00	1.43	1.37
32	A	5212	SQD	C8-C7	2.00	1.56	1.49
33	m	216	LMT	C1'-C2'	2.01	1.58	1.52
23	A	558	CLA	CAA-C2A	2.01	1.58	1.54
23	c	5502	CLA	CMB-C2B	2.01	1.55	1.51
23	C	503	CLA	C4-C3	2.01	1.56	1.50
23	C	501	CLA	C4-C3	2.01	1.55	1.50
23	B	521	CLA	C1C-C2C	2.01	1.48	1.44
23	B	517	CLA	CMB-C2B	2.01	1.55	1.51
29	i	5201	MGE	C3G-C2G	2.01	1.56	1.50
28	T	5104	BCR	C37-C22	2.02	1.55	1.50
32	A	568	SQD	C24-C23	2.02	1.56	1.50
25	f	5051	HEM	C2A-C3A	2.02	1.43	1.37
28	d	5357	BCR	C14-C13	2.03	1.38	1.35
28	B	528	BCR	C24-C23	2.03	1.39	1.33
25	V	552	HEM	C2A-C3A	2.03	1.43	1.37
23	C	493	CLA	C4-C3	2.03	1.55	1.50
30	H	208	DGD	C4E-C3E	2.03	1.57	1.52
24	A	562	PHO	CHD-C1D	2.03	1.42	1.38
29	i	5201	MGE	C3D-C2D	2.03	1.57	1.52
29	l	5210	MGE	O6D-C5D	2.03	1.49	1.44
23	c	5503	CLA	CHC-C1C	2.03	1.41	1.35
30	h	5208	DGD	C4E-C5E	2.04	1.57	1.53
30	C	508	DGD	O6D-C5D	2.04	1.49	1.44
28	b	5528	BCR	C24-C23	2.04	1.39	1.33
30	C	509	DGD	C3D-C2D	2.04	1.57	1.52
29	D	358	MGE	O2G-C1B	2.04	1.40	1.34
23	b	5514	CLA	C4-C3	2.04	1.55	1.50
23	C	500	CLA	CMD-C2D	2.04	1.56	1.51
24	a	5562	PHO	CMD-C2D	2.05	1.55	1.50
23	b	5512	CLA	CHC-C1C	2.05	1.41	1.35
23	B	511	CLA	CHC-C1C	2.05	1.41	1.35
30	H	208	DGD	O6E-C5E	2.05	1.49	1.44
23	B	526	CLA	C1-C2	2.05	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	513	CLA	C2-C3	2.06	1.37	1.33
28	c	5506	BCR	C14-C13	2.06	1.38	1.35
29	I	201	MGE	C3G-C2G	2.06	1.56	1.50
23	C	492	CLA	C5-C3	2.06	1.56	1.51
29	d	5361	MGE	O2G-C1B	2.07	1.40	1.34
23	A	563	CLA	CAA-C2A	2.07	1.58	1.54
23	B	519	CLA	C4-C3	2.07	1.55	1.50
23	b	5520	CLA	C4-C3	2.07	1.55	1.50
23	B	517	CLA	C2-C3	2.08	1.37	1.33
23	C	498	CLA	C4-C3	2.08	1.55	1.50
33	m	216	LMT	C4B-C3B	2.08	1.57	1.52
23	B	524	CLA	CAA-C2A	2.08	1.58	1.54
23	A	560	CLA	C4-C3	2.08	1.55	1.50
23	D	354	CLA	C1C-C2C	2.08	1.48	1.44
23	c	5491	CLA	CHC-C1C	2.09	1.41	1.35
28	X	130	BCR	C10-C9	2.09	1.38	1.35
23	b	5523	CLA	C5-C3	2.09	1.56	1.51
33	M	5216	LMT	C4B-C5B	2.09	1.57	1.53
30	H	208	DGD	C1D-C2D	2.09	1.58	1.52
33	a	5568	LMT	O5B-C5B	2.09	1.49	1.44
23	c	5492	CLA	CAA-C2A	2.09	1.58	1.54
32	L	5213	SQD	C8-C7	2.10	1.56	1.50
29	D	359	MGE	O6D-C5D	2.10	1.49	1.44
23	C	500	CLA	C4-C3	2.10	1.55	1.50
30	h	5208	DGD	C4E-C3E	2.10	1.57	1.52
23	b	5511	CLA	CHC-C1C	2.10	1.41	1.35
23	c	5499	CLA	C1C-C2C	2.10	1.48	1.44
23	c	5503	CLA	C1-C2	2.10	1.55	1.49
23	C	491	CLA	CHC-C1C	2.10	1.41	1.35
32	A	568	SQD	O6-C1	2.10	1.43	1.40
23	C	502	CLA	CMB-C2B	2.10	1.56	1.51
28	t	104	BCR	C35-C13	2.11	1.55	1.50
33	a	5568	LMT	C1B-C2B	2.11	1.58	1.52
30	C	509	DGD	O2G-C1B	2.11	1.40	1.34
23	c	5499	CLA	CHC-C1C	2.11	1.41	1.35
23	C	495	CLA	C4C-C3C	2.11	1.48	1.45
28	C	506	BCR	C35-C13	2.11	1.55	1.50
33	m	216	LMT	O5'-C5'	2.11	1.49	1.44
29	b	5530	MGE	C1D-C2D	2.12	1.58	1.52
33	M	5216	LMT	O5B-C1B	2.12	1.47	1.41
23	b	5520	CLA	C1C-C2C	2.12	1.48	1.44
23	B	523	CLA	CAA-C2A	2.12	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	519	CLA	CMD-C2D	2.12	1.56	1.51
23	B	515	CLA	CAA-C2A	2.12	1.58	1.54
23	c	5502	CLA	CMD-C2D	2.12	1.56	1.51
23	C	495	CLA	C4-C3	2.13	1.55	1.50
23	A	560	CLA	CHC-C1C	2.13	1.42	1.35
30	c	5508	DGD	O6D-C5D	2.13	1.49	1.44
23	C	496	CLA	C1C-C2C	2.13	1.48	1.44
32	t	213	SQD	O6-C1	2.13	1.44	1.40
23	B	518	CLA	C2-C3	2.13	1.37	1.33
26	D	356	PQ9	C3-C4	2.13	1.50	1.44
24	a	5561	PHO	C2-C3	2.13	1.37	1.33
29	d	5359	MGE	C4D-C5D	2.13	1.57	1.53
23	c	5503	CLA	C4-C3	2.14	1.56	1.50
23	B	511	CLA	CMC-C2C	2.14	1.55	1.50
23	b	5513	CLA	C5-C3	2.14	1.56	1.51
28	D	357	BCR	C14-C13	2.14	1.38	1.35
29	D	359	MGE	O1G-C1A	2.14	1.39	1.33
28	x	5130	BCR	C24-C23	2.14	1.39	1.33
33	M	5216	LMT	C1'-C2'	2.14	1.59	1.52
28	D	357	BCR	C38-C26	2.14	1.54	1.51
23	b	5515	CLA	CHC-C1C	2.14	1.42	1.35
29	b	5530	MGE	O2G-C1B	2.14	1.40	1.34
28	X	130	BCR	C24-C23	2.14	1.39	1.33
23	D	355	CLA	C1C-C2C	2.15	1.48	1.44
23	B	512	CLA	CHC-C1C	2.15	1.42	1.35
23	c	5498	CLA	C1C-C2C	2.15	1.48	1.44
23	a	5563	CLA	C4-C3	2.15	1.55	1.50
29	L	210	MGE	C4D-C3D	2.15	1.58	1.52
30	c	5507	DGD	C4D-C5D	2.15	1.57	1.53
23	c	5493	CLA	CMB-C2B	2.16	1.56	1.51
23	b	5520	CLA	CHC-C1C	2.16	1.42	1.35
23	b	5522	CLA	C4-C3	2.16	1.56	1.50
32	a	212	SQD	O48-C23	2.16	1.44	1.33
23	b	5523	CLA	CHC-C1C	2.16	1.42	1.35
33	M	5216	LMT	C3B-C2B	2.17	1.58	1.52
29	i	5201	MGE	O3G-C1D	2.17	1.44	1.40
23	B	523	CLA	CHC-C1C	2.17	1.42	1.35
23	C	492	CLA	CAA-C2A	2.17	1.58	1.54
23	B	515	CLA	CHC-C1C	2.17	1.42	1.35
30	h	5208	DGD	C3E-C2E	2.17	1.58	1.52
33	M	5216	LMT	C1B-C2B	2.17	1.59	1.52
29	d	5360	MGE	O3G-C1D	2.17	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	5530	MGE	C4D-C3D	2.17	1.58	1.52
23	b	5516	CLA	CHC-C1C	2.18	1.42	1.35
28	B	527	BCR	C38-C26	2.18	1.54	1.51
23	B	521	CLA	C4-C3	2.18	1.56	1.50
30	h	5208	DGD	C1D-C2D	2.18	1.59	1.52
29	l	5210	MGE	C4D-C3D	2.20	1.58	1.52
29	B	530	MGE	C4D-C5D	2.20	1.57	1.53
30	C	507	DGD	O6E-C5E	2.20	1.49	1.44
23	B	514	CLA	CHC-C1C	2.20	1.42	1.35
28	X	130	BCR	C14-C13	2.20	1.38	1.35
23	B	515	CLA	C4-C3	2.21	1.56	1.50
23	C	500	CLA	CHC-C1C	2.21	1.42	1.35
23	c	5500	CLA	CHC-C1C	2.21	1.42	1.35
28	C	506	BCR	C14-C13	2.21	1.38	1.35
23	c	5496	CLA	CHC-C1C	2.21	1.42	1.35
23	d	5355	CLA	C1C-C2C	2.21	1.49	1.44
23	b	5520	CLA	C4C-C3C	2.22	1.49	1.45
28	c	5504	BCR	C5-C6	2.22	1.37	1.34
28	B	527	BCR	C1-C6	2.22	1.56	1.53
23	b	5519	CLA	CHC-C1C	2.22	1.42	1.35
28	T	5104	BCR	C30-C25	2.22	1.56	1.53
30	h	5208	DGD	O6D-C1D	2.22	1.47	1.41
23	c	5499	CLA	C4C-C3C	2.23	1.49	1.45
24	a	5561	PHO	CHD-C1D	2.23	1.43	1.38
23	B	518	CLA	C4-C3	2.23	1.56	1.50
28	C	504	BCR	C14-C13	2.23	1.38	1.35
23	C	499	CLA	OBD-CAD	2.23	1.25	1.22
29	D	360	MGE	O6D-C5D	2.24	1.50	1.44
23	c	5502	CLA	C2-C3	2.24	1.37	1.33
30	c	5508	DGD	C4E-C3E	2.24	1.58	1.52
23	b	5526	CLA	CHC-C1C	2.24	1.42	1.35
23	B	519	CLA	CHC-C1C	2.24	1.42	1.35
25	v	5552	HEM	CMA-C3A	2.24	1.56	1.51
23	b	5519	CLA	C1C-C2C	2.24	1.49	1.44
23	C	502	CLA	C4-C3	2.24	1.56	1.50
23	a	5560	CLA	C4-C3	2.25	1.56	1.50
23	C	496	CLA	CHC-C1C	2.25	1.42	1.35
30	c	5507	DGD	O6E-C5E	2.25	1.50	1.44
33	a	5568	LMT	O5B-C1B	2.25	1.47	1.41
28	T	5104	BCR	C26-C25	2.25	1.37	1.34
23	a	5563	CLA	CHC-C1C	2.25	1.42	1.35
23	A	563	CLA	C5-C3	2.26	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	493	CLA	CHC-C1C	2.26	1.42	1.35
23	c	5495	CLA	C4-C3	2.27	1.56	1.50
23	B	511	CLA	C4C-NC	2.27	1.41	1.37
32	d	5358	SQD	C24-C23	2.27	1.57	1.50
23	B	516	CLA	CHC-C1C	2.27	1.42	1.35
30	C	509	DGD	O1G-C1A	2.27	1.40	1.33
23	C	494	CLA	CHC-C1C	2.28	1.42	1.35
32	a	212	SQD	C44-C45	2.28	1.57	1.50
23	b	5511	CLA	CMD-C2D	2.28	1.56	1.51
32	A	5212	SQD	C44-C45	2.28	1.57	1.50
28	a	5566	BCR	C14-C13	2.28	1.38	1.35
32	A	568	SQD	C8-C7	2.28	1.57	1.50
29	i	5201	MGE	C2A-C1A	2.29	1.57	1.50
28	b	5527	BCR	C1-C6	2.29	1.57	1.53
29	I	201	MGE	C4D-C3D	2.30	1.58	1.52
29	d	5361	MGE	O6D-C5D	2.30	1.50	1.44
30	c	5508	DGD	O5D-C1E	2.30	1.44	1.40
29	b	5530	MGE	C4D-C5D	2.30	1.58	1.53
25	v	5552	HEM	C2A-C3A	2.31	1.44	1.37
23	b	5516	CLA	OBD-CAD	2.32	1.25	1.22
29	I	201	MGE	O3G-C1D	2.32	1.44	1.40
23	C	503	CLA	CHC-C1C	2.32	1.42	1.35
25	V	552	HEM	CMA-C3A	2.33	1.56	1.51
30	C	507	DGD	C4D-C5D	2.33	1.58	1.53
23	B	525	CLA	CHC-C1C	2.33	1.42	1.35
23	c	5498	CLA	C4-C3	2.33	1.56	1.50
30	c	5507	DGD	O6D-C5D	2.33	1.50	1.44
23	c	5495	CLA	C1C-C2C	2.34	1.49	1.44
30	c	5509	DGD	C4E-C5E	2.34	1.58	1.53
23	C	500	CLA	C4C-C3C	2.34	1.49	1.45
23	c	5497	CLA	CHC-C1C	2.34	1.42	1.35
28	b	5528	BCR	C26-C25	2.34	1.38	1.34
23	b	5520	CLA	CAA-C2A	2.35	1.58	1.54
23	c	5498	CLA	CAA-C2A	2.35	1.58	1.54
28	c	5506	BCR	C10-C9	2.36	1.38	1.35
23	c	5491	CLA	C4-C3	2.36	1.56	1.50
25	f	5051	HEM	FE-NB	2.36	2.10	1.97
28	X	130	BCR	C33-C5	2.36	1.54	1.51
32	d	5358	SQD	C8-C7	2.36	1.57	1.50
24	A	561	PHO	C4-C3	2.36	1.56	1.50
33	m	216	LMT	O5B-C1B	2.36	1.47	1.41
23	C	497	CLA	CHC-C1C	2.37	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	517	CLA	CHC-C1C	2.37	1.42	1.35
23	d	5354	CLA	CHC-C1C	2.37	1.42	1.35
33	a	5568	LMT	C1'-C2'	2.38	1.59	1.52
28	c	5504	BCR	C10-C9	2.38	1.38	1.35
23	c	5497	CLA	C4-C3	2.38	1.56	1.50
28	a	5566	BCR	C29-C30	2.38	1.59	1.54
23	b	5517	CLA	C2-C3	2.38	1.37	1.33
33	A	569	LMT	C1B-C2B	2.38	1.59	1.52
24	a	5562	PHO	C4-C3	2.39	1.56	1.50
33	m	216	LMT	O5'-C1'	2.39	1.48	1.41
23	B	511	CLA	CMD-C2D	2.39	1.56	1.51
23	A	559	CLA	CAA-C2A	2.39	1.58	1.54
33	t	5217	LMT	C1B-C2B	2.40	1.59	1.52
33	M	5216	LMT	O5'-C1'	2.41	1.48	1.41
23	D	355	CLA	CHC-C1C	2.41	1.42	1.35
28	h	5107	BCR	C14-C13	2.41	1.38	1.35
23	B	525	CLA	CAA-C2A	2.42	1.58	1.54
23	c	5501	CLA	C1C-C2C	2.42	1.49	1.44
25	F	51	HEM	FE-NB	2.42	2.10	1.97
23	a	5563	CLA	C5-C3	2.42	1.56	1.51
32	A	568	SQD	O5-C1	2.42	1.48	1.41
25	f	5051	HEM	CAD-CBD	2.42	1.64	1.52
23	B	511	CLA	C1C-C2C	2.42	1.49	1.44
29	B	530	MGE	O2G-C1B	2.43	1.41	1.34
23	b	5526	CLA	C2-C3	2.43	1.37	1.33
24	a	5562	PHO	CHC-C1C	2.43	1.43	1.38
29	I	201	MGE	O6D-C1D	2.44	1.48	1.41
23	B	524	CLA	CHC-C1C	2.44	1.42	1.35
23	C	501	CLA	CAA-C2A	2.44	1.59	1.54
23	b	5511	CLA	C3C-C2C	2.44	1.41	1.36
23	b	5524	CLA	CHC-C1C	2.44	1.42	1.35
29	B	530	MGE	C1D-C2D	2.45	1.59	1.52
23	C	501	CLA	CHC-C1C	2.45	1.43	1.35
29	B	530	MGE	O6D-C5D	2.45	1.50	1.44
23	C	496	CLA	C2-C3	2.45	1.37	1.33
23	B	521	CLA	CHC-C1C	2.45	1.43	1.35
23	c	5496	CLA	C4-C3	2.46	1.56	1.50
23	B	511	CLA	C3C-C2C	2.46	1.42	1.36
32	a	212	SQD	C8-C7	2.46	1.58	1.49
23	C	496	CLA	CAA-C2A	2.47	1.59	1.54
24	A	561	PHO	CHD-C1D	2.47	1.43	1.38
23	a	5558	CLA	CAA-C2A	2.47	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	514	CLA	C4-C3	2.47	1.56	1.50
23	B	513	CLA	C4-C3	2.47	1.56	1.50
23	C	491	CLA	C4-C3	2.47	1.56	1.50
23	c	5502	CLA	C4-C3	2.48	1.56	1.50
25	F	51	HEM	CHC-C1C	2.48	1.42	1.36
33	A	569	LMT	O5B-C1B	2.48	1.48	1.41
23	c	5502	CLA	CAA-C2A	2.48	1.59	1.54
32	A	5212	SQD	C6-S	2.48	1.81	1.77
30	c	5508	DGD	C1E-C2E	2.49	1.60	1.52
28	a	5566	BCR	C26-C25	2.49	1.38	1.34
23	b	5517	CLA	CHC-C1C	2.49	1.43	1.35
23	B	520	CLA	C4C-C3C	2.49	1.49	1.45
23	C	492	CLA	C4-C3	2.49	1.56	1.50
23	c	5493	CLA	CHC-C1C	2.49	1.43	1.35
30	C	507	DGD	O6D-C5D	2.49	1.50	1.44
23	B	518	CLA	CHC-C1C	2.50	1.43	1.35
23	c	5501	CLA	CHC-C1C	2.50	1.43	1.35
33	T	217	LMT	O1B-C4'	2.50	1.50	1.43
23	b	5525	CLA	CHC-C1C	2.50	1.43	1.35
24	A	562	PHO	C3B-C4B	2.51	1.49	1.43
23	C	493	CLA	CAA-C2A	2.51	1.59	1.54
28	T	5104	BCR	C29-C30	2.51	1.60	1.54
23	A	563	CLA	CHC-C1C	2.51	1.43	1.35
23	c	5494	CLA	CHC-C1C	2.51	1.43	1.35
23	b	5515	CLA	C4-C3	2.51	1.56	1.50
30	H	208	DGD	O6E-C1E	2.51	1.48	1.41
33	A	569	LMT	O5B-C5B	2.52	1.50	1.44
29	d	5359	MGE	O6D-C5D	2.52	1.50	1.44
23	c	5495	CLA	CHC-C1C	2.52	1.43	1.35
28	h	5107	BCR	C5-C6	2.52	1.38	1.34
23	C	497	CLA	C4-C3	2.52	1.56	1.50
29	D	360	MGE	O6D-C1D	2.52	1.48	1.41
33	t	5217	LMT	O1B-C4'	2.53	1.50	1.43
23	B	520	CLA	C4-C3	2.53	1.56	1.50
30	c	5507	DGD	C1E-C2E	2.53	1.60	1.52
23	B	513	CLA	C5-C3	2.53	1.57	1.51
23	c	5496	CLA	C1C-C2C	2.53	1.49	1.44
23	A	563	CLA	C4-C3	2.53	1.56	1.50
23	C	495	CLA	CAA-C2A	2.53	1.59	1.54
30	H	208	DGD	C1E-C2E	2.54	1.60	1.52
23	b	5525	CLA	CAA-C2A	2.54	1.59	1.54
23	C	502	CLA	CHC-C1C	2.54	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	508	DGD	C4D-C3D	2.54	1.59	1.52
23	b	5518	CLA	CHC-C1C	2.54	1.43	1.35
23	B	514	CLA	CAA-C2A	2.55	1.59	1.54
29	I	201	MGE	O6D-C5D	2.55	1.50	1.44
23	D	354	CLA	CHC-C1C	2.55	1.43	1.35
30	h	5208	DGD	O5D-C1E	2.55	1.44	1.40
29	I	201	MGE	O2G-C1B	2.55	1.41	1.34
32	d	5358	SQD	O5-C1	2.55	1.48	1.41
30	c	5509	DGD	O6D-C5D	2.55	1.50	1.44
23	A	558	CLA	CHC-C1C	2.55	1.43	1.35
23	C	495	CLA	CHC-C1C	2.56	1.43	1.35
24	a	5562	PHO	C3B-C4B	2.56	1.49	1.43
30	H	208	DGD	O6D-C5D	2.56	1.50	1.44
30	C	509	DGD	O6D-C5D	2.57	1.50	1.44
29	D	359	MGE	C4D-C3D	2.57	1.59	1.52
23	c	5497	CLA	CAA-C2A	2.57	1.59	1.54
25	f	5051	HEM	CMA-C3A	2.57	1.56	1.51
23	B	511	CLA	C3B-C2B	2.58	1.43	1.40
23	d	5355	CLA	CHC-C1C	2.58	1.43	1.35
25	f	5051	HEM	CHC-C1C	2.58	1.42	1.36
30	C	508	DGD	C3D-C2D	2.58	1.59	1.52
23	C	496	CLA	C4C-C3C	2.58	1.49	1.45
33	m	216	LMT	O1'-C1'	2.59	1.44	1.40
23	b	5513	CLA	C4-C3	2.59	1.57	1.50
29	d	5360	MGE	O6D-C5D	2.59	1.50	1.44
32	t	213	SQD	O5-C1	2.59	1.48	1.41
29	i	5201	MGE	O6D-C1D	2.60	1.48	1.41
30	C	507	DGD	C3E-C2E	2.60	1.59	1.52
28	A	566	BCR	C29-C30	2.60	1.60	1.54
23	c	5502	CLA	CHC-C1C	2.61	1.43	1.35
23	b	5522	CLA	CHC-C1C	2.61	1.43	1.35
23	b	5514	CLA	CHC-C1C	2.61	1.43	1.35
23	d	5355	CLA	CAA-C2A	2.61	1.59	1.54
23	b	5526	CLA	C1-C2	2.61	1.57	1.49
23	B	511	CLA	C4C-C3C	2.61	1.49	1.45
33	T	217	LMT	O5B-C1B	2.62	1.48	1.41
28	b	5529	BCR	C10-C9	2.62	1.39	1.35
30	C	508	DGD	C1E-C2E	2.62	1.60	1.52
28	B	528	BCR	C5-C6	2.62	1.38	1.34
32	a	212	SQD	O5-C1	2.62	1.48	1.41
23	b	5511	CLA	C4C-NC	2.62	1.42	1.37
28	C	505	BCR	C38-C26	2.62	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	C1C-C2C	2.63	1.49	1.44
33	T	217	LMT	O1B-C1B	2.64	1.48	1.41
30	c	5508	DGD	O1G-C1A	2.64	1.41	1.33
28	B	527	BCR	C2-C1	2.64	1.60	1.54
29	i	5201	MGE	O2G-C1B	2.64	1.42	1.34
23	c	5503	CLA	C1C-C2C	2.65	1.49	1.44
28	B	529	BCR	C10-C9	2.65	1.39	1.35
23	c	5500	CLA	C4-C3	2.66	1.57	1.50
32	A	5212	SQD	O5-C1	2.66	1.48	1.41
30	C	507	DGD	O3G-C1D	2.66	1.44	1.40
23	b	5518	CLA	CAA-C2A	2.67	1.59	1.54
24	A	562	PHO	CHC-C1C	2.67	1.44	1.38
23	c	5498	CLA	CHC-C1C	2.67	1.43	1.35
29	d	5359	MGE	C4D-C3D	2.67	1.59	1.52
23	b	5521	CLA	CAA-C2A	2.67	1.59	1.54
30	c	5507	DGD	O3G-C1D	2.68	1.45	1.40
23	B	526	CLA	C2-C3	2.68	1.38	1.33
23	c	5493	CLA	CAA-C2A	2.68	1.59	1.54
29	d	5360	MGE	O1G-C1A	2.68	1.41	1.33
30	H	208	DGD	O6D-C1D	2.69	1.48	1.41
26	A	564	PQ9	C11-C2	2.69	1.53	1.51
28	x	5130	BCR	C14-C13	2.69	1.39	1.35
23	C	498	CLA	CHC-C1C	2.69	1.43	1.35
23	c	5500	CLA	CAA-C2A	2.70	1.59	1.54
23	c	5491	CLA	CAA-C2A	2.71	1.59	1.54
33	t	5217	LMT	O5B-C1B	2.72	1.48	1.41
24	A	562	PHO	C4-C3	2.72	1.57	1.50
29	b	5530	MGE	O6D-C5D	2.72	1.51	1.44
30	C	508	DGD	O3G-C1D	2.74	1.45	1.40
30	H	208	DGD	O5D-C1E	2.75	1.45	1.40
30	h	5208	DGD	O6D-C5D	2.75	1.51	1.44
30	c	5508	DGD	C4D-C3D	2.75	1.59	1.52
30	h	5208	DGD	O6E-C1E	2.76	1.48	1.41
30	C	508	DGD	C4E-C3E	2.76	1.59	1.52
23	b	5523	CLA	CAA-C2A	2.76	1.59	1.54
28	A	566	BCR	C26-C25	2.76	1.38	1.34
25	f	5051	HEM	C4C-NC	2.77	1.39	1.36
23	c	5492	CLA	C4-C3	2.77	1.57	1.50
23	B	521	CLA	CAA-C2A	2.78	1.59	1.54
30	c	5507	DGD	C3E-C2E	2.78	1.59	1.52
32	L	5213	SQD	O6-C1	2.78	1.45	1.40
23	C	502	CLA	CAA-C2A	2.79	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	526	CLA	CAA-C2A	2.79	1.59	1.54
33	A	569	LMT	C1'-C2'	2.79	1.60	1.52
25	V	552	HEM	C4C-NC	2.79	1.39	1.36
23	b	5519	CLA	CAA-C2A	2.80	1.59	1.54
32	A	5212	SQD	O6-C1	2.80	1.45	1.40
23	a	5560	CLA	CAA-C2A	2.80	1.59	1.54
30	C	509	DGD	O6D-C1D	2.80	1.49	1.41
25	f	5051	HEM	FE-NC	2.81	2.06	1.95
23	c	5496	CLA	C4C-C3C	2.81	1.50	1.45
28	C	506	BCR	C29-C30	2.81	1.60	1.54
23	b	5513	CLA	CAA-C2A	2.82	1.59	1.54
28	t	104	BCR	C29-C30	2.82	1.60	1.54
29	d	5360	MGE	C4D-C3D	2.82	1.59	1.52
23	B	520	CLA	CAA-C2A	2.83	1.59	1.54
29	D	358	MGE	C4D-C3D	2.83	1.59	1.52
29	D	358	MGE	O6D-C5D	2.83	1.51	1.44
23	B	522	CLA	CHC-C1C	2.84	1.44	1.35
23	B	517	CLA	CAA-C2A	2.84	1.59	1.54
23	C	495	CLA	C1C-C2C	2.85	1.50	1.44
28	b	5528	BCR	C2-C1	2.85	1.61	1.54
29	i	5201	MGE	C4D-C5D	2.86	1.59	1.53
23	a	5563	CLA	CAA-C2A	2.87	1.59	1.54
23	b	5511	CLA	C1C-C2C	2.87	1.50	1.44
23	b	5511	CLA	C4C-C3C	2.87	1.50	1.45
28	b	5529	BCR	C14-C13	2.87	1.39	1.35
23	a	5558	CLA	CHC-C1C	2.88	1.44	1.35
23	C	500	CLA	CAA-C2A	2.89	1.59	1.54
33	A	569	LMT	O5'-C1'	2.90	1.49	1.41
30	C	508	DGD	O1G-C1A	2.92	1.42	1.33
28	B	529	BCR	C14-C13	2.92	1.39	1.35
28	b	5527	BCR	C2-C1	2.92	1.61	1.54
23	b	5514	CLA	CAA-C2A	2.92	1.60	1.54
23	b	5515	CLA	CAA-C2A	2.93	1.60	1.54
29	d	5360	MGE	O6D-C1D	2.93	1.49	1.41
28	A	566	BCR	C30-C25	2.93	1.57	1.53
28	C	504	BCR	C2-C1	2.93	1.61	1.54
28	B	529	BCR	C5-C6	2.93	1.39	1.34
28	a	5566	BCR	C2-C1	2.94	1.61	1.54
23	b	5516	CLA	CAA-C2A	2.95	1.60	1.54
33	a	5568	LMT	O5'-C1'	2.96	1.49	1.41
33	t	5217	LMT	O1B-C1B	2.96	1.49	1.41
23	c	5495	CLA	CAA-C2A	2.97	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	5529	BCR	C5-C6	2.98	1.39	1.34
25	F	51	HEM	FE-NC	2.98	2.07	1.95
28	B	529	BCR	C29-C30	2.99	1.61	1.54
23	C	491	CLA	CAA-C2A	3.00	1.60	1.54
28	B	528	BCR	C2-C1	3.00	1.61	1.54
28	b	5528	BCR	C5-C6	3.00	1.39	1.34
28	C	504	BCR	C5-C6	3.00	1.39	1.34
29	d	5361	MGE	O3G-C1D	3.00	1.45	1.40
32	L	5213	SQD	O5-C1	3.00	1.49	1.41
28	c	5505	BCR	C38-C26	3.01	1.56	1.51
23	B	526	CLA	C5-C3	3.01	1.58	1.51
28	b	5529	BCR	C26-C25	3.01	1.39	1.34
33	m	216	LMT	C3B-C2B	3.02	1.60	1.52
25	v	5552	HEM	C4C-NC	3.02	1.39	1.36
29	d	5359	MGE	O3G-C1D	3.04	1.45	1.40
29	d	5359	MGE	O6D-C1D	3.04	1.49	1.41
32	A	568	SQD	O5-C5	3.04	1.52	1.44
30	C	507	DGD	O6D-C1D	3.05	1.49	1.41
29	b	5530	MGE	O3G-C1D	3.05	1.45	1.40
28	d	5357	BCR	C38-C26	3.05	1.56	1.51
32	d	5358	SQD	O3-C3	3.05	1.50	1.43
28	b	5527	BCR	C26-C25	3.06	1.39	1.34
29	D	360	MGE	O3G-C1D	3.07	1.45	1.40
30	C	508	DGD	O5D-C1E	3.07	1.45	1.40
28	t	104	BCR	C2-C1	3.08	1.61	1.54
28	c	5506	BCR	C29-C30	3.08	1.61	1.54
28	X	130	BCR	C2-C1	3.09	1.61	1.54
25	V	552	HEM	CAA-C2A	3.09	1.57	1.52
23	B	526	CLA	C4-C3	3.10	1.58	1.50
32	a	212	SQD	O6-C1	3.10	1.45	1.40
29	l	5210	MGE	O6D-C1D	3.10	1.49	1.41
32	L	5213	SQD	O47-C7	3.11	1.43	1.34
23	b	5517	CLA	CAA-C2A	3.11	1.60	1.54
23	b	5526	CLA	C5-C3	3.12	1.58	1.51
28	H	107	BCR	C5-C6	3.12	1.39	1.34
23	c	5499	CLA	CAA-C2A	3.14	1.60	1.54
28	b	5527	BCR	C5-C6	3.14	1.39	1.34
23	c	5496	CLA	CAA-C2A	3.14	1.60	1.54
29	D	359	MGE	O6D-C1D	3.14	1.49	1.41
24	a	5561	PHO	C4-C3	3.15	1.58	1.50
28	t	104	BCR	C26-C25	3.15	1.39	1.34
28	H	107	BCR	C14-C13	3.15	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	5522	CLA	CAA-C2A	3.17	1.60	1.54
29	i	5201	MGE	O6D-C5D	3.18	1.52	1.44
28	c	5505	BCR	C29-C30	3.18	1.61	1.54
28	b	5529	BCR	C1-C6	3.19	1.58	1.53
28	x	5130	BCR	C26-C25	3.19	1.39	1.34
23	B	522	CLA	CAA-C2A	3.20	1.60	1.54
32	A	568	SQD	C6-S	3.21	1.82	1.77
23	b	5526	CLA	CAA-C2A	3.21	1.60	1.54
31	A	567	LHG	P-O6	3.21	1.73	1.59
30	C	508	DGD	O6D-C1D	3.22	1.50	1.41
28	d	5357	BCR	C2-C1	3.23	1.61	1.54
30	c	5507	DGD	O6D-C1D	3.23	1.50	1.41
33	t	5217	LMT	O1'-C1'	3.23	1.46	1.40
28	B	529	BCR	C2-C1	3.24	1.61	1.54
31	a	5567	LHG	O7-C7	3.26	1.44	1.34
31	A	567	LHG	O7-C7	3.26	1.44	1.34
23	c	5503	CLA	CAA-C2A	3.26	1.60	1.54
23	B	518	CLA	CAA-C2A	3.27	1.60	1.54
28	b	5527	BCR	C29-C30	3.27	1.62	1.54
28	b	5529	BCR	C2-C1	3.28	1.62	1.54
30	c	5509	DGD	O5D-C1E	3.28	1.46	1.40
28	C	505	BCR	C5-C6	3.28	1.39	1.34
23	B	513	CLA	CAA-C2A	3.28	1.60	1.54
28	T	5104	BCR	C1-C6	3.28	1.58	1.53
28	X	130	BCR	C26-C25	3.29	1.39	1.34
32	A	5212	SQD	C1-C2	3.29	1.62	1.52
28	B	527	BCR	C29-C30	3.29	1.62	1.54
28	c	5505	BCR	C2-C1	3.30	1.62	1.54
32	t	213	SQD	O3-C3	3.30	1.50	1.43
28	A	566	BCR	C2-C1	3.31	1.62	1.54
31	a	5567	LHG	P-O6	3.31	1.74	1.59
23	B	516	CLA	CAA-C2A	3.32	1.60	1.54
32	a	212	SQD	O3-C3	3.33	1.50	1.43
25	F	51	HEM	CMA-C3A	3.33	1.58	1.51
29	B	530	MGE	O6D-C1D	3.36	1.50	1.41
23	C	503	CLA	CAA-C2A	3.36	1.60	1.54
28	x	5130	BCR	C2-C1	3.36	1.62	1.54
28	C	505	BCR	C29-C30	3.36	1.62	1.54
32	L	5213	SQD	O3-C3	3.37	1.51	1.43
28	b	5528	BCR	C29-C30	3.37	1.62	1.54
28	b	5529	BCR	C29-C30	3.37	1.62	1.54
28	c	5504	BCR	C26-C25	3.37	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	506	BCR	C1-C6	3.38	1.58	1.53
32	A	5212	SQD	O3-C3	3.38	1.51	1.43
29	L	210	MGE	O3G-C1D	3.39	1.46	1.40
29	D	358	MGE	O3G-C1D	3.39	1.46	1.40
25	F	51	HEM	C4C-NC	3.39	1.40	1.36
32	t	213	SQD	O47-C7	3.40	1.44	1.34
29	b	5530	MGE	O6D-C1D	3.41	1.50	1.41
30	C	509	DGD	O3G-C1D	3.41	1.46	1.40
28	D	357	BCR	C2-C1	3.41	1.62	1.54
32	d	5358	SQD	O5-C5	3.42	1.52	1.44
32	A	5212	SQD	O5-C5	3.42	1.52	1.44
31	A	567	LHG	P-O3	3.43	1.74	1.59
23	c	5501	CLA	CAA-C2A	3.43	1.61	1.54
23	B	519	CLA	CAA-C2A	3.44	1.61	1.54
30	C	507	DGD	O5D-C1E	3.44	1.46	1.40
30	H	208	DGD	C4E-C5E	3.45	1.60	1.53
28	a	5566	BCR	C5-C6	3.45	1.39	1.34
28	D	357	BCR	C1-C6	3.46	1.58	1.53
31	a	5567	LHG	O8-C23	3.47	1.43	1.33
23	C	494	CLA	CAA-C2A	3.49	1.61	1.54
26	a	5564	PQ9	C11-C2	3.51	1.54	1.51
25	V	552	HEM	FE-NC	3.52	2.09	1.95
28	C	504	BCR	C29-C30	3.52	1.62	1.54
29	D	358	MGE	O6D-C1D	3.54	1.50	1.41
23	D	355	CLA	CAA-C2A	3.54	1.61	1.54
28	c	5504	BCR	C2-C1	3.54	1.62	1.54
28	H	107	BCR	C2-C1	3.55	1.62	1.54
28	d	5357	BCR	C30-C25	3.57	1.58	1.53
28	B	528	BCR	C29-C30	3.57	1.62	1.54
30	c	5509	DGD	O6D-C1D	3.58	1.51	1.41
30	C	507	DGD	C4D-C3D	3.59	1.61	1.52
28	t	104	BCR	C1-C6	3.60	1.58	1.53
28	X	130	BCR	C29-C30	3.60	1.62	1.54
28	d	5357	BCR	C29-C30	3.61	1.62	1.54
23	b	5526	CLA	C4-C3	3.61	1.59	1.50
33	T	217	LMT	O1'-C1'	3.62	1.46	1.40
32	A	568	SQD	O3-C3	3.62	1.51	1.43
25	v	5552	HEM	CAA-C2A	3.62	1.58	1.52
31	A	567	LHG	O8-C23	3.64	1.44	1.33
23	c	5494	CLA	CAA-C2A	3.65	1.61	1.54
28	B	527	BCR	C5-C6	3.66	1.40	1.34
29	L	210	MGE	O6D-C1D	3.67	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	212	SQD	O5-C5	3.68	1.53	1.44
25	v	5552	HEM	FE-NC	3.68	2.10	1.95
29	d	5361	MGE	O6D-C1D	3.68	1.51	1.41
32	A	568	SQD	O47-C7	3.68	1.45	1.34
30	c	5508	DGD	O3G-C1D	3.68	1.46	1.40
23	A	560	CLA	CAA-C2A	3.72	1.61	1.54
28	c	5505	BCR	C5-C6	3.72	1.40	1.34
28	T	5104	BCR	C2-C1	3.73	1.63	1.54
28	D	357	BCR	C29-C30	3.75	1.63	1.54
29	D	359	MGE	O3G-C1D	3.76	1.46	1.40
32	d	5358	SQD	O47-C7	3.77	1.45	1.34
25	F	51	HEM	CAA-C2A	3.78	1.58	1.52
28	B	528	BCR	C26-C25	3.79	1.40	1.34
28	C	505	BCR	C2-C1	3.80	1.63	1.54
28	c	5506	BCR	C2-C1	3.80	1.63	1.54
32	t	213	SQD	O48-C23	3.80	1.44	1.33
30	c	5507	DGD	O5D-C1E	3.81	1.47	1.40
30	c	5507	DGD	C4D-C3D	3.81	1.62	1.52
28	C	506	BCR	C26-C25	3.82	1.40	1.34
28	h	5107	BCR	C2-C1	3.82	1.63	1.54
32	L	5213	SQD	C1-C2	3.82	1.64	1.52
28	x	5130	BCR	C29-C30	3.84	1.63	1.54
28	t	104	BCR	C30-C25	3.85	1.59	1.53
32	A	568	SQD	C1-C2	3.85	1.64	1.52
28	t	104	BCR	C5-C6	3.86	1.40	1.34
28	h	5107	BCR	C29-C30	3.86	1.63	1.54
25	f	5051	HEM	CAA-C2A	3.86	1.58	1.52
28	C	505	BCR	C1-C6	3.88	1.59	1.53
32	d	5358	SQD	O48-C23	3.89	1.45	1.33
32	A	568	SQD	O48-C23	3.89	1.45	1.33
28	C	504	BCR	C26-C25	3.90	1.40	1.34
28	c	5504	BCR	C29-C30	3.91	1.63	1.54
32	d	5358	SQD	C1-C2	3.91	1.64	1.52
28	A	566	BCR	C5-C6	3.92	1.40	1.34
32	L	5213	SQD	O5-C5	3.93	1.54	1.44
33	M	5216	LMT	O1'-C1'	3.94	1.47	1.40
28	b	5528	BCR	C1-C6	3.94	1.59	1.53
28	C	506	BCR	C5-C6	3.95	1.40	1.34
33	a	5568	LMT	O1'-C1'	3.95	1.47	1.40
29	B	530	MGE	O3G-C1D	3.96	1.47	1.40
28	C	506	BCR	C2-C1	4.02	1.63	1.54
28	B	529	BCR	C1-C6	4.05	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	5509	DGD	O3G-C1D	4.10	1.47	1.40
28	C	506	BCR	C30-C25	4.10	1.59	1.53
32	a	212	SQD	C1-C2	4.14	1.64	1.52
28	T	5104	BCR	C5-C6	4.15	1.40	1.34
28	a	5566	BCR	C30-C25	4.18	1.59	1.53
31	a	5567	LHG	P-O3	4.18	1.78	1.59
32	d	5358	SQD	O8-S	4.19	1.57	1.46
30	c	5508	DGD	O6D-C1D	4.23	1.52	1.41
32	A	568	SQD	O8-S	4.23	1.57	1.46
32	A	568	SQD	O7-S	4.29	1.58	1.45
25	F	51	HEM	CBC-CAC	4.34	1.54	1.29
32	t	213	SQD	O5-C5	4.36	1.55	1.44
32	L	5213	SQD	O48-C23	4.38	1.46	1.33
33	A	569	LMT	O1'-C1'	4.38	1.48	1.40
25	f	5051	HEM	CBC-CAC	4.40	1.54	1.29
28	c	5506	BCR	C1-C6	4.43	1.60	1.53
25	V	552	HEM	CBC-CAC	4.46	1.55	1.29
28	c	5506	BCR	C26-C25	4.52	1.41	1.34
28	d	5357	BCR	C26-C25	4.54	1.41	1.34
32	a	212	SQD	O7-S	4.55	1.59	1.45
25	v	5552	HEM	CBC-CAC	4.55	1.55	1.29
28	D	357	BCR	C5-C6	4.56	1.41	1.34
32	A	5212	SQD	O47-C7	4.58	1.45	1.35
28	b	5529	BCR	C30-C25	4.59	1.60	1.53
28	X	130	BCR	C30-C25	4.60	1.60	1.53
28	c	5505	BCR	C1-C6	4.60	1.60	1.53
28	c	5506	BCR	C5-C6	4.62	1.41	1.34
28	b	5527	BCR	C30-C25	4.64	1.60	1.53
32	t	213	SQD	C6-S	4.65	1.84	1.77
28	h	5107	BCR	C26-C25	4.66	1.41	1.34
28	H	107	BCR	C26-C25	4.67	1.41	1.34
28	X	130	BCR	C1-C6	4.71	1.60	1.53
28	x	5130	BCR	C30-C25	4.72	1.60	1.53
30	h	5208	DGD	O3G-C1D	4.72	1.48	1.40
28	x	5130	BCR	C1-C6	4.73	1.60	1.53
28	d	5357	BCR	C5-C6	4.73	1.41	1.34
28	B	529	BCR	C30-C25	4.76	1.60	1.53
28	B	529	BCR	C26-C25	4.76	1.41	1.34
28	C	505	BCR	C26-C25	4.80	1.42	1.34
28	C	504	BCR	C30-C25	4.80	1.60	1.53
28	H	107	BCR	C29-C30	4.83	1.65	1.54
28	a	5566	BCR	C1-C6	4.83	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	5506	BCR	C30-C25	4.83	1.60	1.53
32	t	213	SQD	C1-C2	4.83	1.67	1.52
28	c	5505	BCR	C26-C25	4.84	1.42	1.34
32	A	5212	SQD	O7-S	4.94	1.60	1.45
32	a	212	SQD	C6-S	4.94	1.85	1.77
28	B	527	BCR	C26-C25	4.96	1.42	1.34
28	h	5107	BCR	C1-C6	4.98	1.60	1.53
28	D	357	BCR	C30-C25	5.02	1.60	1.53
28	D	357	BCR	C26-C25	5.03	1.42	1.34
28	B	527	BCR	C30-C25	5.14	1.61	1.53
28	x	5130	BCR	C5-C6	5.16	1.42	1.34
28	H	107	BCR	C1-C6	5.23	1.61	1.53
32	A	5212	SQD	O8-S	5.29	1.60	1.46
28	X	130	BCR	C5-C6	5.30	1.42	1.34
30	H	208	DGD	O3G-C1D	5.35	1.49	1.40
28	A	566	BCR	C1-C6	5.36	1.61	1.53
32	a	212	SQD	O8-S	5.39	1.60	1.46
32	L	5213	SQD	O8-S	5.40	1.60	1.46
28	B	528	BCR	C1-C6	5.40	1.61	1.53
32	t	213	SQD	O8-S	5.41	1.60	1.46
32	d	5358	SQD	O7-S	5.41	1.62	1.45
32	a	212	SQD	O47-C7	5.44	1.47	1.35
28	b	5528	BCR	C30-C25	5.47	1.61	1.53
32	t	213	SQD	O7-S	5.49	1.62	1.45
28	C	504	BCR	C1-C6	5.67	1.61	1.53
28	c	5505	BCR	C30-C25	5.74	1.61	1.53
28	C	505	BCR	C30-C25	5.80	1.62	1.53
32	L	5213	SQD	O7-S	5.80	1.63	1.45
28	d	5357	BCR	C1-C6	5.96	1.62	1.53
28	B	528	BCR	C30-C25	6.05	1.62	1.53
28	H	107	BCR	C30-C25	6.38	1.62	1.53
28	h	5107	BCR	C30-C25	6.44	1.62	1.53
28	c	5504	BCR	C30-C25	6.45	1.62	1.53
32	A	5212	SQD	C4-C3	7.01	1.70	1.52
32	L	5213	SQD	C6-S	7.05	1.88	1.77
28	c	5504	BCR	C1-C6	7.39	1.64	1.53
32	L	5213	SQD	C4-C3	7.52	1.72	1.52
32	d	5358	SQD	C4-C3	7.58	1.72	1.52
31	a	5567	LHG	P-O5	7.62	1.79	1.51
31	A	567	LHG	P-O5	7.71	1.79	1.51
32	a	212	SQD	C4-C3	7.84	1.73	1.52
32	t	213	SQD	C4-C3	7.87	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	568	SQD	C4-C3	7.90	1.73	1.52

All (1500) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	v	5552	HEM	C3C-CAC-CBC	-9.32	110.16	124.46
25	V	552	HEM	C3C-CAC-CBC	-8.76	111.03	124.46
25	F	51	HEM	C3C-CAC-CBC	-6.12	115.06	124.46
25	f	5051	HEM	C3C-CAC-CBC	-5.67	115.76	124.46
26	d	5356	PQ9	C11-C2-C3	-5.36	118.97	123.42
26	D	356	PQ9	C11-C2-C3	-5.18	119.12	123.42
23	B	515	CLA	CAA-C2A-C3A	-5.10	98.56	113.22
23	b	5515	CLA	CAA-C2A-C3A	-4.78	99.47	113.22
30	c	5508	DGD	C3G-O3G-C1D	-4.42	104.53	113.82
25	F	51	HEM	CBD-CAD-C3D	-4.29	101.06	113.55
24	A	562	PHO	CBD-CHA-C4D	-4.22	103.73	108.46
28	X	130	BCR	C8-C9-C10	-4.20	112.22	118.98
28	T	5104	BCR	C33-C5-C4	-4.18	105.51	113.43
28	T	5104	BCR	C38-C26-C27	-4.17	105.53	113.43
28	x	5130	BCR	C33-C5-C4	-4.14	105.58	113.43
28	x	5130	BCR	C8-C9-C10	-4.14	112.31	118.98
28	B	529	BCR	C38-C26-C27	-4.14	105.58	113.43
28	D	357	BCR	C38-C26-C27	-4.12	105.62	113.43
28	d	5357	BCR	C38-C26-C27	-4.11	105.63	113.43
29	L	210	MGE	C3G-O3G-C1D	-4.11	105.18	113.82
25	f	5051	HEM	CBD-CAD-C3D	-4.11	101.61	113.55
29	l	5210	MGE	C3G-O3G-C1D	-4.10	105.20	113.82
24	a	5562	PHO	CBD-CHA-C4D	-4.07	103.90	108.46
28	D	357	BCR	C33-C5-C4	-4.07	105.72	113.43
28	X	130	BCR	C33-C5-C4	-4.06	105.73	113.43
28	t	104	BCR	C33-C5-C4	-4.02	105.81	113.43
28	d	5357	BCR	C33-C5-C4	-4.00	105.85	113.43
30	C	508	DGD	C3G-O3G-C1D	-4.00	105.42	113.82
26	a	5564	PQ9	C2-C3-C4	-4.00	120.53	122.97
28	C	504	BCR	C38-C26-C27	-3.96	105.91	113.43
28	C	505	BCR	C33-C5-C4	-3.94	105.95	113.43
25	v	5552	HEM	CBD-CAD-C3D	-3.93	102.11	113.55
28	C	506	BCR	C38-C26-C27	-3.92	105.99	113.43
23	c	5502	CLA	CAA-C2A-C3A	-3.92	101.96	113.22
28	H	107	BCR	C38-C26-C27	-3.90	106.03	113.43
23	C	495	CLA	CAA-C2A-C3A	-3.89	102.03	113.22
28	B	528	BCR	C38-C26-C27	-3.87	106.08	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	563	CLA	OBD-CAD-CBD	-3.87	120.10	125.94
23	c	5495	CLA	CAA-C2A-C3A	-3.87	102.09	113.22
23	B	517	CLA	OBD-CAD-CBD	-3.86	120.12	125.94
33	a	5568	LMT	C1-O1'-C1'	-3.85	107.21	113.94
23	B	511	CLA	CAA-C2A-C3A	-3.84	107.00	116.20
23	b	5511	CLA	CAA-C2A-C3A	-3.84	107.01	116.20
28	C	504	BCR	C33-C5-C4	-3.83	106.16	113.43
23	C	494	CLA	CAA-C2A-C3A	-3.83	102.21	113.22
33	A	569	LMT	C1-O1'-C1'	-3.82	107.27	113.94
24	a	5561	PHO	CBD-CHA-C4D	-3.81	104.19	108.46
23	c	5493	CLA	CAA-C2A-C3A	-3.79	102.32	113.22
28	C	506	BCR	C33-C5-C4	-3.78	106.25	113.43
23	c	5494	CLA	CAA-C2A-C3A	-3.78	102.33	113.22
28	c	5506	BCR	C38-C26-C27	-3.77	106.27	113.43
23	C	493	CLA	CAA-C2A-C3A	-3.77	102.37	113.22
24	A	561	PHO	CBD-CHA-C4D	-3.76	104.25	108.46
28	c	5504	BCR	C38-C26-C27	-3.76	106.30	113.43
28	A	566	BCR	C38-C26-C27	-3.74	106.34	113.43
23	C	502	CLA	CAA-C2A-C3A	-3.74	102.47	113.22
28	b	5527	BCR	C38-C26-C27	-3.73	106.35	113.43
28	A	566	BCR	C33-C5-C4	-3.72	106.37	113.43
28	a	5566	BCR	C38-C26-C27	-3.72	106.37	113.43
28	h	5107	BCR	C38-C26-C27	-3.72	106.37	113.43
28	c	5505	BCR	C38-C26-C27	-3.71	106.39	113.43
28	c	5506	BCR	C33-C5-C4	-3.71	106.39	113.43
32	d	5358	SQD	O9-S-C6	-3.70	103.82	106.94
26	d	5356	PQ9	C2-C3-C4	-3.70	120.72	122.97
28	B	528	BCR	C30-C25-C26	-3.70	117.23	122.66
26	A	564	PQ9	C11-C12-C13	-3.70	120.43	126.70
23	b	5517	CLA	OBD-CAD-CBD	-3.69	120.37	125.94
28	c	5505	BCR	C33-C5-C4	-3.66	106.48	113.43
26	A	564	PQ9	C2-C3-C4	-3.66	120.74	122.97
28	B	527	BCR	C38-C26-C27	-3.66	106.49	113.43
32	A	568	SQD	O9-S-C6	-3.66	103.86	106.94
28	X	130	BCR	C38-C26-C27	-3.66	106.49	113.43
25	V	552	HEM	CBD-CAD-C3D	-3.66	102.91	113.55
28	b	5529	BCR	C38-C26-C27	-3.65	106.51	113.43
28	b	5527	BCR	C33-C5-C4	-3.65	106.52	113.43
28	H	107	BCR	C33-C5-C4	-3.64	106.53	113.43
28	t	104	BCR	C38-C26-C27	-3.63	106.54	113.43
28	B	527	BCR	C33-C5-C4	-3.63	106.55	113.43
28	x	5130	BCR	C38-C26-C27	-3.61	106.58	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	5529	BCR	C33-C5-C4	-3.58	106.63	113.43
23	C	497	CLA	C7-C6-C5	-3.58	102.48	113.06
28	d	5357	BCR	C30-C25-C26	-3.56	117.42	122.66
28	T	5104	BCR	C30-C25-C26	-3.56	117.43	122.66
28	B	529	BCR	C33-C5-C4	-3.56	106.69	113.43
28	d	5357	BCR	C1-C6-C5	-3.54	117.46	122.66
28	a	5566	BCR	C33-C5-C4	-3.54	106.72	113.43
23	B	513	CLA	CAA-C2A-C3A	-3.53	103.06	113.22
28	c	5504	BCR	C33-C5-C4	-3.52	106.76	113.43
23	b	5526	CLA	OBD-CAD-CBD	-3.51	120.65	125.94
23	a	5560	CLA	CAA-C2A-C3A	-3.49	103.19	113.22
28	c	5504	BCR	C1-C6-C5	-3.48	117.55	122.66
28	D	357	BCR	C1-C6-C5	-3.47	117.56	122.66
29	B	530	MGE	C3G-O3G-C1D	-3.47	106.53	113.82
28	h	5107	BCR	C33-C5-C4	-3.47	106.86	113.43
23	A	560	CLA	CAA-C2A-C3A	-3.46	103.26	113.22
28	H	107	BCR	C30-C25-C26	-3.46	117.58	122.66
28	C	504	BCR	C1-C6-C5	-3.46	117.59	122.66
30	C	508	DGD	C3G-C2G-C1G	-3.45	104.00	112.07
28	D	357	BCR	C30-C25-C26	-3.44	117.60	122.66
28	b	5528	BCR	C38-C26-C27	-3.44	106.90	113.43
28	C	505	BCR	C38-C26-C27	-3.44	106.90	113.43
28	b	5528	BCR	C33-C5-C4	-3.44	106.91	113.43
28	b	5528	BCR	C30-C25-C26	-3.43	117.63	122.66
23	b	5514	CLA	OBD-CAD-CBD	-3.42	120.77	125.94
28	c	5506	BCR	C30-C25-C26	-3.40	117.67	122.66
23	B	513	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
30	c	5508	DGD	C3G-C2G-C1G	-3.39	104.14	112.07
23	c	5497	CLA	C7-C6-C5	-3.38	103.09	113.06
28	t	104	BCR	C30-C25-C26	-3.37	117.71	122.66
28	X	130	BCR	C30-C25-C26	-3.37	117.71	122.66
28	x	5130	BCR	C30-C25-C26	-3.36	117.72	122.66
23	D	354	CLA	OBD-CAD-CBD	-3.36	120.86	125.94
23	B	522	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
23	C	503	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
23	b	5513	CLA	CAA-C2A-C3A	-3.35	103.57	113.22
23	B	526	CLA	OBD-CAD-CBD	-3.35	120.88	125.94
23	b	5512	CLA	CAA-C2A-C3A	-3.33	103.65	113.22
24	a	5562	PHO	CAB-C3B-C2B	-3.32	117.27	128.41
23	b	5520	CLA	C7-C6-C5	-3.32	103.25	113.06
28	a	5566	BCR	C30-C25-C26	-3.32	117.78	122.66
23	b	5526	CLA	CAA-C2A-C3A	-3.30	103.72	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	5107	BCR	C30-C25-C26	-3.30	117.81	122.66
23	b	5511	CLA	CMA-C3A-C2A	-3.29	108.33	116.20
23	d	5354	CLA	CAA-C2A-C3A	-3.28	103.78	113.22
24	a	5562	PHO	C7-C6-C5	-3.28	103.37	113.06
23	b	5522	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
23	B	521	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
26	D	356	PQ9	C2-C3-C4	-3.26	120.98	122.97
28	A	566	BCR	C30-C25-C26	-3.26	117.88	122.66
23	B	512	CLA	CAA-C2A-C3A	-3.25	103.86	113.22
23	a	5563	CLA	OBD-CAD-CBD	-3.25	121.04	125.94
24	A	562	PHO	CAB-C3B-C2B	-3.24	117.53	128.41
28	b	5529	BCR	C30-C25-C26	-3.22	117.93	122.66
23	c	5495	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
23	b	5512	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
28	B	529	BCR	C30-C25-C26	-3.22	117.94	122.66
28	x	5130	BCR	C12-C13-C14	-3.21	113.81	118.98
23	B	511	CLA	CMA-C3A-C2A	-3.20	108.53	116.20
23	c	5503	CLA	OBD-CAD-CBD	-3.20	121.10	125.94
26	a	5564	PQ9	C11-C12-C13	-3.20	121.28	126.70
29	b	5530	MGE	C3G-O3G-C1D	-3.20	107.10	113.82
23	A	559	CLA	CAA-C2A-C3A	-3.19	104.04	113.22
23	D	354	CLA	CAA-C2A-C3A	-3.18	104.08	113.22
26	A	564	PQ9	C16-C17-C18	-3.18	120.86	127.76
23	b	5521	CLA	C7-C6-C5	-3.17	103.69	113.06
23	a	5559	CLA	CAA-C2A-C3A	-3.17	104.11	113.22
23	C	492	CLA	OBD-CAD-CBD	-3.15	121.18	125.94
23	B	512	CLA	OBD-CAD-CBD	-3.15	121.19	125.94
28	C	504	BCR	C30-C25-C26	-3.14	118.04	122.66
23	B	521	CLA	C7-C6-C5	-3.14	103.78	113.06
26	a	5564	PQ9	C16-C17-C18	-3.14	120.94	127.76
23	B	520	CLA	C7-C6-C5	-3.13	103.82	113.06
23	c	5494	CLA	OBD-CAD-CBD	-3.12	121.23	125.94
28	C	506	BCR	C30-C25-C26	-3.12	118.08	122.66
28	B	528	BCR	C33-C5-C4	-3.12	107.52	113.43
23	B	524	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
23	A	560	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
23	B	526	CLA	CAA-C2A-C3A	-3.11	104.27	113.22
23	b	5518	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
23	c	5500	CLA	C7-C6-C5	-3.11	103.88	113.06
23	c	5496	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
28	H	107	BCR	C1-C6-C5	-3.10	118.11	122.66
32	A	5212	SQD	C3-C4-C5	-3.10	104.79	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5501	CLA	C7-C6-C5	-3.10	103.91	113.06
32	t	213	SQD	O9-S-C6	-3.09	104.33	106.94
23	d	5355	CLA	OBD-CAD-CBD	-3.08	121.28	125.94
28	b	5528	BCR	C1-C6-C5	-3.08	118.13	122.66
28	h	5107	BCR	C1-C6-C5	-3.08	118.14	122.66
32	a	212	SQD	C3-C4-C5	-3.07	104.84	110.20
28	B	527	BCR	C30-C25-C26	-3.04	118.19	122.66
23	b	5513	CLA	OBD-CAD-CBD	-3.03	121.36	125.94
28	b	5529	BCR	C1-C6-C5	-3.03	118.21	122.66
23	b	5521	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
23	a	5560	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
28	x	5130	BCR	C1-C6-C5	-3.01	118.23	122.66
24	A	561	PHO	CAB-C3B-C2B	-3.00	118.36	128.41
23	B	514	CLA	OBD-CAD-CBD	-3.00	121.42	125.94
28	X	130	BCR	C1-C6-C5	-2.99	118.27	122.66
28	H	107	BCR	C12-C13-C14	-2.99	114.17	118.98
23	D	355	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
23	B	520	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
28	b	5527	BCR	C1-C6-C5	-2.98	118.28	122.66
23	B	518	CLA	CAA-C2A-C3A	-2.97	104.67	113.22
24	A	562	PHO	C7-C6-C5	-2.97	104.28	113.06
23	C	492	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
23	b	5523	CLA	OBD-CAD-CBD	-2.96	121.48	125.94
23	b	5516	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
28	B	529	BCR	C1-C6-C5	-2.94	118.34	122.66
23	C	502	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
23	c	5498	CLA	CAA-C2A-C3A	-2.93	104.80	113.22
23	b	5522	CLA	C7-C6-C5	-2.92	104.42	113.06
24	a	5562	PHO	C2A-C1A-NA	-2.92	108.34	112.08
23	c	5496	CLA	CAA-C2A-C3A	-2.92	104.83	113.22
23	B	516	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
23	C	497	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
23	b	5518	CLA	CAA-C2A-C3A	-2.91	104.85	113.22
23	B	525	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
28	c	5504	BCR	C30-C25-C26	-2.90	118.40	122.66
24	a	5561	PHO	CAB-C3B-C2B	-2.90	118.69	128.41
26	D	356	PQ9	C16-C17-C18	-2.90	121.46	127.76
28	c	5505	BCR	C1-C6-C5	-2.89	118.41	122.66
23	d	5354	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
23	A	563	CLA	CAA-C2A-C3A	-2.89	104.92	113.22
28	c	5506	BCR	C40-C30-C29	-2.88	98.46	108.79
23	C	501	CLA	C7-C6-C5	-2.88	104.56	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	499	CLA	OBD-CAD-CBD	-2.88	121.60	125.94
23	A	558	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
23	c	5499	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
23	b	5519	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
28	C	506	BCR	C1-C6-C5	-2.84	118.49	122.66
33	m	216	LMT	C1-O1'-C1'	-2.84	108.99	113.94
23	c	5492	CLA	O1D-CGD-CBD	-2.82	120.58	124.62
28	C	506	BCR	C40-C30-C29	-2.82	98.68	108.79
30	c	5509	DGD	C3G-C2G-C1G	-2.81	105.49	112.07
28	B	528	BCR	C1-C6-C5	-2.81	118.53	122.66
28	h	5107	BCR	C12-C13-C14	-2.81	114.46	118.98
23	C	495	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
28	b	5527	BCR	C30-C25-C26	-2.80	118.55	122.66
23	C	496	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
23	C	495	CLA	C7-C6-C5	-2.79	104.83	113.06
28	X	130	BCR	C12-C13-C14	-2.78	114.50	118.98
28	D	357	BCR	C12-C13-C14	-2.78	114.50	118.98
23	c	5498	CLA	OBD-CAD-CBD	-2.77	121.75	125.94
23	a	5558	CLA	C7-C6-C5	-2.77	104.87	113.06
24	A	562	PHO	CAA-C2A-C3A	-2.77	105.25	113.22
23	B	525	CLA	C7-C6-C5	-2.77	104.87	113.06
32	a	212	SQD	O9-S-C6	-2.77	104.61	106.94
23	B	511	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
24	a	5561	PHO	C7-C6-C5	-2.77	104.89	113.06
23	C	495	CLA	CMB-C2B-C1B	-2.76	123.79	128.36
23	B	522	CLA	C7-C6-C5	-2.76	104.90	113.06
24	a	5562	PHO	CAA-C2A-C3A	-2.75	105.30	113.22
23	a	5563	CLA	CAA-C2A-C3A	-2.75	105.30	113.22
23	b	5520	CLA	OBD-CAD-CBD	-2.75	121.78	125.94
28	T	5104	BCR	C40-C30-C29	-2.75	98.95	108.79
29	I	201	MGE	O1G-C1G-C2G	-2.74	101.33	108.69
29	i	5201	MGE	O1G-C1G-C2G	-2.74	101.33	108.69
23	c	5493	CLA	C7-C6-C5	-2.73	104.99	113.06
23	A	558	CLA	C7-C6-C5	-2.73	104.99	113.06
24	A	561	PHO	O1D-CGD-CBD	-2.73	120.71	124.62
23	C	498	CLA	CAA-C2A-C3A	-2.73	105.37	113.22
28	c	5505	BCR	C30-C25-C26	-2.73	118.66	122.66
23	b	5525	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
23	C	491	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
33	T	217	LMT	C1-O1'-C1'	-2.72	109.19	113.94
23	C	496	CLA	CAA-C2A-C3A	-2.72	105.40	113.22
30	C	509	DGD	C3G-C2G-C1G	-2.72	105.72	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	505	BCR	C1-C6-C5	-2.70	118.69	122.66
33	t	5217	LMT	C1-O1'-C1'	-2.70	109.23	113.94
24	A	562	PHO	C2A-C1A-NA	-2.70	108.63	112.08
23	c	5495	CLA	C7-C6-C5	-2.69	105.10	113.06
23	C	494	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
28	t	104	BCR	C1-C6-C5	-2.69	118.70	122.66
23	B	515	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
28	T	5104	BCR	C23-C22-C21	-2.69	114.65	118.98
23	B	519	CLA	OBD-CAD-CBD	-2.69	121.89	125.94
23	b	5524	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
23	A	558	CLA	CAA-C2A-C3A	-2.68	105.51	113.22
28	B	527	BCR	C1-C6-C5	-2.68	118.72	122.66
28	T	5104	BCR	C1-C6-C5	-2.68	118.73	122.66
26	d	5356	PQ9	C16-C17-C18	-2.68	121.94	127.76
23	B	517	CLA	CAA-C2A-C3A	-2.67	105.54	113.22
29	B	530	MGE	O1G-C1G-C2G	-2.67	101.51	108.69
23	a	5558	CLA	CAA-C2A-C3A	-2.66	105.55	113.22
23	C	500	CLA	C7-C6-C5	-2.66	105.19	113.06
23	C	493	CLA	C7-C6-C5	-2.66	105.20	113.06
23	c	5498	CLA	O1D-CGD-CBD	-2.65	120.83	124.62
28	C	504	BCR	C32-C1-C2	-2.64	99.33	108.79
26	D	356	PQ9	C21-C22-C23	-2.64	122.03	127.76
24	a	5561	PHO	O1D-CGD-CBD	-2.63	120.85	124.62
23	B	524	CLA	C7-C6-C5	-2.63	105.30	113.06
32	L	5213	SQD	C3-C4-C5	-2.63	105.62	110.20
23	c	5494	CLA	CMB-C2B-C1B	-2.62	124.02	128.36
23	B	515	CLA	C7-C6-C5	-2.62	105.32	113.06
23	C	494	CLA	OBD-CAD-CBD	-2.62	121.98	125.94
28	C	505	BCR	C19-C18-C17	-2.62	114.77	118.98
23	B	519	CLA	CAA-C2A-C3A	-2.61	105.70	113.22
28	X	130	BCR	C32-C1-C2	-2.61	99.44	108.79
23	c	5491	CLA	C7-C6-C5	-2.61	105.36	113.06
23	C	493	CLA	OBD-CAD-CBD	-2.60	122.01	125.94
23	b	5517	CLA	C7-C6-C5	-2.60	105.39	113.06
23	b	5521	CLA	CAA-C2A-C3A	-2.59	105.78	113.22
23	b	5517	CLA	CAA-C2A-C3A	-2.58	105.79	113.22
28	d	5357	BCR	C12-C13-C14	-2.58	114.82	118.98
23	b	5524	CLA	C7-C6-C5	-2.58	105.43	113.06
23	b	5515	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
28	C	505	BCR	C30-C25-C26	-2.57	118.88	122.66
28	C	506	BCR	C19-C18-C17	-2.57	114.85	118.98
28	t	104	BCR	C23-C22-C21	-2.56	114.86	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5495	CLA	CMB-C2B-C1B	-2.56	124.13	128.36
23	C	496	CLA	C7-C6-C5	-2.56	105.51	113.06
28	C	506	BCR	C12-C13-C14	-2.56	114.86	118.98
23	a	5559	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
28	C	504	BCR	C23-C22-C21	-2.55	114.88	118.98
23	b	5525	CLA	C7-C6-C5	-2.55	105.53	113.06
23	a	5560	CLA	CMB-C2B-C1B	-2.53	124.17	128.36
28	t	104	BCR	C40-C30-C29	-2.53	99.73	108.79
23	a	5560	CLA	C7-C6-C5	-2.53	105.60	113.06
29	d	5360	MGE	C3G-O3G-C1D	-2.52	108.52	113.82
26	A	564	PQ9	C21-C22-C23	-2.52	122.28	127.76
28	A	566	BCR	C1-C6-C5	-2.52	118.96	122.66
23	B	512	CLA	C7-C6-C5	-2.52	105.62	113.06
23	b	5511	CLA	CMB-C2B-C1B	-2.52	124.20	128.36
29	b	5530	MGE	O1G-C1G-C2G	-2.51	101.92	108.69
29	d	5359	MGE	C3G-C2G-C1G	-2.51	106.20	112.07
28	c	5506	BCR	C1-C6-C5	-2.51	118.98	122.66
29	l	5210	MGE	O1G-C1G-C2G	-2.51	101.94	108.69
23	c	5493	CLA	OBD-CAD-CBD	-2.51	122.16	125.94
23	c	5496	CLA	C7-C6-C5	-2.50	105.67	113.06
23	b	5524	CLA	CAA-C2A-C3A	-2.50	106.02	113.22
23	c	5492	CLA	OBD-CAD-CBD	-2.50	122.16	125.94
23	A	560	CLA	CMB-C2B-C1B	-2.50	124.23	128.36
23	B	518	CLA	C7-C6-C5	-2.50	105.68	113.06
23	b	5519	CLA	CAA-C2A-C3A	-2.50	106.04	113.22
29	B	530	MGE	C3G-C2G-C1G	-2.49	106.24	112.07
23	B	516	CLA	C7-C6-C5	-2.49	105.70	113.06
23	b	5526	CLA	O1D-CGD-CBD	-2.49	121.05	124.62
23	b	5519	CLA	C7-C6-C5	-2.49	105.71	113.06
23	C	499	CLA	CMB-C2B-C1B	-2.49	124.25	128.36
28	a	5566	BCR	C1-C6-C5	-2.47	119.03	122.66
23	B	523	CLA	OBD-CAD-CBD	-2.47	122.21	125.94
32	A	568	SQD	C3-C4-C5	-2.47	105.89	110.20
28	c	5504	BCR	C32-C1-C2	-2.46	99.96	108.79
23	B	514	CLA	C7-C6-C5	-2.46	105.79	113.06
23	b	5513	CLA	CMB-C2B-C1B	-2.46	124.29	128.36
23	B	519	CLA	C7-C6-C5	-2.46	105.79	113.06
29	L	210	MGE	O1G-C1G-C2G	-2.46	102.07	108.69
23	c	5492	CLA	CAA-C2A-C3A	-2.46	106.15	113.22
23	C	498	CLA	C7-C6-C5	-2.46	105.80	113.06
23	B	517	CLA	C7-C6-C5	-2.46	105.81	113.06
32	t	213	SQD	C3-C4-C5	-2.45	105.93	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	521	CLA	CAA-C2A-C3A	-2.45	106.17	113.22
32	d	5358	SQD	C3-C4-C5	-2.45	105.93	110.20
23	C	503	CLA	CAA-C2A-C3A	-2.45	106.18	113.22
32	L	5213	SQD	O9-S-C6	-2.44	104.88	106.94
26	a	5564	PQ9	C21-C22-C23	-2.44	122.45	127.76
23	C	498	CLA	CMB-C2B-C1B	-2.44	124.33	128.36
33	t	5217	LMT	C3'-C4'-C5'	-2.43	105.33	110.84
23	b	5512	CLA	C7-C6-C5	-2.43	105.89	113.06
24	A	561	PHO	C7-C6-C5	-2.43	105.89	113.06
23	c	5497	CLA	OBD-CAD-CBD	-2.42	122.28	125.94
28	x	5130	BCR	C32-C1-C2	-2.42	100.12	108.79
23	B	518	CLA	OBD-CAD-CBD	-2.41	122.29	125.94
23	B	519	CLA	CMB-C2B-C1B	-2.41	124.37	128.36
23	B	524	CLA	CAA-C2A-C3A	-2.41	106.28	113.22
28	C	505	BCR	C12-C13-C14	-2.41	115.10	118.98
23	C	502	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
32	A	5212	SQD	O9-S-C6	-2.40	104.92	106.94
23	a	5563	CLA	CMB-C2B-C1B	-2.40	124.39	128.36
28	c	5506	BCR	C19-C18-C17	-2.40	115.12	118.98
28	t	104	BCR	C12-C13-C14	-2.40	115.12	118.98
23	b	5518	CLA	C7-C6-C5	-2.40	105.98	113.06
23	c	5502	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
23	c	5491	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
23	b	5512	CLA	O1D-CGD-CBD	-2.39	121.19	124.62
23	B	520	CLA	CMB-C2B-C1B	-2.39	124.41	128.36
23	b	5526	CLA	C7-C6-C5	-2.39	106.01	113.06
23	a	5558	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
23	b	5518	CLA	CMB-C2B-C1B	-2.38	124.42	128.36
23	b	5515	CLA	C7-C6-C5	-2.38	106.03	113.06
23	b	5523	CLA	CMB-C2B-C1B	-2.38	124.43	128.36
23	B	519	CLA	O1D-CGD-CBD	-2.37	121.22	124.62
23	b	5516	CLA	C7-C6-C5	-2.37	106.06	113.06
23	c	5491	CLA	CAA-C2A-C3A	-2.37	106.40	113.22
23	C	500	CLA	CMB-C2B-C1B	-2.37	124.44	128.36
23	A	559	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
23	b	5519	CLA	O1D-CGD-CBD	-2.37	121.23	124.62
23	B	521	CLA	O1D-CGD-CBD	-2.36	121.24	124.62
28	t	104	BCR	C8-C9-C10	-2.35	115.19	118.98
23	A	560	CLA	C7-C6-C5	-2.35	106.13	113.06
28	b	5528	BCR	C32-C1-C2	-2.34	100.39	108.79
23	b	5523	CLA	C7-C6-C5	-2.34	106.14	113.06
29	i	5201	MGE	C3G-O3G-C1D	-2.34	108.90	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	492	CLA	CAA-C2A-C3A	-2.34	106.50	113.22
23	b	5525	CLA	O1D-CGD-CBD	-2.34	121.27	124.62
23	C	498	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
23	c	5503	CLA	CAA-C2A-C3A	-2.33	106.51	113.22
23	c	5500	CLA	CAA-C2A-C3A	-2.32	106.54	113.22
23	C	498	CLA	O1D-CGD-CBD	-2.32	121.30	124.62
23	b	5520	CLA	CMB-C2B-C1B	-2.32	124.53	128.36
28	c	5504	BCR	C23-C22-C21	-2.32	115.25	118.98
23	b	5517	CLA	CMB-C2B-C1B	-2.32	124.53	128.36
28	c	5505	BCR	C12-C13-C14	-2.32	115.25	118.98
23	C	503	CLA	CMB-C2B-C1B	-2.31	124.54	128.36
30	H	208	DGD	C3G-C2G-C1G	-2.31	106.66	112.07
23	C	491	CLA	C7-C6-C5	-2.31	106.23	113.06
29	D	360	MGE	O1G-C1G-C2G	-2.31	102.47	108.69
28	B	527	BCR	C12-C13-C14	-2.31	115.26	118.98
28	c	5504	BCR	C12-C13-C14	-2.31	115.26	118.98
23	B	523	CLA	C7-C6-C5	-2.30	106.28	113.06
23	a	5558	CLA	CMB-C2B-C1B	-2.29	124.57	128.36
23	B	512	CLA	CMB-C2B-C1B	-2.28	124.59	128.36
28	c	5506	BCR	C12-C13-C14	-2.28	115.31	118.98
23	B	512	CLA	O1D-CGD-CBD	-2.28	121.35	124.62
23	D	355	CLA	O1D-CGD-CBD	-2.28	121.36	124.62
28	b	5529	BCR	C12-C13-C14	-2.28	115.31	118.98
28	B	529	BCR	C12-C13-C14	-2.27	115.32	118.98
26	D	356	PQ9	C11-C12-C13	-2.27	122.85	126.70
23	C	493	CLA	O1D-CGD-CBD	-2.27	121.37	124.62
28	T	5104	BCR	C12-C13-C14	-2.26	115.33	118.98
23	b	5519	CLA	CMB-C2B-C1B	-2.26	124.62	128.36
23	c	5498	CLA	CMB-C2B-C1B	-2.26	124.62	128.36
23	c	5498	CLA	C7-C6-C5	-2.26	106.39	113.06
23	b	5512	CLA	CMB-C2B-C1B	-2.25	124.64	128.36
24	A	562	PHO	O1D-CGD-CBD	-2.25	121.40	124.62
23	B	523	CLA	CMB-C2B-C1B	-2.25	124.65	128.36
23	A	559	CLA	CMB-C2B-C1B	-2.24	124.65	128.36
28	A	566	BCR	C19-C18-C17	-2.24	115.37	118.98
23	B	524	CLA	CMB-C2B-C1B	-2.24	124.66	128.36
23	b	5516	CLA	O1D-CGD-CBD	-2.24	121.42	124.62
30	h	5208	DGD	C3G-C2G-C1G	-2.23	106.85	112.07
33	T	217	LMT	C3'-C4'-C5'	-2.23	105.80	110.84
23	c	5501	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
29	d	5361	MGE	O1G-C1G-C2G	-2.22	102.70	108.69
29	D	358	MGE	C3G-C2G-C1G	-2.22	106.87	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5525	CLA	CMB-C2B-C1B	-2.22	124.69	128.36
23	c	5497	CLA	CAA-C2A-C3A	-2.22	106.82	113.22
23	A	563	CLA	CMB-C2B-C1B	-2.22	124.69	128.36
28	c	5506	BCR	C23-C22-C21	-2.22	115.41	118.98
23	B	514	CLA	CAA-C2A-C3A	-2.22	106.85	113.22
25	f	5051	HEM	CBA-CAA-C2A	-2.21	108.56	112.53
23	B	526	CLA	C7-C6-C5	-2.21	106.53	113.06
23	D	355	CLA	CMB-C2B-C1B	-2.20	124.72	128.36
23	b	5513	CLA	O1D-CGD-CBD	-2.20	121.47	124.62
23	d	5354	CLA	C7-C6-C5	-2.20	106.57	113.06
23	b	5515	CLA	C12-C11-C10	-2.20	102.08	112.99
28	D	357	BCR	C23-C22-C21	-2.20	115.44	118.98
23	c	5493	CLA	C12-C11-C10	-2.20	102.09	112.99
23	b	5514	CLA	CAA-C2A-C3A	-2.19	106.91	113.22
23	B	518	CLA	CMB-C2B-C1B	-2.19	124.74	128.36
23	B	513	CLA	C7-C6-C5	-2.18	106.62	113.06
29	I	201	MGE	C3G-O3G-C1D	-2.18	109.25	113.82
23	c	5497	CLA	O1D-CGD-CBD	-2.18	121.50	124.62
28	X	130	BCR	C19-C18-C17	-2.18	115.48	118.98
23	b	5516	CLA	CMB-C2B-C1B	-2.18	124.76	128.36
23	B	520	CLA	CAA-C2A-C3A	-2.17	106.96	113.22
26	D	356	PQ9	C24-C23-C22	-2.17	119.23	123.50
28	C	506	BCR	C23-C22-C21	-2.17	115.48	118.98
23	C	501	CLA	OBD-CAD-CBD	-2.17	122.66	125.94
28	a	5566	BCR	C12-C13-C14	-2.17	115.49	118.98
30	C	508	DGD	C6E-C5E-C4E	-2.17	107.67	113.02
29	b	5530	MGE	C3G-C2G-C1G	-2.17	107.01	112.07
28	B	528	BCR	C32-C1-C2	-2.16	101.03	108.79
23	b	5521	CLA	O1D-CGD-CBD	-2.16	121.52	124.62
28	C	504	BCR	C12-C13-C14	-2.16	115.50	118.98
23	c	5500	CLA	CMB-C2B-C1B	-2.16	124.79	128.36
28	A	566	BCR	C12-C13-C14	-2.16	115.50	118.98
33	M	5216	LMT	C1-O1'-C1'	-2.16	110.17	113.94
23	A	558	CLA	CMB-C2B-C1B	-2.16	124.80	128.36
23	C	499	CLA	CAA-C2A-C3A	-2.15	107.04	113.22
29	D	359	MGE	C3G-O3G-C1D	-2.14	109.32	113.82
28	d	5357	BCR	C19-C18-C17	-2.14	115.53	118.98
28	x	5130	BCR	C40-C30-C29	-2.14	101.13	108.79
23	C	491	CLA	CAA-C2A-C3A	-2.13	107.08	113.22
23	D	354	CLA	C7-C6-C5	-2.13	106.76	113.06
32	a	212	SQD	O10-C23-C24	-2.13	116.98	124.85
23	c	5492	CLA	C7-C6-C5	-2.13	106.78	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5502	CLA	CMB-C2B-C1B	-2.13	124.85	128.36
23	B	515	CLA	C12-C11-C10	-2.12	102.46	112.99
23	b	5514	CLA	C7-C6-C5	-2.12	106.80	113.06
23	C	500	CLA	CMA-C3A-C2A	-2.12	104.98	114.35
23	B	513	CLA	CMB-C2B-C1B	-2.11	124.87	128.36
28	b	5527	BCR	C12-C13-C14	-2.11	115.58	118.98
23	C	497	CLA	O1D-CGD-CBD	-2.10	121.61	124.62
28	B	527	BCR	C19-C18-C17	-2.10	115.60	118.98
28	a	5566	BCR	C8-C9-C10	-2.10	115.60	118.98
23	c	5493	CLA	O1D-CGD-CBD	-2.10	121.61	124.62
23	c	5499	CLA	CMB-C2B-C1B	-2.10	124.89	128.36
29	d	5360	MGE	C3G-C2G-C1G	-2.10	107.17	112.07
28	d	5357	BCR	C23-C22-C21	-2.09	115.61	118.98
28	X	130	BCR	C40-C30-C29	-2.09	101.30	108.79
28	C	505	BCR	C40-C30-C29	-2.09	101.32	108.79
23	c	5493	CLA	CMB-C2B-C1B	-2.08	124.92	128.36
23	a	5559	CLA	CMB-C2B-C1B	-2.08	124.92	128.36
25	F	51	HEM	CBA-CAA-C2A	-2.08	108.80	112.53
28	h	5107	BCR	C40-C30-C29	-2.08	101.35	108.79
23	b	5511	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
23	B	517	CLA	CMB-C2B-C1B	-2.07	124.93	128.36
23	c	5497	CLA	CMB-C2B-C1B	-2.07	124.94	128.36
23	C	500	CLA	CAA-C2A-C3A	-2.07	107.26	113.22
28	c	5505	BCR	C40-C30-C29	-2.07	101.37	108.79
28	b	5529	BCR	C40-C30-C29	-2.07	101.39	108.79
23	c	5501	CLA	C12-C11-C10	-2.06	102.75	112.99
28	B	528	BCR	C40-C30-C29	-2.06	101.40	108.79
23	B	513	CLA	O1D-CGD-CBD	-2.06	121.67	124.62
23	B	518	CLA	C2C-C1C-NC	-2.06	108.71	110.24
23	A	563	CLA	CMA-C3A-C2A	-2.06	105.25	114.35
24	A	561	PHO	C3A-C4A-NA	-2.05	109.98	113.57
23	b	5518	CLA	O1D-CGD-CBD	-2.05	121.68	124.62
33	T	217	LMT	C1B-O1B-C4'	-2.05	112.65	118.01
26	d	5356	PQ9	C24-C23-C22	-2.05	119.48	123.50
28	T	5104	BCR	C8-C9-C10	-2.04	115.69	118.98
23	B	515	CLA	CMB-C2B-C1B	-2.04	125.00	128.36
23	C	502	CLA	CMB-C2B-C1B	-2.04	125.00	128.36
23	B	522	CLA	CAA-C2A-C3A	-2.03	107.37	113.22
23	A	558	CLA	CMA-C3A-C2A	-2.03	105.36	114.35
23	b	5515	CLA	CMA-C3A-C2A	-2.03	105.36	114.35
23	C	501	CLA	C12-C11-C10	-2.03	102.92	112.99
23	B	525	CLA	O1D-CGD-CBD	-2.03	121.72	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	493	CLA	C12-C11-C10	-2.03	102.94	112.99
29	d	5361	MGE	C3G-C2G-C1G	-2.02	107.35	112.07
32	t	213	SQD	O6-C44-C45	-2.02	106.19	110.99
23	d	5355	CLA	CMB-C2B-C1B	-2.02	125.03	128.36
23	B	516	CLA	CMB-C2B-C1B	-2.01	125.03	128.36
28	c	5505	BCR	C19-C18-C17	-2.01	115.74	118.98
23	A	558	CLA	C2C-C1C-NC	-2.01	108.75	110.24
23	c	5500	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
30	C	509	DGD	C3G-O3G-C1D	-2.00	109.61	113.82
23	C	499	CLA	O1D-CGD-CBD	-2.00	121.75	124.62
29	l	5210	MGE	O1G-C1A-C2A	2.00	117.99	111.90
32	L	5213	SQD	O8-S-O7	2.00	116.26	111.61
28	b	5529	BCR	C28-C27-C26	2.00	117.04	113.87
28	B	529	BCR	C36-C18-C19	2.00	121.43	118.10
28	B	529	BCR	C16-C17-C18	2.01	130.09	127.20
28	b	5528	BCR	C35-C13-C12	2.01	121.44	118.10
28	b	5529	BCR	C11-C10-C9	2.01	130.10	127.20
23	c	5494	CLA	C2A-C1A-CHA	2.01	127.58	123.89
23	b	5516	CLA	C16-C15-C13	2.01	122.15	115.49
28	C	505	BCR	C28-C27-C26	2.01	117.06	113.87
28	B	529	BCR	C1-C6-C7	2.02	121.46	115.82
28	h	5107	BCR	C36-C18-C19	2.02	121.45	118.10
28	c	5505	BCR	C34-C9-C8	2.02	121.45	118.10
23	b	5520	CLA	CMB-C2B-C3B	2.02	129.03	125.09
23	B	511	CLA	C2A-C1A-CHA	2.02	127.60	123.89
28	c	5504	BCR	C28-C27-C26	2.02	117.07	113.87
30	c	5508	DGD	O3G-C3G-C2G	2.02	115.80	110.99
29	b	5530	MGE	O1G-C1A-C2A	2.02	118.06	111.90
29	L	210	MGE	O1G-C1A-C2A	2.03	118.08	111.90
28	T	5104	BCR	C34-C9-C8	2.03	121.47	118.10
24	a	5562	PHO	C2A-C3A-C4A	2.03	105.75	101.10
28	T	5104	BCR	C16-C17-C18	2.03	130.13	127.20
23	B	525	CLA	C2A-C1A-CHA	2.03	127.63	123.89
25	F	51	HEM	C3B-C4B-CHC	2.03	126.03	123.16
23	c	5495	CLA	O2D-CGD-CBD	2.04	114.09	111.30
25	F	51	HEM	C1D-CHD-C4C	2.04	129.23	125.82
28	A	566	BCR	C30-C25-C24	2.04	121.53	115.82
23	b	5517	CLA	OBD-CAD-C3D	2.04	132.52	128.35
23	B	515	CLA	C2A-C1A-CHA	2.04	127.64	123.89
23	A	558	CLA	C16-C15-C13	2.04	122.26	115.49
28	x	5130	BCR	C24-C23-C22	2.04	129.33	126.22
24	A	562	PHO	CBA-CAA-C2A	2.05	119.51	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	562	PHO	CMD-C2D-C1D	2.05	128.39	125.06
30	C	507	DGD	O6D-C1D-C2D	2.05	114.48	110.28
32	A	568	SQD	C17-C16-C15	2.05	125.13	114.53
28	H	107	BCR	C37-C22-C23	2.05	121.51	118.10
23	b	5513	CLA	CBA-CAA-C2A	2.05	119.53	113.73
23	A	560	CLA	C6-C7-C8	2.05	122.30	115.49
23	c	5495	CLA	CMB-C2B-C3B	2.06	129.12	125.09
23	c	5494	CLA	CMB-C2B-C3B	2.06	129.12	125.09
28	A	566	BCR	C32-C1-C6	2.06	113.53	110.30
23	b	5519	CLA	C2A-C1A-CHA	2.06	127.69	123.89
23	c	5493	CLA	C2A-C1A-CHA	2.07	127.69	123.89
23	B	518	CLA	C1C-NC-C4C	2.07	108.78	106.27
28	A	566	BCR	C1-C6-C7	2.07	121.61	115.82
28	a	5566	BCR	C34-C9-C8	2.07	121.54	118.10
30	C	508	DGD	O1G-C1A-C2A	2.08	118.22	111.90
33	A	569	LMT	O1'-C1'-C2'	2.08	110.66	108.04
23	B	520	CLA	CMB-C2B-C3B	2.08	129.15	125.09
23	c	5503	CLA	O2D-CGD-CBD	2.08	114.15	111.30
23	b	5525	CLA	C6-C5-C3	2.08	117.05	112.48
23	a	5559	CLA	CAA-CBA-CGA	2.08	119.41	113.32
23	B	514	CLA	C2A-C1A-CHA	2.08	127.72	123.89
23	C	500	CLA	CBA-CAA-C2A	2.08	119.61	113.73
24	A	562	PHO	C2A-C3A-C4A	2.08	105.87	101.10
24	A	561	PHO	C2A-C3A-C4A	2.08	105.87	101.10
28	H	107	BCR	C30-C25-C24	2.09	121.66	115.82
23	c	5491	CLA	CBA-CAA-C2A	2.09	119.62	113.73
23	b	5517	CLA	C2A-C1A-CHA	2.09	127.73	123.89
23	C	499	CLA	C1-O2A-CGA	2.09	123.32	116.73
23	b	5514	CLA	C2A-C1A-CHA	2.09	127.73	123.89
28	b	5528	BCR	C30-C25-C24	2.09	121.67	115.82
30	c	5508	DGD	O2D-C2D-C1D	2.09	114.60	110.02
23	B	511	CLA	CMB-C2B-C3B	2.09	129.18	125.09
28	x	5130	BCR	C36-C18-C19	2.09	121.58	118.10
32	t	213	SQD	O8-S-O7	2.09	116.48	111.61
23	B	523	CLA	O2D-CGD-CBD	2.10	114.17	111.30
23	b	5518	CLA	C16-C15-C13	2.10	122.45	115.49
28	x	5130	BCR	C37-C22-C23	2.10	121.59	118.10
23	a	5563	CLA	C6-C5-C3	2.10	117.09	112.48
23	b	5517	CLA	CBA-CAA-C2A	2.10	119.66	113.73
23	C	494	CLA	CMB-C2B-C3B	2.10	129.20	125.09
28	h	5107	BCR	C30-C25-C24	2.10	121.71	115.82
23	C	503	CLA	CBA-CAA-C2A	2.10	119.67	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5511	CLA	O2D-CGD-CBD	2.10	114.18	111.30
33	a	5568	LMT	O1'-C1'-C2'	2.11	110.70	108.04
25	V	552	HEM	CBA-CAA-C2A	2.11	116.31	112.53
28	X	130	BCR	C36-C18-C19	2.11	121.61	118.10
30	c	5508	DGD	O1G-C1A-C2A	2.11	118.33	111.90
28	c	5505	BCR	C40-C30-C25	2.11	113.61	110.30
23	A	559	CLA	O2D-CGD-CBD	2.11	114.20	111.30
28	t	104	BCR	C23-C24-C25	2.12	133.67	127.32
23	A	558	CLA	C6-C5-C3	2.12	117.13	112.48
28	C	505	BCR	C7-C8-C9	2.12	129.44	126.22
23	b	5513	CLA	CMB-C2B-C3B	2.12	129.24	125.09
23	b	5523	CLA	CMB-C2B-C3B	2.12	129.24	125.09
29	d	5360	MGE	O1G-C1A-C2A	2.12	118.37	111.90
28	T	5104	BCR	C23-C24-C25	2.12	133.69	127.32
28	b	5529	BCR	C1-C6-C7	2.12	121.77	115.82
28	a	5566	BCR	C7-C8-C9	2.12	129.45	126.22
28	h	5107	BCR	C34-C9-C8	2.13	121.64	118.10
23	C	495	CLA	C2A-C1A-CHA	2.14	127.82	123.89
23	B	522	CLA	CBA-CAA-C2A	2.14	119.77	113.73
28	C	504	BCR	C30-C25-C24	2.14	121.81	115.82
28	B	529	BCR	C11-C10-C9	2.14	130.29	127.20
32	A	568	SQD	C34-C33-C32	2.14	125.59	114.53
28	t	104	BCR	C34-C9-C8	2.14	121.66	118.10
30	C	508	DGD	O3G-C3G-C2G	2.14	116.08	110.99
23	C	493	CLA	C2A-C1A-CHA	2.15	127.84	123.89
23	b	5520	CLA	C6-C5-C3	2.15	117.20	112.48
23	C	495	CLA	CMB-C2B-C3B	2.15	129.29	125.09
28	b	5528	BCR	C7-C8-C9	2.15	129.50	126.22
23	A	560	CLA	CMB-C2B-C3B	2.15	129.30	125.09
23	C	496	CLA	CBA-CAA-C2A	2.15	119.81	113.73
23	c	5491	CLA	C6-C5-C3	2.15	117.21	112.48
23	B	519	CLA	C2A-C1A-CHA	2.16	127.86	123.89
28	b	5529	BCR	C15-C14-C13	2.16	130.31	127.20
23	C	501	CLA	C2A-C1A-CHA	2.16	127.86	123.89
28	d	5357	BCR	C32-C1-C6	2.16	113.69	110.30
23	B	523	CLA	CBA-CAA-C2A	2.16	119.83	113.73
28	a	5566	BCR	C35-C13-C12	2.16	121.69	118.10
28	H	107	BCR	C36-C18-C19	2.16	121.70	118.10
28	X	130	BCR	C28-C27-C26	2.16	117.30	113.87
32	a	212	SQD	O47-C45-C44	2.16	115.99	108.36
29	D	360	MGE	O1G-C1A-C2A	2.17	118.50	111.90
28	c	5505	BCR	C36-C18-C19	2.17	121.70	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5523	CLA	CBA-CAA-C2A	2.17	119.85	113.73
32	t	213	SQD	C15-C14-C13	2.17	125.74	114.53
28	t	104	BCR	C16-C17-C18	2.17	130.34	127.20
32	d	5358	SQD	C17-C16-C15	2.17	125.75	114.53
23	B	514	CLA	C6-C5-C3	2.17	117.26	112.48
23	b	5511	CLA	CED-O2D-CGD	2.18	121.09	115.99
23	A	560	CLA	O2A-CGA-CBA	2.18	118.55	111.90
28	c	5504	BCR	C7-C8-C9	2.18	129.54	126.22
28	C	504	BCR	C16-C17-C18	2.18	130.35	127.20
28	B	528	BCR	C40-C30-C25	2.18	113.73	110.30
28	T	5104	BCR	C36-C18-C19	2.19	121.73	118.10
23	C	500	CLA	CED-O2D-CGD	2.19	121.12	115.99
28	c	5506	BCR	C36-C18-C19	2.19	121.74	118.10
28	c	5505	BCR	C7-C8-C9	2.19	129.55	126.22
28	C	506	BCR	C32-C1-C6	2.19	113.74	110.30
32	d	5358	SQD	C34-C33-C32	2.19	125.85	114.53
28	D	357	BCR	C7-C8-C9	2.19	129.56	126.22
23	A	559	CLA	CAA-CBA-CGA	2.20	119.75	113.32
28	h	5107	BCR	C37-C22-C23	2.20	121.75	118.10
32	a	212	SQD	O8-S-O7	2.20	116.73	111.61
30	c	5508	DGD	O3G-C1D-C2D	2.20	110.82	108.04
23	B	511	CLA	CED-O2D-CGD	2.20	121.16	115.99
28	t	104	BCR	C37-C22-C23	2.20	121.77	118.10
28	t	104	BCR	C36-C18-C19	2.21	121.77	118.10
28	H	107	BCR	C7-C8-C9	2.21	129.58	126.22
25	f	5051	HEM	C3B-C4B-CHC	2.21	126.27	123.16
24	a	5561	PHO	C6-C5-C3	2.21	117.34	112.48
23	c	5493	CLA	C6-C5-C3	2.21	117.34	112.48
23	B	525	CLA	C6-C5-C3	2.21	117.34	112.48
23	C	493	CLA	CBA-CAA-C2A	2.22	119.99	113.73
23	C	494	CLA	O2A-CGA-CBA	2.22	121.61	112.36
23	B	515	CLA	CBA-CAA-C2A	2.22	119.99	113.73
23	b	5518	CLA	C6-C7-C8	2.22	122.85	115.49
28	A	566	BCR	C8-C7-C6	2.22	133.99	127.32
28	H	107	BCR	C35-C13-C12	2.22	121.79	118.10
28	C	505	BCR	C8-C7-C6	2.23	134.00	127.32
30	C	508	DGD	O3G-C1D-C2D	2.23	110.86	108.04
23	C	491	CLA	CBA-CAA-C2A	2.23	120.03	113.73
23	c	5496	CLA	C6-C5-C3	2.23	117.38	112.48
32	L	5213	SQD	C15-C14-C13	2.23	126.05	114.53
28	C	506	BCR	C24-C23-C22	2.23	129.62	126.22
23	c	5494	CLA	O2A-CGA-CBA	2.23	121.67	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	5212	SQD	O47-C45-C44	2.23	116.23	108.36
23	B	523	CLA	CED-O2D-CGD	2.24	121.24	115.99
23	b	5517	CLA	O2D-CGD-CBD	2.24	114.37	111.30
23	c	5499	CLA	C2A-C1A-CHA	2.24	128.01	123.89
23	C	496	CLA	C6-C5-C3	2.24	117.40	112.48
24	a	5561	PHO	O2A-CGA-CBA	2.24	118.73	111.90
23	b	5514	CLA	CED-O2D-CGD	2.24	121.25	115.99
23	D	355	CLA	CBA-CAA-C2A	2.25	120.07	113.73
28	d	5357	BCR	C35-C13-C12	2.25	121.83	118.10
23	C	503	CLA	C1-C2-C3	2.25	130.40	126.71
25	v	5552	HEM	CBA-CAA-C2A	2.25	116.57	112.53
23	B	514	CLA	CED-O2D-CGD	2.25	121.28	115.99
23	C	502	CLA	CBA-CAA-C2A	2.25	120.09	113.73
23	C	493	CLA	C6-C5-C3	2.25	117.43	112.48
28	C	506	BCR	C37-C22-C23	2.25	121.85	118.10
23	c	5493	CLA	CBA-CAA-C2A	2.26	120.10	113.73
23	c	5500	CLA	CED-O2D-CGD	2.26	121.29	115.99
23	c	5501	CLA	O2D-CGD-CBD	2.26	114.40	111.30
23	B	526	CLA	O2D-CGD-CBD	2.26	114.40	111.30
23	b	5524	CLA	C6-C5-C3	2.26	117.45	112.48
28	c	5504	BCR	C11-C10-C9	2.26	130.47	127.20
24	a	5562	PHO	C6-C5-C3	2.27	117.46	112.48
23	c	5495	CLA	CED-O2D-CGD	2.27	121.32	115.99
29	i	5201	MGE	O3G-C1D-C2D	2.27	110.91	108.04
23	a	5560	CLA	O2A-CGA-CBA	2.28	118.83	111.90
23	B	519	CLA	O2A-CGA-CBA	2.28	118.84	111.90
28	C	506	BCR	C36-C18-C19	2.28	121.89	118.10
23	B	524	CLA	C6-C5-C3	2.28	117.49	112.48
28	T	5104	BCR	C37-C22-C23	2.28	121.90	118.10
23	B	518	CLA	C6-C7-C8	2.28	123.07	115.49
23	b	5521	CLA	O2A-CGA-CBA	2.29	118.88	111.90
33	T	217	LMT	O1B-C1B-C2B	2.29	113.68	108.10
28	C	505	BCR	C36-C18-C19	2.29	121.91	118.10
23	c	5502	CLA	C2A-C1A-CHA	2.29	128.11	123.89
23	B	511	CLA	O2D-CGD-CBD	2.29	114.44	111.30
32	A	5212	SQD	O8-S-O7	2.30	116.95	111.61
28	A	566	BCR	C37-C22-C23	2.30	121.92	118.10
28	X	130	BCR	C37-C22-C23	2.30	121.92	118.10
28	x	5130	BCR	C28-C27-C26	2.30	117.52	113.87
23	C	502	CLA	C2A-C1A-CHA	2.30	128.13	123.89
23	B	518	CLA	CBA-CAA-C2A	2.31	120.24	113.73
23	C	494	CLA	C2A-C1A-CHA	2.31	128.13	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	517	CLA	CBA-CAA-C2A	2.31	120.24	113.73
28	D	357	BCR	C40-C30-C25	2.31	113.92	110.30
28	a	5566	BCR	C30-C25-C24	2.31	122.29	115.82
23	b	5515	CLA	CBA-CAA-C2A	2.31	120.25	113.73
28	X	130	BCR	C35-C13-C12	2.31	121.94	118.10
23	D	354	CLA	CED-O2D-CGD	2.31	121.42	115.99
23	B	516	CLA	O2D-CGD-CBD	2.32	114.47	111.30
28	C	504	BCR	C11-C10-C9	2.32	130.54	127.20
28	x	5130	BCR	C30-C25-C24	2.32	122.30	115.82
28	H	107	BCR	C1-C6-C7	2.32	122.31	115.82
23	B	521	CLA	O2A-CGA-CBA	2.32	118.96	111.90
25	F	51	HEM	C2D-C3D-C4D	2.32	105.43	101.50
28	B	529	BCR	C15-C14-C13	2.32	130.55	127.20
32	d	5358	SQD	C44-O6-C1	2.32	118.70	113.82
23	c	5502	CLA	CBA-CAA-C2A	2.33	120.30	113.73
28	B	527	BCR	C36-C18-C19	2.33	121.97	118.10
23	c	5500	CLA	CBA-CAA-C2A	2.33	120.31	113.73
23	C	500	CLA	C6-C5-C3	2.33	117.60	112.48
23	C	495	CLA	O2D-CGD-CBD	2.33	114.50	111.30
23	C	491	CLA	C6-C5-C3	2.33	117.61	112.48
23	b	5518	CLA	CBA-CAA-C2A	2.33	120.32	113.73
33	t	5217	LMT	O1B-C1B-C2B	2.34	113.79	108.10
23	c	5495	CLA	C2A-C1A-CHA	2.34	128.19	123.89
23	c	5496	CLA	CBA-CAA-C2A	2.34	120.33	113.73
26	D	356	PQ9	C14-C13-C15	2.34	118.98	115.41
28	b	5528	BCR	C1-C6-C7	2.34	122.38	115.82
28	b	5527	BCR	C8-C7-C6	2.35	134.38	127.32
28	b	5527	BCR	C35-C13-C12	2.35	122.01	118.10
28	D	357	BCR	C37-C22-C23	2.36	122.02	118.10
23	B	517	CLA	C2A-C1A-CHA	2.36	128.23	123.89
28	c	5504	BCR	C30-C25-C24	2.36	122.44	115.82
28	c	5505	BCR	C8-C7-C6	2.36	134.42	127.32
28	B	528	BCR	C1-C6-C7	2.37	122.45	115.82
32	A	568	SQD	C15-C14-C13	2.37	126.76	114.53
25	f	5051	HEM	C2D-C3D-C4D	2.38	105.53	101.50
25	V	552	HEM	C2D-C3D-C4D	2.38	105.53	101.50
23	B	519	CLA	C6-C5-C3	2.38	117.71	112.48
23	a	5560	CLA	C6-C5-C3	2.38	117.72	112.48
23	B	524	CLA	O2D-CGD-CBD	2.38	114.57	111.30
28	a	5566	BCR	C36-C18-C19	2.39	122.07	118.10
29	B	530	MGE	O6D-C5D-C6D	2.39	112.39	106.36
28	b	5528	BCR	C32-C1-C6	2.39	114.05	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5503	CLA	O2A-CGA-CBA	2.39	119.18	111.90
28	B	529	BCR	C32-C1-C6	2.39	114.05	110.30
23	b	5519	CLA	O2A-CGA-CBA	2.39	119.19	111.90
23	A	563	CLA	C6-C5-C3	2.39	117.74	112.48
32	A	568	SQD	C44-O6-C1	2.40	118.86	113.82
23	b	5512	CLA	C6-C5-C3	2.40	117.75	112.48
23	C	495	CLA	CED-O2D-CGD	2.40	121.63	115.99
28	a	5566	BCR	C32-C1-C6	2.41	114.08	110.30
28	C	506	BCR	C30-C25-C24	2.41	122.57	115.82
28	c	5504	BCR	C37-C22-C23	2.41	122.11	118.10
28	B	529	BCR	C40-C30-C25	2.41	114.09	110.30
28	C	504	BCR	C40-C30-C25	2.42	114.10	110.30
32	d	5358	SQD	O8-S-O7	2.42	117.25	111.61
28	X	130	BCR	C30-C25-C24	2.42	122.61	115.82
23	A	558	CLA	O2D-CGD-CBD	2.43	114.62	111.30
28	C	504	BCR	C37-C22-C23	2.43	122.14	118.10
24	A	561	PHO	O2A-CGA-CBA	2.43	119.31	111.90
32	L	5213	SQD	C31-C30-C29	2.44	132.59	113.44
28	A	566	BCR	C2-C1-C6	2.44	114.22	110.36
28	T	5104	BCR	C7-C8-C9	2.44	129.93	126.22
28	C	504	BCR	C7-C8-C9	2.44	129.94	126.22
28	B	529	BCR	C35-C13-C12	2.44	122.17	118.10
23	c	5501	CLA	O2A-CGA-CBA	2.45	119.38	111.90
25	v	5552	HEM	C2D-C3D-C4D	2.45	105.66	101.50
23	c	5498	CLA	C6-C5-C3	2.45	117.87	112.48
23	B	518	CLA	O2D-CGD-CBD	2.46	114.67	111.30
23	B	516	CLA	C1D-CHD-C4C	2.46	126.32	122.60
23	d	5354	CLA	CED-O2D-CGD	2.46	121.76	115.99
28	a	5566	BCR	C37-C22-C23	2.46	122.19	118.10
23	A	563	CLA	CED-O2D-CGD	2.46	121.77	115.99
28	h	5107	BCR	C35-C13-C12	2.47	122.21	118.10
28	B	527	BCR	C8-C7-C6	2.47	134.74	127.32
28	c	5504	BCR	C35-C13-C12	2.47	122.21	118.10
30	C	508	DGD	O6D-C5D-C6D	2.47	111.66	106.61
23	c	5502	CLA	O2D-CGD-CBD	2.47	114.69	111.30
28	A	566	BCR	C35-C13-C12	2.47	122.21	118.10
28	a	5566	BCR	C2-C1-C6	2.48	114.29	110.36
28	c	5506	BCR	C37-C22-C23	2.48	122.22	118.10
23	C	498	CLA	C6-C5-C3	2.48	117.93	112.48
28	h	5107	BCR	C1-C6-C7	2.48	122.77	115.82
28	A	566	BCR	C36-C18-C19	2.48	122.23	118.10
29	b	5530	MGE	O3G-C1D-C2D	2.48	111.17	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5492	CLA	O2A-CGA-CBA	2.49	119.48	111.90
28	D	357	BCR	C16-C17-C18	2.49	130.79	127.20
28	d	5357	BCR	C16-C17-C18	2.49	130.79	127.20
28	b	5529	BCR	C7-C8-C9	2.49	130.01	126.22
24	A	561	PHO	C6-C5-C3	2.49	117.96	112.48
28	a	5566	BCR	C8-C7-C6	2.49	134.81	127.32
28	x	5130	BCR	C35-C13-C12	2.50	122.26	118.10
23	c	5500	CLA	C6-C5-C3	2.50	117.97	112.48
28	a	5566	BCR	C16-C17-C18	2.50	130.81	127.20
32	a	212	SQD	O48-C23-C24	2.50	123.76	112.42
26	d	5356	PQ9	C19-C18-C20	2.51	119.23	115.41
23	a	5560	CLA	CED-O2D-CGD	2.51	121.87	115.99
28	B	528	BCR	C32-C1-C6	2.51	114.24	110.30
23	B	519	CLA	O2D-CGD-CBD	2.51	114.74	111.30
28	h	5107	BCR	C16-C17-C18	2.51	130.83	127.20
28	D	357	BCR	C35-C13-C12	2.51	122.28	118.10
23	B	518	CLA	C6-C5-C3	2.52	118.00	112.48
23	b	5519	CLA	O2D-CGD-CBD	2.52	114.75	111.30
23	b	5517	CLA	C6-C5-C3	2.52	118.01	112.48
25	f	5051	HEM	CMD-C2D-C3D	2.52	125.51	114.35
28	A	566	BCR	C7-C8-C9	2.53	130.08	126.22
23	a	5560	CLA	O2D-CGD-CBD	2.54	114.78	111.30
23	c	5500	CLA	O2A-CGA-CBA	2.54	119.63	111.90
28	b	5529	BCR	C35-C13-C12	2.54	122.32	118.10
28	h	5107	BCR	C28-C27-C26	2.54	117.89	113.87
24	A	561	PHO	CBD-CHA-C1A	2.54	132.34	126.36
23	C	498	CLA	O2A-CGA-CBA	2.54	119.65	111.90
23	C	496	CLA	O2D-CGD-CBD	2.54	114.79	111.30
23	b	5524	CLA	O2A-CGA-CBA	2.55	119.66	111.90
23	b	5516	CLA	C1D-CHD-C4C	2.55	126.46	122.60
32	d	5358	SQD	C15-C14-C13	2.55	127.69	114.53
23	C	499	CLA	CED-O2D-CGD	2.55	121.97	115.99
32	A	5212	SQD	O48-C23-C24	2.55	123.98	112.42
32	t	213	SQD	C31-C30-C29	2.55	133.50	113.44
28	X	130	BCR	C24-C23-C22	2.56	130.11	126.22
23	b	5521	CLA	CED-O2D-CGD	2.56	121.99	115.99
29	d	5359	MGE	O6D-C5D-C6D	2.56	112.83	106.36
28	c	5506	BCR	C35-C13-C12	2.56	122.36	118.10
23	C	501	CLA	O2D-CGD-CBD	2.57	114.82	111.30
28	H	107	BCR	C16-C17-C18	2.58	130.92	127.20
28	c	5506	BCR	C24-C23-C22	2.58	130.14	126.22
28	b	5529	BCR	C32-C1-C6	2.58	114.35	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	5357	BCR	C7-C8-C9	2.59	130.16	126.22
28	B	529	BCR	C8-C7-C6	2.59	135.09	127.32
28	d	5357	BCR	C36-C18-C19	2.59	122.41	118.10
23	a	5558	CLA	CBA-CAA-C2A	2.60	121.06	113.73
23	c	5496	CLA	O2D-CGD-CBD	2.60	114.86	111.30
23	B	517	CLA	C6-C5-C3	2.60	118.19	112.48
28	C	505	BCR	C35-C13-C12	2.60	122.43	118.10
23	c	5499	CLA	C1D-CHD-C4C	2.60	126.54	122.60
23	B	512	CLA	C6-C5-C3	2.61	118.20	112.48
24	a	5561	PHO	CBD-CHA-C1A	2.61	132.50	126.36
28	H	107	BCR	C28-C27-C26	2.61	118.00	113.87
23	B	520	CLA	O2D-CGD-CBD	2.61	114.88	111.30
23	c	5494	CLA	CBA-CAA-C2A	2.61	121.10	113.73
23	C	499	CLA	C2A-C1A-CHA	2.61	128.70	123.89
23	C	503	CLA	O2D-CGD-CBD	2.62	114.89	111.30
23	b	5515	CLA	C1D-CHD-C4C	2.62	126.56	122.60
28	t	104	BCR	C7-C8-C9	2.62	130.21	126.22
23	d	5355	CLA	O2A-CGA-CBA	2.62	119.89	111.90
28	c	5506	BCR	C30-C25-C24	2.63	123.17	115.82
26	A	564	PQ9	C14-C13-C15	2.63	119.42	115.41
26	a	5564	PQ9	C14-C13-C15	2.63	119.42	115.41
23	c	5498	CLA	O2A-CGA-CBA	2.63	119.92	111.90
23	B	515	CLA	C1D-CHD-C4C	2.63	126.58	122.60
28	b	5528	BCR	C8-C7-C6	2.63	135.22	127.32
23	c	5500	CLA	O2D-CGD-CBD	2.64	114.92	111.30
30	H	208	DGD	O6D-C5D-C4D	2.64	114.63	109.68
30	c	5508	DGD	O6D-C5D-C6D	2.64	112.00	106.61
28	c	5506	BCR	C16-C17-C18	2.64	131.01	127.20
23	C	498	CLA	CED-O2D-CGD	2.64	122.19	115.99
29	b	5530	MGE	O6D-C5D-C6D	2.64	113.03	106.36
23	c	5496	CLA	O2A-CGA-CBA	2.64	119.96	111.90
30	h	5208	DGD	O6D-C5D-C4D	2.64	114.64	109.68
23	a	5563	CLA	C1D-CHD-C4C	2.65	126.61	122.60
25	F	51	HEM	CMD-C2D-C3D	2.65	126.07	114.35
28	B	527	BCR	C16-C17-C18	2.65	131.03	127.20
23	C	501	CLA	O2A-CGA-CBA	2.65	119.98	111.90
23	A	558	CLA	CBA-CAA-C2A	2.66	121.22	113.73
28	C	504	BCR	C1-C6-C7	2.66	123.26	115.82
23	A	560	CLA	C6-C5-C3	2.66	118.32	112.48
24	A	562	PHO	C6-C5-C3	2.66	118.33	112.48
23	A	560	CLA	O2D-CGD-CBD	2.66	114.95	111.30
23	C	500	CLA	O2A-CGA-CBA	2.66	120.01	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5511	CLA	C1D-CHD-C4C	2.67	126.64	122.60
28	A	566	BCR	C16-C17-C18	2.67	131.05	127.20
28	b	5528	BCR	C24-C23-C22	2.67	130.28	126.22
24	A	562	PHO	CED-O2D-CGD	2.67	122.25	115.99
28	d	5357	BCR	C37-C22-C23	2.67	122.54	118.10
23	B	515	CLA	CED-O2D-CGD	2.67	122.25	115.99
23	C	501	CLA	CED-O2D-CGD	2.67	122.26	115.99
32	A	568	SQD	O8-S-O7	2.67	117.83	111.61
23	A	558	CLA	C1D-CHD-C4C	2.68	126.65	122.60
23	B	517	CLA	O2D-CGD-CBD	2.68	114.98	111.30
23	b	5515	CLA	O2D-CGD-CBD	2.68	114.98	111.30
24	a	5562	PHO	O2D-CGD-CBD	2.69	114.99	111.30
28	C	504	BCR	C23-C24-C25	2.69	135.40	127.32
23	A	559	CLA	O2A-CGA-CBA	2.69	120.11	111.90
23	B	512	CLA	C1D-CHD-C4C	2.70	126.68	122.60
28	B	528	BCR	C8-C7-C6	2.70	135.42	127.32
28	C	504	BCR	C35-C13-C12	2.70	122.58	118.10
32	A	568	SQD	C36-C35-C34	2.70	128.47	114.53
23	c	5497	CLA	C1D-CHD-C4C	2.70	126.69	122.60
28	B	527	BCR	C24-C23-C22	2.70	130.33	126.22
23	b	5519	CLA	C6-C5-C3	2.70	118.42	112.48
28	c	5504	BCR	C23-C24-C25	2.70	135.44	127.32
28	D	357	BCR	C24-C23-C22	2.70	130.34	126.22
23	B	523	CLA	O2A-CGA-CBA	2.71	120.15	111.90
23	a	5558	CLA	C1D-CHD-C4C	2.71	126.70	122.60
29	l	5210	MGE	O2G-C1B-C2B	2.71	117.42	111.53
23	A	560	CLA	CAA-CBA-CGA	2.71	121.26	113.32
23	b	5520	CLA	CED-O2D-CGD	2.71	122.35	115.99
28	T	5104	BCR	C35-C13-C12	2.71	122.61	118.10
23	A	560	CLA	CED-O2D-CGD	2.71	122.36	115.99
23	B	513	CLA	CED-O2D-CGD	2.72	122.37	115.99
32	d	5358	SQD	C36-C35-C34	2.72	128.58	114.53
23	B	524	CLA	O2A-CGA-CBA	2.72	120.20	111.90
23	b	5516	CLA	O2D-CGD-CBD	2.73	115.04	111.30
28	a	5566	BCR	C23-C24-C25	2.73	135.51	127.32
23	c	5501	CLA	CED-O2D-CGD	2.74	122.41	115.99
23	d	5354	CLA	C1D-CHD-C4C	2.74	126.75	122.60
26	d	5356	PQ9	C14-C13-C15	2.74	119.59	115.41
23	C	494	CLA	CBA-CAA-C2A	2.74	121.47	113.73
23	c	5497	CLA	CED-O2D-CGD	2.74	122.42	115.99
24	A	562	PHO	CBD-CHA-C1A	2.74	132.82	126.36
28	X	130	BCR	C16-C17-C18	2.74	131.16	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5492	CLA	C1D-CHD-C4C	2.74	126.75	122.60
25	V	552	HEM	CMD-C2D-C3D	2.75	126.50	114.35
23	A	559	CLA	CED-O2D-CGD	2.75	122.44	115.99
24	a	5562	PHO	CBD-CHA-C1A	2.75	132.83	126.36
23	C	497	CLA	CED-O2D-CGD	2.75	122.44	115.99
23	b	5513	CLA	CED-O2D-CGD	2.76	122.45	115.99
23	B	511	CLA	C1D-CHD-C4C	2.76	126.77	122.60
28	d	5357	BCR	C8-C7-C6	2.76	135.60	127.32
32	a	212	SQD	O47-C7-C8	2.76	116.30	111.10
29	L	210	MGE	O2G-C1B-C2B	2.76	117.53	111.53
23	b	5526	CLA	O2A-CGA-CBA	2.76	120.31	111.90
23	A	558	CLA	CED-O2D-CGD	2.77	122.48	115.99
23	c	5491	CLA	O2D-CGD-CBD	2.77	115.10	111.30
23	b	5512	CLA	C1D-CHD-C4C	2.77	126.79	122.60
23	c	5493	CLA	O2D-CGD-CBD	2.77	115.10	111.30
28	A	566	BCR	C23-C24-C25	2.77	135.65	127.32
28	b	5529	BCR	C8-C7-C6	2.78	135.65	127.32
23	B	525	CLA	CED-O2D-CGD	2.78	122.51	115.99
23	A	563	CLA	O2D-CGD-CBD	2.78	115.11	111.30
23	b	5525	CLA	CED-O2D-CGD	2.78	122.52	115.99
23	a	5560	CLA	C1D-CHD-C4C	2.78	126.81	122.60
23	c	5492	CLA	O2D-CGD-CBD	2.79	115.12	111.30
23	b	5523	CLA	O2D-CGD-CBD	2.79	115.12	111.30
28	T	5104	BCR	C2-C1-C6	2.79	114.78	110.36
32	A	5212	SQD	O47-C7-C8	2.79	116.36	111.10
28	T	5104	BCR	C11-C10-C9	2.79	131.22	127.20
28	h	5107	BCR	C15-C14-C13	2.79	131.23	127.20
23	b	5520	CLA	C1D-CHD-C4C	2.79	126.83	122.60
23	B	519	CLA	C1D-CHD-C4C	2.79	126.83	122.60
23	D	355	CLA	CED-O2D-CGD	2.80	122.55	115.99
23	b	5526	CLA	C6-C5-C3	2.80	118.63	112.48
23	C	491	CLA	O2A-CGA-CBA	2.80	120.44	111.90
28	b	5527	BCR	C16-C17-C18	2.80	131.24	127.20
32	d	5358	SQD	C32-C31-C30	2.80	129.01	114.53
23	C	502	CLA	O2D-CGD-CBD	2.80	115.14	111.30
28	t	104	BCR	C35-C13-C12	2.81	122.77	118.10
28	B	527	BCR	C23-C24-C25	2.81	135.75	127.32
23	b	5520	CLA	O2D-CGD-CBD	2.81	115.15	111.30
23	B	526	CLA	C1D-CHD-C4C	2.81	126.85	122.60
23	B	526	CLA	C6-C5-C3	2.81	118.65	112.48
28	H	107	BCR	C8-C7-C6	2.81	135.76	127.32
23	C	494	CLA	C1D-CHD-C4C	2.81	126.86	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	5518	CLA	CED-O2D-CGD	2.81	122.59	115.99
23	A	559	CLA	C1D-CHD-C4C	2.82	126.86	122.60
23	C	493	CLA	C1D-CHD-C4C	2.82	126.86	122.60
23	a	5558	CLA	O2A-CGA-CBA	2.82	120.49	111.90
23	C	492	CLA	C1D-CHD-C4C	2.82	126.87	122.60
23	C	498	CLA	C1D-CHD-C4C	2.82	126.87	122.60
28	c	5505	BCR	C16-C17-C18	2.82	131.27	127.20
25	v	5552	HEM	CMD-C2D-C3D	2.82	126.83	114.35
23	B	515	CLA	O2D-CGD-CBD	2.82	115.17	111.30
29	D	358	MGE	O6D-C5D-C6D	2.82	113.49	106.36
28	B	527	BCR	C35-C13-C12	2.83	122.80	118.10
23	d	5355	CLA	O2D-CGD-CBD	2.83	115.18	111.30
28	b	5529	BCR	C24-C23-C22	2.83	130.53	126.22
23	b	5512	CLA	O2D-CGD-CBD	2.83	115.18	111.30
23	a	5560	CLA	CAA-CBA-CGA	2.83	121.60	113.32
28	X	130	BCR	C34-C9-C8	2.83	122.81	118.10
28	d	5357	BCR	C23-C24-C25	2.84	135.83	127.32
23	D	355	CLA	O2A-CGA-CBA	2.84	120.54	111.90
23	c	5493	CLA	C1D-CHD-C4C	2.84	126.90	122.60
23	C	500	CLA	O2D-CGD-CBD	2.84	115.19	111.30
23	B	512	CLA	O2D-CGD-CBD	2.84	115.20	111.30
23	c	5499	CLA	CED-O2D-CGD	2.84	122.66	115.99
32	L	5213	SQD	C44-O6-C1	2.84	119.80	113.82
23	b	5513	CLA	C6-C5-C3	2.85	118.73	112.48
23	c	5494	CLA	C1D-CHD-C4C	2.85	126.91	122.60
23	b	5518	CLA	C6-C5-C3	2.85	118.73	112.48
23	c	5498	CLA	CED-O2D-CGD	2.85	122.68	115.99
28	B	529	BCR	C7-C8-C9	2.86	130.57	126.22
23	A	558	CLA	O2A-CGA-CBA	2.86	120.61	111.90
23	B	520	CLA	C1D-CHD-C4C	2.86	126.93	122.60
23	D	354	CLA	C1D-CHD-C4C	2.87	126.94	122.60
23	c	5496	CLA	C1D-CHD-C4C	2.87	126.94	122.60
28	D	357	BCR	C8-C7-C6	2.87	135.93	127.32
23	b	5525	CLA	C1D-CHD-C4C	2.87	126.94	122.60
28	c	5504	BCR	C1-C6-C7	2.87	123.86	115.82
23	b	5526	CLA	C1D-CHD-C4C	2.88	126.95	122.60
23	b	5516	CLA	CBA-CAA-C2A	2.88	121.86	113.73
31	a	5567	LHG	O7-C7-C8	2.88	117.79	111.53
32	A	568	SQD	C45-O47-C7	2.88	124.81	117.89
23	b	5524	CLA	O2D-CGD-CBD	2.88	115.26	111.30
23	B	526	CLA	O2A-CGA-CBA	2.89	120.70	111.90
28	C	504	BCR	C32-C1-C6	2.89	114.83	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	497	CLA	C1D-CHD-C4C	2.89	126.97	122.60
23	A	563	CLA	O2A-CGA-CBA	2.89	120.71	111.90
23	b	5523	CLA	O2A-CGA-CBA	2.89	120.71	111.90
28	x	5130	BCR	C34-C9-C8	2.89	122.91	118.10
23	B	525	CLA	O2A-CGA-CBA	2.90	120.73	111.90
23	b	5521	CLA	O2D-CGD-CBD	2.90	115.27	111.30
23	a	5563	CLA	CED-O2D-CGD	2.90	122.79	115.99
23	C	503	CLA	O2A-CGA-CBA	2.90	120.74	111.90
23	a	5559	CLA	O2A-CGA-CBA	2.90	120.74	111.90
28	c	5504	BCR	C29-C30-C25	2.90	114.96	110.36
23	a	5563	CLA	O2A-CGA-CBA	2.90	120.75	111.90
28	B	528	BCR	C24-C23-C22	2.91	130.64	126.22
28	H	107	BCR	C32-C1-C6	2.91	114.86	110.30
23	C	491	CLA	C1D-CHD-C4C	2.91	127.01	122.60
23	B	512	CLA	O2A-CGA-CBA	2.91	120.77	111.90
23	c	5498	CLA	C1D-CHD-C4C	2.91	127.01	122.60
28	b	5529	BCR	C23-C24-C25	2.91	136.07	127.32
23	d	5355	CLA	C1D-CHD-C4C	2.91	127.01	122.60
23	d	5355	CLA	CED-O2D-CGD	2.92	122.83	115.99
28	c	5505	BCR	C35-C13-C12	2.92	122.96	118.10
23	C	502	CLA	CED-O2D-CGD	2.92	122.85	115.99
24	a	5562	PHO	CED-O2D-CGD	2.93	122.85	115.99
23	C	492	CLA	O2D-CGD-CBD	2.93	115.31	111.30
23	B	524	CLA	C1D-CHD-C4C	2.93	127.03	122.60
24	a	5561	PHO	CED-O2D-CGD	2.93	122.86	115.99
23	B	513	CLA	O2D-CGD-CBD	2.93	115.32	111.30
28	C	506	BCR	C35-C13-C12	2.93	122.98	118.10
23	B	516	CLA	CBA-CAA-C2A	2.94	122.02	113.73
23	a	5559	CLA	C1D-CHD-C4C	2.94	127.05	122.60
23	a	5563	CLA	O2D-CGD-CBD	2.94	115.33	111.30
23	C	503	CLA	C1D-CHD-C4C	2.94	127.05	122.60
29	i	5201	MGE	O6D-C5D-C6D	2.94	113.80	106.36
23	B	514	CLA	O2A-CGA-CBA	2.94	120.87	111.90
23	b	5524	CLA	CED-O2D-CGD	2.94	122.90	115.99
23	b	5526	CLA	O2D-CGD-CBD	2.95	115.34	111.30
23	b	5514	CLA	C1D-CHD-C4C	2.95	127.06	122.60
23	b	5524	CLA	C1D-CHD-C4C	2.95	127.07	122.60
23	c	5502	CLA	C1D-CHD-C4C	2.95	127.07	122.60
28	t	104	BCR	C2-C1-C6	2.96	115.04	110.36
23	c	5495	CLA	O2A-CGA-CBA	2.96	120.91	111.90
23	b	5519	CLA	C1D-CHD-C4C	2.96	127.08	122.60
23	B	521	CLA	CED-O2D-CGD	2.96	122.93	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	5506	BCR	C23-C24-C25	2.96	136.21	127.32
28	c	5504	BCR	C40-C30-C25	2.96	114.94	110.30
23	C	493	CLA	CED-O2D-CGD	2.96	122.94	115.99
23	B	515	CLA	O2A-CGA-CBA	2.96	120.92	111.90
23	C	492	CLA	O2A-CGA-CBA	2.96	120.93	111.90
23	C	497	CLA	C6-C5-C3	2.97	119.00	112.48
23	B	520	CLA	CED-O2D-CGD	2.97	122.95	115.99
28	B	529	BCR	C23-C24-C25	2.97	136.24	127.32
23	c	5499	CLA	O2A-CGA-CBA	2.98	120.97	111.90
23	B	512	CLA	CED-O2D-CGD	2.98	122.97	115.99
23	C	499	CLA	O2A-CGA-CBA	2.98	120.97	111.90
28	B	528	BCR	C23-C24-C25	2.98	136.26	127.32
23	B	520	CLA	O2A-CGA-CBA	2.98	120.98	111.90
23	b	5518	CLA	O2D-CGD-CBD	2.98	115.39	111.30
23	B	513	CLA	C6-C5-C3	2.98	119.03	112.48
23	B	516	CLA	CED-O2D-CGD	2.98	122.99	115.99
28	b	5528	BCR	C23-C24-C25	2.99	136.29	127.32
23	b	5522	CLA	CED-O2D-CGD	2.99	123.00	115.99
32	A	568	SQD	C32-C31-C30	2.99	129.96	114.53
31	A	567	LHG	O7-C7-C8	2.99	118.02	111.53
23	B	522	CLA	CED-O2D-CGD	2.99	123.00	115.99
23	c	5503	CLA	C1D-CHD-C4C	2.99	127.12	122.60
24	a	5561	PHO	O2D-CGD-CBD	2.99	115.40	111.30
23	b	5518	CLA	C1D-CHD-C4C	2.99	127.13	122.60
23	B	514	CLA	C1D-CHD-C4C	2.99	127.13	122.60
23	C	496	CLA	O2A-CGA-CBA	3.00	121.03	111.90
26	A	564	PQ9	C24-C23-C25	3.00	119.98	115.41
23	c	5497	CLA	C6-C5-C3	3.00	119.06	112.48
26	A	564	PQ9	C19-C18-C20	3.00	119.98	115.41
23	C	493	CLA	O2D-CGD-CBD	3.00	115.41	111.30
23	C	499	CLA	C1D-CHD-C4C	3.00	127.14	122.60
26	D	356	PQ9	C19-C18-C20	3.00	119.99	115.41
23	b	5525	CLA	O2A-CGA-CBA	3.00	121.04	111.90
28	h	5107	BCR	C24-C23-C22	3.00	130.79	126.22
23	D	354	CLA	O2A-CGA-CBA	3.00	121.05	111.90
23	c	5501	CLA	C1D-CHD-C4C	3.01	127.15	122.60
23	c	5491	CLA	C1D-CHD-C4C	3.01	127.16	122.60
28	B	527	BCR	C29-C30-C25	3.01	115.13	110.36
23	C	491	CLA	O2D-CGD-CBD	3.01	115.43	111.30
23	D	354	CLA	O2D-CGD-CBD	3.02	115.44	111.30
28	h	5107	BCR	C8-C7-C6	3.02	136.37	127.32
23	B	521	CLA	C1D-CHD-C4C	3.02	127.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	518	CLA	CED-O2D-CGD	3.02	123.07	115.99
30	H	208	DGD	C1E-O6E-C5E	3.02	119.60	113.75
23	b	5521	CLA	C1D-CHD-C4C	3.02	127.17	122.60
30	C	509	DGD	O2G-C1B-C2B	3.03	118.10	111.53
23	b	5512	CLA	O2A-CGA-CBA	3.03	121.13	111.90
23	B	518	CLA	C1D-CHD-C4C	3.03	127.19	122.60
30	H	208	DGD	O6D-C5D-C6D	3.04	112.81	106.61
23	b	5513	CLA	C1D-CHD-C4C	3.04	127.20	122.60
23	b	5517	CLA	C1D-CHD-C4C	3.04	127.20	122.60
28	B	529	BCR	C24-C23-C22	3.04	130.85	126.22
28	t	104	BCR	C11-C10-C9	3.04	131.59	127.20
28	b	5527	BCR	C23-C24-C25	3.04	136.46	127.32
28	b	5527	BCR	C29-C30-C25	3.04	115.18	110.36
23	C	491	CLA	CED-O2D-CGD	3.05	123.13	115.99
23	C	495	CLA	C1D-CHD-C4C	3.05	127.21	122.60
32	t	213	SQD	C44-O6-C1	3.05	120.23	113.82
23	A	560	CLA	C1D-CHD-C4C	3.05	127.22	122.60
29	d	5360	MGE	O2G-C1B-C2B	3.05	118.16	111.53
23	A	563	CLA	C1D-CHD-C4C	3.05	127.22	122.60
30	h	5208	DGD	O5D-C1E-C2E	3.05	111.90	108.04
30	C	508	DGD	C1E-O6E-C5E	3.06	119.68	113.75
30	c	5509	DGD	O2G-C1B-C2B	3.06	118.18	111.53
28	D	357	BCR	C23-C24-C25	3.06	136.51	127.32
28	H	107	BCR	C23-C24-C25	3.06	136.52	127.32
23	C	495	CLA	O2A-CGA-CBA	3.06	121.23	111.90
23	b	5515	CLA	CED-O2D-CGD	3.07	123.18	115.99
23	C	496	CLA	C1D-CHD-C4C	3.07	127.24	122.60
26	a	5564	PQ9	C19-C18-C20	3.07	120.10	115.41
26	a	5564	PQ9	C24-C23-C25	3.07	120.10	115.41
23	B	524	CLA	CED-O2D-CGD	3.08	123.20	115.99
23	c	5495	CLA	C1D-CHD-C4C	3.08	127.26	122.60
23	B	525	CLA	C1D-CHD-C4C	3.08	127.26	122.60
23	c	5502	CLA	CED-O2D-CGD	3.08	123.22	115.99
23	b	5522	CLA	C1D-CHD-C4C	3.09	127.28	122.60
28	H	107	BCR	C24-C23-C22	3.09	130.93	126.22
29	L	210	MGE	O6D-C5D-C6D	3.10	114.19	106.36
29	I	201	MGE	O6D-C5D-C6D	3.10	114.19	106.36
23	D	355	CLA	C1D-CHD-C4C	3.11	127.31	122.60
28	B	527	BCR	C2-C1-C6	3.11	115.29	110.36
23	b	5523	CLA	C6-C5-C3	3.12	119.33	112.48
28	h	5107	BCR	C32-C1-C6	3.12	115.20	110.30
23	c	5491	CLA	O2A-CGA-CBA	3.12	121.41	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	506	BCR	C16-C17-C18	3.12	131.71	127.20
23	b	5514	CLA	O2A-CGA-CBA	3.12	121.42	111.90
23	C	500	CLA	C1D-CHD-C4C	3.13	127.34	122.60
23	d	5354	CLA	O2A-CGA-CBA	3.13	121.45	111.90
23	b	5520	CLA	O2A-CGA-CBA	3.13	121.45	111.90
24	A	562	PHO	O2D-CGD-CBD	3.13	115.60	111.30
30	h	5208	DGD	O2G-C1B-C2B	3.14	118.34	111.53
30	c	5507	DGD	O2G-C1B-C2B	3.14	118.35	111.53
23	C	502	CLA	C1D-CHD-C4C	3.14	127.36	122.60
28	h	5107	BCR	C2-C1-C6	3.14	115.34	110.36
28	C	504	BCR	C29-C30-C25	3.14	115.34	110.36
23	B	515	CLA	C6-C5-C3	3.15	119.39	112.48
23	C	501	CLA	C1D-CHD-C4C	3.15	127.36	122.60
30	c	5507	DGD	C1E-O6E-C5E	3.15	119.87	113.75
28	c	5504	BCR	C32-C1-C6	3.15	115.25	110.30
23	C	497	CLA	O2A-CGA-CBA	3.16	121.53	111.90
28	h	5107	BCR	C23-C24-C25	3.16	136.82	127.32
23	B	521	CLA	O2D-CGD-CBD	3.17	115.64	111.30
30	c	5508	DGD	C1E-O6E-C5E	3.17	119.90	113.75
23	b	5512	CLA	CED-O2D-CGD	3.17	123.43	115.99
28	C	505	BCR	C16-C17-C18	3.18	131.78	127.20
23	b	5525	CLA	O2D-CGD-CBD	3.18	115.66	111.30
23	c	5495	CLA	C6-C5-C3	3.18	119.46	112.48
23	D	355	CLA	C1-C2-C3	3.18	131.93	126.71
28	H	107	BCR	C15-C14-C13	3.19	131.80	127.20
28	c	5506	BCR	C2-C1-C6	3.19	115.41	110.36
30	c	5507	DGD	O5D-C6D-C5D	3.19	114.86	109.08
30	C	507	DGD	O2G-C1B-C2B	3.20	118.48	111.53
29	b	5530	MGE	O2G-C1B-C2B	3.20	118.48	111.53
28	A	566	BCR	C24-C23-C22	3.20	131.10	126.22
32	d	5358	SQD	C45-O47-C7	3.20	125.58	117.89
23	c	5492	CLA	C6-C5-C3	3.20	119.52	112.48
24	A	561	PHO	CED-O2D-CGD	3.21	123.51	115.99
23	B	522	CLA	C1D-CHD-C4C	3.21	127.46	122.60
23	B	513	CLA	C1D-CHD-C4C	3.22	127.47	122.60
28	C	506	BCR	C23-C24-C25	3.22	136.99	127.32
29	l	5210	MGE	O6D-C5D-C6D	3.23	114.52	106.36
28	H	107	BCR	C2-C1-C6	3.23	115.48	110.36
23	B	521	CLA	C6-C5-C3	3.24	119.58	112.48
23	a	5559	CLA	CED-O2D-CGD	3.24	123.59	115.99
23	b	5522	CLA	O2A-CGA-CBA	3.24	121.77	111.90
28	t	104	BCR	C24-C23-C22	3.24	131.16	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	358	MGE	O2G-C1B-C2B	3.24	118.58	111.53
28	d	5357	BCR	C24-C23-C22	3.25	131.16	126.22
29	D	359	MGE	O2G-C1B-C2B	3.25	118.59	111.53
28	C	504	BCR	C2-C1-C6	3.25	115.51	110.36
23	b	5515	CLA	O2A-CGA-CBA	3.25	121.81	111.90
29	B	530	MGE	O2G-C1B-C2B	3.25	118.60	111.53
23	C	495	CLA	CBA-CAA-C2A	3.26	122.93	113.73
29	D	359	MGE	O6D-C5D-C6D	3.27	114.62	106.36
28	B	528	BCR	C29-C30-C25	3.27	115.55	110.36
23	c	5500	CLA	C1D-CHD-C4C	3.28	127.56	122.60
24	A	562	PHO	O2A-CGA-CBA	3.28	121.89	111.90
30	C	507	DGD	O5D-C6D-C5D	3.28	115.02	109.08
23	c	5495	CLA	CBA-CAA-C2A	3.28	123.00	113.73
23	D	355	CLA	O2D-CGD-CBD	3.29	115.81	111.30
28	a	5566	BCR	C24-C23-C22	3.29	131.22	126.22
30	h	5208	DGD	O6D-C5D-C6D	3.29	113.33	106.61
23	b	5515	CLA	C6-C5-C3	3.29	119.71	112.48
28	B	528	BCR	C2-C1-C6	3.30	115.59	110.36
29	I	201	MGE	O2G-C1B-C2B	3.30	118.70	111.53
29	i	5201	MGE	O2G-C1B-C2B	3.30	118.70	111.53
30	H	208	DGD	O2G-C1B-C2B	3.30	118.71	111.53
23	a	5558	CLA	CED-O2D-CGD	3.30	123.74	115.99
24	a	5562	PHO	O2A-CGA-CBA	3.31	121.98	111.90
23	b	5516	CLA	CED-O2D-CGD	3.31	123.75	115.99
23	b	5513	CLA	O2D-CGD-CBD	3.31	115.84	111.30
23	B	526	CLA	CED-O2D-CGD	3.31	123.76	115.99
24	A	561	PHO	O2D-CGD-CBD	3.31	115.84	111.30
23	c	5497	CLA	O2A-CGA-CBA	3.32	122.00	111.90
23	B	519	CLA	CED-O2D-CGD	3.32	123.77	115.99
23	b	5513	CLA	O2A-CGA-CBA	3.32	122.01	111.90
23	C	503	CLA	CED-O2D-CGD	3.32	123.78	115.99
23	c	5498	CLA	O2D-CGD-CBD	3.32	115.86	111.30
28	D	357	BCR	C29-C30-C25	3.33	115.64	110.36
23	C	493	CLA	O2A-CGA-CBA	3.33	122.06	111.90
23	c	5493	CLA	O2A-CGA-CBA	3.33	122.06	111.90
23	c	5502	CLA	O2A-CGA-CBA	3.34	122.07	111.90
28	c	5504	BCR	C2-C1-C6	3.34	115.65	110.36
30	C	508	DGD	O2G-C1B-C2B	3.34	118.80	111.53
23	B	517	CLA	C1D-CHD-C4C	3.35	127.67	122.60
23	c	5493	CLA	CED-O2D-CGD	3.35	123.85	115.99
30	H	208	DGD	O5D-C1E-C2E	3.35	112.27	108.04
32	a	212	SQD	C45-O47-C7	3.35	124.24	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	523	CLA	C6-C5-C3	3.35	119.85	112.48
23	B	513	CLA	O2A-CGA-CBA	3.36	122.13	111.90
23	B	525	CLA	O2D-CGD-CBD	3.36	115.91	111.30
23	c	5496	CLA	CED-O2D-CGD	3.36	123.87	115.99
30	C	509	DGD	C1E-O6E-C5E	3.36	120.27	113.75
28	T	5104	BCR	C8-C7-C6	3.36	137.42	127.32
30	c	5507	DGD	O6D-C5D-C6D	3.37	113.49	106.61
30	C	507	DGD	O6D-C5D-C6D	3.37	113.50	106.61
23	B	522	CLA	O2A-CGA-CBA	3.38	122.19	111.90
23	C	502	CLA	O2A-CGA-CBA	3.39	122.24	111.90
28	b	5527	BCR	C2-C1-C6	3.41	115.76	110.36
23	c	5497	CLA	O2D-CGD-CBD	3.41	115.98	111.30
28	C	506	BCR	C29-C30-C25	3.42	115.77	110.36
32	L	5213	SQD	C11-C10-C9	3.42	132.18	114.53
23	B	523	CLA	C1D-CHD-C4C	3.42	127.77	122.60
23	b	5517	CLA	O2A-CGA-CBA	3.42	122.33	111.90
23	d	5355	CLA	C1-C2-C3	3.42	132.32	126.71
28	c	5505	BCR	C2-C1-C6	3.43	115.80	110.36
30	c	5509	DGD	C1E-O6E-C5E	3.44	120.42	113.75
23	C	495	CLA	C6-C5-C3	3.44	120.04	112.48
23	C	492	CLA	CED-O2D-CGD	3.44	124.07	115.99
23	C	492	CLA	C6-C5-C3	3.44	120.04	112.48
23	a	5558	CLA	C4A-NA-C1A	3.45	110.82	106.36
23	B	516	CLA	O2A-CGA-CBA	3.46	122.46	111.90
28	d	5357	BCR	C2-C1-C6	3.47	115.85	110.36
28	C	506	BCR	C2-C1-C6	3.47	115.86	110.36
29	B	530	MGE	O3G-C1D-C2D	3.48	112.43	108.04
30	c	5508	DGD	O2G-C1B-C2B	3.49	119.11	111.53
32	A	5212	SQD	C45-O47-C7	3.49	124.50	117.92
23	b	5521	CLA	C6-C5-C3	3.49	120.15	112.48
23	D	354	CLA	C4A-NA-C1A	3.49	110.88	106.36
25	f	5051	HEM	CAA-CBA-CGA	3.50	119.16	112.75
28	t	104	BCR	C8-C7-C6	3.51	137.84	127.32
32	A	568	SQD	O48-C23-C24	3.51	122.58	111.90
23	d	5354	CLA	O2D-CGD-CBD	3.51	116.11	111.30
31	a	5567	LHG	O8-C23-C24	3.51	122.60	111.90
30	C	508	DGD	O5D-C6D-C5D	3.52	115.45	109.08
29	d	5359	MGE	O2G-C1B-C2B	3.52	119.19	111.53
28	c	5506	BCR	C8-C7-C6	3.54	137.95	127.32
28	c	5506	BCR	C29-C30-C25	3.54	115.97	110.36
28	B	529	BCR	C2-C1-C6	3.55	115.98	110.36
23	c	5503	CLA	CED-O2D-CGD	3.56	124.34	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	529	BCR	C29-C30-C25	3.56	116.00	110.36
30	C	507	DGD	C1E-O6E-C5E	3.56	120.66	113.75
23	b	5512	CLA	C4A-NA-C1A	3.57	110.98	106.36
32	d	5358	SQD	C11-C10-C9	3.57	132.98	114.53
23	C	499	CLA	O2D-CGD-CBD	3.57	116.20	111.30
23	c	5492	CLA	CED-O2D-CGD	3.57	124.37	115.99
28	x	5130	BCR	C16-C17-C18	3.58	132.36	127.20
32	t	213	SQD	C11-C10-C9	3.58	133.00	114.53
23	B	517	CLA	O2A-CGA-CBA	3.58	122.80	111.90
28	H	107	BCR	C29-C30-C25	3.58	116.03	110.36
28	D	357	BCR	C2-C1-C6	3.58	116.04	110.36
29	d	5360	MGE	O6D-C5D-C6D	3.59	115.42	106.36
28	X	130	BCR	C23-C24-C25	3.59	138.10	127.32
25	F	51	HEM	CAA-CBA-CGA	3.59	119.33	112.75
23	C	496	CLA	CED-O2D-CGD	3.60	124.42	115.99
28	x	5130	BCR	C23-C24-C25	3.60	138.13	127.32
23	A	558	CLA	C4A-NA-C1A	3.61	111.03	106.36
23	c	5499	CLA	O2D-CGD-CBD	3.62	116.27	111.30
28	A	566	BCR	C29-C30-C25	3.62	116.10	110.36
23	c	5491	CLA	CED-O2D-CGD	3.63	124.50	115.99
28	b	5528	BCR	C2-C1-C6	3.63	116.12	110.36
23	b	5513	CLA	C4A-NA-C1A	3.64	111.06	106.36
30	h	5208	DGD	C1E-O6E-C5E	3.64	120.81	113.75
30	c	5508	DGD	O5D-C6D-C5D	3.64	115.68	109.08
23	C	497	CLA	O2D-CGD-CBD	3.65	116.30	111.30
32	A	568	SQD	C11-C10-C9	3.65	133.38	114.53
23	b	5516	CLA	O2A-CGA-CBA	3.65	123.03	111.90
23	a	5563	CLA	C4A-NA-C1A	3.66	111.09	106.36
28	b	5529	BCR	C2-C1-C6	3.67	116.17	110.36
28	H	107	BCR	C11-C10-C9	3.67	132.50	127.20
28	h	5107	BCR	C11-C10-C9	3.68	132.51	127.20
32	d	5358	SQD	O48-C23-C24	3.68	123.12	111.90
28	c	5504	BCR	C24-C23-C22	3.68	131.83	126.22
23	b	5519	CLA	CED-O2D-CGD	3.68	124.63	115.99
23	b	5518	CLA	O2A-CGA-CBA	3.69	123.15	111.90
23	b	5515	CLA	C4A-NA-C1A	3.69	111.13	106.36
28	x	5130	BCR	C2-C1-C6	3.69	116.21	110.36
28	a	5566	BCR	C29-C30-C25	3.70	116.22	110.36
28	T	5104	BCR	C24-C23-C22	3.70	131.85	126.22
28	b	5528	BCR	C29-C30-C25	3.71	116.24	110.36
23	B	518	CLA	O2A-CGA-CBA	3.72	123.22	111.90
28	c	5505	BCR	C29-C30-C25	3.72	116.25	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	505	BCR	C29-C30-C25	3.72	116.25	110.36
32	A	568	SQD	C31-C30-C29	3.72	133.77	114.53
28	C	505	BCR	C2-C1-C6	3.73	116.26	110.36
28	X	130	BCR	C29-C30-C25	3.73	116.27	110.36
23	B	512	CLA	C4A-NA-C1A	3.75	111.20	106.36
31	A	567	LHG	O8-C23-C24	3.76	123.35	111.90
28	C	506	BCR	C8-C7-C6	3.76	138.60	127.32
23	C	498	CLA	O2D-CGD-CBD	3.77	116.47	111.30
28	C	505	BCR	C23-C24-C25	3.79	138.71	127.32
32	d	5358	SQD	C31-C30-C29	3.81	134.21	114.53
28	X	130	BCR	C2-C1-C6	3.81	116.40	110.36
28	h	5107	BCR	C29-C30-C25	3.82	116.41	110.36
23	d	5354	CLA	C4A-NA-C1A	3.82	111.30	106.36
30	c	5507	DGD	O5D-C1E-C2E	3.83	112.88	108.04
23	B	515	CLA	C4A-NA-C1A	3.83	111.31	106.36
26	D	356	PQ9	C24-C23-C25	3.83	121.26	115.41
28	C	504	BCR	C24-C23-C22	3.84	132.07	126.22
23	B	513	CLA	C4A-NA-C1A	3.85	111.34	106.36
29	d	5361	MGE	O2G-C1B-C2B	3.85	119.90	111.53
29	d	5361	MGE	O6D-C5D-C6D	3.86	116.12	106.36
28	c	5505	BCR	C23-C24-C25	3.87	138.93	127.32
23	A	563	CLA	C4A-NA-C1A	3.87	111.36	106.36
23	b	5523	CLA	C1D-CHD-C4C	3.87	128.46	122.60
28	x	5130	BCR	C29-C30-C25	3.88	116.50	110.36
24	a	5562	PHO	C4A-NA-C1A	3.88	111.68	108.21
24	A	562	PHO	C4A-NA-C1A	3.90	111.69	108.21
23	A	559	CLA	C4A-NA-C1A	3.90	111.40	106.36
32	t	213	SQD	O48-C23-C24	3.90	123.78	111.90
23	b	5520	CLA	C4A-NA-C1A	3.90	111.41	106.36
28	d	5357	BCR	C29-C30-C25	3.91	116.56	110.36
23	C	491	CLA	C4A-NA-C1A	3.92	111.43	106.36
30	C	507	DGD	O5D-C1E-C2E	3.92	112.99	108.04
30	c	5509	DGD	O6D-C5D-C6D	3.92	114.62	106.61
23	a	5559	CLA	C4A-NA-C1A	3.94	111.45	106.36
24	a	5561	PHO	C4A-NA-C1A	3.94	111.73	108.21
26	d	5356	PQ9	C24-C23-C25	3.94	121.42	115.41
32	L	5213	SQD	O48-C23-C24	3.95	123.94	111.90
23	b	5526	CLA	CED-O2D-CGD	3.95	125.26	115.99
29	D	360	MGE	O2G-C1B-C2B	3.97	120.16	111.53
23	B	520	CLA	C4A-NA-C1A	3.98	111.50	106.36
32	A	5212	SQD	C44-O6-C1	3.98	122.17	113.82
24	A	561	PHO	C4A-NA-C1A	3.98	111.77	108.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	5494	CLA	CED-O2D-CGD	3.98	125.33	115.99
23	c	5494	CLA	C4A-NA-C1A	3.99	111.52	106.36
23	A	560	CLA	C4A-NA-C1A	3.99	111.52	106.36
30	C	509	DGD	O6D-C5D-C6D	4.03	114.84	106.61
23	B	522	CLA	C4A-NA-C1A	4.03	111.57	106.36
28	t	104	BCR	C29-C30-C25	4.06	116.79	110.36
23	c	5500	CLA	C4A-NA-C1A	4.06	111.61	106.36
23	b	5526	CLA	C4A-NA-C1A	4.08	111.64	106.36
23	C	500	CLA	C4A-NA-C1A	4.09	111.64	106.36
23	B	511	CLA	C4A-NA-C1A	4.10	111.66	106.36
23	c	5497	CLA	C4A-NA-C1A	4.12	111.68	106.36
23	a	5560	CLA	C4A-NA-C1A	4.14	111.71	106.36
23	b	5519	CLA	C4A-NA-C1A	4.15	111.72	106.36
28	b	5529	BCR	C29-C30-C25	4.15	116.94	110.36
23	b	5522	CLA	C4A-NA-C1A	4.17	111.75	106.36
23	B	519	CLA	C4A-NA-C1A	4.17	111.75	106.36
23	c	5496	CLA	C4A-NA-C1A	4.19	111.77	106.36
25	V	552	HEM	CMC-C2C-C3C	4.19	126.98	116.53
23	c	5499	CLA	C4A-NA-C1A	4.20	111.79	106.36
23	B	526	CLA	C4A-NA-C1A	4.22	111.82	106.36
29	D	360	MGE	O6D-C5D-C6D	4.24	117.08	106.36
25	v	5552	HEM	CMC-C2C-C3C	4.25	127.14	116.53
23	C	495	CLA	C4A-NA-C1A	4.26	111.87	106.36
23	c	5493	CLA	C4A-NA-C1A	4.26	111.87	106.36
23	b	5517	CLA	C4A-NA-C1A	4.27	111.89	106.36
23	b	5521	CLA	C4A-NA-C1A	4.28	111.89	106.36
23	C	499	CLA	C4A-NA-C1A	4.30	111.92	106.36
23	B	525	CLA	C4A-NA-C1A	4.31	111.94	106.36
23	b	5524	CLA	C4A-NA-C1A	4.31	111.94	106.36
23	C	496	CLA	C4A-NA-C1A	4.32	111.94	106.36
23	C	498	CLA	C4A-NA-C1A	4.32	111.95	106.36
23	C	492	CLA	C4A-NA-C1A	4.33	111.96	106.36
23	b	5511	CLA	C4A-NA-C1A	4.34	111.97	106.36
30	c	5508	DGD	O5D-C1E-C2E	4.35	113.53	108.04
23	C	493	CLA	C4A-NA-C1A	4.36	112.00	106.36
23	C	502	CLA	C4A-NA-C1A	4.38	112.02	106.36
23	C	494	CLA	CED-O2D-CGD	4.38	126.25	115.99
23	D	355	CLA	C4A-NA-C1A	4.38	112.03	106.36
32	a	212	SQD	C44-O6-C1	4.40	123.07	113.82
23	b	5518	CLA	C4A-NA-C1A	4.41	112.07	106.36
25	F	51	HEM	CMC-C2C-C3C	4.42	127.57	116.53
23	d	5355	CLA	C4A-NA-C1A	4.44	112.10	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	5104	BCR	C29-C30-C25	4.44	117.39	110.36
23	C	494	CLA	C4A-NA-C1A	4.45	112.11	106.36
23	B	516	CLA	C4A-NA-C1A	4.46	112.13	106.36
23	c	5495	CLA	C4A-NA-C1A	4.47	112.14	106.36
23	b	5523	CLA	C4A-NA-C1A	4.48	112.15	106.36
23	c	5498	CLA	C4A-NA-C1A	4.48	112.15	106.36
23	B	523	CLA	C4A-NA-C1A	4.49	112.17	106.36
23	c	5492	CLA	C4A-NA-C1A	4.51	112.19	106.36
25	f	5051	HEM	CMC-C2C-C3C	4.51	127.79	116.53
23	B	517	CLA	C4A-NA-C1A	4.51	112.19	106.36
23	c	5502	CLA	C4A-NA-C1A	4.51	112.20	106.36
23	b	5525	CLA	C4A-NA-C1A	4.52	112.20	106.36
23	B	521	CLA	C4A-NA-C1A	4.53	112.21	106.36
23	B	518	CLA	C4A-NA-C1A	4.53	112.22	106.36
23	C	503	CLA	C4A-NA-C1A	4.54	112.23	106.36
23	b	5516	CLA	C4A-NA-C1A	4.55	112.25	106.36
23	C	497	CLA	C4A-NA-C1A	4.55	112.25	106.36
23	c	5503	CLA	C4A-NA-C1A	4.60	112.31	106.36
25	F	51	HEM	CMB-C2B-C3B	4.61	128.03	116.53
23	c	5491	CLA	C4A-NA-C1A	4.63	112.35	106.36
25	f	5051	HEM	CMB-C2B-C3B	4.66	128.16	116.53
30	C	508	DGD	O5D-C1E-C2E	4.66	113.92	108.04
23	B	524	CLA	C4A-NA-C1A	4.67	112.39	106.36
23	B	514	CLA	C4A-NA-C1A	4.74	112.49	106.36
23	C	501	CLA	C4A-NA-C1A	4.78	112.54	106.36
23	b	5514	CLA	C4A-NA-C1A	4.80	112.56	106.36
23	c	5501	CLA	C4A-NA-C1A	4.82	112.59	106.36
28	x	5130	BCR	C11-C10-C9	4.84	134.19	127.20
30	H	208	DGD	O3G-C1D-C2D	4.88	114.21	108.04
25	V	552	HEM	CMB-C2B-C3B	4.97	128.94	116.53
32	L	5213	SQD	O7-S-C6	5.02	111.17	106.94
28	B	528	BCR	C33-C5-C6	5.09	129.60	124.61
28	c	5504	BCR	C33-C5-C6	5.12	129.64	124.61
30	h	5208	DGD	O3G-C1D-C2D	5.14	114.53	108.04
25	v	5552	HEM	CMB-C2B-C3B	5.15	129.38	116.53
28	X	130	BCR	C11-C10-C9	5.30	134.85	127.20
28	b	5528	BCR	C33-C5-C6	5.37	129.88	124.61
28	x	5130	BCR	C7-C8-C9	5.37	134.40	126.22
32	A	568	SQD	C25-C24-C23	5.38	134.74	113.59
32	L	5213	SQD	C25-C24-C23	5.39	134.76	113.59
28	C	504	BCR	C33-C5-C6	5.41	129.92	124.61
32	t	213	SQD	C25-C24-C23	5.46	135.06	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	5107	BCR	C33-C5-C6	5.48	129.99	124.61
28	X	130	BCR	C7-C8-C9	5.52	134.63	126.22
28	b	5529	BCR	C33-C5-C6	5.52	130.03	124.61
28	c	5505	BCR	C33-C5-C6	5.55	130.06	124.61
28	H	107	BCR	C33-C5-C6	5.63	130.13	124.61
31	a	5567	LHG	C25-C24-C23	5.64	135.74	113.59
32	d	5358	SQD	C25-C24-C23	5.72	136.09	113.59
31	A	567	LHG	C25-C24-C23	5.73	136.10	113.59
28	X	130	BCR	C38-C26-C25	5.79	130.29	124.61
28	c	5506	BCR	C33-C5-C6	5.85	130.35	124.61
28	x	5130	BCR	C38-C26-C25	5.86	130.36	124.61
32	L	5213	SQD	C10-C9-C8	5.91	134.96	113.29
28	C	505	BCR	C33-C5-C6	5.91	130.41	124.61
32	d	5358	SQD	C10-C9-C8	5.92	135.02	113.29
32	t	213	SQD	C10-C9-C8	5.94	135.07	113.29
28	C	506	BCR	C33-C5-C6	5.99	130.48	124.61
32	A	568	SQD	C10-C9-C8	5.99	135.25	113.29
28	b	5527	BCR	C38-C26-C25	5.99	130.49	124.61
28	c	5504	BCR	C38-C26-C25	6.01	130.51	124.61
28	H	107	BCR	C38-C26-C25	6.06	130.56	124.61
28	a	5566	BCR	C33-C5-C6	6.07	130.57	124.61
28	B	529	BCR	C33-C5-C6	6.10	130.59	124.61
28	A	566	BCR	C38-C26-C25	6.13	130.62	124.61
28	b	5529	BCR	C38-C26-C25	6.13	130.63	124.61
28	a	5566	BCR	C38-C26-C25	6.14	130.63	124.61
28	T	5104	BCR	C33-C5-C6	6.20	130.69	124.61
28	b	5528	BCR	C38-C26-C25	6.21	130.70	124.61
28	t	104	BCR	C33-C5-C6	6.21	130.70	124.61
28	b	5527	BCR	C33-C5-C6	6.22	130.71	124.61
28	C	504	BCR	C38-C26-C25	6.23	130.73	124.61
28	A	566	BCR	C33-C5-C6	6.24	130.73	124.61
28	B	527	BCR	C33-C5-C6	6.28	130.77	124.61
28	c	5506	BCR	C38-C26-C25	6.28	130.77	124.61
28	h	5107	BCR	C38-C26-C25	6.38	130.87	124.61
28	C	506	BCR	C38-C26-C25	6.41	130.90	124.61
28	C	505	BCR	C38-C26-C25	6.51	131.00	124.61
28	B	528	BCR	C38-C26-C25	6.51	131.00	124.61
28	B	527	BCR	C38-C26-C25	6.61	131.09	124.61
28	D	357	BCR	C33-C5-C6	6.74	131.22	124.61
32	A	5212	SQD	O7-S-C6	6.78	112.66	106.94
32	d	5358	SQD	O7-S-C6	6.78	112.66	106.94
30	h	5208	DGD	O6E-C5E-C4E	6.91	122.65	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	t	104	BCR	C38-C26-C25	6.91	131.39	124.61
30	c	5509	DGD	O6E-C5E-C4E	6.92	122.66	109.68
32	t	213	SQD	O7-S-C6	6.92	112.78	106.94
30	C	509	DGD	O6E-C5E-C4E	6.94	122.70	109.68
28	x	5130	BCR	C33-C5-C6	7.00	131.48	124.61
30	C	508	DGD	O6E-C5E-C4E	7.03	122.87	109.68
30	C	507	DGD	O6E-C5E-C4E	7.03	122.88	109.68
28	B	529	BCR	C38-C26-C25	7.04	131.51	124.61
28	d	5357	BCR	C38-C26-C25	7.06	131.54	124.61
28	c	5505	BCR	C38-C26-C25	7.07	131.55	124.61
28	d	5357	BCR	C33-C5-C6	7.11	131.58	124.61
30	c	5508	DGD	O6E-C5E-C4E	7.19	123.17	109.68
30	H	208	DGD	O6E-C5E-C4E	7.25	123.29	109.68
28	T	5104	BCR	C38-C26-C25	7.29	131.77	124.61
28	X	130	BCR	C33-C5-C6	7.32	131.79	124.61
28	D	357	BCR	C38-C26-C25	7.33	131.80	124.61
30	c	5507	DGD	O6E-C5E-C4E	7.42	123.60	109.68
32	t	213	SQD	O5-C1-O6	7.57	128.28	110.05
32	L	5213	SQD	O5-C1-O6	7.91	129.09	110.05
32	d	5358	SQD	O5-C1-O6	7.93	129.16	110.05
32	a	212	SQD	O7-S-C6	7.98	113.66	106.94
32	A	5212	SQD	O6-C1-C2	8.17	118.36	108.04
32	A	568	SQD	O5-C1-O6	8.20	129.81	110.05
32	a	212	SQD	O5-C1-O6	8.23	129.88	110.05
32	A	568	SQD	O7-S-C6	8.42	114.04	106.94
32	a	212	SQD	O6-C1-C2	8.45	118.71	108.04
32	A	5212	SQD	O5-C1-O6	8.60	130.76	110.05
32	A	568	SQD	O6-C1-C2	8.89	119.27	108.04
32	d	5358	SQD	O6-C1-C2	9.10	119.53	108.04
32	L	5213	SQD	O6-C1-C2	9.20	119.65	108.04
32	t	213	SQD	O6-C1-C2	9.65	120.22	108.04
25	v	5552	HEM	CAD-C3D-C2D	9.97	141.87	113.22
25	V	552	HEM	CAD-C3D-C2D	10.05	142.12	113.22
25	F	51	HEM	CAD-C3D-C2D	10.10	142.26	113.22
25	f	5051	HEM	CAD-C3D-C2D	10.24	142.66	113.22

All (234) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	512	CLA	NC
23	B	512	CLA	ND
23	B	512	CLA	NA
23	c	5495	CLA	NC
23	c	5495	CLA	ND
23	c	5495	CLA	NA
23	B	522	CLA	NC
23	B	522	CLA	ND
23	B	522	CLA	NA
23	B	526	CLA	NC
23	B	526	CLA	ND
23	B	526	CLA	NA
23	C	495	CLA	NC
23	C	495	CLA	ND
23	C	495	CLA	NA
23	d	5354	CLA	NC
23	d	5354	CLA	ND
23	d	5354	CLA	NA
23	c	5492	CLA	NC
23	c	5492	CLA	ND
23	c	5492	CLA	NA
23	B	518	CLA	NC
23	B	518	CLA	ND
23	B	518	CLA	NA
23	c	5497	CLA	NC
23	c	5497	CLA	ND
23	c	5497	CLA	NA
23	a	5559	CLA	NC
23	a	5559	CLA	ND
23	a	5559	CLA	NA
23	b	5517	CLA	NC
23	b	5517	CLA	ND
23	b	5517	CLA	NA
23	c	5503	CLA	NC
23	c	5503	CLA	ND
23	c	5503	CLA	NA
23	C	496	CLA	NC
23	C	496	CLA	ND
23	C	496	CLA	NA
23	B	520	CLA	NC
23	B	520	CLA	ND
23	B	520	CLA	NA

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Mol	Chain	Res	Type	Atom
23	C	494	CLA	NC
23	C	494	CLA	ND
23	C	494	CLA	NA
23	C	491	CLA	NC
23	C	491	CLA	ND
23	C	491	CLA	NA
23	b	5520	CLA	NC
23	b	5520	CLA	ND
23	b	5520	CLA	NA
23	C	500	CLA	NC
23	C	500	CLA	ND
23	C	500	CLA	NA
23	C	493	CLA	NC
23	C	493	CLA	ND
23	C	493	CLA	NA
23	b	5514	CLA	NC
23	b	5514	CLA	ND
23	b	5514	CLA	NA
23	B	519	CLA	NC
23	B	519	CLA	ND
23	B	519	CLA	NA
23	D	354	CLA	NC
23	D	354	CLA	ND
23	D	354	CLA	NA
23	B	516	CLA	NC
23	B	516	CLA	ND
23	B	516	CLA	NA
23	b	5512	CLA	NC
23	b	5512	CLA	ND
23	b	5512	CLA	NA
23	B	513	CLA	NC
23	B	513	CLA	ND
23	B	513	CLA	NA
23	c	5499	CLA	NC
23	c	5499	CLA	ND
23	c	5499	CLA	NA
23	A	560	CLA	NC
23	A	560	CLA	ND
23	A	560	CLA	NA
23	d	5355	CLA	NC
23	d	5355	CLA	ND
23	d	5355	CLA	NA

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Mol	Chain	Res	Type	Atom
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D
30	c	5507	DGD	C5E
23	b	5521	CLA	NC
23	b	5521	CLA	ND
23	b	5521	CLA	NA
23	c	5500	CLA	NC
23	c	5500	CLA	ND
23	c	5500	CLA	NA
23	b	5518	CLA	NC
23	b	5518	CLA	ND
23	b	5518	CLA	NA
23	c	5496	CLA	NC
23	c	5496	CLA	ND
23	c	5496	CLA	NA
23	B	524	CLA	NC
23	B	524	CLA	ND
23	B	524	CLA	NA
23	B	515	CLA	NC
23	B	515	CLA	ND
23	B	515	CLA	NA
30	h	5208	DGD	C2D
30	h	5208	DGD	C5D
30	h	5208	DGD	C5E
23	b	5525	CLA	NC
23	b	5525	CLA	ND
23	b	5525	CLA	NA
30	C	508	DGD	C2D
30	C	508	DGD	C5D
30	C	508	DGD	C5E
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	a	5558	CLA	NC
23	a	5558	CLA	ND
23	a	5558	CLA	NA
23	B	511	CLA	NC
23	B	511	CLA	ND
23	B	511	CLA	NA
23	b	5522	CLA	NC
23	b	5522	CLA	ND
23	b	5522	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	5519	CLA	NC
23	b	5519	CLA	ND
23	b	5519	CLA	NA
23	b	5526	CLA	NC
23	b	5526	CLA	ND
23	b	5526	CLA	NA
23	b	5516	CLA	NC
23	b	5516	CLA	ND
23	b	5516	CLA	NA
23	b	5513	CLA	NC
23	b	5513	CLA	ND
23	b	5513	CLA	NA
30	C	507	DGD	C2D
30	C	507	DGD	C5D
30	C	507	DGD	C5E
23	c	5502	CLA	NC
23	c	5502	CLA	ND
23	c	5502	CLA	NA
23	b	5523	CLA	NC
23	b	5523	CLA	ND
23	b	5523	CLA	NA
23	a	5563	CLA	NC
23	a	5563	CLA	ND
23	a	5563	CLA	NA
30	c	5509	DGD	C2D
30	c	5509	DGD	C5D
30	c	5509	DGD	C5E
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
30	c	5508	DGD	C2D
30	c	5508	DGD	C5D
30	c	5508	DGD	C5E
23	b	5515	CLA	NC
23	b	5515	CLA	ND
23	b	5515	CLA	NA
23	c	5493	CLA	NC
23	c	5493	CLA	ND
23	c	5493	CLA	NA
23	B	523	CLA	NC
23	B	523	CLA	ND
23	B	523	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	5511	CLA	NC
23	b	5511	CLA	ND
23	b	5511	CLA	NA
23	C	498	CLA	NC
23	C	498	CLA	ND
23	C	498	CLA	NA
30	C	509	DGD	C2D
30	C	509	DGD	C5D
30	C	509	DGD	C5E
23	A	563	CLA	NC
23	A	563	CLA	ND
23	A	563	CLA	NA
23	B	525	CLA	NC
23	B	525	CLA	ND
23	B	525	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA
23	A	559	CLA	NC
23	A	559	CLA	ND
23	A	559	CLA	NA
23	A	558	CLA	NC
23	A	558	CLA	ND
23	A	558	CLA	NA
23	B	517	CLA	NC
23	B	517	CLA	ND
23	B	517	CLA	NA
23	c	5494	CLA	NC
23	c	5494	CLA	ND
23	c	5494	CLA	NA
23	a	5560	CLA	NC
23	a	5560	CLA	ND
23	a	5560	CLA	NA
23	b	5524	CLA	NC
23	b	5524	CLA	ND
23	b	5524	CLA	NA
23	D	355	CLA	NC
23	D	355	CLA	ND
23	D	355	CLA	NA
23	C	499	CLA	NC
23	C	499	CLA	ND
23	C	499	CLA	NA

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

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	d	5354	CLA	C1-C2-C3-C4
23	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
23	A	558	CLA	10	0
23	A	559	CLA	5	0
23	A	560	CLA	1	0
24	A	561	PHO	7	0
24	A	562	PHO	5	0
26	A	564	PQ9	2	0
28	A	566	BCR	1	0
31	A	567	LHG	4	0
23	B	511	CLA	1	0
23	B	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	513	CLA	8	0
23	B	514	CLA	5	0
23	B	515	CLA	12	0
23	B	516	CLA	6	0
23	B	517	CLA	9	0
23	B	518	CLA	11	0
23	B	519	CLA	5	0
23	B	520	CLA	6	0
23	B	521	CLA	2	0
23	B	522	CLA	4	0
23	B	523	CLA	2	0
23	B	524	CLA	4	0
23	B	525	CLA	4	0
23	B	526	CLA	2	0
28	B	527	BCR	2	0
28	B	528	BCR	2	0
28	B	529	BCR	2	0
29	B	530	MGE	1	0
23	C	491	CLA	4	0
23	C	492	CLA	2	0
23	C	493	CLA	7	0
23	C	494	CLA	2	0
23	C	495	CLA	9	0
23	C	496	CLA	2	0
23	C	497	CLA	5	0
23	C	498	CLA	6	0
23	C	499	CLA	2	0
23	C	500	CLA	3	0
23	C	501	CLA	13	0
23	C	502	CLA	2	0
23	C	503	CLA	1	0
28	C	504	BCR	7	0
28	C	505	BCR	6	0
28	C	506	BCR	7	0
30	C	507	DGD	6	0
30	C	508	DGD	2	0
30	C	509	DGD	10	0
23	D	354	CLA	5	0
23	D	355	CLA	3	0
26	D	356	PQ9	7	0
28	D	357	BCR	4	0
29	D	358	MGE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	359	MGE	1	0
29	D	360	MGE	7	0
25	F	51	HEM	3	0
28	H	107	BCR	3	0
30	H	208	DGD	3	0
29	I	201	MGE	1	0
29	L	210	MGE	2	0
33	T	217	LMT	3	0
28	T	5104	BCR	5	0
25	V	552	HEM	2	0
28	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.58	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.53	5 (1%) 76 49	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.52	2 (0%) 93 80	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.49	1 (0%) 95 87	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.51	3 (0%) 89 70	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.33	6 (1%) 79 53	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 94 84	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.56	1 (0%) 94 84	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.17	1 (1%) 81 55	55, 70, 86, 94	0
5	e	82/84 (97%)	0.01	3 (3%) 45 19	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.20	2 (5%) 27 10	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.09	3 (8%) 13 4	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.36	1 (1%) 74 47	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.19	3 (4%) 35 14	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.46	1 (2%) 55 26	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.32	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.59	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.49	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.53	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.40	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.12	1 (2%) 58 28	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.33	3 (8%) 15 5	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.41	1 (2%) 56 27	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.35	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.37	4 (1%) 73 45	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.29	9 (3%) 45 19	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.47	1 (3%) 50 22	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.72	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.38	1 (1%) 84 60	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.40	3 (3%) 52 24	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.46	2 (1%) 76 49	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.21	5 (3%) 46 20	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.24	4 (6%) 22 8	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.18	2 (3%) 51 23	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.44	69 (1%) 78 51	35, 66, 85, 101	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	5010	SER	4.8
3	c	5473	ASP	4.5
13	o	5049	ASP	4.4
4	D	13	GLY	4.2
11	l	5001	MET	4.2
13	O	114	ASN	4.1
6	f	5013	TYR	3.8
11	L	5	PRO	3.7
7	h	5065	LEU	3.6
15	U	37	GLU	3.5
1	a	5011	ALA	3.5
1	a	5015	GLU	3.4
5	e	5003	GLY	3.4
6	f	5011	VAL	3.4
5	e	5060	GLN	3.2
5	E	84	LYS	3.2
18	Z	30	PRO	3.1
13	o	5050	ASP	3.0
5	e	5017	VAL	2.9
3	C	192	GLY	2.9
16	V	27	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
18	z	5062	VAL	2.8
3	c	5029	GLU	2.8
7	h	5064	ALA	2.8
6	f	5012	SER	2.8
13	O	87	GLN	2.8
13	o	5060	SER	2.7
6	F	12	SER	2.7
12	M	36	SER	2.7
18	Z	60	PHE	2.7
13	O	59	ASP	2.7
3	C	182	PHE	2.7
18	z	5003	ILE	2.7
16	v	5111	GLU	2.6
16	v	5041	GLU	2.5
7	h	5006	TRP	2.5
13	o	5030	THR	2.5
15	u	5053	GLU	2.5
13	o	5061	SER	2.5
3	C	460	ASP	2.4
11	l	5003	PRO	2.4
3	c	5472	LEU	2.4
16	V	81	ARG	2.4
1	a	5227	THR	2.3
13	o	5048	LEU	2.3
2	b	5294	SER	2.3
18	Z	29	SER	2.3
2	B	130	GLU	2.3
2	B	129	GLY	2.3
7	H	26	GLY	2.3
3	c	5033	PHE	2.2
18	Z	34	ASP	2.2
4	d	5226	GLY	2.2
15	u	5052	GLY	2.2
13	o	5082	PRO	2.2
13	o	5089	ALA	2.2
8	I	35	LYS	2.2
15	u	5086	GLU	2.1
11	l	5002	GLU	2.1
16	v	5043	LYS	2.1
16	v	5027	ALA	2.1
13	o	5088	GLU	2.1
13	O	234	THR	2.1

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Mol	Chain	Res	Type	RSRZ
16	v	5039	ASN	2.1
14	T	30	THR	2.0
6	F	11	VAL	2.0
3	c	5214	LEU	2.0
3	c	5142	GLU	2.0
1	a	5262	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	LMT	A	569	35/35	0.72	0.47	7.88	80,89,92,93	0
22	UNK	c	5484	5/-	0.84	0.53	6.25	69,69,70,72	0
33	LMT	a	5568	35/35	0.81	0.43	6.11	79,92,94,96	0
33	LMT	t	5217	35/35	0.68	0.46	6.09	76,95,104,105	0
23	CLA	B	511	41/65	0.73	0.41	6.08	88,90,92,98	0
22	UNK	C	489	7/-	0.78	0.44	5.92	75,76,77,78	0
28	BCR	H	107	40/40	0.82	0.29	5.88	77,83,88,89	0
22	UNK	c	5489	7/-	0.78	0.41	5.88	73,73,74,74	0
22	UNK	c	5485	5/-	0.85	0.39	5.11	68,69,69,70	0
23	CLA	c	5503	50/65	0.85	0.28	4.60	88,91,92,93	0
22	UNK	c	5477	7/-	0.89	0.33	4.59	67,68,70,70	0
26	PQ9	a	5564	30/45	0.87	0.32	4.57	51,55,62,62	30
23	CLA	b	5511	41/65	0.64	0.40	4.31	88,92,95,96	0
26	PQ9	A	564	30/45	0.77	0.37	4.07	54,57,63,64	30
22	UNK	C	481	13/-	0.73	0.36	4.07	61,64,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	BCR	C	505	40/40	0.81	0.43	4.04	75,81,91,92	0
33	LMT	T	217	35/35	0.75	0.31	3.67	83,93,96,97	0
28	BCR	x	5130	40/40	0.79	0.42	3.65	77,81,85,86	0
22	UNK	c	5474	15/-	0.89	0.24	3.37	39,50,56,56	0
23	CLA	a	5560	65/65	0.90	0.22	3.30	62,68,100,101	0
28	BCR	h	5107	40/40	0.86	0.28	3.04	74,79,82,83	0
28	BCR	X	130	40/40	0.84	0.32	3.04	68,71,80,81	0
28	BCR	d	5357	40/40	0.83	0.37	2.98	61,72,86,88	0
29	MGE	d	5359	47/48	0.76	0.30	2.84	72,81,96,98	0
28	BCR	B	528	40/40	0.84	0.25	2.73	54,68,74,75	0
23	CLA	a	5563	55/65	0.84	0.31	2.72	59,65,102,103	0
28	BCR	c	5504	40/40	0.86	0.29	2.71	73,80,88,89	0
28	BCR	b	5529	40/40	0.86	0.34	2.68	69,72,74,74	0
28	BCR	C	504	40/40	0.91	0.27	2.49	57,64,70,70	0
28	BCR	D	357	40/40	0.89	0.26	2.25	61,66,78,80	0
22	UNK	C	482	13/-	0.84	0.25	2.08	64,66,67,67	0
33	LMT	M	5216	35/35	0.77	0.31	2.02	58,83,90,90	0
23	CLA	A	563	55/65	0.88	0.26	1.96	43,49,75,78	0
23	CLA	B	519	65/65	0.88	0.26	1.93	73,82,85,87	0
28	BCR	T	5104	40/40	0.88	0.25	1.90	67,71,78,79	0
23	CLA	c	5498	65/65	0.85	0.25	1.86	81,90,93,93	0
29	MGE	D	358	47/48	0.82	0.24	1.85	65,72,79,81	0
23	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
28	BCR	c	5505	40/40	0.88	0.31	1.80	84,87,91,92	0
29	MGE	d	5361	48/48	0.89	0.22	1.78	61,68,78,83	0
23	CLA	c	5501	65/65	0.88	0.26	1.77	82,91,94,95	0
23	CLA	b	5516	65/65	0.82	0.28	1.77	62,66,84,86	0
33	LMT	m	216	35/35	0.80	0.28	1.68	62,87,89,91	0
22	UNK	c	5476	9/-	0.79	0.33	1.68	58,60,62,62	0
23	CLA	D	355	50/65	0.91	0.22	1.60	63,65,68,70	0
23	CLA	B	515	65/65	0.93	0.21	1.59	55,66,71,72	0
23	CLA	b	5519	65/65	0.89	0.24	1.59	70,75,80,81	0
24	PHO	a	5562	64/64	0.91	0.22	1.57	70,75,81,82	0
32	SQD	A	568	54/54	0.84	0.32	1.57	76,82,90,90	0
23	CLA	C	495	65/65	0.92	0.21	1.55	58,68,74,76	0
23	CLA	B	520	65/65	0.90	0.23	1.53	62,67,76,79	0
23	CLA	b	5520	65/65	0.90	0.24	1.49	63,72,74,76	0
28	BCR	c	5506	40/40	0.76	0.32	1.44	75,81,86,86	0
28	BCR	A	566	40/40	0.92	0.24	1.43	50,57,64,66	0
28	BCR	t	104	40/40	0.91	0.20	1.43	65,72,84,85	0
31	LHG	A	567	39/49	0.92	0.23	1.40	57,73,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	C	498	65/65	0.88	0.22	1.39	64,74,98,101	0
23	CLA	c	5497	65/65	0.89	0.23	1.38	66,82,84,87	0
23	CLA	C	501	65/65	0.89	0.25	1.38	70,78,83,85	0
26	PQ9	D	356	30/45	0.91	0.21	1.30	49,67,80,83	0
23	CLA	B	512	65/65	0.91	0.24	1.29	68,75,78,79	0
28	BCR	a	5566	40/40	0.90	0.25	1.27	59,75,78,79	0
25	HEM	f	5051	43/43	0.94	0.28	1.25	80,84,97,101	0
23	CLA	B	522	65/65	0.94	0.21	1.25	54,65,75,77	0
29	MGE	b	5530	48/48	0.89	0.18	1.23	59,64,71,73	0
22	UNK	C	485	5/-	0.90	0.23	1.23	57,59,61,61	0
23	CLA	b	5515	65/65	0.94	0.21	1.21	46,51,74,76	0
23	CLA	c	5495	65/65	0.91	0.21	1.21	74,81,86,88	0
23	CLA	A	560	65/65	0.91	0.20	1.19	49,57,86,88	0
23	CLA	C	503	50/65	0.86	0.26	1.17	83,86,88,94	0
23	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
23	CLA	C	497	65/65	0.88	0.24	1.07	74,78,80,82	0
29	MGE	D	359	41/48	0.88	0.23	1.03	60,67,76,79	0
26	PQ9	d	5356	30/45	0.93	0.20	1.02	51,57,66,66	0
28	BCR	B	529	40/40	0.89	0.24	1.00	62,69,80,80	0
23	CLA	B	516	65/65	0.82	0.27	0.98	61,76,92,97	0
23	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
22	UNK	c	5481	13/-	0.87	0.23	0.96	60,62,66,66	0
23	CLA	c	5496	65/65	0.82	0.27	0.95	79,83,95,97	0
29	MGE	l	5210	48/48	0.90	0.21	0.95	59,69,78,81	0
23	CLA	b	5513	65/65	0.94	0.20	0.95	54,61,84,90	0
29	MGE	d	5360	41/48	0.90	0.21	0.93	68,72,78,80	0
22	UNK	C	474	15/-	0.89	0.18	0.91	26,37,40,40	0
25	HEM	F	51	43/43	0.95	0.25	0.91	78,84,92,95	0
29	MGE	L	210	48/48	0.88	0.24	0.88	59,68,73,75	0
31	LHG	a	5567	39/49	0.90	0.26	0.87	65,68,74,80	0
32	SQD	a	212	26/54	0.79	0.26	0.87	82,94,101,103	0
25	HEM	v	5552	43/43	0.96	0.22	0.85	65,67,70,70	0
29	MGE	D	360	48/48	0.91	0.20	0.85	52,60,63,68	0
28	BCR	b	5527	40/40	0.92	0.20	0.85	58,63,72,72	0
23	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
29	MGE	i	5201	48/48	0.84	0.27	0.74	67,83,88,90	0
30	DGD	H	208	54/66	0.90	0.20	0.73	61,69,75,76	0
32	SQD	A	5212	26/54	0.81	0.24	0.73	75,100,107,107	0
32	SQD	d	5358	54/54	0.80	0.29	0.72	74,85,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	UNK	C	476	9/-	0.81	0.29	0.72	61,62,63,64	0
29	MGE	I	201	48/48	0.87	0.23	0.71	73,81,89,90	0
23	CLA	C	496	65/65	0.84	0.26	0.70	71,78,88,89	0
23	CLA	B	513	65/65	0.94	0.18	0.68	56,61,67,67	0
23	CLA	C	502	51/65	0.88	0.21	0.67	74,80,83,84	0
24	PHO	a	5561	64/64	0.94	0.18	0.67	51,55,66,68	0
25	HEM	V	552	43/43	0.97	0.18	0.63	37,54,58,59	0
23	CLA	B	525	65/65	0.93	0.20	0.62	67,84,91,92	0
32	SQD	L	5213	47/54	0.80	0.27	0.60	52,85,106,108	0
32	SQD	t	213	47/54	0.85	0.26	0.60	61,95,116,117	0
22	UNK	C	477	7/-	0.96	0.16	0.58	47,49,51,51	0
29	MGE	B	530	48/48	0.88	0.19	0.58	55,64,70,72	0
23	CLA	b	5522	65/65	0.94	0.20	0.58	60,66,75,76	0
30	DGD	C	509	57/66	0.91	0.20	0.55	52,60,69,70	0
21	BCT	D	353	4/4	0.96	0.19	0.54	72,73,73,74	0
23	CLA	c	5502	51/65	0.87	0.24	0.51	93,96,97,98	0
22	UNK	c	5482	13/-	0.90	0.19	0.51	60,61,71,72	0
23	CLA	d	5355	50/65	0.87	0.23	0.48	74,77,80,81	0
28	BCR	b	5528	40/40	0.93	0.18	0.48	61,64,72,73	0
24	PHO	A	562	64/64	0.94	0.17	0.48	47,53,63,66	0
23	CLA	c	5500	65/65	0.92	0.20	0.43	64,69,82,83	0
23	CLA	C	500	65/65	0.94	0.16	0.41	59,63,73,74	0
23	CLA	b	5526	65/65	0.79	0.28	0.38	66,71,92,95	0
23	CLA	D	354	65/65	0.95	0.17	0.36	35,43,63,66	0
23	CLA	b	5514	65/65	0.94	0.18	0.32	41,51,74,75	0
23	CLA	C	499	47/65	0.95	0.17	0.31	57,60,66,69	0
28	BCR	C	506	40/40	0.88	0.22	0.30	68,72,79,80	0
28	BCR	B	527	40/40	0.91	0.18	0.30	58,65,68,69	0
23	CLA	C	491	65/65	0.95	0.18	0.27	63,70,77,79	0
22	UNK	C	484	5/-	0.86	0.21	0.27	47,51,52,53	0
23	CLA	B	518	65/65	0.93	0.19	0.27	53,64,79,79	0
23	CLA	C	492	60/65	0.95	0.17	0.23	53,58,76,77	0
23	CLA	B	521	65/65	0.95	0.17	0.21	58,63,66,68	0
24	PHO	A	561	64/64	0.95	0.16	0.18	32,52,55,59	0
23	CLA	C	493	65/65	0.94	0.18	0.17	67,71,77,79	0
23	CLA	c	5491	65/65	0.92	0.20	0.16	70,78,81,86	0
23	CLA	b	5525	65/65	0.93	0.19	0.13	71,77,80,82	0
23	CLA	c	5493	65/65	0.90	0.21	0.05	67,81,86,86	0
23	CLA	a	5559	65/65	0.95	0.16	-0.02	42,49,60,60	0
30	DGD	c	5508	47/66	0.91	0.18	-0.04	66,76,82,84	0
23	CLA	c	5499	47/65	0.92	0.20	-0.04	60,69,76,78	0
23	CLA	b	5517	65/65	0.95	0.15	-0.05	54,58,66,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	523	65/65	0.95	0.16	-0.06	47,56,73,74	0
23	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
23	CLA	b	5523	65/65	0.95	0.15	-0.12	45,52,74,75	0
23	CLA	C	494	46/65	0.95	0.15	-0.21	59,66,68,72	0
23	CLA	a	5558	65/65	0.95	0.16	-0.22	41,50,55,61	0
23	CLA	b	5524	56/65	0.93	0.18	-0.23	63,68,89,91	0
23	CLA	A	559	65/65	0.96	0.14	-0.31	39,43,49,52	0
23	CLA	B	517	65/65	0.96	0.14	-0.35	37,44,56,57	0
23	CLA	c	5492	60/65	0.93	0.17	-0.38	57,61,83,84	0
23	CLA	b	5518	65/65	0.95	0.16	-0.38	60,64,69,75	0
23	CLA	c	5494	46/65	0.93	0.16	-0.47	72,77,86,88	0
27	OEC	a	5565	5/9	0.96	0.13	-0.51	63,64,71,87	0
23	CLA	b	5521	65/65	0.94	0.15	-0.63	48,57,63,64	0
23	CLA	A	558	65/65	0.97	0.14	-0.73	41,46,50,51	0
27	OEC	A	565	5/9	0.96	0.13	-0.75	62,63,65,66	0
21	BCT	d	5353	4/4	0.97	0.15	-1.05	75,75,76,77	0
20	FE2	a	5557	1/1	1.00	0.11	-2.31	75,75,75,75	0
20	FE2	A	557	1/1	0.95	0.05	-3.62	60,60,60,60	0
22	UNK	C	478	11/-	0.85	0.23	-	58,65,66,66	0
22	UNK	c	5486	8/-	0.89	0.30	-	63,64,65,66	0
22	UNK	C	480	7/-	0.92	0.21	-	35,36,38,38	0
22	UNK	C	490	4/-	0.96	0.15	-	67,67,68,68	0
22	UNK	C	475	12/-	0.73	0.32	-	68,69,72,73	0
22	UNK	c	5475	12/-	0.75	0.34	-	74,78,84,84	0
22	UNK	c	5487	7/-	0.88	0.20	-	57,57,58,58	0
19	CA	K	56	1/1	0.96	0.09	-	119,119,119,119	0
22	UNK	C	488	5/-	0.87	0.16	-	41,45,47,47	0
22	UNK	C	486	8/-	0.80	0.36	-	55,56,59,60	0
22	UNK	C	483	13/-	0.89	0.22	-	61,68,78,78	0
19	CA	k	5056	1/1	0.94	0.19	-	119,119,119,119	0
22	UNK	c	5480	7/-	0.89	0.27	-	65,66,66,67	0
22	UNK	C	487	7/-	0.86	0.23	-	49,52,52,53	0
22	UNK	c	5483	13/-	0.88	0.25	-	71,75,80,82	0
22	UNK	C	479	11/-	0.85	0.26	-	58,64,67,67	0
22	UNK	c	5488	5/-	0.92	0.21	-	59,59,59,60	0
22	UNK	c	5479	11/-	0.85	0.23	-	76,77,77,77	0
22	UNK	c	5478	11/-	0.70	0.39	-	76,79,81,81	0
22	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.