



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 07:09 PM BST

PDB ID : 3BZ1
Title : Crystal Structure of cyanobacterial Photosystem II (part 1 of 2). This file contains first monomer of PSII dimer
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 Å(reported)

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

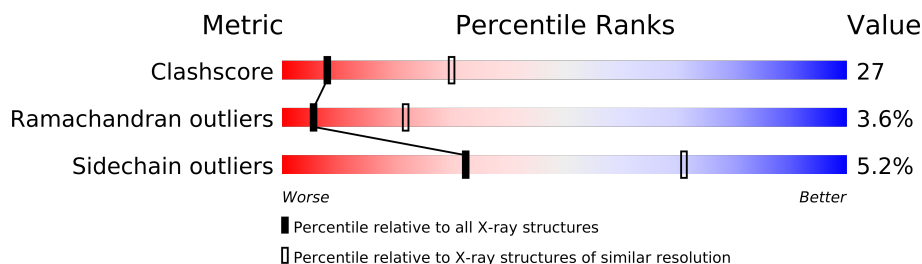
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	344	
2	B	510	
3	C	473	
4	D	352	
5	E	84	
6	F	45	
7	H	66	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	36	
13	O	247	
14	T	32	
15	U	104	
16	V	137	
17	y	46	

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Mol	Chain	Length	Quality of chain
18	X	50	
19	Y	28	
20	Z	62	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 25117 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	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
			3444	2256	576	599	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
C	3	THR	-	SEE REMARK 999	UNP Q8DIF8
C	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
C	5	SER	-	SEE REMARK 999	UNP Q8DIF8
C	6	SER	-	SEE REMARK 999	UNP Q8DIF8
C	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
C	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
C	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
C	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
C	11	SER	-	SEE REMARK 999	UNP Q8DIF8
C	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
C	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

- 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
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O		0	0	0
			666	434	108	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	S	0	0	0
			774	491	129	154				

- 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
			1060	673	177	206	4			

- Molecule 17 is a protein called Protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

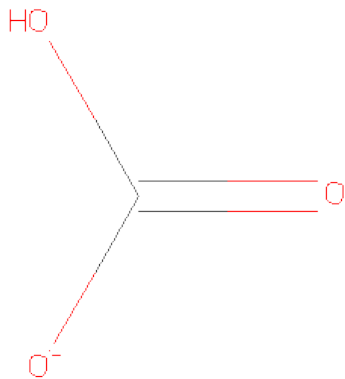
- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	O	1	Total	Ca	0	0
			1	1		
21	K	1	Total	Ca	0	0
			1	1		

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

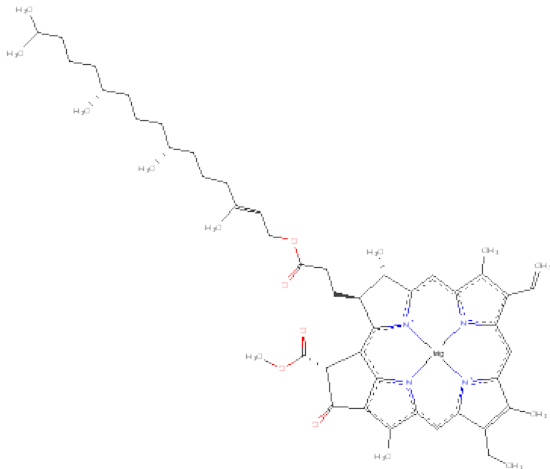
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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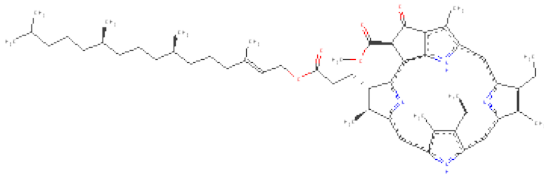
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N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

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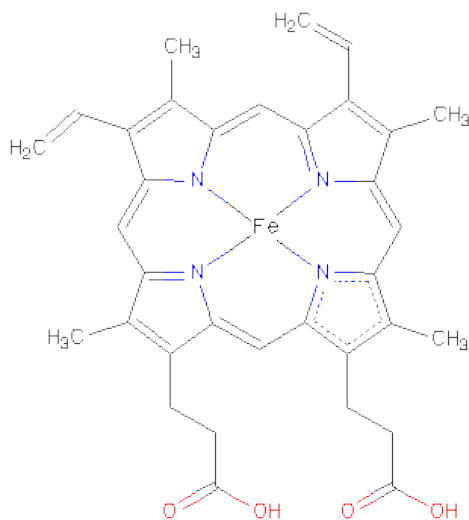
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



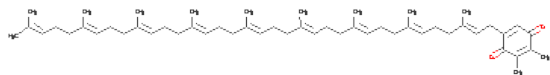
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



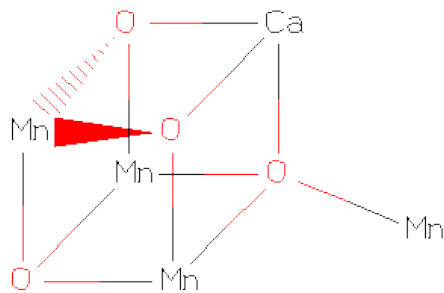
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
26	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



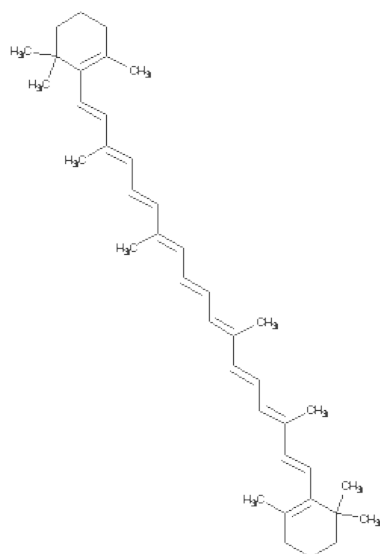
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	D	1	Total	C	O	0	0
			55	53	2		
27	A	1	Total	C	O	0	0
			45	43	2		
27	J	1	Total	C	O	0	0
			35	33	2		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



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

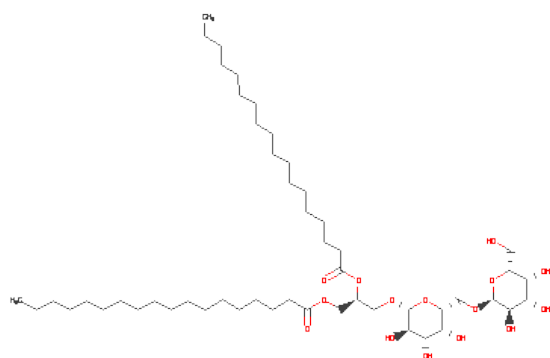
- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

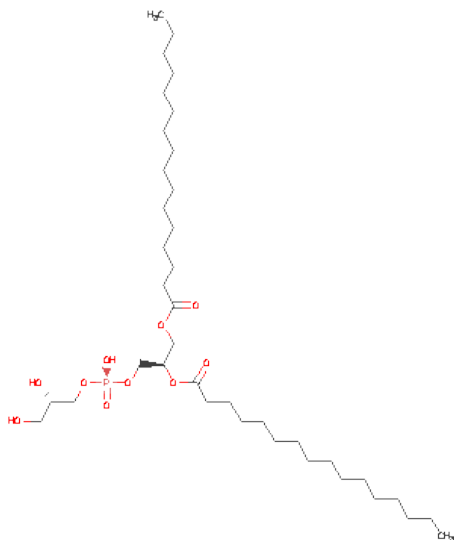
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C₅₁H₉₆O₁₅).



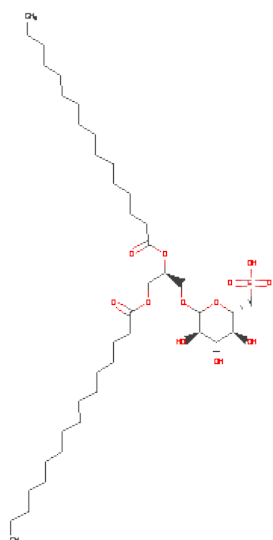
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			56	41	15		
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			62	47	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			58	43	15		
30	A	1	Total	C	O	0	0
			52	37	15		
30	D	1	Total	C	O	0	0
			63	48	15		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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
			37	26	10	1		

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



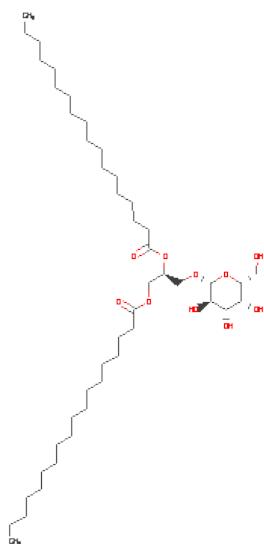
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			51	38	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			54	41	12	1		
32	T	1	Total	C	O	S	0	0
			47	34	12	1		
32	D	1	Total	C	O	S	0	0
			43	30	12	1		
32	F	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



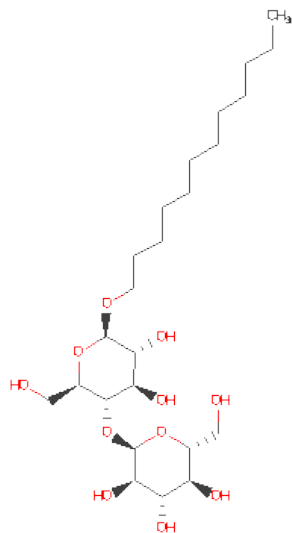
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			46	36	10		
33	B	1	Total	C	O	0	0
			49	39	10		
33	A	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			48	38	10		
33	B	1	Total	C	O	0	0
			49	39	10		
33	B	1	Total	C	O	0	0
			42	32	10		
33	M	1	Total	C	O	0	0
			42	32	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	E	1	Total	C	O	0	0
			44	34	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	I	1	Total	C	O	0	0
			43	33	10		
33	C	1	Total	C	O	0	0
			45	35	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			35	24	11		
34	D	1	Total	C	O	0	0
			31	20	11		
34	I	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			35	24	11		
34	O	1	Total	C	O	0	0
			35	24	11		

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

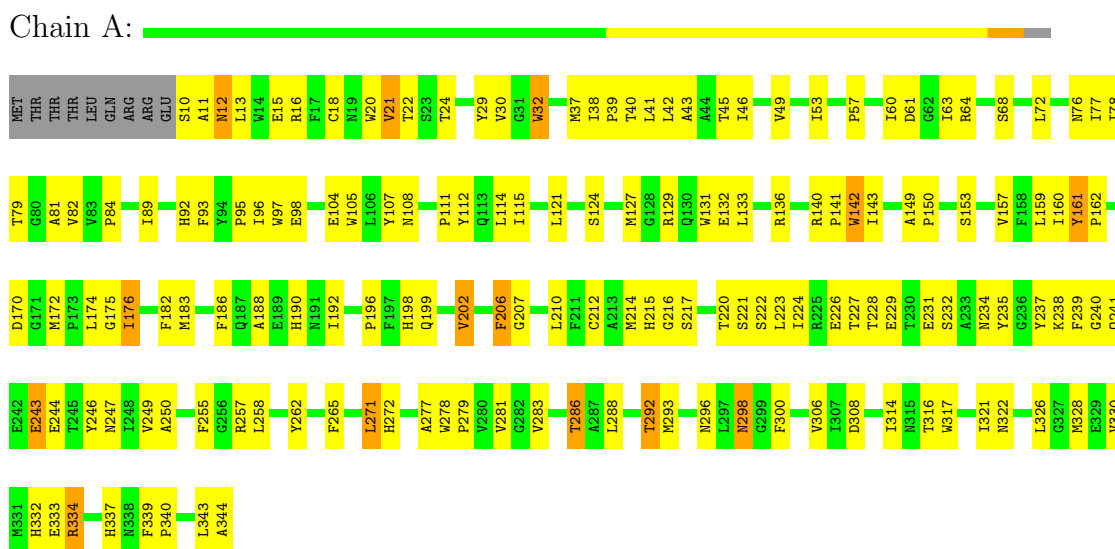
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

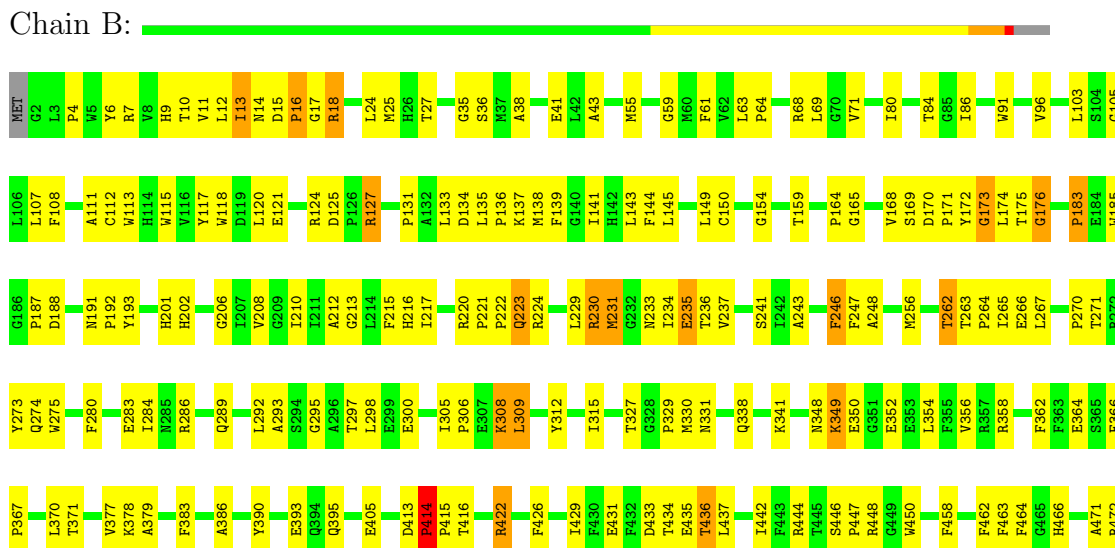
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

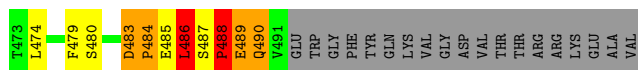
Note EDS was not executed.

• Molecule 1: Photosystem Q(B) protein



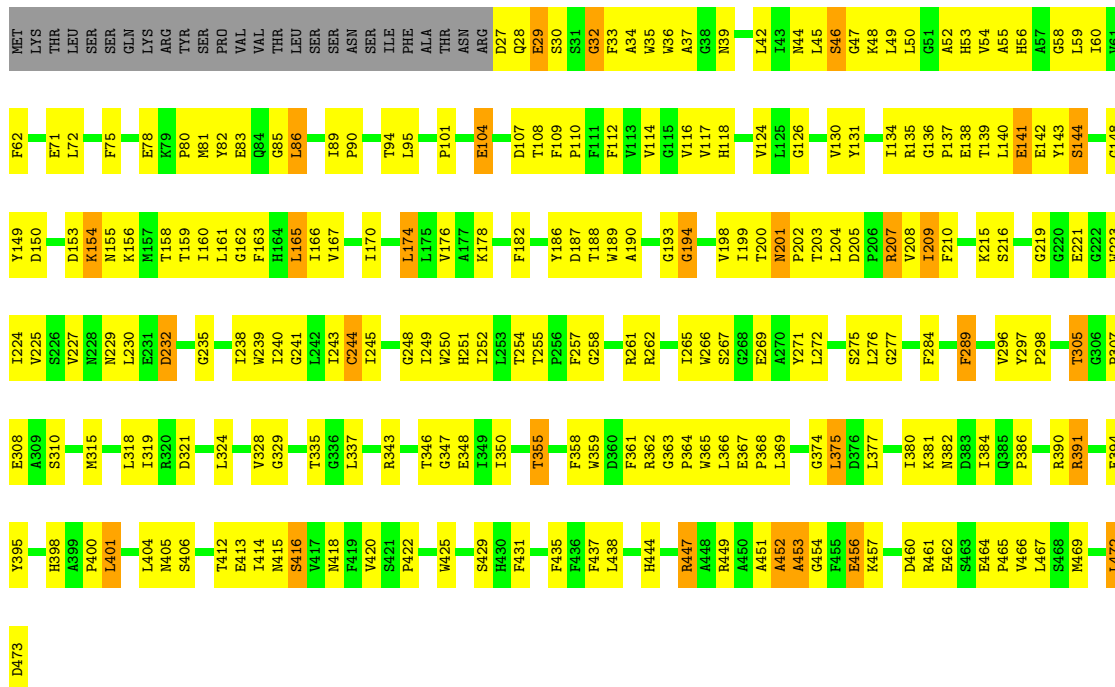
• Molecule 2: Photosystem II core light harvesting protein





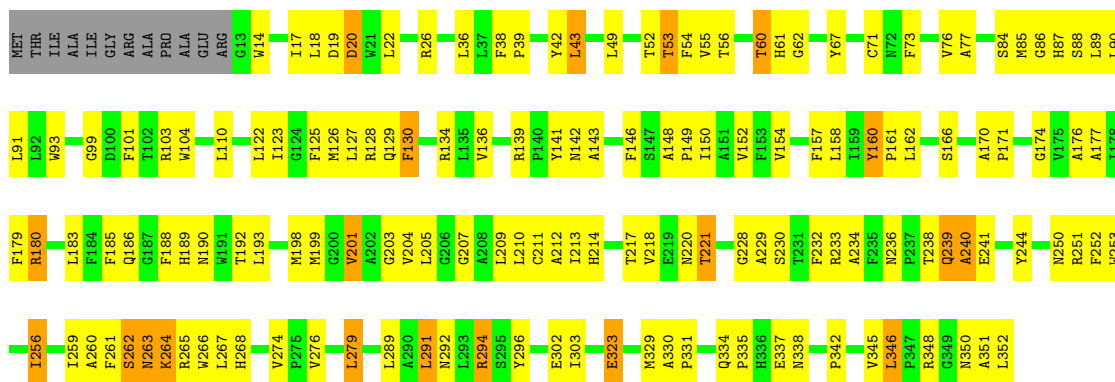
• Molecule 3: Photosystem II CP43 protein

Chain C:



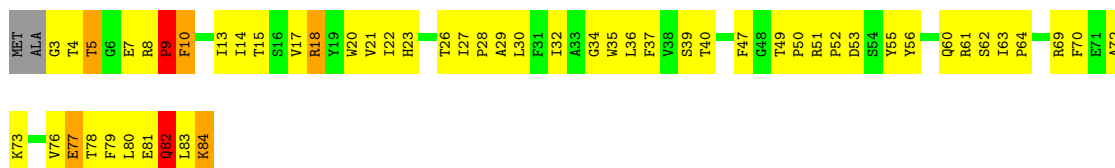
• Molecule 4: Photosystem II reaction center D2 protein

Chain D:



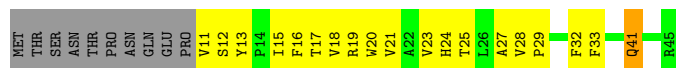
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 



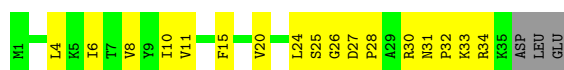
- Molecule 7: Photosystem II reaction center protein H

Chain H: 



- Molecule 8: Photosystem II reaction center protein I

Chain I: 



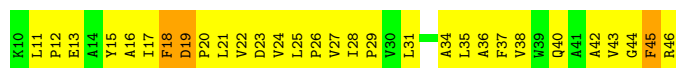
- Molecule 9: Photosystem II reaction center protein J

Chain J: 



- Molecule 10: Photosystem II reaction center protein K

Chain K: 



- Molecule 11: Photosystem II reaction center protein L

Chain L: 



- Molecule 12: Photosystem II reaction center protein M

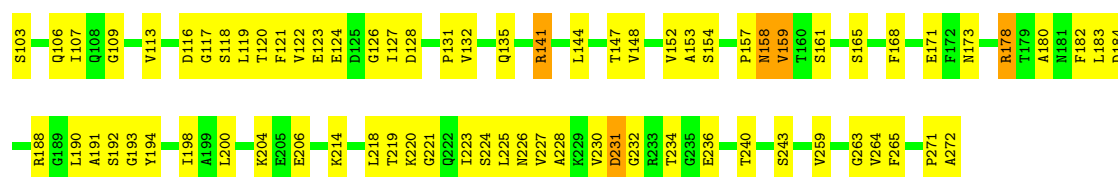
Chain M: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 





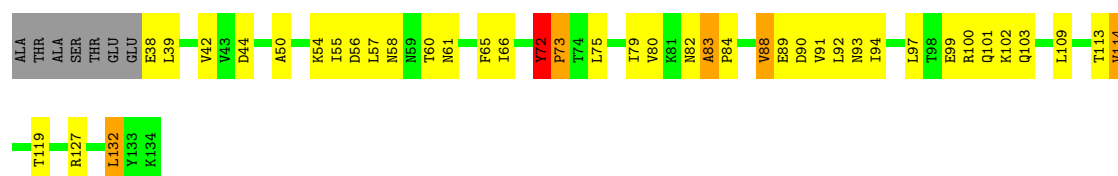
- Molecule 14: Photosystem II reaction center protein T

Chain T:



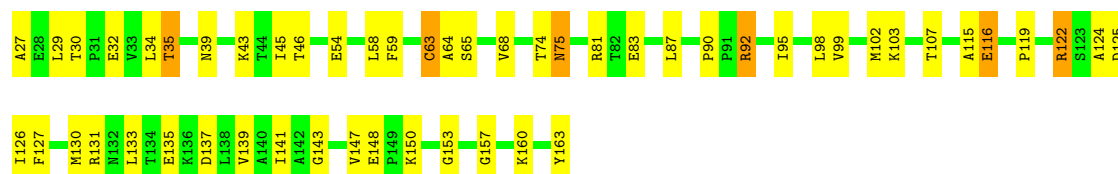
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



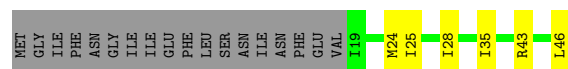
- Molecule 16: Cytochrome c-550

Chain V:



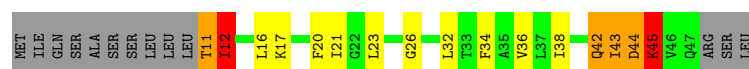
- Molecule 17: Protein ycf12

Chain y:



- Molecule 18: Photosystem II PsbX protein

Chain X:



- Molecule 19: Photosystem II protein Y

Chain Y:



- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

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 – 2.90	Depositor
% Data completeness (in resolution range)	97.7 (10.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292	Depositor
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 193457 reflections (0.001%)	Xtriage
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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	0.44	0/2713	0.66	0/3700
2	B	0.44	0/3986	0.67	3/5433 (0.1%)
3	C	0.41	0/3556	0.64	1/4842 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.45	0/685	0.71	0/933
6	F	0.45	0/291	0.59	0/397
7	H	0.42	0/520	0.73	1/709 (0.1%)
8	I	0.51	0/293	0.68	0/395
9	J	0.43	0/255	0.69	0/346
10	K	0.43	0/303	0.63	0/416
11	L	0.39	0/311	0.65	0/422
12	M	0.44	0/270	0.70	0/367
13	O	0.44	0/1876	0.70	0/2548
14	T	0.50	0/284	0.62	0/381
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.38	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.43	0/273	0.63	0/370
20	Z	0.45	0/490	0.69	0/669
All	All	0.44	0/20975	0.67	6/28550 (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
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	B	488	PRO	N-CA-C	5.86	127.33	112.10
2	B	489	GLU	N-CA-C	5.76	126.56	111.00
7	H	65	LEU	CA-CB-CG	5.72	128.45	115.30
3	C	32	GLY	N-CA-C	-5.54	99.24	113.10
15	U	72	TYR	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	175	0
2	B	3850	0	3718	224	0
3	C	3444	0	3365	258	0
4	D	2706	0	2608	177	0
5	E	666	0	651	71	0
6	F	282	0	291	28	0
7	H	507	0	521	52	0
8	I	286	0	308	15	0
9	J	249	0	262	28	0
10	K	293	0	305	42	0
11	L	304	0	316	15	0
12	M	267	0	289	15	0
13	O	1845	0	1801	113	0
14	T	275	0	288	18	0
15	U	774	0	773	46	0
16	V	1060	0	1068	42	0
17	y	201	0	226	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	X	270	0	299	27	0
19	Y	140	0	32	4	0
20	Z	479	0	516	54	0
21	K	1	0	0	0	0
21	O	1	0	0	0	0
22	A	1	0	0	0	0
23	D	4	0	0	1	0
24	A	195	0	216	16	0
24	B	1040	0	1152	77	0
24	C	845	0	936	61	0
24	D	195	0	216	12	0
25	A	64	0	74	5	0
25	D	64	0	74	2	0
26	E	43	0	30	5	0
26	V	43	0	30	3	0
27	A	45	0	61	5	0
27	D	55	0	80	9	0
27	J	35	0	45	0	0
28	A	5	0	0	0	0
29	A	40	0	56	3	0
29	B	160	0	224	9	0
29	C	80	0	112	15	0
29	D	40	0	56	3	0
29	H	40	0	56	5	0
29	J	40	0	56	5	0
29	K	40	0	56	13	0
29	Z	40	0	56	5	0
30	A	108	0	132	3	0
30	C	181	0	245	19	0
30	D	63	0	87	0	0
30	H	58	0	74	1	0
31	A	76	0	95	8	0
32	A	51	0	68	5	0
32	B	54	0	77	1	0
32	D	43	0	49	2	0
32	F	45	0	53	2	0
32	T	47	0	60	2	0
33	A	51	0	72	1	0
33	B	140	0	190	3	0
33	C	93	0	126	6	0
33	D	94	0	128	8	0
33	E	44	0	58	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	I	43	0	56	3	0
33	M	42	0	54	4	0
34	B	70	0	92	3	0
34	D	31	0	35	2	0
34	I	35	0	46	4	0
34	M	35	0	46	0	0
34	O	35	0	46	3	0
34	T	35	0	46	3	0
35	A	1	0	0	0	0
All	All	25117	0	25682	1330	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (1330) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:63:CYS:SG	26:V:164:HEM:HAB	1.85	1.16
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.23	1.16
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.22	1.09
2:B:68:ARG:HH22	24:B:514:CLA:HED1	1.12	1.07
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.19	1.06
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.36	1.04
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.18	1.04
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.37	1.03
3:C:254:THR:HG22	3:C:255:THR:H	1.18	1.03
2:B:149:LEU:HG	24:B:513:CLA:HBC1	1.44	1.00
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	1.95	0.99
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.47	0.97
13:O:230:VAL:HG12	13:O:231:ASP:H	1.30	0.97
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.49	0.94
15:U:83:ALA:HB1	15:U:84:PRO:CD	1.98	0.93
14:T:29:ILE:HD12	14:T:29:ILE:H	1.33	0.92
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.53	0.89
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.37	0.89
24:D:356:CLA:H42	18:X:26:GLY:HA3	1.53	0.89
3:C:224:ILE:O	3:C:227:VAL:HG23	1.73	0.88
2:B:68:ARG:NH2	24:B:514:CLA:HED1	1.88	0.88
13:O:178:ARG:CG	13:O:178:ARG:HH11	1.88	0.87
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.57	0.87
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.55	0.87
24:B:518:CLA:HMD1	24:B:520:CLA:HAB	1.55	0.86
24:B:518:CLA:HAB	4:D:123:ILE:HG23	1.58	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:271:THR:HG22	2:B:273:TYR:H	1.39	0.86
3:C:305:THR:HG22	3:C:308:GLU:H	1.40	0.86
4:D:129:GLN:NE2	4:D:143:ALA:HA	1.92	0.85
13:O:69:LEU:HD12	13:O:70:CYS:H	1.39	0.85
3:C:447:ARG:HH11	3:C:447:ARG:HG2	1.40	0.85
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.56	0.85
7:H:12:ARG:HD3	7:H:12:ARG:O	1.76	0.84
26:E:85:HEM:HBC2	6:F:27:ALA:HB1	1.59	0.84
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.60	0.84
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.39	0.84
3:C:155:ASN:HD21	3:C:255:THR:HB	1.40	0.84
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.60	0.84
11:L:8:GLN:HE21	11:L:8:GLN:N	1.75	0.83
3:C:39:ASN:HB2	24:C:481:CLA:HBA1	1.58	0.83
3:C:449:ARG:HE	24:C:478:CLA:HED1	1.43	0.83
2:B:68:ARG:HH22	24:B:514:CLA:CED	1.92	0.83
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.43	0.82
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.61	0.81
2:B:489:GLU:HB2	5:E:3:GLY:N	1.96	0.80
13:O:83:LYS:HG2	13:O:84:ASN:H	1.46	0.80
24:A:362:CLA:H152	25:A:365:PHO:H51	1.63	0.80
20:Z:36:SER:HA	20:Z:39:LEU:HG	1.64	0.80
29:D:358:BCR:H403	9:J:25:VAL:HG21	1.64	0.80
1:A:41:LEU:HD13	25:A:365:PHO:H2	1.62	0.79
3:C:254:THR:HG22	3:C:255:THR:N	1.96	0.79
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.63	0.79
13:O:230:VAL:HG12	13:O:231:ASP:N	1.98	0.79
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.65	0.78
2:B:187:PRO:HB3	24:B:511:CLA:HMB2	1.65	0.78
2:B:24:LEU:HD21	24:B:526:CLA:HAB	1.65	0.78
1:A:12:ASN:HD22	1:A:15:GLU:HB2	1.49	0.78
5:E:84:LYS:NZ	5:E:84:LYS:HB2	1.97	0.78
2:B:271:THR:HG22	2:B:273:TYR:N	1.98	0.78
2:B:120:LEU:HD13	24:B:526:CLA:HMD2	1.64	0.78
27:A:367:PL9:H33	4:D:38:PHE:HD1	1.48	0.77
2:B:329:PRO:HB3	24:B:517:CLA:HED1	1.65	0.76
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.67	0.76
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.66	0.76
3:C:42:LEU:HD13	24:C:484:CLA:HMA3	1.68	0.76
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.66	0.76
20:Z:32:ASP:HB2	20:Z:35:ARG:HG2	1.67	0.76
2:B:134:ASP:OD2	2:B:137:LYS:HE3	1.86	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:ILE:HA	1:A:293:MET:HE3	1.68	0.75
3:C:391:ARG:HB2	3:C:391:ARG:NH1	2.02	0.75
18:X:12:ILE:O	18:X:12:ILE:HG23	1.85	0.75
24:C:474:CLA:HMB3	29:C:488:BCR:H403	1.69	0.75
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.07	0.75
20:Z:49:ALA:O	20:Z:53:VAL:HG23	1.86	0.75
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.00	0.74
3:C:155:ASN:HA	3:C:158:THR:HG22	1.69	0.74
3:C:241:GLY:O	3:C:245:ILE:HG13	1.88	0.74
1:A:214:MET:HA	1:A:214:MET:CE	2.17	0.74
2:B:137:LYS:HD2	7:H:14:LEU:O	1.87	0.74
4:D:244:TYR:OH	4:D:264:LYS:HE3	1.88	0.74
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.70	0.74
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.70	0.74
6:F:17:THR:HG23	6:F:20:TRP:H	1.53	0.74
5:E:18:ARG:HB3	5:E:18:ARG:HH11	1.52	0.73
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.23	0.73
3:C:240:ILE:O	3:C:244:CYS:HB2	1.88	0.73
29:C:487:BCR:H353	29:K:112:BCR:H321	1.69	0.73
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.69	0.73
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.17	0.73
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.19	0.73
5:E:17:VAL:O	5:E:21:VAL:HG23	1.88	0.73
18:X:34:PHE:O	18:X:38:ILE:HG12	1.88	0.73
3:C:254:THR:CG2	3:C:255:THR:H	2.00	0.72
1:A:41:LEU:O	1:A:45:THR:HG22	1.88	0.72
3:C:305:THR:CG2	3:C:308:GLU:H	2.02	0.72
3:C:415:ASN:O	3:C:416:SER:HB3	1.89	0.72
3:C:405:ASN:HD22	30:C:491:DGD:HD5	1.54	0.72
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.01	0.72
20:Z:32:ASP:CG	20:Z:33:TRP:H	1.90	0.72
3:C:361:PHE:HA	30:C:489:DGD:HE61	1.72	0.72
13:O:69:LEU:HD12	13:O:70:CYS:N	2.05	0.72
13:O:86:ARG:NH1	13:O:87:GLN:HA	2.05	0.72
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.55	0.71
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.04	0.71
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.72	0.71
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.04	0.71
5:E:56:TYR:O	16:V:27:ALA:HB2	1.90	0.71
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.72	0.71
24:D:356:CLA:H43	18:X:23:LEU:HA	1.71	0.71
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.55	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:T:29:ILE:CD1	14:T:29:ILE:H	1.95	0.71
2:B:150:CYS:HB2	24:B:513:CLA:HMC3	1.72	0.70
3:C:348:GLU:OE2	13:O:37:VAL:HA	1.91	0.70
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.73	0.70
7:H:38:PHE:HB2	29:H:107:BCR:H10C	1.74	0.70
15:U:38:GLU:HG2	15:U:39:LEU:N	2.05	0.70
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.06	0.70
16:V:63:CYS:SG	26:V:164:HEM:CAB	2.74	0.70
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.74	0.70
13:O:35:ASP:C	13:O:36:ILE:HD12	2.12	0.70
13:O:87:GLN:O	13:O:88:GLU:HB3	1.91	0.70
16:V:115:ALA:CB	16:V:122:ARG:HD2	2.22	0.70
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.26	0.69
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.74	0.69
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.69
4:D:122:LEU:HD11	25:D:355:PHO:H92	1.74	0.69
13:O:33:TYR:O	13:O:37:VAL:HG23	1.92	0.69
3:C:158:THR:O	3:C:251:HIS:HB3	1.92	0.69
5:E:26:THR:HB	26:E:85:HEM:HBB2	1.74	0.69
3:C:85:GLY:N	30:C:490:DGD:HE4	2.07	0.69
5:E:81:GLU:O	5:E:83:LEU:N	2.24	0.69
4:D:39:PRO:O	4:D:43:LEU:HD22	1.93	0.69
4:D:129:GLN:HE22	4:D:143:ALA:HA	1.55	0.69
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.58	0.69
4:D:261:PHE:HB2	27:D:357:PL9:H522	1.74	0.68
5:E:15:THR:HG23	9:J:8:ILE:O	1.92	0.68
20:Z:30:PRO:HG3	20:Z:33:TRP:HZ3	1.58	0.68
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.27	0.68
4:D:192:THR:HG23	24:D:354:CLA:HBC2	1.74	0.68
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.73	0.68
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.74	0.68
20:Z:32:ASP:HB3	20:Z:35:ARG:NH1	2.08	0.68
10:K:19:ASP:N	10:K:20:PRO:HD2	2.09	0.68
2:B:135:LEU:HA	2:B:138:MET:HE3	1.74	0.68
13:O:206:GLU:CD	13:O:206:GLU:H	1.97	0.68
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.27	0.68
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.76	0.68
24:D:354:CLA:H72	24:D:364:CLA:HAB	1.76	0.68
20:Z:28:ALA:O	20:Z:30:PRO:HD3	1.93	0.68
2:B:284:ILE:HG12	2:B:309:LEU:CD1	2.23	0.68
4:D:279:LEU:HG	25:D:355:PHO:HBC3	1.76	0.68
5:E:81:GLU:C	5:E:83:LEU:H	1.96	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:180:ARG:CG	4:D:180:ARG:HH11	2.08	0.67
3:C:42:LEU:HD21	24:C:484:CLA:H2A	1.74	0.67
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.48	0.67
2:B:483:ASP:OD2	2:B:484:PRO:HD2	1.94	0.67
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.75	0.67
2:B:135:LEU:HD23	2:B:138:MET:CE	2.25	0.67
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.59	0.67
3:C:472:LEU:HD12	3:C:473:ASP:H	1.59	0.67
3:C:166:ILE:O	3:C:170:ILE:HG13	1.94	0.67
1:A:183:MET:HA	24:A:362:CLA:HMD2	1.76	0.67
12:M:31:SER:HB3	33:M:217:LMG:HC71	1.77	0.67
6:F:11:VAL:HG12	6:F:12:SER:H	1.59	0.67
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.77	0.67
2:B:271:THR:CG2	2:B:273:TYR:H	2.08	0.67
2:B:133:LEU:HB3	2:B:138:MET:CE	2.24	0.67
24:B:512:CLA:H42	7:H:45:ILE:HD11	1.76	0.67
3:C:377:LEU:O	3:C:381:LYS:HB2	1.95	0.67
5:E:78:THR:O	5:E:81:GLU:HB2	1.94	0.67
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.77	0.66
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.59	0.66
24:C:480:CLA:H112	29:C:488:BCR:H362	1.78	0.66
12:M:23:ILE:HD13	33:M:217:LMG:H182	1.78	0.66
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.77	0.66
2:B:141:ILE:CG2	24:B:525:CLA:HBB1	2.26	0.66
24:C:478:CLA:HBD	24:C:478:CLA:HBA1	1.77	0.66
15:U:83:ALA:CB	15:U:84:PRO:HD2	2.14	0.66
6:F:11:VAL:HG12	6:F:12:SER:N	2.09	0.66
3:C:305:THR:HG22	3:C:308:GLU:CB	2.26	0.66
3:C:277:GLY:C	24:C:478:CLA:HBC2	2.15	0.66
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.26	0.66
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.62	0.65
20:Z:33:TRP:O	20:Z:37:LYS:HB2	1.95	0.65
27:A:367:PL9:H33	4:D:38:PHE:CD1	2.31	0.65
2:B:224:ARG:HG2	7:H:24:GLY:O	1.96	0.65
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.78	0.65
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.78	0.65
3:C:89:ILE:N	3:C:90:PRO:HD2	2.11	0.65
3:C:55:ALA:HB1	29:C:487:BCR:H373	1.78	0.65
2:B:331:ASN:HB3	2:B:437:LEU:HD12	1.79	0.65
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.31	0.65
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.78	0.65
3:C:155:ASN:HD21	3:C:255:THR:CB	2.07	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.78	0.65
3:C:30:SER:HB2	10:K:46:ARG:O	1.95	0.65
9:J:14:ALA:CB	29:K:112:BCR:H393	2.27	0.65
2:B:222:PRO:HG3	7:H:27:THR:H	1.61	0.65
2:B:271:THR:HB	2:B:274:GLN:HG3	1.78	0.65
2:B:248:ALA:HA	24:B:513:CLA:H42	1.79	0.65
11:L:7:ARG:HD2	11:L:7:ARG:O	1.97	0.65
13:O:120:THR:HG22	13:O:154:SER:OG	1.96	0.65
2:B:490:GLN:OE1	2:B:490:GLN:O	2.15	0.65
2:B:247:PHE:HE1	24:B:512:CLA:H101	1.62	0.64
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.62	0.64
2:B:86:ILE:O	2:B:86:ILE:HD12	1.97	0.64
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.32	0.64
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.11	0.64
3:C:449:ARG:HE	24:C:478:CLA:CED	2.08	0.64
13:O:86:ARG:HD2	13:O:86:ARG:C	2.18	0.64
2:B:103:LEU:HD21	24:B:515:CLA:HMC3	1.78	0.64
2:B:327:THR:HG22	24:B:517:CLA:H12	1.78	0.64
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.79	0.64
24:C:484:CLA:H151	20:Z:20:VAL:HG13	1.78	0.64
1:A:174:LEU:HD22	25:A:365:PHO:H151	1.78	0.64
15:U:66:ILE:HG22	15:U:66:ILE:O	1.98	0.64
7:H:35:MET:HE2	29:H:107:BCR:HC21	1.80	0.64
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.80	0.64
1:A:57:PRO:HG3	1:A:68:SER:CB	2.28	0.64
13:O:117:GLY:O	13:O:159:VAL:HG12	1.98	0.64
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.80	0.64
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.62	0.64
2:B:284:ILE:HG23	2:B:305:ILE:HD12	1.80	0.63
16:V:143:GLY:O	16:V:147:VAL:HG23	1.97	0.63
3:C:209:ILE:HG23	29:C:488:BCR:H382	1.81	0.63
3:C:310:SER:OG	3:C:355:THR:HG23	1.98	0.63
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.80	0.63
5:E:36:LEU:O	5:E:40:THR:HG23	1.98	0.63
4:D:186:GLN:HB2	24:D:354:CLA:HBC1	1.80	0.63
24:B:512:CLA:H61	7:H:46:LEU:HD13	1.80	0.63
2:B:486:LEU:O	2:B:486:LEU:HD13	1.98	0.63
32:A:372:SQD:H311	24:C:481:CLA:H71	1.81	0.63
30:C:491:DGD:HD2	9:J:32:ALA:O	1.99	0.63
24:C:484:CLA:H171	20:Z:20:VAL:HA	1.79	0.63
3:C:107:ASP:OD2	3:C:110:PRO:HD3	1.99	0.63
2:B:297:THR:OG1	2:B:300:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:18:PHE:HD2	10:K:18:PHE:N	1.97	0.63
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.81	0.63
13:O:230:VAL:CG1	13:O:231:ASP:H	2.10	0.62
24:B:515:CLA:HMB3	24:B:516:CLA:H11	1.81	0.62
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.80	0.62
5:E:26:THR:O	5:E:29:ALA:HB3	1.98	0.62
3:C:337:LEU:HD12	13:O:131:PRO:HG3	1.81	0.62
7:H:19:GLY:O	7:H:21:VAL:HG13	1.99	0.62
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.34	0.62
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.82	0.62
24:C:478:CLA:CMD	24:C:480:CLA:HAB	2.29	0.62
14:T:29:ILE:HD12	14:T:29:ILE:N	2.10	0.62
1:A:142:TRP:HB2	4:D:220:ASN:OD1	1.99	0.62
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.81	0.62
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.30	0.62
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.81	0.62
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.13	0.62
33:D:360:LMG:HC62	11:L:15:THR:HG21	1.82	0.62
5:E:64:PRO:HB3	5:E:84:LYS:HE2	1.82	0.62
3:C:44:ASN:C	3:C:45:LEU:HD12	2.20	0.62
4:D:267:LEU:HD23	4:D:267:LEU:C	2.20	0.62
4:D:26:ARG:CD	6:F:18:VAL:HG11	2.27	0.62
29:C:487:BCR:H312	20:Z:9:LEU:HD11	1.80	0.61
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.15	0.61
7:H:58:VAL:HG13	7:H:58:VAL:O	2.00	0.61
15:U:94:ILE:O	15:U:97:LEU:HG	2.00	0.61
1:A:93:PHE:HZ	24:A:366:CLA:HAA1	1.64	0.61
16:V:102:MET:HE3	16:V:141:ILE:HG21	1.81	0.61
1:A:18:CYS:O	1:A:22:THR:HG22	2.00	0.61
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.82	0.61
1:A:228:THR:HG22	1:A:229:GLU:H	1.65	0.61
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.82	0.61
2:B:371:THR:HG22	2:B:377:VAL:HA	1.81	0.61
24:C:485:CLA:H143	24:C:486:CLA:H162	1.82	0.61
3:C:44:ASN:O	3:C:45:LEU:HD12	1.99	0.61
3:C:248:GLY:O	3:C:252:ILE:HG12	2.00	0.61
1:A:343:LEU:O	1:A:344:ALA:HB2	2.00	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.82	0.61
15:U:97:LEU:O	15:U:102:LYS:HE2	2.01	0.61
3:C:52:ALA:HA	24:C:484:CLA:HMB3	1.82	0.61
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.31	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:342:PRO:O	4:D:345:VAL:HG12	2.01	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	0.61
4:D:209:LEU:HD23	4:D:209:LEU:C	2.21	0.61
16:V:90:PRO:O	16:V:92:ARG:HD3	2.01	0.61
24:B:518:CLA:HMA1	4:D:130:PHE:CE1	2.36	0.61
5:E:18:ARG:O	5:E:22:ILE:HG13	2.00	0.60
10:K:17:ILE:HD12	10:K:17:ILE:N	2.17	0.60
13:O:39:THR:OG1	13:O:41:LEU:HB2	2.01	0.60
13:O:234:THR:OG1	13:O:236:GLU:HG2	2.00	0.60
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.83	0.60
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.60
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.36	0.60
3:C:143:TYR:O	3:C:144:SER:HB2	2.00	0.60
3:C:461:ARG:HG3	3:C:461:ARG:HH11	1.65	0.60
5:E:23:HIS:HA	5:E:26:THR:OG1	2.00	0.60
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.36	0.60
4:D:199:MET:HB3	27:D:357:PL9:H28	1.84	0.60
29:K:112:BCR:H331	29:K:112:BCR:HC8	1.83	0.60
20:Z:32:ASP:CB	20:Z:35:ARG:HG2	2.30	0.60
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.60
2:B:208:VAL:HG21	24:B:512:CLA:HMC1	1.84	0.60
5:E:4:THR:HG22	5:E:5:THR:N	2.17	0.60
2:B:213:GLY:O	2:B:217:ILE:HG13	2.02	0.60
13:O:31:LEU:N	13:O:31:LEU:HD12	2.17	0.60
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.37	0.60
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.82	0.60
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.82	0.60
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.02	0.60
20:Z:33:TRP:O	20:Z:33:TRP:HD1	1.84	0.60
3:C:114:VAL:HG22	33:C:493:LMG:H152	1.83	0.60
1:A:153:SER:CB	24:A:362:CLA:H11	2.32	0.60
1:A:202:VAL:HG11	24:D:364:CLA:OBD	2.02	0.60
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.84	0.60
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.37	0.59
1:A:306:VAL:HG13	1:A:314:ILE:O	2.01	0.59
5:E:79:PHE:O	5:E:84:LYS:HB3	2.01	0.59
1:A:214:MET:HA	1:A:214:MET:HE3	1.83	0.59
5:E:18:ARG:HB3	5:E:18:ARG:NH1	2.17	0.59
24:D:356:CLA:HMD2	34:D:363:LMT:H22	1.85	0.59
24:C:475:CLA:H111	24:C:476:CLA:HMB2	1.84	0.59
10:K:21:LEU:HD11	29:K:112:BCR:HC32	1.84	0.59
10:K:18:PHE:CD2	10:K:18:PHE:N	2.69	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.83	0.59
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.83	0.59
1:A:257:ARG:HH11	1:A:257:ARG:HG3	1.66	0.59
11:L:7:ARG:C	11:L:8:GLN:HE21	2.06	0.59
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.68	0.59
3:C:124:VAL:HB	29:Z:116:BCR:H362	1.84	0.59
15:U:113:THR:O	15:U:114:VAL:HG23	2.02	0.59
5:E:26:THR:HB	26:E:85:HEM:CBB	2.33	0.59
5:E:76:VAL:O	5:E:80:LEU:HD22	2.03	0.59
4:D:55:VAL:HG21	4:D:110:LEU:CD1	2.33	0.58
24:B:525:CLA:H143	24:B:526:CLA:HMA3	1.85	0.58
3:C:305:THR:HG23	3:C:307:PRO:CD	2.32	0.58
1:A:13:LEU:HD12	1:A:13:LEU:H	1.69	0.58
3:C:318:LEU:C	3:C:318:LEU:HD23	2.24	0.58
13:O:123:GLU:HG2	13:O:124:GLU:N	2.18	0.58
3:C:204:LEU:HD21	3:C:238:ILE:HG21	1.84	0.58
2:B:212:ALA:HB2	24:B:519:CLA:HMC3	1.85	0.58
3:C:112:PHE:O	3:C:116:VAL:HG13	2.03	0.58
3:C:141:GLU:H	3:C:141:GLU:CD	2.05	0.58
6:F:19:ARG:O	6:F:23:VAL:HG23	2.03	0.58
24:B:517:CLA:HAC2	29:B:528:BCR:H393	1.84	0.58
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.03	0.58
15:U:38:GLU:HG2	15:U:39:LEU:H	1.68	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
3:C:369:LEU:HD21	3:C:384:ILE:HD13	1.85	0.58
3:C:380:ILE:HA	3:C:384:ILE:HD11	1.85	0.58
7:H:12:ARG:HD3	7:H:12:ARG:C	2.24	0.58
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.68	0.58
2:B:329:PRO:HD3	24:B:517:CLA:HED2	1.86	0.58
4:D:18:LEU:HD22	18:X:38:ILE:CD1	2.34	0.58
4:D:239:GLN:O	4:D:240:ALA:HB3	2.03	0.58
20:Z:16:SER:O	20:Z:20:VAL:HG23	2.04	0.58
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.37	0.58
16:V:74:THR:O	16:V:75:ASN:HB2	2.04	0.58
3:C:447:ARG:NH1	3:C:447:ARG:HG2	2.16	0.57
5:E:84:LYS:HZ2	5:E:84:LYS:HB2	1.68	0.57
1:A:238:LYS:O	1:A:241:GLN:HG3	2.03	0.57
2:B:6:TYR:HA	24:B:521:CLA:H11	1.85	0.57
2:B:149:LEU:HG	24:B:513:CLA:CBC	2.29	0.57
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.34	0.57
2:B:172:TYR:O	2:B:174:LEU:HG	2.02	0.57
4:D:188:PHE:HE2	4:D:329:MET:CE	2.17	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:36:LEU:O	4:D:39:PRO:HD2	2.05	0.57
20:Z:14:ILE:O	20:Z:18:VAL:HG23	2.04	0.57
11:L:11:GLU:HG2	11:L:12:LEU:N	2.19	0.57
10:K:17:ILE:HD12	10:K:17:ILE:H	1.69	0.57
18:X:45:LYS:HD3	18:X:45:LYS:N	2.20	0.57
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.57
10:K:31:LEU:O	10:K:34:ALA:HB3	2.04	0.57
4:D:252:PHE:O	4:D:256:ILE:HG22	2.05	0.57
13:O:80:GLU:O	13:O:89:ALA:HB1	2.05	0.57
1:A:38:ILE:O	1:A:42:LEU:HG	2.05	0.57
4:D:18:LEU:O	4:D:22:LEU:HG	2.05	0.57
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.87	0.57
3:C:37:ALA:HA	24:C:481:CLA:O1A	2.04	0.57
24:C:478:CLA:H92	24:C:478:CLA:HAB	1.87	0.57
1:A:11:ALA:O	1:A:12:ASN:CB	2.53	0.57
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.86	0.57
12:M:29:THR:O	12:M:32:GLN:HG3	2.05	0.57
10:K:26:PRO:O	10:K:29:PRO:HD2	2.05	0.57
10:K:18:PHE:CE1	20:Z:9:LEU:HG	2.40	0.57
5:E:7:GLU:H	5:E:7:GLU:CD	2.07	0.57
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.87	0.57
2:B:256:MET:HA	2:B:263:THR:HG21	1.87	0.57
3:C:343:ARG:NH1	3:C:347:GLY:O	2.38	0.57
5:E:84:LYS:HB2	5:E:84:LYS:HZ3	1.70	0.57
3:C:165:LEU:HD21	24:C:479:CLA:HHC	1.85	0.56
27:D:357:PL9:H13	33:D:360:LMG:H132	1.87	0.56
4:D:266:TRP:CD1	33:D:360:LMG:HC3	2.40	0.56
2:B:191:ASN:ND2	7:H:60:VAL:HA	2.20	0.56
15:U:89:GLU:CD	15:U:89:GLU:H	2.09	0.56
2:B:230:ARG:O	2:B:233:ASN:HB3	2.05	0.56
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.87	0.56
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.40	0.56
2:B:61:PHE:CE1	24:B:517:CLA:HMB3	2.41	0.56
16:V:87:LEU:HD12	16:V:87:LEU:N	2.20	0.56
20:Z:55:GLY:HA2	29:Z:116:BCR:H312	1.87	0.56
4:D:274:VAL:HA	27:D:357:PL9:H253	1.86	0.56
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.41	0.56
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.86	0.56
4:D:152:VAL:HG21	4:D:279:LEU:CD1	2.35	0.56
7:H:58:VAL:O	7:H:58:VAL:CG1	2.53	0.56
3:C:374:GLY:O	3:C:375:LEU:C	2.44	0.56
1:A:244:GLU:HG3	1:A:246:TYR:H	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:ARG:HH22	31:A:371:LHG:P	2.28	0.56
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.88	0.56
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.88	0.56
4:D:199:MET:HG2	27:D:357:PL9:H322	1.86	0.56
2:B:191:ASN:HD21	7:H:60:VAL:HA	1.70	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
2:B:112:CYS:HB3	29:B:530:BCR:H393	1.88	0.56
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.87	0.56
18:X:12:ILE:HG12	18:X:16:LEU:CD1	2.31	0.56
20:Z:29:SER:HB2	20:Z:31:GLN:HG3	1.88	0.56
13:O:31:LEU:HD12	13:O:31:LEU:H	1.71	0.56
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.36	0.56
9:J:14:ALA:HB1	29:K:112:BCR:H393	1.88	0.56
1:A:104:GLU:OE2	13:O:99:ARG:HD3	2.06	0.56
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.70	0.56
20:Z:23:VAL:O	20:Z:26:ALA:HB3	2.07	0.55
3:C:199:ILE:N	3:C:199:ILE:HD12	2.22	0.55
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.21	0.55
4:D:267:LEU:HD23	4:D:267:LEU:O	2.06	0.55
20:Z:26:ALA:CB	20:Z:40:ILE:HD11	2.36	0.55
8:I:11:VAL:O	8:I:15:PHE:HD2	1.89	0.55
2:B:43:ALA:HA	33:B:534:LMG:H112	1.87	0.55
14:T:7:VAL:HG12	34:T:227:LMT:H122	1.89	0.55
3:C:305:THR:HG22	3:C:308:GLU:N	2.16	0.55
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.36	0.55
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.88	0.55
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.41	0.55
33:D:359:LMG:O3	9:J:37:GLY:HA3	2.07	0.55
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.41	0.55
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.42	0.55
24:B:518:CLA:H42	4:D:127:LEU:HD11	1.88	0.55
3:C:95:LEU:HD13	24:C:475:CLA:H143	1.89	0.55
1:A:37:MET:HG2	1:A:41:LEU:HD12	1.89	0.55
5:E:55:TYR:O	5:E:84:LYS:HE3	2.07	0.55
1:A:131:TRP:CE3	1:A:132:GLU:N	2.75	0.55
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.89	0.55
20:Z:36:SER:HA	20:Z:39:LEU:CG	2.35	0.55
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.88	0.55
16:V:59:PHE:HA	16:V:63:CYS:SG	2.47	0.55
4:D:180:ARG:CG	4:D:180:ARG:NH1	2.70	0.55
3:C:107:ASP:OD2	3:C:109:PHE:HB3	2.06	0.55
18:X:32:LEU:N	18:X:32:LEU:HD23	2.22	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:J:14:ALA:HB3	29:K:112:BCR:H393	1.89	0.54
1:A:217:SER:HA	1:A:220:THR:HG22	1.88	0.54
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.89	0.54
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.70	0.54
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.89	0.54
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.22	0.54
20:Z:21:ILE:O	20:Z:25:VAL:HG22	2.07	0.54
1:A:64:ARG:NH1	13:O:98:THR:HG21	2.22	0.54
3:C:155:ASN:O	3:C:158:THR:HG22	2.07	0.54
20:Z:35:ARG:O	20:Z:38:GLN:HB3	2.07	0.54
4:D:86:GLY:O	4:D:166:SER:HB2	2.08	0.54
15:U:100:ARG:O	15:U:103:GLN:HB3	2.07	0.54
3:C:425:TRP:CE2	24:C:477:CLA:HBA1	2.42	0.54
3:C:239:TRP:CE3	3:C:243:ILE:HD11	2.42	0.54
4:D:18:LEU:HD22	18:X:38:ILE:HD13	1.89	0.54
2:B:235:GLU:O	2:B:235:GLU:HG2	2.08	0.54
13:O:227:VAL:HG12	13:O:228:ALA:N	2.22	0.54
13:O:141:ARG:HH11	13:O:141:ARG:HG2	1.71	0.54
2:B:150:CYS:HA	24:B:513:CLA:HBC2	1.89	0.54
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	1.89	0.54
13:O:86:ARG:C	13:O:86:ARG:HH11	2.11	0.54
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.90	0.54
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.07	0.54
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.88	0.54
2:B:487:SER:N	2:B:488:PRO:HD2	2.23	0.54
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.07	0.54
3:C:155:ASN:HA	3:C:158:THR:CG2	2.38	0.54
13:O:154:SER:O	13:O:168:PHE:HA	2.07	0.54
30:A:375:DGD:HD3	34:O:274:LMT:H32	1.89	0.54
7:H:12:ARG:N	7:H:13:PRO:HD2	2.23	0.54
16:V:35:THR:HG23	16:V:46:THR:OG1	2.08	0.54
33:D:360:LMG:H111	11:L:19:LEU:HD21	1.88	0.54
20:Z:32:ASP:CG	20:Z:33:TRP:N	2.60	0.54
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.90	0.54
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.73	0.53
20:Z:36:SER:OG	20:Z:39:LEU:HD12	2.07	0.53
3:C:30:SER:OG	4:D:233:ARG:NH2	2.40	0.53
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.37	0.53
16:V:116:GLU:O	16:V:116:GLU:HG3	2.08	0.53
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.90	0.53
12:M:25:LEU:O	12:M:28:GLN:HG3	2.08	0.53
3:C:453:ALA:O	8:I:34:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:42:LEU:CD1	24:C:484:CLA:HMA3	2.37	0.53
4:D:279:LEU:HD11	24:D:354:CLA:O1A	2.09	0.53
3:C:118:HIS:CE1	33:C:493:LMG:H192	2.43	0.53
13:O:83:LYS:HG2	13:O:84:ASN:N	2.19	0.53
2:B:434:THR:HG23	13:O:204:LYS:HE3	1.91	0.53
4:D:180:ARG:HG3	4:D:180:ARG:NH1	2.23	0.53
3:C:473:ASP:HB2	14:T:26:PRO:CB	2.33	0.53
3:C:36:TRP:O	24:C:481:CLA:H11	2.08	0.53
4:D:239:GLN:O	4:D:240:ALA:CB	2.55	0.53
3:C:174:LEU:HG	24:C:485:CLA:H92	1.90	0.53
1:A:143:ILE:HD11	4:D:217:THR:HA	1.89	0.53
13:O:178:ARG:NH1	13:O:178:ARG:CG	2.55	0.53
30:C:490:DGD:HB62	29:J:115:BCR:H352	1.91	0.53
15:U:66:ILE:CG2	15:U:66:ILE:O	2.56	0.53
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.91	0.53
9:J:15:THR:O	9:J:19:MET:HG3	2.08	0.53
10:K:37:PHE:HB3	29:K:112:BCR:C40	2.39	0.53
24:C:474:CLA:H42	24:C:475:CLA:HMD1	1.90	0.53
4:D:238:THR:O	4:D:239:GLN:O	2.27	0.53
24:B:518:CLA:H12	4:D:127:LEU:HD21	1.91	0.53
6:F:21:VAL:O	6:F:25:THR:HG23	2.09	0.53
29:A:369:BCR:H312	8:I:15:PHE:CE1	2.44	0.53
20:Z:30:PRO:C	20:Z:32:ASP:H	2.12	0.52
3:C:391:ARG:CB	3:C:391:ARG:HH11	2.19	0.52
7:H:55:LEU:O	7:H:58:VAL:HG12	2.09	0.52
15:U:100:ARG:HH11	15:U:103:GLN:HG2	1.73	0.52
2:B:341:LYS:HD2	2:B:429:ILE:HG22	1.90	0.52
3:C:60:ILE:HG23	24:C:483:CLA:HMC2	1.91	0.52
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.91	0.52
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.91	0.52
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.90	0.52
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.09	0.52
1:A:49:VAL:O	1:A:53:ILE:HG13	2.10	0.52
4:D:334:GLN:N	4:D:335:PRO:HD3	2.24	0.52
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.90	0.52
6:F:18:VAL:HG13	6:F:19:ARG:N	2.25	0.52
15:U:66:ILE:HG13	15:U:72:TYR:CD1	2.44	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.90	0.52
3:C:33:PHE:CE1	4:D:229:ALA:CB	2.92	0.52
3:C:429:SER:HB3	30:C:490:DGD:HA81	1.91	0.52
13:O:141:ARG:HG2	13:O:141:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:452:ALA:O	3:C:454:GLY:N	2.42	0.52
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.90	0.52
1:A:326:LEU:HD21	3:C:412:THR:HB	1.91	0.52
16:V:135:GLU:O	16:V:139:VAL:HG23	2.08	0.52
2:B:10:THR:C	2:B:12:LEU:H	2.12	0.52
3:C:163:PHE:CD1	24:C:485:CLA:HAB	2.45	0.52
4:D:85:MET:HE2	5:E:69:ARG:HA	1.90	0.52
10:K:24:VAL:O	10:K:27:VAL:HG12	2.10	0.52
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.52
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.10	0.52
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.92	0.52
3:C:337:LEU:CD1	13:O:131:PRO:HG3	2.39	0.52
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.45	0.52
24:B:514:CLA:H101	24:B:525:CLA:H42	1.91	0.52
10:K:43:VAL:O	10:K:43:VAL:HG13	2.09	0.52
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.40	0.52
16:V:147:VAL:O	16:V:150:LYS:HB2	2.10	0.52
1:A:78:ILE:O	1:A:176:ILE:HB	2.10	0.52
20:Z:32:ASP:C	20:Z:34:ASP:N	2.60	0.52
3:C:415:ASN:O	3:C:416:SER:CB	2.57	0.52
1:A:322:ASN:OD1	3:C:412:THR:HA	2.09	0.52
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.75	0.52
3:C:193:GLY:O	3:C:194:GLY:C	2.49	0.52
3:C:47:GLY:O	3:C:50:LEU:HB3	2.10	0.52
20:Z:17:PHE:CE2	20:Z:21:ILE:HD11	2.45	0.52
18:X:17:LYS:O	18:X:21:ILE:HG13	2.10	0.52
4:D:266:TRP:HD1	33:D:360:LMG:HC3	1.74	0.52
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.91	0.52
2:B:224:ARG:NE	7:H:25:TRP:NE1	2.58	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.92	0.52
24:B:513:CLA:H193	7:H:42:LEU:HD12	1.92	0.51
1:A:227:THR:HA	1:A:231:GLU:OE2	2.10	0.51
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.40	0.51
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.01	0.51
3:C:418:ASN:HD21	30:C:490:DGD:HD4	1.74	0.51
31:A:374:LHG:H162	29:J:115:BCR:H313	1.91	0.51
1:A:43:ALA:HB1	29:A:369:BCR:H362	1.92	0.51
20:Z:3:ILE:O	20:Z:7:LEU:HG	2.09	0.51
3:C:239:TRP:HE3	3:C:243:ILE:HD11	1.74	0.51
4:D:76:VAL:O	4:D:77:ALA:HB2	2.10	0.51
4:D:85:MET:CE	5:E:69:ARG:HA	2.41	0.51
1:A:228:THR:HG22	1:A:229:GLU:N	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.07	0.51
4:D:221:THR:HG23	4:D:221:THR:O	2.10	0.51
20:Z:31:GLN:O	20:Z:32:ASP:HB3	2.10	0.51
20:Z:32:ASP:OD1	20:Z:36:SER:HB2	2.11	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.45	0.51
13:O:271:PRO:HG2	13:O:272:ALA:H	1.76	0.51
2:B:293:ALA:C	2:B:295:GLY:H	2.14	0.51
2:B:229:LEU:O	2:B:231:MET:N	2.43	0.51
3:C:250:TRP:CD1	3:C:250:TRP:C	2.84	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
4:D:136:VAL:O	4:D:136:VAL:HG12	2.10	0.51
2:B:12:LEU:CD2	2:B:18:ARG:HB2	2.40	0.51
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.76	0.51
2:B:125:ASP:OD2	2:B:127:ARG:HB3	2.11	0.51
3:C:117:VAL:HG12	33:C:493:LMG:H191	1.92	0.51
2:B:36:SER:HB2	29:B:528:BCR:C40	2.40	0.51
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.40	0.51
24:B:520:CLA:H12	24:B:520:CLA:H112	1.93	0.51
24:C:486:CLA:HMC2	29:Z:116:BCR:H372	1.93	0.51
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.92	0.51
4:D:86:GLY:HA2	4:D:166:SER:HB3	1.93	0.51
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.46	0.51
13:O:240:THR:HA	13:O:264:VAL:HA	1.91	0.51
34:B:536:LMT:H102	7:H:35:MET:SD	2.51	0.51
18:X:16:LEU:HD13	18:X:16:LEU:C	2.31	0.51
18:X:12:ILE:CG1	18:X:16:LEU:HD12	2.33	0.51
13:O:118:SER:HB3	13:O:157:PRO:HA	1.93	0.51
6:F:16:PHE:CD2	32:F:224:SQD:H262	2.46	0.51
1:A:29:TYR:OH	1:A:132:GLU:OE2	2.25	0.51
2:B:12:LEU:HB2	24:B:522:CLA:HMC2	1.93	0.51
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.46	0.51
15:U:83:ALA:CB	15:U:84:PRO:CD	2.77	0.50
3:C:116:VAL:HG21	29:Z:116:BCR:H323	1.92	0.50
2:B:183:PRO:HB2	2:B:185:TRP:CH2	2.46	0.50
8:I:27:ASP:N	8:I:28:PRO:CD	2.74	0.50
10:K:17:ILE:H	10:K:17:ILE:CD1	2.24	0.50
3:C:158:THR:HG21	3:C:254:THR:O	2.10	0.50
3:C:116:VAL:CG2	29:Z:116:BCR:H323	2.41	0.50
4:D:346:LEU:O	4:D:348:ARG:HG3	2.10	0.50
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.41	0.50
20:Z:5:PHE:HA	20:Z:57:LEU:CD2	2.40	0.50
18:X:12:ILE:O	18:X:12:ILE:CG2	2.58	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:167:VAL:HG12	24:C:485:CLA:H2	1.94	0.50
1:A:283:VAL:O	1:A:286:THR:HG22	2.11	0.50
13:O:86:ARG:HH11	13:O:87:GLN:HA	1.75	0.50
13:O:223:ILE:HG12	13:O:224:SER:N	2.27	0.50
10:K:25:LEU:HB2	10:K:26:PRO:HD3	1.93	0.50
15:U:72:TYR:O	15:U:73:PRO:C	2.48	0.50
24:C:477:CLA:H202	30:C:491:DGD:HAF2	1.94	0.50
3:C:159:THR:HG23	3:C:252:ILE:HD13	1.93	0.50
4:D:53:THR:HG22	4:D:67:TYR:CE2	2.47	0.50
2:B:134:ASP:OD2	2:B:137:LYS:HB2	2.11	0.50
24:B:515:CLA:HBB1	24:B:516:CLA:H51	1.92	0.50
32:A:372:SQD:H223	30:C:491:DGD:HAE1	1.92	0.50
3:C:418:ASN:HB2	30:C:491:DGD:HE2	1.92	0.50
24:B:517:CLA:H42	33:B:533:LMG:H131	1.92	0.50
3:C:81:MET:CE	3:C:89:ILE:HG22	2.42	0.50
20:Z:5:PHE:CE1	20:Z:54:VAL:HG13	2.46	0.50
5:E:34:GLY:HA2	6:F:32:PHE:CE1	2.46	0.50
20:Z:12:LEU:HB2	20:Z:50:LEU:HD22	1.93	0.50
24:B:522:CLA:H171	24:B:523:CLA:HBB2	1.94	0.50
24:B:519:CLA:HMC2	29:H:107:BCR:H343	1.92	0.50
24:A:363:CLA:HED2	4:D:198:MET:SD	2.51	0.50
2:B:9:HIS:HB2	24:B:521:CLA:HBA1	1.93	0.50
33:I:220:LMG:H181	34:I:230:LMT:H42	1.94	0.50
20:Z:47:TRP:O	20:Z:50:LEU:HB2	2.11	0.50
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.50
24:C:478:CLA:HMD1	24:C:480:CLA:HAB	1.92	0.50
3:C:117:VAL:CG1	33:C:493:LMG:H191	2.41	0.50
3:C:89:ILE:N	3:C:90:PRO:CD	2.75	0.50
1:A:20:TRP:O	1:A:21:VAL:C	2.50	0.50
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.11	0.50
13:O:59:ASP:HB3	13:O:62:GLN:HB3	1.93	0.50
2:B:55:MET:CE	2:B:80:ILE:HD12	2.42	0.50
24:B:526:CLA:H43	32:B:532:SQD:H2	1.94	0.50
5:E:81:GLU:C	5:E:83:LEU:N	2.64	0.50
2:B:286:ARG:NH1	2:B:286:ARG:HG2	2.26	0.50
16:V:95:ILE:O	16:V:99:VAL:HG23	2.12	0.50
2:B:141:ILE:HG23	24:B:525:CLA:HBB1	1.92	0.50
3:C:269:GLU:OE1	24:C:481:CLA:HED1	2.12	0.50
3:C:265:ILE:HG12	24:C:478:CLA:HED1	1.94	0.50
33:I:220:LMG:HC2	34:O:274:LMT:H11	1.93	0.50
1:A:235:TYR:C	1:A:237:TYR:H	2.16	0.50
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.12	0.49
6:F:11:VAL:CG1	6:F:12:SER:H	2.25	0.49
1:A:107:TYR:CD1	13:O:141:ARG:NH1	2.80	0.49
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.47	0.49
9:J:18:GLY:HA3	29:K:112:BCR:H371	1.93	0.49
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.78	0.49
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.38	0.49
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.47	0.49
3:C:315:MET:O	3:C:319:ILE:HG13	2.12	0.49
18:X:42:GLN:O	18:X:43:ILE:HG13	2.12	0.49
3:C:137:PRO:HB2	3:C:139:THR:O	2.12	0.49
4:D:350:ASN:O	4:D:352:LEU:N	2.42	0.49
3:C:72:LEU:HD11	3:C:108:THR:HB	1.93	0.49
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.36	0.49
2:B:462:PHE:CZ	24:B:523:CLA:HMB3	2.47	0.49
3:C:135:ARG:HE	20:Z:33:TRP:HE1	1.59	0.49
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.93	0.49
16:V:29:LEU:HD11	16:V:34:LEU:HD21	1.92	0.49
1:A:224:ILE:O	1:A:226:GLU:OE2	2.30	0.49
3:C:275:SER:HB3	24:C:482:CLA:HED3	1.94	0.49
6:F:23:VAL:O	6:F:27:ALA:CB	2.60	0.49
7:H:35:MET:HE2	29:H:107:BCR:H322	1.93	0.49
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.95	0.49
11:L:12:LEU:HD22	12:M:25:LEU:HD12	1.93	0.49
29:C:487:BCR:H391	10:K:36:ALA:HB2	1.95	0.49
24:B:518:CLA:H151	24:B:519:CLA:H203	1.93	0.49
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.94	0.49
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.93	0.49
13:O:59:ASP:C	13:O:61:SER:H	2.14	0.49
24:B:518:CLA:H51	24:B:519:CLA:H101	1.94	0.49
3:C:413:GLU:HG3	3:C:414:ILE:N	2.28	0.49
13:O:43:ASN:OD1	13:O:103:SER:HB2	2.12	0.49
18:X:43:ILE:O	18:X:43:ILE:HG22	2.12	0.49
2:B:137:LYS:O	2:B:141:ILE:HG13	2.11	0.49
24:D:356:CLA:C4	18:X:26:GLY:HA3	2.34	0.49
3:C:405:ASN:HD22	30:C:491:DGD:C5D	2.25	0.49
27:A:367:PL9:H301	4:D:42:TYR:HA	1.94	0.49
3:C:126:GLY:O	3:C:130:VAL:HG23	2.12	0.49
3:C:154:LYS:HE2	3:C:261:ARG:HD2	1.94	0.49
3:C:155:ASN:CA	3:C:158:THR:HG22	2.39	0.49
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.34	0.49
3:C:135:ARG:HB2	20:Z:27:TYR:CG	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:HIS:O	1:A:298:ASN:HB3	2.13	0.49
13:O:126:GLY:O	13:O:128:ASP:N	2.45	0.49
1:A:300:PHE:CZ	3:C:404:LEU:HD23	2.48	0.49
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.12	0.49
3:C:346:THR:O	13:O:40:GLY:HA2	2.13	0.49
3:C:447:ARG:CG	3:C:447:ARG:NH1	2.74	0.49
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.49
16:V:45:ILE:HG12	16:V:46:THR:N	2.28	0.49
2:B:55:MET:HE2	2:B:80:ILE:HD12	1.94	0.49
5:E:9:PRO:HB3	33:E:218:LMG:HC4	1.95	0.49
9:J:11:TRP:CG	10:K:42:ALA:HA	2.48	0.49
2:B:69:LEU:HD21	24:B:513:CLA:HED3	1.95	0.49
3:C:405:ASN:HB2	30:C:491:DGD:HG31	1.95	0.49
24:A:363:CLA:HED1	27:D:357:PL9:H372	1.95	0.49
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.49
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.43	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
3:C:347:GLY:HA3	13:O:43:ASN:HB2	1.95	0.49
10:K:15:TYR:HE2	20:Z:62:VAL:HG21	1.78	0.49
2:B:69:LEU:HD12	24:B:515:CLA:HBA1	1.95	0.48
13:O:94:THR:HB	13:O:135:GLN:O	2.12	0.48
7:H:30:LEU:HD11	7:H:34:PHE:HE1	1.78	0.48
34:B:536:LMT:H3'	32:D:361:SQD:H62	1.95	0.48
24:A:362:CLA:H202	24:A:363:CLA:H93	1.96	0.48
13:O:159:VAL:O	13:O:159:VAL:HG13	2.12	0.48
20:Z:5:PHE:HA	20:Z:57:LEU:HD21	1.95	0.48
29:B:527:BCR:HC31	12:M:10:ALA:HB2	1.94	0.48
2:B:35:GLY:O	2:B:38:ALA:HB3	2.13	0.48
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.35	0.48
4:D:134:ARG:HA	4:D:134:ARG:HE	1.78	0.48
7:H:35:MET:HE2	29:H:107:BCR:C32	2.44	0.48
5:E:28:PRO:O	5:E:32:ILE:HG13	2.13	0.48
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.48	0.48
4:D:201:VAL:O	4:D:205:LEU:HB2	2.13	0.48
2:B:175:THR:O	2:B:176:GLY:O	2.31	0.48
3:C:425:TRP:CZ2	24:C:477:CLA:HBA1	2.48	0.48
24:C:477:CLA:H151	30:C:490:DGD:HBW1	1.95	0.48
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.96	0.48
3:C:413:GLU:HG3	3:C:414:ILE:H	1.79	0.48
2:B:256:MET:O	2:B:448:ARG:NH1	2.42	0.48
1:A:221:SER:HB2	4:D:139:ARG:O	2.13	0.48
13:O:226:ASN:N	13:O:226:ASN:HD22	2.11	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:154:GLY:O	2:B:159:THR:HG23	2.13	0.48
4:D:193:LEU:HG	4:D:193:LEU:O	2.14	0.48
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.44	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.31	0.48
26:V:164:HEM:HAD2	26:V:164:HEM:HHA	1.61	0.48
24:C:477:CLA:HED1	33:C:492:LMG:O3	2.13	0.48
4:D:62:GLY:HA3	5:E:63:ILE:HD13	1.96	0.48
3:C:71:GLU:OE1	3:C:89:ILE:HG13	2.13	0.48
29:A:369:BCR:H312	8:I:15:PHE:HE1	1.79	0.48
10:K:20:PRO:O	10:K:23:ASP:HB2	2.13	0.48
13:O:86:ARG:O	13:O:86:ARG:NH1	2.37	0.48
4:D:337:GLU:O	4:D:338:ASN:C	2.51	0.48
2:B:137:LYS:HZ1	7:H:17:GLU:H	1.61	0.48
2:B:224:ARG:HG3	7:H:25:TRP:CD1	2.48	0.48
3:C:315:MET:CE	3:C:366:LEU:HD13	2.44	0.48
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.95	0.48
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.94	0.48
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.95	0.48
2:B:172:TYR:O	2:B:173:GLY:C	2.52	0.48
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.49	0.48
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.49	0.48
24:C:476:CLA:H172	24:C:483:CLA:HBB2	1.95	0.48
1:A:13:LEU:CD1	1:A:13:LEU:H	2.27	0.48
2:B:434:THR:CG2	13:O:204:LYS:HE3	2.44	0.48
13:O:225:LEU:C	13:O:226:ASN:HD22	2.17	0.48
11:L:24:ILE:HD12	11:L:24:ILE:N	2.29	0.48
1:A:114:LEU:HD23	1:A:114:LEU:C	2.34	0.48
4:D:126:MET:CE	4:D:150:ILE:HG13	2.43	0.48
20:Z:32:ASP:C	20:Z:34:ASP:H	2.17	0.48
2:B:329:PRO:CB	24:B:517:CLA:HED1	2.39	0.48
4:D:87:HIS:ND1	30:H:208:DGD:HD2	2.29	0.48
1:A:111:PRO:O	1:A:115:ILE:HG13	2.14	0.48
3:C:116:VAL:HG23	3:C:117:VAL:N	2.28	0.47
1:A:215:HIS:O	1:A:216:GLY:C	2.53	0.47
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.14	0.47
13:O:36:ILE:N	13:O:36:ILE:HD12	2.29	0.47
18:X:32:LEU:O	18:X:36:VAL:HG23	2.13	0.47
5:E:8:ARG:HB2	6:F:13:TYR:HB3	1.95	0.47
5:E:22:ILE:O	5:E:26:THR:HG23	2.14	0.47
2:B:246:PHE:CD1	2:B:246:PHE:C	2.88	0.47
31:A:371:LHG:HC12	24:C:481:CLA:O1D	2.13	0.47
2:B:265:ILE:HG13	2:B:266:GLU:N	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.47	0.47
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.49	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.47	0.47
19:Y:11:UNK:C	19:Y:13:UNK:N	2.75	0.47
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.96	0.47
2:B:124:ARG:NH1	2:B:124:ARG:HG3	2.26	0.47
1:A:10:SER:C	1:A:12:ASN:H	2.16	0.47
1:A:12:ASN:O	1:A:16:ARG:HG3	2.15	0.47
20:Z:5:PHE:HE1	20:Z:54:VAL:HG13	1.80	0.47
5:E:9:PRO:O	5:E:10:PHE:C	2.53	0.47
14:T:23:PHE:CD1	32:T:213:SQD:H45	2.49	0.47
1:A:124:SER:O	1:A:127:MET:HB3	2.15	0.47
2:B:141:ILE:HG21	24:B:525:CLA:HBB1	1.97	0.47
6:F:23:VAL:O	6:F:27:ALA:HB2	2.14	0.47
20:Z:29:SER:C	20:Z:31:GLN:H	2.17	0.47
3:C:135:ARG:NE	20:Z:33:TRP:HE1	2.12	0.47
8:I:30:ARG:O	8:I:31:ASN:HB3	2.14	0.47
2:B:458:PHE:HB3	24:B:514:CLA:HBC2	1.97	0.47
3:C:250:TRP:HE1	24:C:479:CLA:HED1	1.80	0.47
2:B:124:ARG:HD3	2:B:131:PRO:N	2.30	0.47
1:A:206:PHE:CE2	24:D:354:CLA:HBA1	2.50	0.47
2:B:7:ARG:NH2	33:B:531:LMG:O3	2.46	0.47
3:C:94:THR:HG22	3:C:298:PRO:HD2	1.96	0.47
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.15	0.47
16:V:148:GLU:HA	16:V:148:GLU:OE1	2.15	0.47
15:U:56:ASP:HB3	15:U:60:THR:H	1.80	0.47
24:B:515:CLA:HMA1	24:B:516:CLA:HBA2	1.96	0.47
32:A:372:SQD:H5	4:D:232:PHE:HB3	1.96	0.47
4:D:49:LEU:HD13	29:D:358:BCR:C15	2.45	0.47
1:A:190:HIS:HB3	1:A:293:MET:CE	2.43	0.47
5:E:4:THR:CG2	5:E:5:THR:N	2.77	0.47
3:C:27:ASP:OD1	3:C:28:GLN:HG2	2.14	0.47
24:B:517:CLA:H193	11:L:27:LEU:HD11	1.95	0.47
3:C:365:TRP:CB	3:C:391:ARG:HG2	2.45	0.47
5:E:15:THR:O	9:J:8:ILE:HD12	2.15	0.47
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.47
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.27	0.47
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.44	0.47
3:C:56:HIS:C	3:C:58:GLY:N	2.68	0.47
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.49	0.47
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.45	0.47
4:D:261:PHE:O	4:D:262:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:274:VAL:HG13	27:D:357:PL9:H211	1.97	0.47
1:A:306:VAL:HG11	1:A:316:THR:HG23	1.96	0.47
3:C:193:GLY:O	3:C:194:GLY:O	2.33	0.47
4:D:93:TRP:HA	4:D:99:GLY:H	1.80	0.47
3:C:53:HIS:HB3	24:C:485:CLA:OBD	2.15	0.46
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.43	0.46
4:D:14:TRP:CE3	18:X:38:ILE:HD12	2.50	0.46
1:A:32:TRP:HE3	1:A:32:TRP:HA	1.76	0.46
5:E:8:ARG:HB2	6:F:13:TYR:CB	2.45	0.46
13:O:135:GLN:HG2	13:O:141:ARG:HG3	1.97	0.46
3:C:258:GLY:CA	3:C:262:ARG:HH12	2.28	0.46
24:B:516:CLA:H72	29:B:530:BCR:H311	1.97	0.46
2:B:216:HIS:HE1	24:B:519:CLA:C1A	2.29	0.46
13:O:83:LYS:CG	13:O:84:ASN:H	2.23	0.46
4:D:60:THR:HG23	4:D:61:HIS:HD2	1.75	0.46
3:C:328:VAL:HG23	3:C:329:GLY:N	2.31	0.46
3:C:452:ALA:C	3:C:454:GLY:N	2.68	0.46
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.46	0.46
16:V:68:VAL:O	16:V:68:VAL:HG13	2.15	0.46
2:B:462:PHE:CE1	24:B:523:CLA:HMB3	2.50	0.46
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.46
31:A:374:LHG:H151	30:C:490:DGD:HBV1	1.98	0.46
4:D:146:PHE:O	4:D:150:ILE:HG12	2.14	0.46
20:Z:36:SER:C	20:Z:38:GLN:N	2.69	0.46
1:A:214:MET:O	1:A:215:HIS:C	2.54	0.46
30:A:375:DGD:HD5	30:A:375:DGD:HE1	1.66	0.46
1:A:334:ARG:NH1	13:O:184:ASP:C	2.69	0.46
10:K:35:LEU:HA	10:K:38:VAL:HG23	1.96	0.46
1:A:239:PHE:O	14:T:29:ILE:HA	2.14	0.46
1:A:283:VAL:HG21	25:A:365:PHO:HBC3	1.97	0.46
7:H:25:TRP:O	7:H:26:GLY:C	2.53	0.46
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.98	0.46
13:O:113:VAL:HA	13:O:119:LEU:HD23	1.97	0.46
2:B:10:THR:O	2:B:13:ILE:HG13	2.16	0.46
20:Z:35:ARG:HG3	20:Z:36:SER:N	2.30	0.46
1:A:216:GLY:O	1:A:220:THR:HG22	2.16	0.46
5:E:17:VAL:HG22	9:J:8:ILE:HD11	1.97	0.46
3:C:258:GLY:HA3	3:C:262:ARG:HH12	1.81	0.46
3:C:34:ALA:HB2	4:D:230:SER:CB	2.46	0.46
2:B:96:VAL:HG22	24:B:516:CLA:HBA1	1.97	0.46
2:B:229:LEU:O	2:B:230:ARG:C	2.54	0.46
4:D:217:THR:O	4:D:221:THR:HB	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:59:GLY:HA3	24:B:517:CLA:HED1	1.98	0.46
20:Z:23:VAL:HB	20:Z:24:PRO:HD3	1.97	0.46
12:M:18:PRO:O	12:M:21:PHE:HB3	2.16	0.46
8:I:24:LEU:O	8:I:26:GLY:N	2.41	0.46
10:K:37:PHE:HB3	29:K:112:BCR:H402	1.97	0.46
1:A:40:THR:HG23	24:A:366:CLA:HBB1	1.98	0.46
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
1:A:330:VAL:HG11	4:D:348:ARG:HG2	1.98	0.46
24:C:482:CLA:HBD	24:C:482:CLA:H121	1.97	0.46
16:V:54:GLU:HA	16:V:54:GLU:OE1	2.16	0.46
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.98	0.46
2:B:329:PRO:HD3	24:B:517:CLA:CED	2.46	0.46
2:B:444:ARG:HH11	2:B:444:ARG:HG3	1.81	0.46
14:T:23:PHE:HD1	32:T:213:SQD:H45	1.81	0.46
24:B:518:CLA:H92	32:D:361:SQD:H172	1.97	0.45
1:A:214:MET:CE	4:D:142:ASN:ND2	2.79	0.45
13:O:86:ARG:HD2	13:O:87:GLN:N	2.31	0.45
1:A:262:TYR:O	33:E:218:LMG:H112	2.16	0.45
3:C:114:VAL:HG13	24:C:476:CLA:HMA3	1.97	0.45
2:B:450:TRP:NE1	24:B:517:CLA:HBA1	2.32	0.45
7:H:21:VAL:HG23	7:H:22:ALA:O	2.16	0.45
3:C:318:LEU:O	3:C:318:LEU:HD23	2.16	0.45
3:C:210:PHE:HZ	3:C:243:ILE:HD11	1.81	0.45
3:C:49:LEU:O	3:C:53:HIS:ND1	2.43	0.45
1:A:10:SER:C	1:A:12:ASN:N	2.69	0.45
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.99	0.45
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.51	0.45
2:B:241:SER:HB3	24:B:522:CLA:HED3	1.97	0.45
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.42	0.45
29:J:115:BCR:H361	29:J:115:BCR:H20C	1.83	0.45
1:A:45:THR:HG23	1:A:46:ILE:N	2.31	0.45
33:D:360:LMG:O10	11:L:18:TYR:HB3	2.16	0.45
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.45
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.52	0.45
5:E:7:GLU:HB3	6:F:19:ARG:CZ	2.47	0.45
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.45	0.45
4:D:213:ILE:HG23	4:D:214:HIS:N	2.30	0.45
15:U:100:ARG:NH1	15:U:103:GLN:HG2	2.31	0.45
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.97	0.45
5:E:10:PHE:HB2	33:E:218:LMG:O2	2.16	0.45
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.45
3:C:284:PHE:HB3	30:C:489:DGD:HA51	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.51	0.45
1:A:202:VAL:O	1:A:206:PHE:HB2	2.17	0.45
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.17	0.45
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.45
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.31	0.45
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.99	0.45
13:O:56:TYR:O	13:O:161:SER:HA	2.17	0.45
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.45
7:H:9:ASP:O	7:H:12:ARG:HB3	2.17	0.45
1:A:317:TRP:HZ3	4:D:180:ARG:CD	2.19	0.45
1:A:258:LEU:O	4:D:128:ARG:NH1	2.49	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.98	0.45
4:D:19:ASP:O	4:D:20:ASP:C	2.55	0.45
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
4:D:36:LEU:C	4:D:39:PRO:HD2	2.37	0.45
3:C:176:VAL:HG11	3:C:238:ILE:HG12	1.99	0.45
1:A:72:LEU:HD21	34:T:227:LMT:H31	1.99	0.45
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.79	0.45
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.34	0.45
2:B:474:LEU:HD11	24:B:518:CLA:HAA1	1.98	0.45
3:C:245:ILE:O	3:C:249:ILE:HG12	2.16	0.45
24:B:517:CLA:H3A	24:B:517:CLA:HBA2	1.68	0.45
15:U:80:VAL:HG22	15:U:127:ARG:HH21	1.82	0.45
5:E:51:ARG:O	5:E:53:ASP:N	2.49	0.45
3:C:457:LYS:HE3	4:D:228:GLY:O	2.17	0.45
4:D:303:ILE:HD13	12:M:2:GLU:HG2	1.97	0.45
2:B:141:ILE:O	2:B:144:PHE:HB3	2.17	0.45
13:O:120:THR:HG22	13:O:154:SER:CB	2.47	0.45
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.52	0.45
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.99	0.45
2:B:169:SER:O	7:H:65:LEU:HG	2.16	0.45
3:C:435:PHE:O	3:C:438:LEU:N	2.49	0.45
16:V:63:CYS:O	16:V:64:ALA:C	2.55	0.44
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.44
3:C:110:PRO:O	3:C:114:VAL:HG23	2.17	0.44
1:A:183:MET:HG2	24:A:363:CLA:HBC1	1.98	0.44
5:E:64:PRO:HD3	5:E:84:LYS:HE2	1.98	0.44
30:A:375:DGD:HA21	34:O:274:LMT:H121	1.98	0.44
24:C:478:CLA:H42	29:C:488:BCR:H342	1.99	0.44
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.99	0.44
2:B:191:ASN:HB2	7:H:58:VAL:HG22	1.98	0.44
3:C:452:ALA:O	3:C:453:ALA:C	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:39:ASN:HD21	16:V:43:LYS:HB3	1.82	0.44
13:O:173:ASN:ND2	13:O:220:LYS:HD3	2.32	0.44
8:I:4:LEU:O	8:I:8:VAL:HG23	2.17	0.44
3:C:276:LEU:CD1	3:C:444:HIS:HD2	2.30	0.44
3:C:425:TRP:HE1	30:C:490:DGD:HE62	1.81	0.44
33:C:492:LMG:H172	10:K:27:VAL:HG11	1.99	0.44
18:X:16:LEU:HD11	18:X:20:PHE:CE2	2.53	0.44
3:C:170:ILE:HD13	24:C:486:CLA:H201	1.98	0.44
24:A:362:CLA:HBB1	24:D:354:CLA:NC	2.32	0.44
13:O:218:LEU:HD22	15:U:119:THR:CG2	2.45	0.44
13:O:86:ARG:O	13:O:86:ARG:HG3	2.18	0.44
18:X:44:ASP:O	18:X:45:LYS:HB3	2.17	0.44
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.98	0.44
13:O:72:GLN:O	13:O:263:GLY:HA3	2.17	0.44
1:A:243:GLU:CD	1:A:243:GLU:H	2.16	0.44
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.17	0.44
3:C:33:PHE:CE1	4:D:229:ALA:HB3	2.53	0.44
24:B:524:CLA:H51	29:B:527:BCR:H372	1.99	0.44
2:B:15:ASP:O	2:B:17:GLY:N	2.50	0.44
2:B:71:VAL:HG21	2:B:96:VAL:CG2	2.47	0.44
3:C:449:ARG:NE	24:C:478:CLA:HED1	2.22	0.44
3:C:243:ILE:O	24:C:479:CLA:HMC1	2.18	0.44
3:C:235:GLY:O	3:C:238:ILE:HB	2.18	0.44
8:I:11:VAL:HG22	34:I:230:LMT:H82	2.00	0.44
13:O:116:ASP:OD1	13:O:157:PRO:HB3	2.18	0.44
7:H:28:THR:O	7:H:31:MET:HB3	2.18	0.44
1:A:296:ASN:HB2	3:C:400:PRO:O	2.17	0.44
3:C:363:GLY:O	3:C:364:PRO:C	2.56	0.44
16:V:59:PHE:CD1	16:V:63:CYS:SG	3.08	0.44
13:O:230:VAL:CG1	13:O:231:ASP:N	2.70	0.44
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.52	0.44
2:B:271:THR:CG2	2:B:273:TYR:HB2	2.48	0.44
31:A:374:LHG:H271	31:A:374:LHG:H101	2.00	0.44
29:J:115:BCR:H24C	29:J:115:BCR:H371	1.79	0.44
3:C:163:PHE:CD1	3:C:252:ILE:HD11	2.52	0.44
4:D:209:LEU:O	4:D:213:ILE:HG22	2.18	0.44
6:F:16:PHE:O	32:F:224:SQD:H461	2.18	0.44
2:B:25:MET:HE2	29:B:527:BCR:H393	1.98	0.44
2:B:435:GLU:O	2:B:436:THR:C	2.56	0.44
3:C:55:ALA:HB1	29:C:487:BCR:C37	2.46	0.44
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.45	0.44
1:A:107:TYR:HD1	13:O:141:ARG:NH1	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:C:487:BCR:H11C	29:K:112:BCR:H322	2.00	0.44
1:A:42:LEU:HA	1:A:45:THR:HG22	2.00	0.44
2:B:185:TRP:CE3	24:B:511:CLA:H61	2.53	0.44
3:C:143:TYR:O	3:C:144:SER:CB	2.64	0.44
2:B:263:THR:HB	2:B:448:ARG:HH12	1.82	0.44
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.44
2:B:422:ARG:HG2	2:B:422:ARG:HH11	1.81	0.44
2:B:206:GLY:O	2:B:210:ILE:HG13	2.18	0.44
4:D:253:TRP:HB2	4:D:260:ALA:HB2	2.00	0.44
1:A:64:ARG:O	13:O:178:ARG:NH2	2.51	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:208:VAL:O	3:C:209:ILE:C	2.56	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.18	0.44
16:V:81:ARG:HH11	16:V:81:ARG:HG2	1.83	0.44
3:C:82:TYR:HA	3:C:422:PRO:HG2	2.00	0.44
1:A:247:ASN:HB3	1:A:250:ALA:HB3	2.00	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.75	0.44
10:K:17:ILE:C	10:K:18:PHE:HD2	2.21	0.43
26:E:85:HEM:HBC2	6:F:27:ALA:CB	2.39	0.43
3:C:472:LEU:HD12	3:C:473:ASP:N	2.28	0.43
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.53	0.43
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.86	0.43
7:H:18:TYR:CG	7:H:19:GLY:N	2.85	0.43
20:Z:5:PHE:CG	20:Z:61:VAL:HG21	2.53	0.43
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.43
16:V:64:ALA:O	16:V:65:SER:C	2.56	0.43
29:C:487:BCR:HC22	10:K:18:PHE:HD1	1.83	0.43
1:A:217:SER:O	1:A:220:THR:HG22	2.18	0.43
2:B:484:PRO:O	2:B:485:GLU:HG2	2.18	0.43
18:X:32:LEU:HD23	18:X:32:LEU:H	1.83	0.43
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.00	0.43
4:D:303:ILE:CD1	12:M:2:GLU:HG2	2.48	0.43
2:B:442:ILE:HD11	13:O:200:LEU:HD23	2.00	0.43
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.43
10:K:17:ILE:HG22	10:K:17:ILE:O	2.17	0.43
15:U:54:LYS:HD2	15:U:113:THR:CG2	2.49	0.43
2:B:10:THR:C	2:B:12:LEU:N	2.71	0.43
2:B:229:LEU:HD11	24:B:519:CLA:O1A	2.18	0.43
3:C:362:ARG:H	30:C:489:DGD:HE4	1.83	0.43
4:D:152:VAL:HG12	24:D:354:CLA:H43	2.00	0.43
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.43
5:E:72:ALA:O	5:E:76:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:33:GLN:HG2	12:M:34:LYS:N	2.33	0.43
2:B:164:PRO:HG2	2:B:165:GLY:H	1.82	0.43
15:U:73:PRO:HG2	16:V:107:THR:HB	2.01	0.43
2:B:348:ASN:OD1	2:B:352:GLU:HB2	2.18	0.43
24:B:512:CLA:H122	24:B:512:CLA:H162	1.79	0.43
2:B:86:ILE:C	2:B:86:ILE:HD12	2.38	0.43
5:E:69:ARG:HG3	5:E:70:PHE:N	2.34	0.43
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.43
1:A:60:ILE:HG23	1:A:61:ASP:N	2.32	0.43
3:C:318:LEU:HG	3:C:328:VAL:CG1	2.48	0.43
8:I:6:ILE:CD1	34:I:230:LMT:H5'	2.48	0.43
7:H:63:LYS:C	7:H:65:LEU:N	2.70	0.43
14:T:25:GLU:O	14:T:26:PRO:C	2.54	0.43
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.53	0.43
24:B:517:CLA:CAC	29:B:528:BCR:H393	2.49	0.43
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.82	0.43
10:K:46:ARG:HB2	10:K:46:ARG:NH1	2.34	0.43
1:A:39:PRO:HB2	24:A:366:CLA:CBB	2.48	0.43
2:B:284:ILE:HG23	2:B:305:ILE:CD1	2.48	0.43
33:A:373:LMG:H421	24:B:521:CLA:H142	2.00	0.43
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.43
4:D:154:VAL:O	4:D:158:LEU:HB2	2.18	0.43
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.53	0.43
1:A:198:HIS:O	1:A:202:VAL:HG12	2.18	0.43
20:Z:36:SER:HA	20:Z:39:LEU:CD1	2.48	0.43
1:A:214:MET:HE2	1:A:214:MET:HA	1.97	0.43
1:A:159:LEU:C	1:A:162:PRO:HD2	2.38	0.43
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.01	0.43
3:C:162:GLY:O	3:C:166:ILE:HG13	2.18	0.43
3:C:163:PHE:CG	24:C:485:CLA:HAB	2.54	0.43
1:A:153:SER:HB2	24:A:362:CLA:H43	2.00	0.43
4:D:126:MET:HE3	4:D:150:ILE:HG13	2.00	0.43
4:D:263:ASN:O	4:D:265:ARG:N	2.52	0.43
20:Z:30:PRO:C	20:Z:32:ASP:N	2.72	0.43
29:D:358:BCR:H363	6:F:33:PHE:HB3	2.00	0.43
5:E:20:TRP:CD1	9:J:8:ILE:HD13	2.53	0.43
3:C:460:ASP:O	3:C:461:ARG:C	2.55	0.43
4:D:101:PHE:O	4:D:104:TRP:HB3	2.18	0.43
13:O:171:GLU:HA	13:O:221:GLY:O	2.19	0.43
6:F:24:HIS:HA	6:F:27:ALA:HB3	2.00	0.43
2:B:349:LYS:HG2	2:B:395:GLN:O	2.19	0.43
12:M:31:SER:HA	33:M:217:LMG:HC3	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:39:LEU:HD23	7:H:39:LEU:C	2.39	0.43
13:O:70:CYS:O	13:O:265:PHE:HB2	2.18	0.43
10:K:43:VAL:O	10:K:46:ARG:HG3	2.19	0.43
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
3:C:464:GLU:O	3:C:467:LEU:HB2	2.19	0.43
10:K:44:GLY:O	10:K:45:PHE:C	2.57	0.43
4:D:203:GLY:O	4:D:207:GLY:N	2.52	0.43
4:D:180:ARG:HH11	4:D:180:ARG:HG3	1.79	0.43
1:A:222:SER:O	1:A:246:TYR:HB2	2.19	0.43
13:O:227:VAL:CG1	13:O:228:ALA:N	2.82	0.43
13:O:225:LEU:HD12	13:O:225:LEU:N	2.33	0.43
2:B:289:GLN:OE1	2:B:292:LEU:HD12	2.19	0.43
3:C:394:GLU:OE2	3:C:398:HIS:CD2	2.71	0.43
3:C:28:GLN:HB2	24:C:484:CLA:HED3	2.00	0.42
10:K:21:LEU:HD11	29:K:112:BCR:C3	2.47	0.42
4:D:217:THR:HG21	27:D:357:PL9:C1	2.49	0.42
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.42
7:H:41:PHE:O	7:H:45:ILE:HG23	2.18	0.42
2:B:222:PRO:CG	7:H:27:THR:H	2.28	0.42
15:U:82:ASN:ND2	15:U:94:ILE:HG23	2.34	0.42
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.54	0.42
9:J:15:THR:HG23	29:K:112:BCR:H392	2.01	0.42
24:C:481:CLA:H172	30:C:490:DGD:HBW2	2.01	0.42
3:C:437:PHE:CZ	24:C:483:CLA:HMB3	2.55	0.42
1:A:215:HIS:CD2	4:D:268:HIS:HD2	2.37	0.42
1:A:255:PHE:CE2	27:A:367:PL9:H111	2.54	0.42
3:C:48:LYS:CD	3:C:138:GLU:HG3	2.49	0.42
2:B:464:PHE:HD2	24:B:521:CLA:HAC2	1.84	0.42
12:M:33:GLN:CG	12:M:34:LYS:N	2.82	0.42
4:D:291:LEU:O	4:D:292:ASN:HB2	2.18	0.42
13:O:109:GLY:HA3	13:O:122:VAL:O	2.18	0.42
9:J:12:ILE:O	9:J:16:VAL:HG23	2.19	0.42
2:B:471:ALA:HB2	4:D:130:PHE:CE2	2.53	0.42
24:C:485:CLA:H162	24:C:485:CLA:HMA2	2.01	0.42
1:A:42:LEU:HA	1:A:45:THR:CG2	2.49	0.42
4:D:52:THR:HG22	4:D:67:TYR:CE2	2.54	0.42
4:D:56:THR:HB	5:E:49:THR:HG23	2.01	0.42
1:A:92:HIS:HD2	3:C:219:GLY:HA3	1.84	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.84	0.42
3:C:406:SER:HA	3:C:420:VAL:CG2	2.49	0.42
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:456:GLU:OE1	3:C:456:GLU:N	2.53	0.42
2:B:145:LEU:CD1	24:B:525:CLA:HMB2	2.49	0.42
13:O:69:LEU:HB3	13:O:107:ILE:CB	2.35	0.42
15:U:72:TYR:CG	15:U:73:PRO:N	2.87	0.42
2:B:234:ILE:C	2:B:236:THR:H	2.23	0.42
3:C:174:LEU:HD12	24:C:485:CLA:H71	2.01	0.42
4:D:221:THR:CG2	4:D:244:TYR:HB2	2.48	0.42
2:B:327:THR:O	2:B:444:ARG:NE	2.46	0.42
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.49	0.42
4:D:160:TYR:CB	4:D:161:PRO:CD	2.96	0.42
5:E:34:GLY:O	5:E:37:PHE:HB3	2.19	0.42
3:C:205:ASP:OD1	3:C:207:ARG:HB3	2.19	0.42
5:E:35:TRP:CD1	5:E:35:TRP:C	2.93	0.42
10:K:19:ASP:N	10:K:20:PRO:CD	2.80	0.42
1:A:228:THR:HB	1:A:231:GLU:HB3	2.01	0.42
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.54	0.42
20:Z:5:PHE:CD2	20:Z:61:VAL:HG21	2.54	0.42
1:A:207:GLY:O	1:A:210:LEU:HB3	2.19	0.42
4:D:89:LEU:HG	7:H:50:ASN:OD1	2.20	0.42
26:E:85:HEM:HAD2	26:E:85:HEM:HHA	1.57	0.42
3:C:276:LEU:HD21	24:C:481:CLA:HBB1	2.01	0.42
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.42
2:B:354:LEU:HD12	2:B:378:LYS:HB2	2.02	0.42
9:J:7:ARG:HE	9:J:7:ARG:HA	1.83	0.42
5:E:15:THR:CG2	9:J:7:ARG:HG3	2.49	0.42
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.42
2:B:472:ARG:HG2	2:B:472:ARG:HH11	1.84	0.42
2:B:215:PHE:C	2:B:215:PHE:CD2	2.93	0.42
2:B:413:ASP:O	2:B:414:PRO:C	2.57	0.42
2:B:237:VAL:HG12	24:B:522:CLA:HMD1	2.02	0.42
24:B:522:CLA:H162	24:B:522:CLA:H122	1.84	0.42
4:D:125:PHE:O	4:D:128:ARG:HB3	2.19	0.42
10:K:16:ALA:O	10:K:19:ASP:HB2	2.20	0.42
4:D:204:VAL:HG22	4:D:279:LEU:HD21	2.01	0.42
2:B:59:GLY:HA3	24:B:517:CLA:CED	2.50	0.42
1:A:22:THR:HG21	8:I:30:ARG:CD	2.50	0.42
6:F:16:PHE:CD1	6:F:16:PHE:N	2.88	0.42
14:T:22:PHE:C	14:T:23:PHE:CD2	2.93	0.42
12:M:1:MET:HG2	12:M:2:GLU:H	1.84	0.42
15:U:91:VAL:HG13	15:U:92:LEU:N	2.33	0.42
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.01	0.42
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:390:ARG:CZ	16:V:126:ILE:HD13	2.50	0.42
31:A:371:LHG:HC92	32:A:372:SQD:O10	2.20	0.42
5:E:30:LEU:HD11	6:F:28:VAL:HG13	2.02	0.42
6:F:25:THR:O	6:F:29:PRO:HG2	2.19	0.42
4:D:17:ILE:HG21	18:X:42:GLN:HG3	2.02	0.42
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.16	0.42
20:Z:17:PHE:HE2	20:Z:21:ILE:HD11	1.83	0.42
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.42
2:B:377:VAL:HG11	4:D:342:PRO:HG2	2.01	0.42
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.00	0.42
6:F:15:ILE:HG22	6:F:16:PHE:N	2.34	0.42
13:O:59:ASP:O	13:O:61:SER:N	2.53	0.42
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.55	0.42
16:V:130:MET:SD	16:V:133:LEU:HD12	2.60	0.42
3:C:140:LEU:HB2	3:C:148:GLY:HA2	2.02	0.42
9:J:11:TRP:CE2	9:J:12:ILE:HG12	2.55	0.42
7:H:13:PRO:HG2	7:H:14:LEU:H	1.85	0.42
2:B:237:VAL:HG22	24:B:520:CLA:HBC2	2.01	0.42
2:B:348:ASN:O	2:B:349:LYS:C	2.57	0.42
1:A:12:ASN:O	1:A:15:GLU:HB3	2.20	0.42
24:B:517:CLA:HMD3	29:B:528:BCR:H271	2.02	0.42
33:I:220:LMG:H132	34:I:230:LMT:O2'	2.20	0.42
1:A:96:ILE:C	1:A:98:GLU:H	2.23	0.42
33:E:218:LMG:O9	33:E:218:LMG:HC71	2.19	0.42
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.55	0.42
2:B:330:MET:SD	2:B:446:SER:HB3	2.59	0.42
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.42
24:C:484:CLA:HMB2	29:C:487:BCR:H382	2.02	0.41
15:U:50:ALA:HB1	15:U:113:THR:HG21	2.01	0.41
24:B:525:CLA:H162	7:H:7:LEU:HD21	2.02	0.41
18:X:12:ILE:HD13	18:X:12:ILE:C	2.40	0.41
1:A:214:MET:HE1	4:D:142:ASN:ND2	2.35	0.41
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.84	0.41
13:O:157:PRO:O	13:O:158:ASN:O	2.38	0.41
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.01	0.41
2:B:12:LEU:O	2:B:14:ASN:N	2.53	0.41
3:C:188:THR:CG2	3:C:298:PRO:HB3	2.51	0.41
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.55	0.41
3:C:45:LEU:O	3:C:46:SER:C	2.58	0.41
15:U:75:LEU:O	15:U:79:ILE:HG13	2.21	0.41
33:D:359:LMG:O4	9:J:31:GLY:O	2.39	0.41
9:J:36:LEU:C	9:J:38:SER:H	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:80:GLU:O	13:O:89:ALA:CB	2.66	0.41
1:A:317:TRP:O	1:A:321:ILE:HG13	2.20	0.41
2:B:413:ASP:OD1	2:B:416:THR:HB	2.20	0.41
19:Y:21:UNK:O	19:Y:22:UNK:C	2.68	0.41
24:C:474:CLA:HMB3	29:C:488:BCR:C40	2.46	0.41
3:C:365:TRP:HB3	3:C:391:ARG:HG2	2.02	0.41
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.02	0.41
1:A:343:LEU:O	1:A:344:ALA:CB	2.66	0.41
2:B:448:ARG:HH11	2:B:448:ARG:HG3	1.84	0.41
3:C:199:ILE:CD1	3:C:199:ILE:N	2.83	0.41
34:T:227:LMT:H1B	34:T:227:LMT:H3'	1.64	0.41
13:O:147:THR:OG1	13:O:148:VAL:N	2.54	0.41
3:C:189:TRP:O	3:C:190:ALA:C	2.59	0.41
1:A:206:PHE:HA	1:A:206:PHE:HD2	1.76	0.41
1:A:45:THR:HB	25:A:365:PHO:H93	2.02	0.41
7:H:53:LEU:HD21	7:H:55:LEU:HD21	2.03	0.41
5:E:78:THR:HA	5:E:81:GLU:HG2	2.02	0.41
7:H:10:ILE:HG13	7:H:10:ILE:H	1.70	0.41
3:C:142:GLU:C	3:C:144:SER:H	2.24	0.41
2:B:105:GLY:O	2:B:108:PHE:HB3	2.19	0.41
10:K:11:LEU:O	10:K:12:PRO:C	2.59	0.41
10:K:28:ILE:O	10:K:31:LEU:HB2	2.20	0.41
1:A:172:MET:SD	24:A:363:CLA:HMC3	2.61	0.41
1:A:215:HIS:HA	27:A:367:PL9:O1	2.21	0.41
5:E:15:THR:O	9:J:8:ILE:CD1	2.69	0.41
33:M:217:LMG:HC72	33:M:217:LMG:HC2	1.96	0.41
3:C:202:PRO:HB2	3:C:235:GLY:HA2	2.01	0.41
15:U:89:GLU:CD	15:U:89:GLU:N	2.73	0.41
11:L:22:LEU:O	11:L:26:VAL:HG13	2.21	0.41
2:B:383:PHE:O	13:O:192:SER:HA	2.20	0.41
16:V:83:GLU:H	16:V:83:GLU:CD	2.23	0.41
5:E:82:GLN:HG3	5:E:82:GLN:H	1.54	0.41
2:B:24:LEU:HD13	2:B:111:ALA:N	2.36	0.41
4:D:26:ARG:HD3	6:F:18:VAL:CG1	2.32	0.41
30:C:491:DGD:HG2	9:J:33:TYR:OH	2.21	0.41
3:C:116:VAL:CG2	3:C:117:VAL:N	2.84	0.41
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.33	0.41
2:B:191:ASN:OD1	2:B:193:TYR:N	2.52	0.41
13:O:120:THR:HA	13:O:153:ALA:O	2.21	0.41
5:E:49:THR:HA	5:E:50:PRO:HD3	1.86	0.41
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.56	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:192:SER:OG	13:O:193:GLY:N	2.54	0.41
2:B:463:PHE:CD2	2:B:463:PHE:C	2.94	0.41
29:C:487:BCR:H341	29:K:112:BCR:H322	2.02	0.41
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.03	0.41
20:Z:36:SER:C	20:Z:38:GLN:H	2.24	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.41
1:A:277:ALA:O	1:A:281:VAL:HG23	2.21	0.41
2:B:479:PHE:O	2:B:480:SER:CB	2.68	0.41
13:O:73:PRO:HG2	13:O:102:THR:HB	2.03	0.41
3:C:101:PRO:O	3:C:104:GLU:HB2	2.19	0.41
10:K:34:ALA:O	10:K:37:PHE:HB2	2.20	0.41
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.56	0.41
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.56	0.41
4:D:128:ARG:O	4:D:129:GLN:C	2.59	0.41
29:J:115:BCR:H15C	29:J:115:BCR:H351	1.91	0.41
19:Y:23:UNK:O	19:Y:24:UNK:C	2.68	0.41
3:C:165:LEU:HG	24:C:480:CLA:HED1	2.03	0.41
1:A:183:MET:HB3	24:A:362:CLA:HBC2	2.02	0.41
1:A:215:HIS:CD2	4:D:268:HIS:CD2	3.08	0.41
4:D:268:HIS:CE1	23:D:353:BCT:O3	2.74	0.41
3:C:414:ILE:HG22	3:C:415:ASN:N	2.35	0.41
15:U:57:LEU:HD22	15:U:79:ILE:CG2	2.51	0.41
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.51	0.41
13:O:116:ASP:C	13:O:116:ASP:OD2	2.58	0.41
3:C:267:SER:O	3:C:271:TYR:CD2	2.74	0.41
14:T:22:PHE:C	14:T:23:PHE:HD2	2.24	0.41
3:C:258:GLY:C	3:C:262:ARG:NH1	2.74	0.41
1:A:288:LEU:O	1:A:292:THR:HB	2.21	0.41
3:C:198:VAL:HG12	3:C:200:THR:HG23	2.03	0.41
2:B:91:TRP:HE1	34:B:535:LMT:H12	1.86	0.41
2:B:393:GLU:HG2	15:U:44:ASP:O	2.20	0.41
2:B:137:LYS:NZ	7:H:14:LEU:O	2.54	0.41
1:A:129:ARG:C	1:A:131:TRP:H	2.23	0.41
24:C:485:CLA:H2A	24:C:485:CLA:HED2	2.03	0.41
24:A:363:CLA:H62	24:A:363:CLA:H41	1.91	0.41
1:A:10:SER:OG	1:A:13:LEU:HD12	2.20	0.41
2:B:331:ASN:HB3	2:B:437:LEU:CD1	2.49	0.41
16:V:81:ARG:CG	16:V:157:GLY:HA3	2.51	0.41
2:B:447:PRO:O	2:B:448:ARG:C	2.59	0.41
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.56	0.41
2:B:168:VAL:O	2:B:176:GLY:HA2	2.20	0.41
1:A:114:LEU:O	1:A:114:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:ARG:NH1	13:O:183:LEU:O	2.54	0.41
16:V:30:THR:OG1	16:V:32:GLU:HB3	2.21	0.41
15:U:55:ILE:HG21	15:U:65:PHE:CE1	2.56	0.41
2:B:113:TRP:CE2	2:B:117:TYR:CD2	3.09	0.41
19:Y:23:UNK:O	19:Y:25:UNK:N	2.54	0.40
24:A:363:CLA:HAA1	27:D:357:PL9:C36	2.51	0.40
5:E:64:PRO:HB3	5:E:84:LYS:CD	2.50	0.40
2:B:280:PHE:O	2:B:284:ILE:HG13	2.20	0.40
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.02	0.40
2:B:16:PRO:HG3	2:B:133:LEU:HD11	2.03	0.40
3:C:461:ARG:NH1	3:C:461:ARG:HG3	2.33	0.40
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.03	0.40
1:A:105:TRP:CZ3	1:A:111:PRO:HG3	2.55	0.40
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.03	0.40
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.40
34:D:363:LMT:O3'	18:X:21:ILE:HG21	2.21	0.40
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.35	0.40
5:E:14:ILE:O	5:E:14:ILE:HG22	2.20	0.40
7:H:63:LYS:C	7:H:65:LEU:H	2.24	0.40
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.21	0.40
3:C:42:LEU:HD11	24:C:484:CLA:C1A	2.51	0.40
24:C:475:CLA:HBD	24:C:476:CLA:H43	2.03	0.40
29:C:488:BCR:C33	8:I:20:VAL:HG13	2.52	0.40
4:D:43:LEU:HD12	4:D:43:LEU:HA	1.94	0.40
15:U:94:ILE:HB	15:U:97:LEU:HD11	2.03	0.40
18:X:43:ILE:O	18:X:43:ILE:CG2	2.70	0.40
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.72	0.40
15:U:88:VAL:HG13	15:U:109:LEU:HD22	2.03	0.40
1:A:24:THR:OG1	3:C:469:MET:CE	2.70	0.40
15:U:90:ASP:HA	15:U:93:ASN:HD22	1.87	0.40
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.40
4:D:302:GLU:HA	4:D:302:GLU:OE1	2.20	0.40
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.40
7:H:11:LEU:C	7:H:13:PRO:HD2	2.42	0.40
2:B:233:ASN:O	2:B:236:THR:HG22	2.22	0.40
32:A:372:SQD:H132	31:A:374:LHG:H132	2.02	0.40
31:A:374:LHG:O9	31:A:374:LHG:HC41	2.21	0.40
3:C:59:LEU:HD13	24:C:483:CLA:HMD2	2.04	0.40
3:C:414:ILE:CG2	3:C:415:ASN:N	2.84	0.40
2:B:222:PRO:O	2:B:223:GLN:C	2.59	0.40
3:C:94:THR:CG2	3:C:298:PRO:HD2	2.51	0.40
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.71	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:O:226:ASN:ND2	13:O:226:ASN:N	2.69	0.40
3:C:451:ALA:HA	3:C:456:GLU:CD	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	39
2	B	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	7	28
3	C	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	5	22
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	8	30
5	E	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	3	11
6	F	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	27
7	H	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	1	2
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	7
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	6
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	8
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	3	11
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	24
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	16
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	30	72
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	1
18	X	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	1	1
20	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	11
All	All	2569/2740 (94%)	2133 (83%)	344 (13%)	92 (4%)	5	22

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	141	PRO
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
2	B	488	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
3	C	452	ALA
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
5	E	82	GLN
7	H	18	TYR
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
14	T	30	THR
15	U	72	TYR
15	U	83	ALA
16	V	75	ASN
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	209	ILE
3	C	456	GLU
4	D	234	ALA
4	D	264	LYS
7	H	26	GLY
9	J	38	SER
13	O	231	ASP
15	U	73	PRO
17	y	25	ILE
18	X	43	ILE
2	B	127	ARG
2	B	183	PRO

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Mol	Chain	Res	Type
2	B	414	PRO
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	375	LEU
3	C	453	ALA
4	D	263	ASN
5	E	9	PRO
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
13	O	60	SER
13	O	158	ASN
13	O	165	SER
20	Z	24	PRO
20	Z	28	ALA
2	B	13	ILE
2	B	173	GLY
2	B	231	MET
2	B	235	GLU
3	C	154	LYS
4	D	73	PHE
5	E	10	PHE
13	O	51	THR
13	O	82	PRO
17	y	24	MET
18	X	44	ASP
1	A	97	TRP
3	C	462	GLU
6	F	41	GLN
7	H	6	TRP
15	U	42	VAL
18	X	12	ILE
1	A	334	ARG
4	D	351	ALA
7	H	14	LEU
13	O	88	GLU
1	A	21	VAL
2	B	16	PRO
13	O	159	VAL
3	C	201	ASN
17	y	35	ILE

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Mol	Chain	Res	Type
5	E	52	PRO
7	H	60	VAL
8	I	32	PRO
13	O	232	GLY
1	A	176	ILE
4	D	160	TYR
13	O	127	ILE
13	O	152	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	258 (95%)	13 (5%)	35	74
2	B	390/407 (96%)	374 (96%)	16 (4%)	41	80
3	C	347/374 (93%)	329 (95%)	18 (5%)	32	71
4	D	275/283 (97%)	256 (93%)	19 (7%)	22	54
5	E	72/73 (99%)	66 (92%)	6 (8%)	16	43
6	F	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	29	66
8	I	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	J	24/28 (86%)	23 (96%)	1 (4%)	40	79
10	K	30/30 (100%)	28 (93%)	2 (7%)	23	56
11	L	35/35 (100%)	31 (89%)	4 (11%)	8	24
12	M	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	195 (96%)	7 (4%)	48	85
14	T	29/29 (100%)	28 (97%)	1 (3%)	49	86
15	U	84/89 (94%)	80 (95%)	4 (5%)	35	74
16	V	116/117 (99%)	111 (96%)	5 (4%)	40	78
17	y	20/37 (54%)	18 (90%)	2 (10%)	11	32
18	X	30/42 (71%)	26 (87%)	4 (13%)	6	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Z	52/52 (100%)	47 (90%)	5 (10%)	12	35
All	All	2122/2246 (94%)	2011 (95%)	111 (5%)	32	71

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	170	ASP
1	A	202	VAL
1	A	206	PHE
1	A	234	ASN
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	298	ASN
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	223	GLN
2	B	246	PHE
2	B	262	THR
2	B	308	LYS
2	B	309	LEU
2	B	362	PHE
2	B	414	PRO
2	B	422	ARG
2	B	433	ASP
2	B	483	ASP
2	B	486	LEU
2	B	488	PRO
2	B	490	GLN
3	C	29	GLU
3	C	78	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	201	ASN

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Mol	Chain	Res	Type
3	C	207	ARG
3	C	232	ASP
3	C	244	CYS
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	401	LEU
3	C	447	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	60	THR
4	D	84	SER
4	D	91	LEU
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	221	THR
4	D	236	ASN
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	5	THR
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
10	K	18	PHE

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Mol	Chain	Res	Type
10	K	19	ASP
11	L	7	ARG
11	L	8	GLN
11	L	11	GLU
11	L	15	THR
13	O	31	LEU
13	O	86	ARG
13	O	97	VAL
13	O	106	GLN
13	O	141	ARG
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	35	THR
16	V	63	CYS
16	V	92	ARG
16	V	116	GLU
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	42	GLN
18	X	45	LYS
20	Z	14	ILE
20	Z	25	VAL
20	Z	33	TRP
20	Z	58	ASN
20	Z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	234	ASN
1	A	241	GLN
2	B	201	HIS

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Mol	Chain	Res	Type
2	B	216	HIS
2	B	490	GLN
3	C	155	ASN
3	C	398	HIS
3	C	418	ASN
3	C	444	HIS
4	D	98	GLN
4	D	117	HIS
4	D	129	GLN
4	D	142	ASN
4	D	239	GLN
4	D	250	ASN
7	H	59	ASN
11	L	6	ASN
11	L	8	GLN
12	M	33	GLN
13	O	87	GLN
13	O	106	GLN
13	O	114	ASN
13	O	135	GLN
13	O	150	ASN
13	O	173	ASN
13	O	222	GLN
13	O	226	ASN
15	U	82	ASN
15	U	93	ASN
17	y	21	GLN
18	X	42	GLN
20	Z	6	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 92 ligands modelled in this entry, 4 are monoatomic - leaving 88 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$
24	CLA	A	362	1	73,73,73	1.48	13 (17%)	95,113,113	1.54	18 (18%)
24	CLA	A	363	-	73,73,73	1.43	12 (16%)	95,113,113	1.66	18 (18%)
25	PHO	A	365	-	69,69,69	1.86	6 (8%)	91,99,99	1.51	15 (16%)
24	CLA	A	366	1	73,73,73	1.44	10 (13%)	95,113,113	1.48	18 (18%)
27	PL9	A	367	-	45,45,55	1.00	2 (4%)	55,57,69	1.86	16 (29%)
28	OEC	A	368	1,3	0,0,13	0.00	-	0,0,27	0.00	-
29	BCR	A	369	-	41,41,41	1.61	7 (17%)	56,56,56	2.06	20 (35%)
30	DGD	A	370	-	57,57,67	2.09	14 (24%)	71,71,81	1.49	9 (12%)
31	LHG	A	371	-	38,38,48	1.93	6 (15%)	44,44,54	1.31	4 (9%)
32	SQD	A	372	-	51,51,54	6.80	25 (49%)	62,62,65	2.90	21 (33%)
33	LMG	A	373	-	51,51,55	1.41	4 (7%)	59,59,63	1.02	4 (6%)
31	LHG	A	374	-	36,36,48	1.72	4 (11%)	42,42,54	1.12	3 (7%)
30	DGD	A	375	-	53,53,67	2.50	19 (35%)	67,67,81	1.64	8 (11%)
24	CLA	B	511	-	73,73,73	1.70	12 (16%)	95,113,113	1.48	18 (18%)
24	CLA	B	512	2	73,73,73	1.48	13 (17%)	95,113,113	1.49	19 (20%)
24	CLA	B	513	2	73,73,73	1.48	11 (15%)	95,113,113	1.54	19 (20%)
24	CLA	B	514	2	73,73,73	1.57	12 (16%)	95,113,113	1.49	18 (18%)
24	CLA	B	515	-	73,73,73	1.55	12 (16%)	95,113,113	1.48	17 (17%)
24	CLA	B	516	2	73,73,73	1.51	12 (16%)	95,113,113	1.45	18 (18%)
24	CLA	B	517	-	73,73,73	1.49	15 (20%)	95,113,113	1.55	18 (18%)
24	CLA	B	518	2	73,73,73	1.50	11 (15%)	95,113,113	1.54	19 (20%)
24	CLA	B	519	2	73,73,73	1.65	14 (19%)	95,113,113	1.48	18 (18%)
24	CLA	B	520	-	73,73,73	1.46	11 (15%)	95,113,113	1.53	21 (22%)
24	CLA	B	521	2	73,73,73	1.40	9 (12%)	95,113,113	1.49	19 (20%)
24	CLA	B	522	-	73,73,73	1.51	11 (15%)	95,113,113	1.51	18 (18%)
24	CLA	B	523	-	73,73,73	1.39	10 (13%)	95,113,113	1.49	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	524	2	73,73,73	1.55	13 (17%)	95,113,113	1.59	25 (26%)
24	CLA	B	525	-	73,73,73	1.57	13 (17%)	95,113,113	1.55	20 (21%)
24	CLA	B	526	-	73,73,73	1.56	13 (17%)	95,113,113	1.57	21 (22%)
29	BCR	B	527	-	41,41,41	1.68	7 (17%)	56,56,56	1.96	14 (25%)
29	BCR	B	528	-	41,41,41	1.69	6 (14%)	56,56,56	2.17	27 (48%)
29	BCR	B	529	-	41,41,41	1.91	8 (19%)	56,56,56	2.05	15 (26%)
29	BCR	B	530	-	41,41,41	1.82	7 (17%)	56,56,56	2.03	17 (30%)
33	LMG	B	531	-	49,49,55	1.53	7 (14%)	57,57,63	1.05	4 (7%)
32	SQD	B	532	-	54,54,54	2.99	29 (53%)	65,65,65	2.70	20 (30%)
33	LMG	B	533	-	49,49,55	1.81	6 (12%)	57,57,63	1.07	5 (8%)
33	LMG	B	534	-	42,42,55	2.11	9 (21%)	50,50,63	1.05	3 (6%)
34	LMT	B	535	-	36,36,36	1.42	7 (19%)	47,47,47	1.20	3 (6%)
34	LMT	B	536	-	36,36,36	1.36	7 (19%)	47,47,47	0.96	3 (6%)
24	CLA	C	474	3	73,73,73	1.49	10 (13%)	95,113,113	1.50	20 (21%)
24	CLA	C	475	3	73,73,73	1.56	12 (16%)	95,113,113	1.46	17 (17%)
24	CLA	C	476	3	73,73,73	1.65	14 (19%)	95,113,113	1.48	17 (17%)
24	CLA	C	477	-	73,73,73	1.55	11 (15%)	95,113,113	1.53	18 (18%)
24	CLA	C	478	3	73,73,73	1.60	13 (17%)	95,113,113	1.56	20 (21%)
24	CLA	C	479	3	73,73,73	1.51	13 (17%)	95,113,113	1.50	19 (20%)
24	CLA	C	480	-	73,73,73	1.46	13 (17%)	95,113,113	1.53	22 (23%)
24	CLA	C	481	3	73,73,73	1.57	15 (20%)	95,113,113	1.55	20 (21%)
24	CLA	C	482	-	73,73,73	1.54	11 (15%)	95,113,113	1.55	19 (20%)
24	CLA	C	483	-	73,73,73	1.59	12 (16%)	95,113,113	1.51	17 (17%)
24	CLA	C	484	3	73,73,73	1.66	11 (15%)	95,113,113	1.51	20 (21%)
24	CLA	C	485	-	73,73,73	1.66	13 (17%)	95,113,113	1.57	20 (21%)
24	CLA	C	486	3	73,73,73	1.64	13 (17%)	95,113,113	1.49	19 (20%)
29	BCR	C	487	-	41,41,41	1.73	6 (14%)	56,56,56	2.10	21 (37%)
29	BCR	C	488	-	41,41,41	1.66	6 (14%)	56,56,56	2.13	18 (32%)
30	DGD	C	489	-	54,54,67	1.57	10 (18%)	68,68,81	1.60	8 (11%)
30	DGD	C	490	-	63,63,67	1.28	6 (9%)	77,77,81	1.64	9 (11%)
30	DGD	C	491	-	67,67,67	1.02	6 (8%)	81,81,81	1.27	4 (4%)
33	LMG	C	492	-	48,48,55	1.90	7 (14%)	56,56,63	0.87	3 (5%)
33	LMG	C	493	-	45,45,55	2.01	10 (22%)	53,53,63	1.06	4 (7%)
23	BCT	D	353	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	D	354	4	73,73,73	1.57	13 (17%)	95,113,113	1.51	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	D	355	-	69,69,69	1.95	6 (8%)	91,99,99	1.54	14 (15%)
24	CLA	D	356	-	73,73,73	1.57	12 (16%)	95,113,113	1.49	18 (18%)
27	PL9	D	357	-	55,55,55	0.54	0	69,69,69	1.81	18 (26%)
29	BCR	D	358	-	41,41,41	1.81	7 (17%)	56,56,56	2.27	19 (33%)
33	LMG	D	359	-	46,46,55	2.07	6 (13%)	54,54,63	0.95	2 (3%)
33	LMG	D	360	-	48,48,55	1.68	5 (10%)	56,56,63	1.06	3 (5%)
32	SQD	D	361	-	43,43,54	7.80	23 (53%)	54,54,65	3.30	18 (33%)
30	DGD	D	362	-	64,64,67	1.90	18 (28%)	78,78,81	1.42	7 (8%)
34	LMT	D	363	-	32,32,36	1.72	5 (15%)	43,43,47	1.03	2 (4%)
24	CLA	D	364	-	73,73,73	1.44	9 (12%)	95,113,113	1.47	16 (16%)
33	LMG	E	218	-	44,44,55	1.88	7 (15%)	52,52,63	1.12	5 (9%)
26	HEM	E	85	5,6	49,50,50	3.00	27 (55%)	46,82,82	2.53	11 (23%)
32	SQD	F	224	-	45,45,54	10.24	25 (55%)	56,56,65	3.17	20 (35%)
29	BCR	H	107	-	41,41,41	1.85	8 (19%)	56,56,56	2.22	21 (37%)
30	DGD	H	208	-	59,59,67	2.10	9 (15%)	73,73,81	1.48	7 (9%)
33	LMG	I	220	-	43,43,55	2.18	10 (23%)	51,51,63	1.11	4 (7%)
34	LMT	I	230	-	36,36,36	1.39	4 (11%)	47,47,47	0.95	1 (2%)
29	BCR	J	115	-	41,41,41	2.04	8 (19%)	56,56,56	3.23	22 (39%)
27	PL9	J	59	-	35,35,55	1.41	5 (14%)	43,45,69	1.88	14 (32%)
29	BCR	K	112	-	41,41,41	1.82	7 (17%)	56,56,56	2.50	25 (44%)
33	LMG	M	217	-	42,42,55	2.34	8 (19%)	50,50,63	1.24	6 (12%)
34	LMT	M	226	-	36,36,36	1.17	3 (8%)	47,47,47	0.95	2 (4%)
34	LMT	O	274	-	36,36,36	1.42	6 (16%)	47,47,47	1.05	3 (6%)
32	SQD	T	213	-	47,47,54	3.29	24 (51%)	58,58,65	3.03	16 (27%)
34	LMT	T	227	-	36,36,36	1.34	5 (13%)	47,47,47	1.08	4 (8%)
26	HEM	V	164	16	49,50,50	3.53	26 (53%)	46,82,82	2.39	13 (28%)
29	BCR	Z	116	-	41,41,41	1.81	7 (17%)	56,56,56	2.06	18 (32%)

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
24	CLA	A	362	1	-	0/37/135/135	0/0/9/9
24	CLA	A	363	-	-	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	A	365	-	3/3/17/22	1/48/103/103	0/0/6/6
24	CLA	A	366	1	-	0/37/135/135	0/0/9/9
27	PL9	A	367	-	-	0/41/61/73	0/1/1/1
28	OEC	A	368	1,3	-	0/0/0/54	0/0/0/5
29	BCR	A	369	-	-	0/29/63/63	0/2/2/2
30	DGD	A	370	-	3/3/13/13	0/45/85/95	0/2/2/2
31	LHG	A	371	-	-	0/43/43/53	0/0/0/0
32	SQD	A	372	-	-	0/46/66/69	0/1/1/1
33	LMG	A	373	-	2/2/8/8	0/46/66/70	0/1/1/1
31	LHG	A	374	-	-	0/41/41/53	0/0/0/0
30	DGD	A	375	-	3/3/13/13	0/41/81/95	0/2/2/2
24	CLA	B	511	-	-	0/37/135/135	0/0/9/9
24	CLA	B	512	2	-	1/37/135/135	0/0/9/9
24	CLA	B	513	2	-	0/37/135/135	0/0/9/9
24	CLA	B	514	2	-	0/37/135/135	0/0/9/9
24	CLA	B	515	-	-	0/37/135/135	0/0/9/9
24	CLA	B	516	2	-	1/37/135/135	0/0/9/9
24	CLA	B	517	-	-	0/37/135/135	0/0/9/9
24	CLA	B	518	2	-	0/37/135/135	0/0/9/9
24	CLA	B	519	2	-	0/37/135/135	0/0/9/9
24	CLA	B	520	-	-	0/37/135/135	0/0/9/9
24	CLA	B	521	2	-	1/37/135/135	0/0/9/9
24	CLA	B	522	-	-	0/37/135/135	0/0/9/9
24	CLA	B	523	-	-	0/37/135/135	0/0/9/9
24	CLA	B	524	2	-	0/37/135/135	0/0/9/9
24	CLA	B	525	-	-	0/37/135/135	0/0/9/9
24	CLA	B	526	-	-	0/37/135/135	0/0/9/9
29	BCR	B	527	-	-	0/29/63/63	0/2/2/2
29	BCR	B	528	-	-	0/29/63/63	0/2/2/2
29	BCR	B	529	-	-	0/29/63/63	0/2/2/2
29	BCR	B	530	-	-	0/29/63/63	0/2/2/2
33	LMG	B	531	-	2/2/8/8	0/44/64/70	0/1/1/1
32	SQD	B	532	-	-	0/49/69/69	0/1/1/1
33	LMG	B	533	-	2/2/8/8	0/44/64/70	0/1/1/1
33	LMG	B	534	-	2/2/8/8	0/37/57/70	0/1/1/1
34	LMT	B	535	-	-	0/21/61/61	0/2/2/2
34	LMT	B	536	-	-	0/21/61/61	0/2/2/2
24	CLA	C	474	3	-	0/37/135/135	0/0/9/9
24	CLA	C	475	3	-	1/37/135/135	0/0/9/9
24	CLA	C	476	3	-	0/37/135/135	0/0/9/9
24	CLA	C	477	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	478	3	-	0/37/135/135	0/0/9/9
24	CLA	C	479	3	-	0/37/135/135	0/0/9/9
24	CLA	C	480	-	-	0/37/135/135	0/0/9/9
24	CLA	C	481	3	-	0/37/135/135	0/0/9/9
24	CLA	C	482	-	-	1/37/135/135	0/0/9/9
24	CLA	C	483	-	-	1/37/135/135	0/0/9/9
24	CLA	C	484	3	-	0/37/135/135	0/0/9/9
24	CLA	C	485	-	-	0/37/135/135	0/0/9/9
24	CLA	C	486	3	-	1/37/135/135	0/0/9/9
29	BCR	C	487	-	-	0/29/63/63	0/2/2/2
29	BCR	C	488	-	-	0/29/63/63	0/2/2/2
30	DGD	C	489	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	490	-	3/3/13/13	0/51/91/95	0/2/2/2
30	DGD	C	491	-	3/3/13/13	0/55/95/95	0/2/2/2
33	LMG	C	492	-	2/2/8/8	0/43/63/70	0/1/1/1
33	LMG	C	493	-	2/2/8/8	0/40/60/70	0/1/1/1
23	BCT	D	353	22	-	0/0/0/0	0/0/0/0
24	CLA	D	354	4	-	0/37/135/135	0/0/9/9
25	PHO	D	355	-	3/3/17/22	0/48/103/103	0/0/6/6
24	CLA	D	356	-	-	0/37/135/135	0/0/9/9
27	PL9	D	357	-	-	0/53/73/73	0/1/1/1
29	BCR	D	358	-	-	0/29/63/63	0/2/2/2
33	LMG	D	359	-	2/2/8/8	0/41/61/70	0/1/1/1
33	LMG	D	360	-	2/2/8/8	1/43/63/70	0/1/1/1
32	SQD	D	361	-	-	2/38/58/69	0/1/1/1
30	DGD	D	362	-	3/3/13/13	0/52/92/95	0/2/2/2
34	LMT	D	363	-	-	0/17/57/61	0/2/2/2
24	CLA	D	364	-	-	0/37/135/135	0/0/9/9
33	LMG	E	218	-	2/2/8/8	0/39/59/70	0/1/1/1
26	HEM	E	85	5,6	-	0/14/114/114	0/0/8/8
32	SQD	F	224	-	-	0/40/60/69	0/1/1/1
29	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/47/87/95	0/2/2/2
33	LMG	I	220	-	2/2/8/8	0/38/58/70	0/1/1/1
34	LMT	I	230	-	-	0/21/61/61	0/2/2/2
29	BCR	J	115	-	-	0/29/63/63	0/2/2/2
27	PL9	J	59	-	-	0/29/49/73	0/1/1/1
29	BCR	K	112	-	-	0/29/63/63	0/2/2/2
33	LMG	M	217	-	2/2/8/8	1/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	M	226	-	-	0/21/61/61	0/2/2/2
34	LMT	O	274	-	-	0/21/61/61	0/2/2/2
32	SQD	T	213	-	-	0/42/62/69	0/1/1/1
34	LMT	T	227	-	-	0/21/61/61	0/2/2/2
26	HEM	V	164	16	-	0/14/114/114	0/0/8/8
29	BCR	Z	116	-	-	0/29/63/63	0/2/2/2

All (912) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	224	SQD	C19-C18	-47.49	1.36	1.55
32	F	224	SQD	C32-C31	-45.64	1.37	1.55
32	D	361	SQD	C18-C17	-45.22	1.37	1.55
32	A	372	SQD	C35-C34	-43.95	1.37	1.55
26	V	164	HEM	C3D-C4D	13.41	1.47	1.44
32	B	532	SQD	C6-C5	-12.06	1.39	1.52
26	V	164	HEM	C2D-C1D	-12.01	1.41	1.44
33	D	359	LMG	C22-C21	-11.81	1.50	1.55
32	D	361	SQD	C31-C30	11.62	1.59	1.55
32	A	372	SQD	C6-C5	-11.60	1.40	1.52
25	D	355	PHO	CHC-C1C	11.25	1.42	1.35
32	T	213	SQD	C31-C30	11.15	1.59	1.55
30	H	208	DGD	CDB-CCB	-11.07	1.50	1.55
30	A	370	DGD	CDB-CCB	-11.07	1.50	1.55
25	A	365	PHO	CHC-C1C	10.75	1.42	1.35
32	D	361	SQD	C6-C5	-10.66	1.41	1.52
32	F	224	SQD	C6-C5	-10.42	1.41	1.52
33	B	533	LMG	C23-C22	-10.30	1.51	1.55
30	A	375	DGD	C9A-C8A	-9.06	1.51	1.55
33	M	217	LMG	C37-C36	-8.92	1.51	1.55
33	C	492	LMG	C23-C22	-8.86	1.51	1.55
33	I	220	LMG	C23-C22	-8.72	1.51	1.55
33	D	360	LMG	C25-C24	-8.70	1.51	1.55
33	C	493	LMG	C22-C21	-8.69	1.51	1.55
30	A	375	DGD	CDB-CCB	-8.64	1.51	1.55
26	E	85	HEM	C2D-C1D	-8.38	1.42	1.44
33	E	218	LMG	C22-C21	-8.27	1.51	1.55
32	T	213	SQD	C6-C5	-8.15	1.43	1.52
33	B	534	LMG	C22-C21	-8.03	1.52	1.55
26	E	85	HEM	C3D-C4D	7.75	1.46	1.44
32	T	213	SQD	C4-C3	7.66	1.72	1.52
32	A	372	SQD	C4-C3	7.61	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	532	SQD	C4-C3	7.56	1.72	1.52
33	A	373	LMG	C25-C24	-7.49	1.52	1.55
31	A	371	LHG	P-O5	7.48	1.79	1.51
33	B	531	LMG	C25-C24	-7.47	1.52	1.55
32	D	361	SQD	C4-C3	7.38	1.72	1.52
30	H	208	DGD	CFA-CEA	-6.98	1.52	1.55
30	C	489	DGD	CEA-CDA	-6.86	1.52	1.55
24	B	511	CLA	C1B-C2B	6.81	1.48	1.40
33	M	217	LMG	C22-C21	-6.78	1.52	1.55
32	F	224	SQD	C4-C3	6.72	1.70	1.52
25	D	355	PHO	C1D-CHD	6.48	1.42	1.35
24	C	483	CLA	C1B-C2B	6.37	1.48	1.40
25	A	365	PHO	C1D-CHD	6.35	1.42	1.35
24	C	484	CLA	MG-NA	6.04	2.25	2.07
33	I	220	LMG	C37-C36	-6.01	1.52	1.55
24	B	525	CLA	C1B-C2B	6.00	1.47	1.40
30	C	490	DGD	CEA-CDA	-5.99	1.52	1.55
24	B	519	CLA	C1B-C2B	5.97	1.47	1.40
29	J	115	BCR	C5-C6	5.96	1.43	1.34
24	C	485	CLA	C1B-C2B	5.93	1.47	1.40
24	C	477	CLA	C3B-C4B	5.92	1.49	1.40
31	A	374	LHG	C30-C29	-5.92	1.52	1.55
33	B	534	LMG	C37-C36	-5.89	1.52	1.55
29	H	107	BCR	C26-C25	5.85	1.43	1.34
31	A	374	LHG	C18-C17	-5.82	1.52	1.55
32	T	213	SQD	C6-S	5.78	1.84	1.77
24	C	484	CLA	C1B-C2B	5.75	1.47	1.40
25	D	355	PHO	C3B-C4B	5.75	1.49	1.40
24	C	483	CLA	C3B-C4B	5.74	1.49	1.40
26	E	85	HEM	C4A-C3A	5.70	1.47	1.40
24	C	475	CLA	C1B-C2B	5.65	1.47	1.40
30	D	362	DGD	CFA-CEA	-5.63	1.52	1.55
24	C	476	CLA	MG-NA	5.61	2.23	2.07
24	C	486	CLA	MG-NA	5.59	2.23	2.07
26	V	164	HEM	CHA-C4D	5.58	1.43	1.35
24	C	476	CLA	C1B-C2B	5.53	1.47	1.40
24	D	354	CLA	MG-NA	5.53	2.23	2.07
32	T	213	SQD	O8-S	5.52	1.59	1.46
32	D	361	SQD	O8-S	5.48	1.59	1.46
24	B	525	CLA	C3B-C4B	5.48	1.49	1.40
29	B	529	BCR	C30-C25	5.45	1.61	1.53
24	C	478	CLA	MG-NA	5.44	2.23	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	532	SQD	O8-S	5.42	1.59	1.46
29	K	112	BCR	C5-C6	5.42	1.43	1.34
24	B	526	CLA	C1B-C2B	5.41	1.46	1.40
30	D	362	DGD	O3G-C1D	5.38	1.50	1.40
24	B	515	CLA	C1B-C2B	5.30	1.46	1.40
29	C	487	BCR	C1-C6	5.26	1.61	1.53
26	V	164	HEM	C2B-C1B	5.26	1.45	1.44
29	K	112	BCR	C30-C25	5.24	1.61	1.53
24	D	356	CLA	C1B-C2B	5.23	1.46	1.40
24	B	512	CLA	C3B-C4B	5.22	1.48	1.40
24	B	519	CLA	C3B-C4B	5.22	1.48	1.40
25	A	365	PHO	C3B-C4B	5.22	1.48	1.40
24	B	516	CLA	C1B-C2B	5.21	1.46	1.40
24	C	474	CLA	C1B-C2B	5.18	1.46	1.40
29	Z	116	BCR	C1-C6	5.16	1.61	1.53
24	C	486	CLA	C1B-C2B	5.15	1.46	1.40
24	C	482	CLA	C1B-C2B	5.15	1.46	1.40
24	B	522	CLA	C1B-C2B	5.12	1.46	1.40
24	A	362	CLA	C3B-C4B	5.10	1.48	1.40
24	B	514	CLA	MG-NA	5.09	2.22	2.07
24	C	481	CLA	MG-NA	5.07	2.22	2.07
29	B	530	BCR	C30-C25	5.06	1.61	1.53
29	D	358	BCR	C26-C25	5.02	1.42	1.34
24	D	354	CLA	C1B-C2B	5.02	1.46	1.40
24	C	485	CLA	C3B-C4B	5.00	1.48	1.40
24	C	481	CLA	C3B-C4B	4.98	1.48	1.40
24	C	477	CLA	C1B-C2B	4.98	1.46	1.40
24	C	475	CLA	C3B-C4B	4.98	1.48	1.40
29	C	487	BCR	C30-C25	4.98	1.60	1.53
24	D	364	CLA	C1B-C2B	4.97	1.46	1.40
29	B	529	BCR	C1-C6	4.97	1.60	1.53
24	B	520	CLA	C1B-C2B	4.97	1.46	1.40
24	B	515	CLA	C3B-C4B	4.96	1.48	1.40
29	B	530	BCR	C1-C6	4.95	1.60	1.53
24	C	479	CLA	C1B-C2B	4.93	1.46	1.40
24	B	513	CLA	C3B-C4B	4.91	1.48	1.40
26	E	85	HEM	C2B-C1B	4.91	1.45	1.44
34	D	363	LMT	C8-C7	-4.89	1.53	1.55
29	Z	116	BCR	C30-C25	4.87	1.60	1.53
32	D	361	SQD	C1-C2	4.84	1.66	1.52
24	C	484	CLA	C3B-C4B	4.84	1.48	1.40
24	B	518	CLA	C1B-C2B	4.83	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	478	CLA	C1B-C2B	4.82	1.46	1.40
24	B	516	CLA	MG-NA	4.82	2.21	2.07
29	J	115	BCR	C26-C25	4.81	1.42	1.34
24	B	512	CLA	C1B-C2B	4.80	1.46	1.40
33	C	492	LMG	C42-C41	-4.80	1.53	1.55
29	J	115	BCR	C30-C25	4.79	1.60	1.53
24	C	482	CLA	C3B-C4B	4.78	1.47	1.40
24	B	514	CLA	C1B-C2B	4.77	1.46	1.40
24	C	481	CLA	C1B-C2B	4.75	1.46	1.40
24	A	366	CLA	C1B-C2B	4.75	1.46	1.40
29	B	529	BCR	C26-C25	4.73	1.41	1.34
24	C	476	CLA	C3B-C4B	4.73	1.47	1.40
24	B	524	CLA	C3B-C4B	4.72	1.47	1.40
24	C	485	CLA	MG-NA	4.69	2.21	2.07
24	B	511	CLA	MG-NA	4.68	2.21	2.07
24	D	356	CLA	C3B-C4B	4.68	1.47	1.40
29	A	369	BCR	C1-C6	4.67	1.60	1.53
24	C	478	CLA	C3B-C4B	4.65	1.47	1.40
29	D	358	BCR	C30-C25	4.65	1.60	1.53
24	B	524	CLA	C1B-C2B	4.65	1.46	1.40
32	D	361	SQD	O5-C5	4.64	1.56	1.44
24	B	526	CLA	C3B-C4B	4.63	1.47	1.40
24	B	523	CLA	C1B-C2B	4.59	1.45	1.40
24	C	486	CLA	C3B-C4B	4.57	1.47	1.40
32	F	224	SQD	O8-S	4.56	1.57	1.46
29	J	115	BCR	C1-C6	4.55	1.60	1.53
24	B	522	CLA	C3B-C4B	4.55	1.47	1.40
24	C	480	CLA	C1B-C2B	4.52	1.45	1.40
29	B	528	BCR	C5-C6	4.50	1.41	1.34
24	D	356	CLA	MG-NA	4.49	2.20	2.07
24	D	364	CLA	C3B-C4B	4.49	1.47	1.40
24	B	521	CLA	C1B-C2B	4.47	1.45	1.40
33	M	217	LMG	O1-C1	4.46	1.48	1.40
24	B	511	CLA	C4B-NB	4.45	1.40	1.34
29	B	528	BCR	C30-C25	4.45	1.60	1.53
24	C	479	CLA	C3B-C4B	4.45	1.47	1.40
29	H	107	BCR	C30-C25	4.44	1.60	1.53
24	B	519	CLA	MG-NA	4.44	2.20	2.07
32	D	361	SQD	C16-C17	-4.43	1.36	1.52
24	B	518	CLA	C3B-C4B	4.42	1.47	1.40
24	B	513	CLA	C1B-C2B	4.42	1.45	1.40
24	B	511	CLA	C3B-C4B	4.41	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	527	BCR	C26-C25	4.40	1.41	1.34
32	D	361	SQD	O48-C23	4.39	1.47	1.33
26	V	164	HEM	C1A-NA	4.39	1.45	1.36
29	C	488	BCR	C30-C25	4.39	1.60	1.53
24	C	474	CLA	MG-NA	4.37	2.20	2.07
24	B	521	CLA	C3B-C4B	4.37	1.47	1.40
29	H	107	BCR	C1-C6	4.37	1.60	1.53
24	B	523	CLA	C3B-C4B	4.37	1.47	1.40
32	B	532	SQD	C6-S	4.36	1.82	1.77
32	T	213	SQD	O5-C5	4.35	1.55	1.44
29	C	488	BCR	C1-C6	4.35	1.60	1.53
32	A	372	SQD	O8-S	4.33	1.56	1.46
29	Z	116	BCR	C26-C25	4.33	1.41	1.34
26	V	164	HEM	CBC-CAC	4.31	1.54	1.28
24	B	524	CLA	MG-NA	4.30	2.20	2.07
31	A	371	LHG	P-O3	4.28	1.78	1.59
24	A	366	CLA	C3B-C4B	4.27	1.47	1.40
32	B	532	SQD	O47-C7	4.27	1.47	1.34
29	D	358	BCR	C5-C6	4.27	1.41	1.34
32	T	213	SQD	O7-S	4.27	1.59	1.45
24	C	485	CLA	C4B-NB	4.26	1.39	1.34
32	D	361	SQD	C6-S	4.24	1.82	1.77
24	A	362	CLA	MG-NA	4.24	2.19	2.07
32	F	224	SQD	O47-C7	4.23	1.47	1.34
24	C	479	CLA	MG-NA	4.23	2.19	2.07
26	E	85	HEM	C3B-C4B	4.22	1.49	1.44
32	B	532	SQD	C1-C2	4.21	1.65	1.52
24	B	516	CLA	C3B-C4B	4.21	1.46	1.40
24	B	520	CLA	C3B-C4B	4.21	1.46	1.40
24	B	514	CLA	C3B-C4B	4.19	1.46	1.40
32	B	532	SQD	O5-C5	4.19	1.54	1.44
24	C	476	CLA	CAA-C2A	4.19	1.61	1.54
33	D	359	LMG	C41-C40	-4.19	1.53	1.55
32	A	372	SQD	C33-C34	-4.14	1.37	1.52
29	K	112	BCR	C1-C6	4.11	1.59	1.53
32	F	224	SQD	O48-C23	4.11	1.46	1.33
26	V	164	HEM	C3C-CAC	4.10	1.53	1.40
29	A	369	BCR	C30-C25	4.10	1.59	1.53
29	B	530	BCR	C5-C6	4.10	1.40	1.34
24	B	515	CLA	MG-NA	4.09	2.19	2.07
29	B	527	BCR	C30-C25	4.09	1.59	1.53
24	B	517	CLA	C1B-C2B	4.09	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	528	BCR	C1-C6	4.08	1.59	1.53
32	D	361	SQD	O7-S	4.07	1.58	1.45
24	A	363	CLA	C3B-C4B	4.06	1.46	1.40
26	E	85	HEM	CBC-CAC	4.05	1.52	1.28
32	F	224	SQD	O5-C5	4.01	1.54	1.44
31	A	374	LHG	O8-C23	4.01	1.45	1.33
30	D	362	DGD	O5D-C1E	4.01	1.47	1.40
24	B	518	CLA	CAA-C2A	4.01	1.61	1.54
24	C	474	CLA	C3B-C4B	4.00	1.46	1.40
32	A	372	SQD	C6-S	4.00	1.82	1.77
29	B	529	BCR	C5-C6	4.00	1.40	1.34
32	A	372	SQD	O47-C7	3.99	1.46	1.34
32	T	213	SQD	C1-C2	3.98	1.64	1.52
24	C	486	CLA	CAA-C2A	3.97	1.61	1.54
24	C	475	CLA	MG-NA	3.97	2.19	2.07
24	D	354	CLA	C3B-C4B	3.93	1.46	1.40
32	D	361	SQD	O6-C1	3.93	1.47	1.40
24	B	517	CLA	MG-NA	3.93	2.18	2.07
24	C	483	CLA	C1A-NA	3.92	1.40	1.32
24	A	362	CLA	C1B-C2B	3.92	1.45	1.40
24	B	513	CLA	MG-NA	3.92	2.18	2.07
30	A	375	DGD	C4E-C3E	3.91	1.62	1.52
32	F	224	SQD	C17-C18	-3.90	1.38	1.52
30	A	370	DGD	O5D-C1E	3.88	1.47	1.40
26	V	164	HEM	C4A-C3A	3.88	1.45	1.40
29	C	488	BCR	C5-C6	3.87	1.40	1.34
32	D	361	SQD	O47-C7	3.87	1.46	1.34
26	E	85	HEM	CAA-C2A	3.85	1.58	1.52
29	D	358	BCR	C1-C6	3.85	1.59	1.53
29	B	527	BCR	C5-C6	3.84	1.40	1.34
32	B	532	SQD	O48-C23	3.83	1.45	1.33
30	D	362	DGD	O6D-C5D	3.83	1.53	1.44
26	E	85	HEM	C1A-NA	3.83	1.44	1.36
31	A	374	LHG	O7-C7	3.83	1.45	1.34
32	B	532	SQD	O7-S	3.81	1.57	1.45
33	C	493	LMG	C4-C3	3.80	1.62	1.52
24	C	474	CLA	CAA-C2A	3.78	1.60	1.54
32	F	224	SQD	O7-S	3.78	1.57	1.45
34	I	230	LMT	O1'-C1'	3.77	1.47	1.40
24	B	517	CLA	C3B-C4B	3.77	1.46	1.40
33	B	534	LMG	O6-C1	3.76	1.51	1.41
29	C	487	BCR	C26-C25	3.75	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	371	LHG	C12-C11	-3.73	1.53	1.55
29	B	527	BCR	C1-C6	3.73	1.59	1.53
32	A	372	SQD	C1-C2	3.72	1.63	1.52
30	A	375	DGD	C4E-C5E	3.71	1.61	1.53
24	A	363	CLA	C1B-C2B	3.69	1.44	1.40
30	D	362	DGD	O6D-C1D	3.69	1.51	1.41
33	M	217	LMG	O7-C10	3.69	1.45	1.34
30	D	362	DGD	O6E-C1E	3.68	1.51	1.41
24	A	363	CLA	CAA-C2A	3.68	1.60	1.54
24	C	480	CLA	C3B-C4B	3.67	1.46	1.40
33	I	220	LMG	O6-C1	3.67	1.51	1.41
24	D	356	CLA	CAA-C2A	3.67	1.60	1.54
24	C	477	CLA	C4B-NB	3.66	1.39	1.34
34	B	535	LMT	O5'-C1'	3.65	1.51	1.41
32	F	224	SQD	C6-S	3.65	1.81	1.77
26	E	85	HEM	CHA-C4D	3.64	1.41	1.35
30	H	208	DGD	O5D-C1E	3.64	1.46	1.40
24	B	520	CLA	MG-NA	3.63	2.18	2.07
24	D	364	CLA	CAA-C2A	3.61	1.60	1.54
24	C	480	CLA	C1A-NA	3.61	1.40	1.32
33	E	218	LMG	O6-C1	3.60	1.51	1.41
30	C	489	DGD	O5D-C1E	3.59	1.46	1.40
29	J	115	BCR	C29-C30	3.59	1.63	1.54
24	B	524	CLA	CAA-C2A	3.57	1.60	1.54
29	H	107	BCR	C29-C30	3.56	1.63	1.54
24	B	525	CLA	C4B-NB	3.56	1.39	1.34
24	C	482	CLA	MG-NA	3.56	2.17	2.07
29	B	530	BCR	C26-C25	3.55	1.40	1.34
30	A	375	DGD	O6E-C1E	3.54	1.50	1.41
32	T	213	SQD	O47-C7	3.54	1.45	1.34
34	D	363	LMT	O1'-C1'	3.53	1.46	1.40
32	T	213	SQD	O48-C23	3.50	1.44	1.33
33	C	493	LMG	O6-C1	3.50	1.50	1.41
33	M	217	LMG	O6-C1	3.50	1.50	1.41
24	C	482	CLA	C1A-NA	3.50	1.39	1.32
24	C	484	CLA	C4B-NB	3.49	1.38	1.34
24	C	477	CLA	C1A-NA	3.49	1.39	1.32
31	A	371	LHG	P-O6	3.48	1.74	1.59
24	C	477	CLA	CAA-C2A	3.47	1.60	1.54
24	A	366	CLA	MG-NA	3.47	2.17	2.07
24	C	483	CLA	C4B-NB	3.46	1.38	1.34
32	D	361	SQD	O3-C3	3.46	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	475	CLA	C1A-NA	3.46	1.39	1.32
24	C	480	CLA	MG-NA	3.46	2.17	2.07
24	B	525	CLA	MG-NA	3.46	2.17	2.07
24	B	525	CLA	C1A-NA	3.46	1.39	1.32
31	A	371	LHG	O7-C7	3.45	1.44	1.34
24	B	514	CLA	CAA-C2A	3.45	1.60	1.54
24	B	515	CLA	C4B-NB	3.45	1.38	1.34
33	D	360	LMG	O1-C1	3.44	1.46	1.40
26	E	85	HEM	FE-NA	3.43	2.07	1.92
26	E	85	HEM	CHC-C1C	3.43	1.42	1.36
33	E	218	LMG	C39-C38	-3.42	1.53	1.55
29	D	358	BCR	C29-C30	3.41	1.62	1.54
33	I	220	LMG	C4-C3	3.41	1.61	1.52
29	A	369	BCR	C26-C25	3.40	1.39	1.34
24	D	354	CLA	CAA-C2A	3.40	1.60	1.54
32	A	372	SQD	O48-C23	3.40	1.44	1.33
24	C	480	CLA	C3B-CAB	-3.40	1.46	1.49
24	B	522	CLA	C1A-NA	3.38	1.39	1.32
24	B	519	CLA	CAA-C2A	3.38	1.60	1.54
24	C	475	CLA	C4B-NB	3.38	1.38	1.34
24	B	522	CLA	MG-NA	3.38	2.17	2.07
24	B	526	CLA	MG-NA	3.37	2.17	2.07
24	B	511	CLA	C1A-NA	3.37	1.39	1.32
26	E	85	HEM	C3C-CAC	3.37	1.50	1.40
24	B	515	CLA	CAA-C2A	3.37	1.60	1.54
27	J	59	PL9	C6-C1	3.34	1.54	1.48
26	E	85	HEM	CAD-CBD	3.34	1.61	1.52
24	B	522	CLA	C4B-NB	3.32	1.38	1.34
33	B	534	LMG	C4-C5	3.33	1.60	1.53
34	M	226	LMT	O1'-C1'	3.32	1.46	1.40
32	F	224	SQD	O6-C1	3.32	1.46	1.40
32	A	372	SQD	O7-S	3.32	1.56	1.45
29	B	529	BCR	C29-C30	3.31	1.62	1.54
24	B	519	CLA	C4B-NB	3.31	1.38	1.34
24	D	364	CLA	MG-NA	3.31	2.17	2.07
32	F	224	SQD	C1-C2	3.30	1.62	1.52
33	A	373	LMG	O6-C1	3.30	1.50	1.41
24	B	526	CLA	CAA-C2A	3.29	1.60	1.54
24	C	486	CLA	C4B-NB	3.29	1.38	1.34
24	B	517	CLA	CAA-C2A	3.28	1.60	1.54
29	Z	116	BCR	C29-C30	3.28	1.62	1.54
30	A	375	DGD	O3G-C1D	3.28	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	478	CLA	CAA-C2A	3.27	1.60	1.54
33	D	360	LMG	O6-C1	3.26	1.50	1.41
24	C	484	CLA	C1A-NA	3.26	1.39	1.32
24	B	512	CLA	C1A-NA	3.25	1.39	1.32
30	A	375	DGD	C4D-C5D	3.25	1.60	1.53
24	B	521	CLA	C1A-NA	3.25	1.39	1.32
33	C	493	LMG	O6-C5	3.23	1.52	1.44
24	C	478	CLA	C1A-NA	3.23	1.39	1.32
24	B	514	CLA	C1A-NA	3.23	1.39	1.32
24	C	486	CLA	C1A-NA	3.23	1.39	1.32
29	B	530	BCR	C29-C30	3.22	1.62	1.54
32	A	372	SQD	O5-C5	3.22	1.52	1.44
29	A	369	BCR	C5-C6	3.21	1.39	1.34
24	B	526	CLA	C1A-NA	3.20	1.39	1.32
33	C	492	LMG	O1-C1	3.20	1.46	1.40
24	C	479	CLA	CAA-C2A	3.18	1.59	1.54
26	V	164	HEM	FE-NA	3.18	2.06	1.92
24	C	485	CLA	C1A-NA	3.18	1.39	1.32
29	A	369	BCR	C2-C1	3.18	1.62	1.54
24	D	364	CLA	C1A-NA	3.17	1.39	1.32
24	C	484	CLA	CAA-C2A	3.17	1.59	1.54
34	O	274	LMT	O1B-C1B	3.17	1.50	1.41
24	C	481	CLA	C1A-NA	3.16	1.39	1.32
34	T	227	LMT	O5B-C1B	3.16	1.49	1.41
26	E	85	HEM	FE-NB	3.15	2.09	1.97
24	B	511	CLA	CHB-C4A	3.15	1.43	1.36
24	B	513	CLA	C1A-NA	3.14	1.39	1.32
30	A	375	DGD	O5D-C1E	3.14	1.45	1.40
24	A	362	CLA	CAA-C2A	3.14	1.59	1.54
29	B	528	BCR	C2-C1	3.14	1.62	1.54
24	B	523	CLA	MG-NA	3.14	2.16	2.07
24	B	518	CLA	C1A-NA	3.14	1.39	1.32
29	B	530	BCR	C2-C1	3.13	1.62	1.54
24	C	485	CLA	C1B-NB	3.13	1.38	1.34
24	C	482	CLA	C4B-NB	3.13	1.38	1.34
32	D	361	SQD	O5-C1	3.12	1.49	1.41
30	A	375	DGD	O6D-C5D	3.12	1.52	1.44
33	B	531	LMG	C41-C40	-3.12	1.53	1.55
29	K	112	BCR	C29-C30	3.11	1.62	1.54
24	A	366	CLA	C1C-NC	-3.11	1.35	1.38
30	D	362	DGD	C4E-C5E	3.11	1.59	1.53
32	T	213	SQD	O5-C1	3.11	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	492	LMG	O6-C1	3.11	1.49	1.41
30	A	370	DGD	O3G-C1D	3.10	1.45	1.40
32	B	532	SQD	O3-C3	3.09	1.50	1.43
33	B	534	LMG	O1-C1	3.09	1.45	1.40
24	D	364	CLA	C1C-NC	-3.09	1.35	1.38
33	C	493	LMG	C4-C5	3.09	1.59	1.53
33	M	217	LMG	O6-C5	3.08	1.52	1.44
24	B	517	CLA	C1A-NA	3.08	1.39	1.32
24	B	521	CLA	CAA-C2A	3.07	1.59	1.54
24	A	363	CLA	C4B-NB	3.07	1.38	1.34
30	A	370	DGD	O6D-C1D	3.07	1.49	1.41
24	C	475	CLA	CAA-C2A	3.07	1.59	1.54
26	V	164	HEM	CAA-C2A	3.07	1.57	1.52
26	V	164	HEM	FE-NB	3.06	2.09	1.97
24	B	513	CLA	CAA-C2A	3.06	1.59	1.54
30	C	489	DGD	C9B-C8B	-3.06	1.53	1.55
33	I	220	LMG	O6-C5	3.06	1.52	1.44
29	Z	116	BCR	C5-C6	3.06	1.39	1.34
24	B	514	CLA	C4B-NB	3.06	1.38	1.34
30	A	370	DGD	C4D-C5D	3.05	1.59	1.53
24	B	516	CLA	CAA-C2A	3.06	1.59	1.54
26	E	85	HEM	C1A-C2A	3.05	1.48	1.43
24	A	362	CLA	C1A-NA	3.05	1.39	1.32
27	A	367	PL9	C7-C3	3.05	1.54	1.51
26	E	85	HEM	C3B-CAB	3.05	1.49	1.40
24	B	523	CLA	C1A-NA	3.04	1.38	1.32
26	V	164	HEM	C3B-C4B	3.04	1.48	1.44
24	B	520	CLA	C1A-NA	3.04	1.38	1.32
29	C	488	BCR	C26-C25	3.03	1.39	1.34
24	A	363	CLA	C1A-NA	3.03	1.38	1.32
32	A	372	SQD	O3-C3	3.03	1.50	1.43
29	B	527	BCR	C29-C30	3.03	1.61	1.54
30	A	375	DGD	O2G-C1B	3.03	1.43	1.34
24	C	474	CLA	C1A-NA	3.02	1.38	1.32
34	O	274	LMT	O5B-C1B	3.02	1.49	1.41
24	C	476	CLA	C4B-NB	3.01	1.38	1.34
33	I	220	LMG	C4-C5	3.01	1.59	1.53
29	B	528	BCR	C26-C25	3.01	1.39	1.34
24	B	518	CLA	MG-NA	3.01	2.16	2.07
24	A	362	CLA	C1C-NC	-3.00	1.35	1.38
24	B	524	CLA	C1A-NA	3.00	1.38	1.32
33	B	533	LMG	O6-C1	2.99	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	360	LMG	C40-C39	-2.99	1.54	1.55
29	C	487	BCR	C29-C30	2.99	1.61	1.54
24	B	512	CLA	C4B-NB	2.98	1.38	1.34
24	B	526	CLA	C4B-NB	2.98	1.38	1.34
29	B	528	BCR	C29-C30	2.97	1.61	1.54
24	C	476	CLA	C1A-NA	2.97	1.38	1.32
24	B	525	CLA	CHB-C4A	2.97	1.43	1.36
30	C	490	DGD	O6D-C1D	2.97	1.49	1.41
24	D	354	CLA	C4B-NB	2.96	1.38	1.34
33	E	218	LMG	O1-C1	2.96	1.45	1.40
34	B	536	LMT	O1'-C1'	2.95	1.45	1.40
24	C	485	CLA	CHB-C4A	2.95	1.43	1.36
24	C	478	CLA	C4B-NB	2.95	1.38	1.34
24	B	516	CLA	C4B-NB	2.94	1.38	1.34
30	A	370	DGD	C4E-C3E	2.94	1.60	1.52
26	V	164	HEM	CAD-CBD	2.94	1.60	1.52
29	B	527	BCR	C2-C1	2.94	1.61	1.54
29	C	488	BCR	C2-C1	2.94	1.61	1.54
29	Z	116	BCR	C2-C1	2.94	1.61	1.54
26	V	164	HEM	C3B-C2B	-2.94	1.38	1.43
24	D	354	CLA	C1A-NA	2.93	1.38	1.32
24	C	481	CLA	C4B-NB	2.93	1.38	1.34
24	B	519	CLA	CHB-C4A	2.93	1.43	1.36
24	C	482	CLA	CAA-C2A	2.92	1.59	1.54
24	B	524	CLA	C4B-NB	2.92	1.38	1.34
24	A	366	CLA	C1A-NA	2.92	1.38	1.32
24	C	484	CLA	CHB-C4A	2.92	1.43	1.36
24	D	356	CLA	CHB-C4A	2.91	1.43	1.36
26	E	85	HEM	C4D-ND	-2.91	1.33	1.39
24	B	518	CLA	C1C-NC	-2.91	1.36	1.38
24	C	477	CLA	MG-NB	2.91	2.11	2.05
29	C	487	BCR	C5-C6	2.91	1.39	1.34
24	C	479	CLA	C1A-NA	2.90	1.38	1.32
27	J	59	PL9	C7-C3	2.89	1.53	1.51
24	B	519	CLA	C1A-NA	2.89	1.38	1.32
30	A	370	DGD	O6E-C1E	2.89	1.49	1.41
24	B	511	CLA	C1B-NB	2.89	1.38	1.34
24	B	519	CLA	C1B-NB	2.89	1.38	1.34
24	C	476	CLA	C3D-CAD	-2.88	1.41	1.47
29	B	529	BCR	C2-C1	2.88	1.61	1.54
32	F	224	SQD	C44-C45	2.88	1.58	1.50
24	B	526	CLA	C1C-NC	-2.87	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	T	213	SQD	O3-C3	2.87	1.49	1.43
30	D	362	DGD	C1D-C2D	2.87	1.61	1.52
32	B	532	SQD	O6-C1	2.86	1.45	1.40
29	K	112	BCR	C2-C1	2.86	1.61	1.54
29	H	107	BCR	C2-C1	2.86	1.61	1.54
30	C	491	DGD	O6D-C1D	2.86	1.49	1.41
29	A	369	BCR	C29-C30	2.86	1.61	1.54
34	D	363	LMT	O5'-C1'	2.86	1.49	1.41
33	I	220	LMG	C3-C2	2.85	1.60	1.52
34	B	535	LMT	O5B-C1B	2.85	1.49	1.41
32	F	224	SQD	O3-C3	2.85	1.49	1.43
30	A	375	DGD	C4D-C3D	2.84	1.59	1.52
24	A	366	CLA	C1B-CHB	-2.84	1.32	1.39
33	M	217	LMG	C3-C2	2.84	1.59	1.52
24	B	515	CLA	C1B-NB	2.83	1.38	1.34
29	D	358	BCR	C2-C1	2.83	1.61	1.54
24	D	356	CLA	C1A-NA	2.83	1.38	1.32
26	V	164	HEM	FE-NC	2.83	2.08	1.97
24	C	476	CLA	CHB-C4A	2.83	1.43	1.36
32	F	224	SQD	C8-C7	2.83	1.59	1.50
24	B	515	CLA	C1A-NA	2.82	1.38	1.32
34	D	363	LMT	O5B-C1B	2.82	1.49	1.41
24	B	517	CLA	C4B-NB	2.82	1.38	1.34
26	E	85	HEM	C2A-C3A	2.82	1.46	1.37
24	B	512	CLA	MG-NA	2.81	2.15	2.07
30	D	362	DGD	C4E-C3E	2.80	1.59	1.52
24	B	516	CLA	C3D-CAD	-2.80	1.41	1.47
30	D	362	DGD	C3D-C2D	2.79	1.59	1.52
31	A	371	LHG	O8-C23	2.79	1.42	1.33
26	V	164	HEM	CMA-C3A	2.79	1.57	1.51
24	B	516	CLA	C1A-NA	2.78	1.38	1.32
29	H	107	BCR	C14-C13	2.78	1.39	1.35
26	E	85	HEM	FE-NC	2.78	2.08	1.97
29	K	112	BCR	C26-C25	2.78	1.38	1.34
24	B	514	CLA	CHB-C4A	2.78	1.43	1.36
33	C	492	LMG	O6-C5	2.78	1.51	1.44
34	O	274	LMT	O5'-C1'	2.78	1.48	1.41
26	V	164	HEM	C3C-C2C	-2.78	1.38	1.43
26	V	164	HEM	CHC-C1C	2.77	1.41	1.36
24	A	363	CLA	C3D-CAD	-2.77	1.41	1.47
34	I	230	LMT	O5B-C1B	2.77	1.48	1.41
24	C	478	CLA	CHB-C4A	2.75	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	512	CLA	C1B-CHB	-2.75	1.32	1.39
34	T	227	LMT	O1B-C1B	2.75	1.49	1.41
24	B	524	CLA	MG-NB	2.75	2.11	2.05
24	B	522	CLA	C1C-NC	-2.74	1.36	1.38
32	B	532	SQD	O5-C1	2.74	1.48	1.41
34	B	536	LMT	O5'-C1'	2.74	1.48	1.41
26	E	85	HEM	C3C-C2C	-2.74	1.39	1.43
25	D	355	PHO	C4B-NB	2.73	1.39	1.36
26	E	85	HEM	C3B-C2B	-2.73	1.39	1.43
30	H	208	DGD	C1E-C2E	2.73	1.60	1.52
29	K	112	BCR	C14-C13	2.73	1.39	1.35
26	E	85	HEM	CMA-C3A	2.72	1.57	1.51
24	B	521	CLA	C1B-CHB	-2.71	1.32	1.39
34	D	363	LMT	C4B-C5B	2.71	1.59	1.53
30	A	370	DGD	C4E-C5E	2.70	1.59	1.53
24	D	354	CLA	CHB-C4A	2.70	1.42	1.36
24	D	356	CLA	C4B-NB	2.70	1.38	1.34
29	C	488	BCR	C29-C30	2.70	1.61	1.54
29	J	115	BCR	C14-C13	2.69	1.39	1.35
24	A	363	CLA	MG-NA	2.69	2.15	2.07
24	C	476	CLA	C1C-NC	-2.69	1.36	1.38
24	C	483	CLA	C4A-NA	-2.69	1.33	1.39
26	V	164	HEM	C1A-C2A	2.68	1.48	1.43
24	B	518	CLA	C4B-NB	2.68	1.38	1.34
30	C	491	DGD	O3G-C1D	2.67	1.45	1.40
32	F	224	SQD	O5-C1	2.67	1.48	1.41
32	A	372	SQD	C32-C31	-2.66	1.35	1.51
30	C	491	DGD	O6D-C5D	2.66	1.51	1.44
24	B	519	CLA	C3D-CAD	-2.66	1.41	1.47
24	A	363	CLA	CHB-C4A	2.66	1.42	1.36
33	B	531	LMG	O6-C1	2.66	1.48	1.41
34	I	230	LMT	O5'-C1'	2.65	1.48	1.41
24	C	482	CLA	CHB-C4A	2.65	1.42	1.36
24	B	515	CLA	C3D-CAD	-2.65	1.42	1.47
24	B	522	CLA	CHB-C4A	2.65	1.42	1.36
32	T	213	SQD	C17-C16	-2.64	1.35	1.51
26	V	164	HEM	CHB-C1B	-2.64	1.32	1.35
33	M	217	LMG	C4-C5	2.64	1.58	1.53
24	C	477	CLA	C1B-CHB	-2.64	1.32	1.39
32	B	532	SQD	C15-C14	-2.64	1.35	1.51
24	C	484	CLA	C1B-NB	2.64	1.37	1.34
24	C	483	CLA	MG-NA	2.63	2.15	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B	533	LMG	C4-C5	2.63	1.58	1.53
24	B	523	CLA	C4A-NA	-2.63	1.33	1.39
33	B	533	LMG	O1-C1	2.63	1.45	1.40
24	B	515	CLA	CHB-C4A	2.62	1.42	1.36
24	B	513	CLA	C1B-CHB	-2.62	1.32	1.39
32	A	372	SQD	O6-C44	-2.62	1.38	1.43
24	C	481	CLA	MG-NB	2.62	2.10	2.05
24	C	481	CLA	C3D-CAD	-2.62	1.42	1.47
24	A	363	CLA	MG-NB	2.62	2.10	2.05
29	B	529	BCR	C14-C13	2.62	1.39	1.35
24	B	517	CLA	CHB-C4A	2.61	1.42	1.36
24	B	520	CLA	C4A-NA	-2.61	1.33	1.39
30	A	370	DGD	C3E-C2E	2.61	1.59	1.52
32	T	213	SQD	O6-C1	2.61	1.44	1.40
26	V	164	HEM	C3B-CAB	2.60	1.48	1.40
24	C	479	CLA	C1C-NC	-2.60	1.36	1.38
32	B	532	SQD	C11-C10	-2.60	1.35	1.51
30	C	489	DGD	O6D-C5D	2.59	1.50	1.44
33	C	492	LMG	C4-C5	2.59	1.58	1.53
24	C	480	CLA	C1B-CHB	-2.59	1.32	1.39
32	T	213	SQD	C19-C18	-2.59	1.35	1.51
32	D	361	SQD	C11-C10	-2.59	1.35	1.51
33	B	533	LMG	O6-C5	2.59	1.50	1.44
30	C	490	DGD	O6D-C5D	2.59	1.50	1.44
30	H	208	DGD	C4E-C5E	2.59	1.58	1.53
24	C	479	CLA	C4B-NB	2.59	1.37	1.34
24	B	511	CLA	C3D-CAD	-2.58	1.42	1.47
32	B	532	SQD	C17-C16	-2.58	1.35	1.51
33	B	534	LMG	C3-C2	2.57	1.59	1.52
32	A	372	SQD	C33-C32	-2.57	1.35	1.51
24	B	513	CLA	C4A-NA	-2.57	1.33	1.39
33	C	493	LMG	C9-C8	2.57	1.57	1.50
29	J	115	BCR	C2-C1	2.57	1.60	1.54
24	C	478	CLA	CHC-C1C	2.56	1.44	1.35
29	H	107	BCR	C5-C6	2.56	1.38	1.34
24	B	516	CLA	C4A-NA	-2.56	1.33	1.39
29	H	107	BCR	C38-C26	2.56	1.55	1.51
24	C	481	CLA	C1B-NB	2.56	1.37	1.34
24	C	478	CLA	C1C-C2C	2.56	1.49	1.44
24	B	525	CLA	CAA-C2A	2.56	1.58	1.54
32	D	361	SQD	C12-C11	-2.56	1.35	1.51
30	C	489	DGD	O6D-C1D	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	362	DGD	O2G-C1B	2.55	1.42	1.34
33	I	220	LMG	O7-C10	2.55	1.42	1.34
30	D	362	DGD	C4D-C3D	2.54	1.59	1.52
26	E	85	HEM	CHB-C1B	-2.54	1.32	1.35
33	B	534	LMG	O6-C5	2.54	1.50	1.44
33	D	360	LMG	O6-C5	2.53	1.50	1.44
32	D	361	SQD	C15-C14	-2.53	1.35	1.51
24	C	474	CLA	C1C-NC	-2.52	1.36	1.38
34	T	227	LMT	O1'-C1'	2.52	1.44	1.40
24	B	526	CLA	C3D-CAD	-2.52	1.42	1.47
29	C	487	BCR	C2-C1	2.52	1.60	1.54
32	T	213	SQD	C16-C15	-2.52	1.36	1.51
24	A	366	CLA	C4-C3	2.52	1.57	1.50
30	C	491	DGD	C4E-C3E	2.52	1.59	1.52
32	D	361	SQD	C16-C15	-2.51	1.36	1.51
32	T	213	SQD	C20-C19	-2.51	1.36	1.51
24	B	514	CLA	MG-NB	2.51	2.10	2.05
24	C	479	CLA	C1B-NB	2.51	1.37	1.34
30	A	375	DGD	O6D-C1D	2.50	1.48	1.41
24	C	481	CLA	CHC-C1C	2.50	1.43	1.35
33	E	218	LMG	O6-C5	2.50	1.50	1.44
32	T	213	SQD	C15-C14	-2.49	1.36	1.51
33	C	493	LMG	O7-C10	2.49	1.41	1.34
24	B	526	CLA	C2-C3	2.49	1.38	1.32
30	A	375	DGD	O6E-C5E	2.49	1.50	1.44
24	B	517	CLA	C1B-CHB	-2.49	1.33	1.39
24	C	474	CLA	CHB-C4A	2.48	1.42	1.36
30	C	490	DGD	C4D-C5D	2.48	1.58	1.53
24	B	523	CLA	C3D-CAD	-2.48	1.42	1.47
32	A	372	SQD	C12-C11	-2.48	1.36	1.51
24	C	483	CLA	CAA-C2A	2.48	1.58	1.54
25	D	355	PHO	C4D-CHA	-2.48	1.42	1.45
24	A	366	CLA	C4A-NA	-2.48	1.33	1.39
32	A	372	SQD	C17-C16	-2.48	1.36	1.51
33	D	359	LMG	O6-C1	2.48	1.48	1.41
24	B	520	CLA	C4B-NB	2.48	1.37	1.34
24	A	363	CLA	C4A-NA	-2.48	1.33	1.39
32	T	213	SQD	C12-C11	-2.47	1.36	1.51
26	V	164	HEM	C2A-C3A	2.47	1.45	1.37
33	B	534	LMG	C4-C3	2.47	1.59	1.52
30	C	489	DGD	C4E-C3E	2.47	1.59	1.52
24	C	478	CLA	C1C-NC	-2.47	1.36	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	481	CLA	C1C-NC	-2.47	1.36	1.38
24	B	515	CLA	MG-NB	2.47	2.10	2.05
30	D	362	DGD	C3E-C2E	2.47	1.59	1.52
32	T	213	SQD	C11-C10	-2.46	1.36	1.51
33	B	531	LMG	O1-C1	2.46	1.44	1.40
24	B	521	CLA	CHB-C4A	2.46	1.42	1.36
24	C	475	CLA	C1B-NB	2.45	1.37	1.34
24	D	354	CLA	MG-NB	2.45	2.10	2.05
32	D	361	SQD	C44-C45	2.45	1.57	1.50
24	B	522	CLA	CAA-C2A	2.45	1.58	1.54
32	A	372	SQD	C15-C14	-2.45	1.36	1.51
32	A	372	SQD	C16-C15	-2.45	1.36	1.51
30	A	375	DGD	C3E-C2E	2.45	1.58	1.52
24	D	356	CLA	C4A-NA	-2.45	1.33	1.39
24	D	356	CLA	C3D-CAD	-2.45	1.42	1.47
24	B	512	CLA	C3D-CAD	-2.45	1.42	1.47
24	B	523	CLA	C1B-CHB	-2.45	1.33	1.39
24	B	519	CLA	C1C-NC	-2.44	1.36	1.38
24	D	364	CLA	C1B-CHB	-2.44	1.33	1.39
29	B	530	BCR	C14-C13	2.44	1.39	1.35
30	D	362	DGD	C4D-C5D	2.44	1.58	1.53
24	C	485	CLA	MG-NB	2.44	2.10	2.05
33	D	359	LMG	C4-C3	2.44	1.58	1.52
24	A	362	CLA	C4B-NB	2.44	1.37	1.34
24	B	517	CLA	C3B-CAB	-2.43	1.47	1.49
24	D	364	CLA	C4A-NA	-2.43	1.33	1.39
32	D	361	SQD	C14-C13	-2.43	1.36	1.51
24	A	362	CLA	C1B-CHB	-2.43	1.33	1.39
32	F	224	SQD	C17-C16	-2.43	1.36	1.51
24	A	366	CLA	C4B-NB	2.42	1.37	1.34
24	C	480	CLA	C1C-NC	-2.42	1.36	1.38
24	C	480	CLA	C3D-CAD	-2.42	1.42	1.47
24	B	525	CLA	MG-NB	2.42	2.10	2.05
24	B	521	CLA	C4B-NB	2.42	1.37	1.34
30	H	208	DGD	O3G-C1D	2.41	1.44	1.40
24	B	526	CLA	CHB-C4A	2.41	1.42	1.36
34	B	536	LMT	O5B-C1B	2.41	1.48	1.41
32	B	532	SQD	C12-C11	-2.41	1.36	1.51
32	F	224	SQD	C15-C14	-2.41	1.36	1.51
24	D	364	CLA	C3D-CAD	-2.41	1.42	1.47
32	B	532	SQD	C19-C18	-2.41	1.36	1.51
24	B	514	CLA	C1B-NB	2.41	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	372	SQD	C14-C13	-2.41	1.36	1.51
32	A	372	SQD	C11-C10	-2.40	1.36	1.51
24	B	524	CLA	C1B-CHB	-2.40	1.33	1.39
33	A	373	LMG	O1-C1	2.40	1.44	1.40
24	C	481	CLA	CHB-C4A	2.40	1.42	1.36
24	A	363	CLA	C1B-CHB	-2.40	1.33	1.39
33	A	373	LMG	C43-C42	-2.40	1.54	1.55
24	B	513	CLA	C4B-NB	2.40	1.37	1.34
24	B	523	CLA	CHB-C4A	2.40	1.42	1.36
24	B	523	CLA	CAA-C2A	2.40	1.58	1.54
33	C	493	LMG	C3-C2	2.39	1.58	1.52
24	B	517	CLA	C2-C3	2.39	1.37	1.32
24	B	516	CLA	CHB-C4A	2.39	1.42	1.36
30	C	491	DGD	O5D-C1E	2.39	1.44	1.40
24	B	513	CLA	C1C-NC	-2.39	1.36	1.38
24	C	486	CLA	C4-C3	2.38	1.56	1.50
24	B	520	CLA	CHB-C4A	2.38	1.42	1.36
33	C	493	LMG	O8-C28	2.38	1.40	1.33
32	D	361	SQD	C13-C12	-2.37	1.36	1.51
24	B	514	CLA	C3D-CAD	-2.37	1.42	1.47
24	C	481	CLA	CAA-C2A	2.37	1.58	1.54
32	T	213	SQD	C18-C17	-2.37	1.36	1.51
32	T	213	SQD	C14-C13	-2.37	1.36	1.51
33	B	531	LMG	C4-C3	2.37	1.58	1.52
33	B	531	LMG	O7-C10	2.37	1.41	1.34
32	B	532	SQD	C16-C15	-2.37	1.36	1.51
24	B	524	CLA	CHB-C4A	2.37	1.42	1.36
26	E	85	HEM	CMD-C2D	2.36	1.54	1.47
24	B	524	CLA	CHC-C1C	2.36	1.43	1.35
24	D	354	CLA	C1C-C2C	2.36	1.49	1.44
26	E	85	HEM	CMB-C2B	2.36	1.54	1.47
32	F	224	SQD	C16-C15	-2.36	1.37	1.51
29	A	369	BCR	C19-C18	-2.36	1.40	1.45
32	B	532	SQD	C14-C13	-2.36	1.37	1.51
24	B	526	CLA	C1B-CHB	-2.36	1.33	1.39
24	C	484	CLA	C3D-CAD	-2.35	1.42	1.47
24	D	354	CLA	C4C-C3C	2.35	1.49	1.45
30	H	208	DGD	C4E-C3E	2.35	1.58	1.52
30	D	362	DGD	O1G-C1A	2.35	1.40	1.33
24	B	513	CLA	C4-C3	2.35	1.56	1.50
33	C	492	LMG	C4-C3	2.35	1.58	1.52
24	B	525	CLA	C3D-CAD	-2.35	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	362	CLA	C3D-CAD	-2.34	1.42	1.47
26	V	164	HEM	CMB-C2B	2.35	1.54	1.47
24	C	486	CLA	C1B-NB	2.34	1.37	1.34
24	C	479	CLA	C3D-CAD	-2.34	1.42	1.47
33	D	359	LMG	O1-C1	2.34	1.44	1.40
24	A	362	CLA	C4A-NA	-2.34	1.34	1.39
32	A	372	SQD	O5-C1	2.34	1.47	1.41
30	H	208	DGD	O6D-C1D	2.33	1.47	1.41
24	B	526	CLA	C4A-NA	-2.33	1.34	1.39
24	B	518	CLA	CHB-C4A	2.33	1.42	1.36
24	C	479	CLA	CHB-C4A	2.33	1.42	1.36
24	C	486	CLA	C4A-NA	-2.33	1.34	1.39
34	B	535	LMT	O1'-C1'	2.33	1.44	1.40
32	B	532	SQD	C18-C17	-2.33	1.37	1.51
24	B	512	CLA	C4A-NA	-2.33	1.34	1.39
26	E	85	HEM	C2C-C1C	2.32	1.50	1.43
24	A	363	CLA	C5-C3	2.32	1.56	1.51
32	A	372	SQD	C20-C19	-2.32	1.37	1.51
24	B	521	CLA	MG-NB	2.32	2.10	2.05
30	D	362	DGD	C1E-C2E	2.32	1.59	1.52
32	A	372	SQD	C19-C18	-2.32	1.37	1.51
24	B	523	CLA	C4B-NB	2.32	1.37	1.34
27	J	59	PL9	C2-C1	2.31	1.51	1.44
24	B	512	CLA	MG-NB	2.31	2.10	2.05
24	B	520	CLA	C4-C3	2.32	1.56	1.50
24	B	514	CLA	CHC-C1C	2.31	1.43	1.35
32	B	532	SQD	C24-C23	2.31	1.57	1.50
27	J	59	PL9	C3-C4	2.31	1.53	1.49
25	D	355	PHO	C4-C3	2.30	1.56	1.50
24	C	477	CLA	CHC-C1C	2.30	1.43	1.35
24	B	524	CLA	C1C-NC	-2.30	1.36	1.38
24	C	478	CLA	C3D-CAD	-2.29	1.42	1.47
32	F	224	SQD	C30-C31	2.29	1.60	1.52
24	C	485	CLA	CHC-C1C	2.29	1.43	1.35
24	C	481	CLA	C4-C3	2.29	1.56	1.50
30	H	208	DGD	O6E-C1E	2.29	1.47	1.41
24	C	486	CLA	CHC-C1C	2.29	1.43	1.35
34	B	536	LMT	C4B-C5B	2.29	1.58	1.53
24	B	517	CLA	C3D-CAD	-2.29	1.42	1.47
32	T	213	SQD	C13-C12	-2.28	1.37	1.51
24	C	486	CLA	CHB-C4A	2.28	1.41	1.36
24	B	512	CLA	CHC-C1C	2.28	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	478	CLA	C4A-NA	-2.28	1.34	1.39
34	T	227	LMT	O1B-C4'	2.28	1.49	1.43
30	C	489	DGD	O6E-C1E	2.28	1.47	1.41
24	B	520	CLA	CAA-C2A	2.28	1.58	1.54
24	B	517	CLA	MG-NB	2.27	2.10	2.05
24	C	478	CLA	C4C-C3C	2.27	1.49	1.45
29	B	529	BCR	C24-C23	2.27	1.39	1.32
30	C	491	DGD	O6E-C1E	2.27	1.47	1.41
24	B	519	CLA	MG-NC	2.27	2.13	2.07
24	B	512	CLA	C1C-NC	-2.27	1.36	1.38
30	D	362	DGD	O6E-C5E	2.27	1.50	1.44
24	D	354	CLA	CHC-C1C	2.27	1.43	1.35
24	C	476	CLA	C1B-NB	2.26	1.37	1.34
24	C	485	CLA	C3D-CAD	-2.26	1.42	1.47
24	C	482	CLA	C4A-NA	-2.26	1.34	1.39
24	C	480	CLA	MG-NC	2.26	2.13	2.07
29	J	115	BCR	C37-C22	2.26	1.54	1.51
32	B	532	SQD	C32-C31	-2.25	1.37	1.51
30	A	370	DGD	CDA-CCA	-2.25	1.54	1.55
24	B	511	CLA	CAA-C2A	2.25	1.58	1.54
32	B	532	SQD	C33-C32	-2.25	1.37	1.51
30	A	370	DGD	C1E-C2E	2.24	1.59	1.52
24	C	482	CLA	C1C-NC	-2.24	1.36	1.38
24	B	518	CLA	C4A-NA	-2.23	1.34	1.39
32	F	224	SQD	C11-C10	-2.23	1.37	1.51
33	D	359	LMG	O6-C5	2.23	1.49	1.44
24	D	354	CLA	C1B-NB	2.23	1.37	1.34
24	B	522	CLA	CHC-C1C	2.23	1.43	1.35
24	C	479	CLA	MG-NB	2.23	2.10	2.05
33	E	218	LMG	O7-C10	2.22	1.41	1.34
33	B	531	LMG	O6-C5	2.22	1.49	1.44
32	B	532	SQD	C44-C45	2.21	1.56	1.50
24	B	511	CLA	C4-C3	2.21	1.56	1.50
24	B	517	CLA	CHC-C1C	2.21	1.42	1.35
24	A	362	CLA	CAA-CBA	-2.21	1.45	1.52
32	A	372	SQD	C13-C12	-2.21	1.37	1.51
24	C	482	CLA	C1B-CHB	-2.20	1.33	1.39
24	C	475	CLA	C1B-CHB	-2.20	1.33	1.39
24	C	480	CLA	C4B-NB	2.20	1.37	1.34
32	B	532	SQD	C13-C12	-2.20	1.38	1.51
29	D	358	BCR	C38-C26	2.19	1.54	1.51
32	F	224	SQD	C12-C11	-2.19	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	477	CLA	C3D-CAD	-2.19	1.42	1.47
33	I	220	LMG	C1-C2	2.19	1.59	1.52
24	B	517	CLA	C1C-C2C	2.19	1.49	1.44
25	A	365	PHO	C4B-NB	2.19	1.38	1.36
24	B	520	CLA	C4C-C3C	2.19	1.49	1.45
24	C	475	CLA	C1C-NC	-2.18	1.36	1.38
30	C	490	DGD	C6D-C5D	2.18	1.58	1.51
32	B	532	SQD	C20-C19	-2.18	1.38	1.51
32	B	532	SQD	C36-C35	-2.18	1.38	1.51
34	M	226	LMT	O5'-C1'	2.18	1.47	1.41
24	A	362	CLA	MG-NB	2.18	2.09	2.05
26	V	164	HEM	CMD-C2D	2.18	1.54	1.47
24	B	512	CLA	CAA-CBA	-2.17	1.45	1.52
24	C	475	CLA	C4A-NA	-2.17	1.34	1.39
24	B	519	CLA	C4A-NA	-2.16	1.34	1.39
24	C	483	CLA	C1B-CHB	-2.16	1.33	1.39
33	B	533	LMG	C4-C3	2.16	1.58	1.52
24	B	516	CLA	MG-NC	2.15	2.13	2.07
24	B	515	CLA	C1B-CHB	-2.15	1.33	1.39
24	C	485	CLA	MG-NC	2.15	2.13	2.07
33	E	218	LMG	C7-C8	2.15	1.56	1.50
24	C	483	CLA	C3D-CAD	-2.15	1.43	1.47
34	O	274	LMT	C4B-C5B	2.15	1.57	1.53
30	C	489	DGD	C4D-C5D	2.14	1.57	1.53
34	B	535	LMT	C4B-C5B	2.14	1.57	1.53
34	O	274	LMT	O1B-C4'	2.14	1.49	1.43
24	C	477	CLA	CHB-C4A	2.13	1.41	1.36
24	D	356	CLA	MG-NB	2.13	2.09	2.05
30	C	489	DGD	O3G-C1D	2.13	1.44	1.40
29	B	527	BCR	C23-C22	-2.13	1.41	1.45
26	V	164	HEM	C2C-C1C	2.13	1.49	1.43
32	D	361	SQD	C8-C7	2.13	1.57	1.50
32	F	224	SQD	C14-C13	-2.13	1.38	1.51
30	A	375	DGD	C1D-C2D	2.12	1.58	1.52
24	B	521	CLA	MG-NC	2.12	2.13	2.07
24	C	486	CLA	C1C-C2C	2.12	1.48	1.44
34	B	536	LMT	O1B-C1B	2.12	1.47	1.41
24	C	485	CLA	C4A-NA	-2.12	1.34	1.39
33	I	220	LMG	O1-C1	2.12	1.44	1.40
24	B	525	CLA	C1B-NB	2.12	1.37	1.34
24	D	356	CLA	CHC-C1C	2.12	1.42	1.35
24	A	362	CLA	CHC-C1C	2.12	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	489	DGD	C4D-C3D	2.12	1.58	1.52
33	C	493	LMG	C40-C39	-2.12	1.54	1.55
24	B	520	CLA	C1B-CHB	-2.12	1.34	1.39
30	A	375	DGD	O1G-C1A	2.12	1.39	1.33
24	C	481	CLA	C1B-CHB	-2.12	1.34	1.39
24	B	513	CLA	C3D-CAD	-2.11	1.43	1.47
24	C	476	CLA	MG-NB	2.11	2.09	2.05
30	A	375	DGD	O5D-C6D	2.11	1.47	1.43
34	B	536	LMT	O5B-C5B	2.11	1.49	1.44
24	C	475	CLA	CHC-C1C	2.11	1.42	1.35
30	C	490	DGD	O3G-C1D	2.11	1.44	1.40
24	B	511	CLA	MG-NC	2.10	2.13	2.07
27	J	59	PL9	C31-C29	2.10	1.51	1.40
24	B	518	CLA	C1B-CHB	-2.11	1.34	1.39
24	B	522	CLA	C3B-CAB	-2.10	1.47	1.49
33	B	534	LMG	C1-C2	2.10	1.58	1.52
24	C	474	CLA	C4B-NB	2.10	1.37	1.34
24	D	354	CLA	C4A-NA	-2.10	1.34	1.39
24	C	476	CLA	C4A-NA	-2.10	1.34	1.39
24	C	482	CLA	CHC-C1C	2.09	1.42	1.35
24	B	517	CLA	C4A-NA	-2.09	1.34	1.39
26	V	164	HEM	CMC-C2C	2.09	1.53	1.47
29	Z	116	BCR	C38-C26	2.09	1.54	1.51
24	B	519	CLA	MG-NB	2.09	2.09	2.05
24	D	356	CLA	C4C-C3C	2.09	1.48	1.45
24	C	480	CLA	C4-C3	2.08	1.56	1.50
24	B	526	CLA	C4-C3	2.08	1.56	1.50
24	C	481	CLA	C4A-NA	-2.08	1.34	1.39
24	C	474	CLA	C1B-CHB	-2.08	1.34	1.39
24	C	485	CLA	CAA-C2A	2.08	1.57	1.54
30	A	370	DGD	O6E-C5E	2.08	1.49	1.44
24	C	474	CLA	C3D-CAD	-2.07	1.43	1.47
24	B	519	CLA	C1C-C2C	2.07	1.48	1.44
24	C	483	CLA	C1C-C2C	2.07	1.48	1.44
24	B	525	CLA	CHC-C1C	2.07	1.42	1.35
24	C	486	CLA	C3D-CAD	-2.07	1.43	1.47
34	I	230	LMT	C4B-C5B	2.07	1.57	1.53
32	B	532	SQD	C8-C7	2.07	1.57	1.50
34	O	274	LMT	C1B-C2B	2.07	1.58	1.52
27	A	367	PL9	C41-C39	2.07	1.51	1.40
24	B	511	CLA	C3C-C2C	2.06	1.41	1.36
30	A	370	DGD	C1G-C2G	2.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	536	LMT	C4'-C5'	2.06	1.58	1.52
32	B	532	SQD	C35-C34	-2.05	1.38	1.51
34	T	227	LMT	C3'-C4'	2.05	1.58	1.52
24	C	480	CLA	MG-NB	2.05	2.09	2.05
24	C	479	CLA	C1B-CHB	-2.05	1.34	1.39
30	A	370	DGD	O2G-C1B	2.04	1.40	1.34
24	A	366	CLA	CHC-C1C	2.04	1.42	1.35
25	A	365	PHO	CAA-CBA	-2.04	1.46	1.52
24	B	516	CLA	C1B-CHB	-2.04	1.34	1.39
24	B	524	CLA	C1B-NB	2.03	1.37	1.34
34	M	226	LMT	O5B-C1B	2.03	1.47	1.41
24	B	522	CLA	MG-NC	2.03	2.13	2.07
24	B	514	CLA	C1C-NC	-2.03	1.36	1.38
24	C	483	CLA	CHB-C4A	2.03	1.41	1.36
24	C	484	CLA	C4-C3	2.02	1.55	1.50
24	C	476	CLA	CHC-C1C	2.02	1.42	1.35
34	B	535	LMT	C6'-C5'	2.02	1.59	1.52
24	B	515	CLA	CHC-C1C	2.02	1.42	1.35
30	A	375	DGD	C3D-C2D	2.01	1.57	1.52
24	B	525	CLA	MG-NC	2.02	2.13	2.07
32	F	224	SQD	C24-C23	2.01	1.56	1.50
24	C	483	CLA	CAA-CBA	-2.01	1.46	1.52
24	C	480	CLA	CHB-C4A	2.01	1.41	1.36
24	C	484	CLA	C1C-NC	-2.01	1.36	1.38
30	A	375	DGD	C1E-C2E	2.01	1.58	1.52
24	B	518	CLA	C5-C3	2.01	1.56	1.51
24	B	524	CLA	C1C-C2C	2.01	1.48	1.44
24	B	525	CLA	C1B-CHB	-2.01	1.34	1.39
30	D	362	DGD	C1G-C2G	2.01	1.56	1.50
24	C	477	CLA	C4-C3	2.01	1.55	1.50
24	C	476	CLA	C1C-C2C	2.01	1.48	1.44
26	E	85	HEM	CHD-C4C	2.01	1.39	1.36
24	B	512	CLA	MG-NC	2.01	2.13	2.07
25	A	365	PHO	C1D-ND	-2.01	1.35	1.38
24	B	516	CLA	C1C-NC	-2.01	1.36	1.38
32	T	213	SQD	C8-C7	2.00	1.56	1.50
34	B	535	LMT	C3B-C2B	2.00	1.57	1.52
34	B	535	LMT	O5B-C5B	2.00	1.49	1.44
24	C	475	CLA	OBD-CAD	2.00	1.25	1.22
24	C	479	CLA	C4A-NA	-2.00	1.34	1.39

All (1217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	115	BCR	C32-C1-C6	-9.81	94.07	110.33
32	D	361	SQD	O6-C1-C2	9.62	120.42	108.18
32	T	213	SQD	O6-C1-C2	9.45	120.21	108.18
32	F	224	SQD	O5-C1-O6	9.28	131.79	109.98
32	T	213	SQD	C5-C6-S	9.23	128.05	114.45
32	B	532	SQD	O6-C1-C2	8.81	119.39	108.18
32	D	361	SQD	O5-C1-O6	8.60	130.18	109.98
32	A	372	SQD	O6-C1-C2	8.56	119.08	108.18
32	A	372	SQD	O5-C1-O6	8.50	129.94	109.98
32	B	532	SQD	O5-C1-O6	8.43	129.78	109.98
29	J	115	BCR	C32-C1-C31	-8.34	79.94	108.44
32	D	361	SQD	C5-C6-S	8.32	126.72	114.45
32	A	372	SQD	C5-C6-S	8.32	126.71	114.45
32	D	361	SQD	C31-C30-C29	8.23	132.96	114.46
32	F	224	SQD	O6-C1-C2	8.15	118.56	108.18
32	T	213	SQD	C31-C30-C29	8.08	132.62	114.46
32	T	213	SQD	O5-C1-O6	8.01	128.79	109.98
32	F	224	SQD	C5-C6-S	7.98	126.21	114.45
32	D	361	SQD	O8-S-C6	-7.52	95.95	105.64
26	E	85	HEM	CAD-C3D-C2D	7.44	143.81	127.25
26	E	85	HEM	CAD-C3D-C4D	-7.41	111.20	124.53
30	C	490	DGD	O6E-C5E-C4E	7.33	123.33	109.76
26	E	85	HEM	C3B-C4B-NB	-7.29	108.78	114.00
30	A	370	DGD	O6E-C5E-C4E	7.28	123.23	109.76
30	H	208	DGD	O6E-C5E-C4E	7.25	123.17	109.76
30	D	362	DGD	O6E-C5E-C4E	6.93	122.59	109.76
29	J	115	BCR	C32-C1-C2	-6.93	80.67	108.73
32	A	372	SQD	O8-S-C6	-6.86	96.80	105.64
32	F	224	SQD	C32-C31-C30	6.85	129.86	114.46
30	A	375	DGD	O6E-C5E-C4E	6.85	122.44	109.76
30	C	491	DGD	O6E-C5E-C4E	6.81	122.36	109.76
29	J	115	BCR	C38-C26-C25	6.75	132.16	124.51
30	C	489	DGD	O6E-C5E-C4E	6.68	122.12	109.76
29	H	107	BCR	C38-C26-C25	6.65	132.05	124.51
26	V	164	HEM	C3B-C4B-NB	-6.64	109.25	114.00
29	J	115	BCR	C33-C5-C6	6.58	131.97	124.51
29	K	112	BCR	C33-C5-C6	6.55	131.94	124.51
26	V	164	HEM	CAD-C3D-C2D	6.55	141.84	127.25
29	J	115	BCR	C2-C1-C6	6.55	121.32	110.44
29	D	358	BCR	C38-C26-C25	6.50	131.88	124.51
26	V	164	HEM	CAD-C3D-C4D	-6.39	113.05	124.53
30	C	490	DGD	O5D-C6D-C5D	6.37	119.90	108.97
29	D	358	BCR	C33-C5-C6	6.26	131.60	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	361	SQD	O7-S-C6	6.14	117.79	107.03
32	F	224	SQD	C10-C9-C8	6.10	136.26	113.28
32	B	532	SQD	C5-C6-S	6.09	123.43	114.45
32	A	372	SQD	C10-C9-C8	6.08	136.20	113.28
29	B	529	BCR	C38-C26-C25	6.04	131.36	124.51
32	F	224	SQD	O8-S-C6	-5.97	97.96	105.64
32	T	213	SQD	C10-C9-C8	5.93	135.62	113.28
30	D	362	DGD	O3G-C1D-C2D	5.90	115.68	108.18
29	Z	116	BCR	C38-C26-C25	5.89	131.18	124.51
32	B	532	SQD	O8-S-C6	-5.82	98.14	105.64
31	A	371	LHG	C25-C24-C23	5.82	136.33	113.51
29	B	527	BCR	C38-C26-C25	5.82	131.10	124.51
32	D	361	SQD	C10-C9-C8	5.79	135.12	113.28
26	E	85	HEM	CBD-CAD-C3D	-5.74	101.85	114.37
29	B	530	BCR	C38-C26-C25	5.68	130.95	124.51
32	B	532	SQD	C10-C9-C8	5.65	134.57	113.28
32	A	372	SQD	O7-S-C6	5.65	116.93	107.03
29	C	488	BCR	C33-C5-C6	5.65	130.91	124.51
32	T	213	SQD	O8-S-C6	-5.64	98.38	105.64
29	B	528	BCR	C33-C5-C6	5.61	130.87	124.51
29	C	488	BCR	C38-C26-C25	5.60	130.86	124.51
25	D	355	PHO	C3D-C4D-CHA	5.58	115.36	109.18
29	B	528	BCR	C38-C26-C25	5.57	130.82	124.51
30	C	489	DGD	O5D-C1E-C2E	5.52	115.20	108.18
29	K	112	BCR	C7-C8-C9	5.51	134.46	126.22
25	A	365	PHO	C3D-C4D-CHA	5.49	115.26	109.18
32	B	532	SQD	C25-C24-C23	5.49	135.03	113.51
29	B	527	BCR	C33-C5-C6	5.42	130.66	124.51
29	C	487	BCR	C38-C26-C25	5.38	130.61	124.51
27	D	357	PL9	C7-C3-C2	-5.37	118.59	123.77
29	B	529	BCR	C33-C5-C6	5.34	130.57	124.51
32	A	372	SQD	C25-C24-C23	5.34	134.46	113.51
29	B	530	BCR	C33-C5-C6	5.34	130.56	124.51
34	B	535	LMT	C1-O1'-C1'	-5.32	104.38	113.96
30	A	375	DGD	O5D-C1E-C2E	5.32	114.95	108.18
32	T	213	SQD	C25-C24-C23	5.24	134.05	113.51
32	F	224	SQD	C25-C24-C23	5.23	134.03	113.51
29	C	487	BCR	C33-C5-C6	5.23	130.44	124.51
29	A	369	BCR	C33-C5-C6	5.23	130.43	124.51
24	A	363	CLA	CAA-C2A-C3A	-5.20	100.76	113.04
32	D	361	SQD	C25-C24-C23	5.17	133.76	113.51
26	V	164	HEM	CBD-CAD-C3D	-5.13	103.18	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	T	213	SQD	O7-S-C6	5.12	116.00	107.03
29	K	112	BCR	C11-C10-C9	5.11	134.66	127.29
32	F	224	SQD	O7-S-C6	5.07	115.91	107.03
29	A	369	BCR	C38-C26-C25	5.05	130.23	124.51
29	Z	116	BCR	C33-C5-C6	5.04	130.22	124.51
32	F	224	SQD	C29-C30-C31	5.04	132.88	113.78
32	F	224	SQD	C44-O6-C1	5.03	123.83	113.81
29	J	115	BCR	C23-C24-C25	5.03	142.16	127.32
24	A	362	CLA	C2B-C3B-CAB	-4.99	117.11	127.33
32	B	532	SQD	O7-S-C6	4.94	115.68	107.03
24	A	363	CLA	C2B-C3B-CAB	-4.87	117.37	127.33
27	J	59	PL9	C7-C3-C2	-4.83	119.11	123.77
24	C	477	CLA	C2B-C3B-CAB	-4.74	117.64	127.33
29	J	115	BCR	C31-C1-C6	4.71	118.14	110.33
30	C	490	DGD	C3G-O3G-C1D	-4.69	104.47	113.81
29	J	115	BCR	C38-C26-C27	-4.68	104.74	113.34
30	H	208	DGD	O5D-C1E-C2E	4.66	114.11	108.18
29	J	115	BCR	C8-C7-C6	4.64	141.01	127.32
24	C	482	CLA	C2B-C3B-CAB	-4.62	117.87	127.33
24	C	483	CLA	C2B-C3B-CAB	-4.61	117.90	127.33
29	K	112	BCR	C38-C26-C25	4.60	129.72	124.51
26	E	85	HEM	CHA-C4D-ND	4.58	130.60	124.31
29	H	107	BCR	C33-C5-C6	4.57	129.69	124.51
26	V	164	HEM	CHA-C4D-ND	4.51	130.51	124.31
24	A	362	CLA	C4B-C3B-CAB	4.51	136.31	127.18
24	A	363	CLA	C4B-C3B-CAB	4.50	136.29	127.18
30	A	370	DGD	O5D-C6D-C5D	4.50	116.69	108.97
24	C	477	CLA	C4B-C3B-CAB	4.49	136.26	127.18
24	B	514	CLA	C4A-NA-C1A	4.46	112.67	106.52
24	B	517	CLA	C2B-C3B-CAB	-4.43	118.26	127.33
24	B	522	CLA	C2B-C3B-CAB	-4.43	118.26	127.33
29	K	112	BCR	C33-C5-C4	-4.39	105.28	113.34
24	C	481	CLA	C2B-C3B-CAB	-4.39	118.35	127.33
24	C	481	CLA	C4A-NA-C1A	4.38	112.56	106.52
29	D	358	BCR	C38-C26-C27	-4.37	105.32	113.34
24	B	521	CLA	C2B-C3B-CAB	-4.35	118.42	127.33
27	D	357	PL9	C7-C3-C4	4.35	121.41	117.10
25	A	365	PHO	C2B-C3B-CAB	-4.34	118.44	127.33
24	C	476	CLA	C4A-NA-C1A	4.32	112.47	106.52
24	B	519	CLA	C2B-C3B-CAB	-4.31	118.50	127.33
24	B	515	CLA	C2B-C3B-CAB	-4.29	118.54	127.33
24	C	484	CLA	C4A-NA-C1A	4.29	112.43	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	479	CLA	C2B-C3B-CAB	-4.28	118.57	127.33
24	B	513	CLA	C2B-C3B-CAB	-4.28	118.57	127.33
24	C	485	CLA	C2B-C3B-CAB	-4.27	118.58	127.33
24	C	482	CLA	C4B-C3B-CAB	4.27	135.83	127.18
32	B	532	SQD	C44-O6-C1	4.24	122.25	113.81
32	D	361	SQD	C44-O6-C1	4.24	122.25	113.81
24	C	474	CLA	C2B-C3B-CAB	-4.23	118.67	127.33
24	B	525	CLA	C2B-C3B-CAB	-4.22	118.70	127.33
24	C	478	CLA	C2B-C3B-CAB	-4.21	118.72	127.33
29	D	358	BCR	C33-C5-C4	-4.20	105.62	113.34
29	H	107	BCR	C38-C26-C27	-4.20	105.63	113.34
29	B	529	BCR	C38-C26-C27	-4.20	105.63	113.34
24	B	525	CLA	C4A-NA-C1A	4.19	112.30	106.52
24	B	511	CLA	C4A-NA-C1A	4.19	112.30	106.52
26	V	164	HEM	C1A-CHA-C4D	-4.19	121.96	127.47
29	K	112	BCR	C2-C1-C6	4.17	117.38	110.44
24	B	514	CLA	C2B-C3B-CAB	-4.17	118.79	127.33
24	B	526	CLA	CAA-C2A-C3A	-4.17	103.18	113.04
27	A	367	PL9	C7-C8-C9	-4.17	119.71	126.76
24	B	518	CLA	C2B-C3B-CAB	-4.17	118.80	127.33
24	D	356	CLA	C2B-C3B-CAB	-4.16	118.82	127.33
24	B	516	CLA	C2B-C3B-CAB	-4.16	118.82	127.33
24	B	526	CLA	C2B-C3B-CAB	-4.15	118.83	127.33
24	C	475	CLA	C2B-C3B-CAB	-4.14	118.85	127.33
24	C	483	CLA	C4B-C3B-CAB	4.12	135.52	127.18
24	C	476	CLA	C2B-C3B-CAB	-4.12	118.90	127.33
24	A	366	CLA	C2B-C3B-CAB	-4.10	118.94	127.33
24	D	364	CLA	C2B-C3B-CAB	-4.09	118.95	127.33
24	D	354	CLA	C4A-NA-C1A	4.07	112.13	106.52
29	J	115	BCR	C1-C6-C5	-4.07	116.71	122.60
24	C	486	CLA	C2B-C3B-CAB	-4.06	119.03	127.33
25	D	355	PHO	C2B-C3B-CAB	-4.04	119.05	127.33
24	C	484	CLA	C2B-C3B-CAB	-4.04	119.06	127.33
24	C	486	CLA	C4A-NA-C1A	4.04	112.09	106.52
24	C	479	CLA	C4A-NA-C1A	4.03	112.08	106.52
32	F	224	SQD	C19-C18-C17	4.02	123.49	114.46
24	B	524	CLA	C4A-NA-C1A	4.02	112.06	106.52
29	B	528	BCR	C33-C5-C4	-4.01	105.97	113.34
24	C	485	CLA	C4A-NA-C1A	4.01	112.05	106.52
29	C	488	BCR	C38-C26-C27	-4.01	105.97	113.34
24	B	513	CLA	CAA-C2A-C3A	-4.00	103.58	113.04
29	C	487	BCR	C33-C5-C4	-4.00	106.00	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	513	CLA	C4B-C3B-CAB	3.99	135.26	127.18
24	C	480	CLA	C4A-NA-C1A	3.99	112.02	106.52
33	M	217	LMG	O7-C10-C11	3.98	120.28	111.56
24	C	478	CLA	C4A-NA-C1A	3.98	112.00	106.52
24	C	480	CLA	C2B-C3B-CAB	-3.98	119.19	127.33
29	B	530	BCR	C38-C26-C27	-3.97	106.05	113.34
24	D	356	CLA	C4A-NA-C1A	3.96	111.98	106.52
30	C	491	DGD	O6D-C5D-C6D	3.96	114.57	106.61
24	B	517	CLA	C4A-NA-C1A	3.96	111.97	106.52
24	B	522	CLA	C4B-C3B-CAB	3.95	135.17	127.18
29	B	528	BCR	C38-C26-C27	-3.95	106.09	113.34
29	K	112	BCR	C8-C9-C10	-3.93	112.93	118.97
31	A	374	LHG	O7-C7-C8	3.93	120.17	111.56
30	C	490	DGD	O2G-C1B-C2B	3.92	120.15	111.56
24	C	474	CLA	C4A-NA-C1A	3.92	111.92	106.52
24	B	512	CLA	C2B-C3B-CAB	-3.91	119.33	127.33
24	B	520	CLA	C4A-NA-C1A	3.90	111.90	106.52
29	H	107	BCR	C24-C23-C22	3.90	132.04	126.22
24	C	475	CLA	C4A-NA-C1A	3.89	111.89	106.52
27	J	59	PL9	C10-C9-C11	3.89	121.30	115.39
32	B	532	SQD	O48-C23-C24	3.88	124.16	111.94
24	B	523	CLA	C4A-NA-C1A	3.87	111.86	106.52
32	T	213	SQD	O48-C23-C24	3.87	124.10	111.94
24	B	516	CLA	C4A-NA-C1A	3.87	111.85	106.52
29	B	529	BCR	C33-C5-C4	-3.85	106.27	113.34
24	C	478	CLA	CAA-C2A-C3A	-3.83	103.98	113.04
29	B	530	BCR	C33-C5-C4	-3.82	106.33	113.34
24	B	520	CLA	C2B-C3B-CAB	-3.82	119.51	127.33
24	C	481	CLA	C4B-C3B-CAB	3.80	134.88	127.18
29	C	488	BCR	C33-C5-C4	-3.80	106.36	113.34
24	B	526	CLA	C4A-NA-C1A	3.79	111.75	106.52
24	A	362	CLA	C4A-NA-C1A	3.79	111.74	106.52
24	B	525	CLA	C4B-C3B-CAB	3.78	134.83	127.18
29	Z	116	BCR	C38-C26-C27	-3.77	106.41	113.34
24	D	364	CLA	CAA-C2A-C3A	-3.77	104.12	113.04
29	C	487	BCR	C38-C26-C27	-3.77	106.41	113.34
24	B	522	CLA	C4A-NA-C1A	3.77	111.72	106.52
24	B	521	CLA	C4B-C3B-CAB	3.77	134.81	127.18
24	D	364	CLA	C4A-NA-C1A	3.76	111.71	106.52
29	A	369	BCR	C38-C26-C27	-3.76	106.43	113.34
29	D	358	BCR	C24-C23-C22	3.76	131.84	126.22
24	B	526	CLA	C4B-C3B-CAB	3.76	134.78	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	356	CLA	C4B-C3B-CAB	3.75	134.77	127.18
24	C	482	CLA	C4A-NA-C1A	3.75	111.69	106.52
24	B	515	CLA	C4B-C3B-CAB	3.75	134.76	127.18
27	J	59	PL9	C7-C3-C4	3.74	120.81	117.10
24	B	515	CLA	C4A-NA-C1A	3.74	111.68	106.52
24	B	524	CLA	C2B-C3B-CAB	-3.74	119.67	127.33
24	D	364	CLA	C4B-C3B-CAB	3.74	134.74	127.18
30	A	375	DGD	C1E-O6E-C5E	3.74	120.99	113.73
24	C	478	CLA	C4B-C3B-CAB	3.73	134.73	127.18
29	Z	116	BCR	C23-C24-C25	3.73	138.34	127.32
24	B	521	CLA	C4A-NA-C1A	3.73	111.66	106.52
24	B	519	CLA	C4B-C3B-CAB	3.73	134.73	127.18
24	C	477	CLA	C4A-NA-C1A	3.73	111.66	106.52
29	B	527	BCR	C38-C26-C27	-3.73	106.49	113.34
30	A	375	DGD	O2G-C1B-C2B	3.72	119.71	111.56
24	B	513	CLA	C4A-NA-C1A	3.72	111.65	106.52
24	A	363	CLA	CBA-CAA-C2A	3.72	125.05	114.01
24	B	517	CLA	CBD-CHA-C1A	3.72	133.63	128.77
33	D	360	LMG	O6-C5-C6	3.71	115.47	106.34
24	B	518	CLA	C4A-NA-C1A	3.71	111.64	106.52
29	A	369	BCR	C33-C5-C4	-3.71	106.52	113.34
24	B	511	CLA	C2B-C3B-CAB	-3.71	119.73	127.33
24	B	518	CLA	C4B-C3B-CAB	3.71	134.69	127.18
29	J	115	BCR	C33-C5-C4	-3.71	106.53	113.34
30	C	489	DGD	C1E-O6E-C5E	3.69	120.91	113.73
24	C	479	CLA	C4B-C3B-CAB	3.68	134.63	127.18
24	C	485	CLA	C4B-C3B-CAB	3.68	134.63	127.18
29	C	488	BCR	C29-C30-C25	3.68	116.56	110.44
24	B	519	CLA	C4A-NA-C1A	3.67	111.58	106.52
29	B	527	BCR	C33-C5-C4	-3.67	106.60	113.34
29	B	528	BCR	C29-C30-C25	3.67	116.53	110.44
24	C	475	CLA	C4B-C3B-CAB	3.67	134.60	127.18
24	B	514	CLA	C4B-C3B-CAB	3.67	134.60	127.18
24	B	517	CLA	C4B-C3B-CAB	3.66	134.58	127.18
29	B	529	BCR	C30-C25-C26	-3.65	117.31	122.60
29	D	358	BCR	C29-C30-C25	3.65	116.50	110.44
24	A	366	CLA	C4A-NA-C1A	3.65	111.55	106.52
24	C	476	CLA	C4B-C3B-CAB	3.65	134.57	127.18
24	C	476	CLA	C1-C2-C3	3.65	132.67	126.19
29	J	115	BCR	C29-C30-C25	3.63	116.47	110.44
27	J	59	PL9	C7-C8-C9	-3.63	120.63	126.76
27	A	367	PL9	C27-C28-C29	-3.63	119.97	127.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	369	BCR	C24-C23-C22	3.62	131.63	126.22
24	B	523	CLA	C2B-C3B-CAB	-3.62	119.92	127.33
34	T	227	LMT	C1-O1'-C1'	-3.61	107.45	113.96
24	B	516	CLA	C4B-C3B-CAB	3.61	134.49	127.18
24	B	512	CLA	C4B-C3B-CAB	3.61	134.49	127.18
27	A	367	PL9	C17-C18-C19	-3.60	120.03	127.80
24	A	366	CLA	C4B-C3B-CAB	3.60	134.47	127.18
24	C	474	CLA	C4B-C3B-CAB	3.60	134.46	127.18
34	I	230	LMT	C1-O1'-C1'	-3.60	107.49	113.96
24	C	474	CLA	CAA-C2A-C3A	-3.59	104.55	113.04
29	B	529	BCR	C24-C23-C22	3.59	131.58	126.22
30	C	489	DGD	O5D-C6D-C5D	3.58	115.11	108.97
29	J	115	BCR	C16-C15-C14	3.58	131.28	123.36
24	C	483	CLA	C4A-NA-C1A	3.58	111.45	106.52
30	C	491	DGD	C1E-O6E-C5E	3.57	120.68	113.73
24	C	484	CLA	C4B-C3B-CAB	3.56	134.39	127.18
29	K	112	BCR	C38-C26-C27	-3.55	106.81	113.34
29	C	488	BCR	C2-C1-C6	3.55	116.34	110.44
24	D	354	CLA	OBD-CAD-CBD	-3.54	120.59	125.94
32	D	361	SQD	O48-C23-C24	3.54	123.07	111.94
24	D	356	CLA	CAA-C2A-C3A	-3.54	104.68	113.04
32	A	372	SQD	C11-C10-C9	3.54	133.75	114.61
24	B	512	CLA	CAA-C2A-C3A	-3.54	104.67	113.04
29	K	112	BCR	C1-C6-C5	-3.53	117.49	122.60
25	D	355	PHO	CAA-C2A-C3A	-3.52	104.72	113.04
27	A	367	PL9	C22-C23-C24	-3.51	120.22	127.80
24	C	478	CLA	CBD-CHA-C1A	3.51	133.35	128.77
29	A	369	BCR	C7-C8-C9	3.50	131.46	126.22
24	A	366	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
25	D	355	PHO	CBD-CHA-C1A	3.50	132.67	126.57
24	C	483	CLA	CBD-CHA-C1A	3.49	133.34	128.77
27	A	367	PL9	C35-C34-C36	3.49	120.69	115.39
24	C	480	CLA	CBD-CHA-C1A	3.49	133.33	128.77
24	C	486	CLA	C4B-C3B-CAB	3.49	134.24	127.18
24	C	477	CLA	CBD-CHA-C1A	3.48	133.31	128.77
29	H	107	BCR	C33-C5-C4	-3.48	106.96	113.34
33	B	531	LMG	O6-C5-C6	3.47	114.86	106.34
24	C	481	CLA	CBD-CHA-C1A	3.47	133.30	128.77
30	H	208	DGD	O6D-C5D-C6D	3.46	113.58	106.61
33	A	373	LMG	O6-C5-C6	3.46	114.84	106.34
29	D	358	BCR	C30-C25-C26	-3.45	117.60	122.60
29	H	107	BCR	C30-C25-C26	-3.45	117.60	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	372	SQD	C31-C30-C29	3.45	133.27	114.61
29	H	107	BCR	C29-C30-C25	3.44	116.16	110.44
24	B	525	CLA	CBD-CHA-C1A	3.43	133.25	128.77
24	A	363	CLA	O2A-CGA-CBA	3.43	122.73	111.94
30	C	489	DGD	O6D-C5D-C6D	3.42	113.49	106.61
24	A	366	CLA	CAA-C2A-C3A	-3.42	104.96	113.04
29	Z	116	BCR	C16-C17-C18	3.42	132.22	127.29
27	A	367	PL9	C12-C13-C14	-3.42	120.42	127.80
33	D	360	LMG	O7-C10-C11	3.41	119.03	111.56
24	C	478	CLA	OBD-CAD-CBD	-3.40	120.80	125.94
24	B	524	CLA	C4B-C3B-CAB	3.40	134.07	127.18
29	K	112	BCR	C29-C30-C25	3.40	116.09	110.44
24	B	523	CLA	CBD-CHA-C1A	3.39	133.21	128.77
24	C	485	CLA	O2A-CGA-CBA	3.39	122.60	111.94
24	B	518	CLA	O2A-CGA-CBA	3.38	122.56	111.94
32	D	361	SQD	C11-C10-C9	3.37	132.86	114.61
32	B	532	SQD	C11-C10-C9	3.37	132.86	114.61
24	B	518	CLA	CAA-C2A-C3A	-3.37	105.07	113.04
32	F	224	SQD	C11-C10-C9	3.37	132.85	114.61
29	B	530	BCR	C29-C30-C25	3.37	116.04	110.44
24	B	512	CLA	C4A-NA-C1A	3.37	111.16	106.52
29	Z	116	BCR	C29-C30-C25	3.36	116.03	110.44
29	C	488	BCR	C30-C25-C26	-3.37	117.73	122.60
32	T	213	SQD	C11-C10-C9	3.36	132.81	114.61
27	A	367	PL9	C30-C29-C31	3.36	120.50	115.39
24	B	517	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
30	H	208	DGD	O2G-C1B-C2B	3.36	118.91	111.56
24	C	484	CLA	CBD-CHA-C1A	3.35	133.15	128.77
29	K	112	BCR	C30-C25-C26	-3.35	117.74	122.60
24	A	363	CLA	C4A-NA-C1A	3.35	111.14	106.52
29	Z	116	BCR	C33-C5-C4	-3.35	107.18	113.34
25	A	365	PHO	CBD-CHA-C1A	3.35	132.41	126.57
24	B	519	CLA	CED-O2D-CGD	3.35	123.99	116.02
33	C	493	LMG	O7-C10-C11	3.35	118.89	111.56
25	D	355	PHO	C7-C6-C5	-3.33	103.19	113.01
24	B	511	CLA	C4B-C3B-CAB	3.33	133.92	127.18
29	D	358	BCR	C1-C6-C5	-3.33	117.78	122.60
24	B	523	CLA	C4B-C3B-CAB	3.33	133.92	127.18
32	B	532	SQD	C31-C30-C29	3.32	132.58	114.61
24	B	521	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
30	D	362	DGD	C1E-O6E-C5E	3.32	120.17	113.73
24	C	483	CLA	C1D-CHD-C4C	3.31	127.74	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	485	CLA	CBD-CHA-C1A	3.31	133.10	128.77
24	C	480	CLA	O2A-CGA-CBA	3.31	122.36	111.94
27	A	367	PL9	C37-C38-C39	-3.31	120.60	128.63
24	B	517	CLA	C2D-C1D-ND	3.31	111.91	109.41
27	J	59	PL9	C25-C24-C26	3.31	120.42	115.39
29	C	488	BCR	C23-C24-C25	3.31	137.08	127.32
30	A	370	DGD	C1E-O6E-C5E	3.30	120.15	113.73
24	B	514	CLA	CBD-CHA-C1A	3.30	133.09	128.77
29	B	528	BCR	C30-C25-C26	-3.30	117.82	122.60
32	F	224	SQD	O48-C23-C24	3.30	122.31	111.94
29	A	369	BCR	C30-C25-C26	-3.30	117.83	122.60
24	B	524	CLA	CBD-CHA-C1A	3.29	133.08	128.77
30	A	375	DGD	O5D-C6D-C5D	3.29	114.62	108.97
31	A	371	LHG	O8-C23-C24	3.29	122.28	111.94
24	B	520	CLA	C4B-C3B-CAB	3.29	133.83	127.18
29	B	530	BCR	C30-C25-C26	-3.28	117.85	122.60
29	H	107	BCR	C12-C13-C14	-3.28	113.94	118.97
24	B	525	CLA	C1D-CHD-C4C	3.27	127.68	122.60
29	C	487	BCR	C24-C23-C22	3.27	131.11	126.22
33	B	533	LMG	C7-O1-C1	-3.27	107.29	113.81
24	B	515	CLA	CAA-C2A-C3A	-3.26	105.34	113.04
29	C	488	BCR	C8-C7-C6	3.26	136.95	127.32
24	C	479	CLA	CED-O2D-CGD	3.25	123.75	116.02
29	K	112	BCR	C24-C23-C22	3.25	131.08	126.22
27	D	357	PL9	C17-C18-C19	-3.25	120.79	127.80
24	B	511	CLA	CBD-CHA-C1A	3.24	133.01	128.77
30	H	208	DGD	C1E-O6E-C5E	3.24	120.02	113.73
29	K	112	BCR	C23-C24-C25	3.24	136.88	127.32
29	B	528	BCR	C8-C7-C6	3.24	136.87	127.32
24	B	522	CLA	CBD-CHA-C1A	3.23	132.99	128.77
24	C	482	CLA	C1D-CHD-C4C	3.23	127.61	122.60
29	J	115	BCR	C30-C25-C26	-3.23	117.93	122.60
29	D	358	BCR	C8-C7-C6	3.22	136.83	127.32
29	B	530	BCR	C24-C23-C22	3.22	131.03	126.22
24	B	517	CLA	CAA-C2A-C3A	-3.22	105.44	113.04
24	C	479	CLA	CAA-C2A-C3A	-3.21	105.45	113.04
24	D	364	CLA	OBD-CAD-CBD	-3.21	121.10	125.94
24	A	363	CLA	C2A-C3A-C4A	3.21	106.33	101.40
24	B	524	CLA	C1-C2-C3	3.21	131.88	126.19
29	Z	116	BCR	C2-C1-C6	3.20	115.76	110.44
33	B	534	LMG	O7-C10-C11	3.20	118.58	111.56
24	D	364	CLA	CBD-CHA-C1A	3.20	132.96	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	107	BCR	C15-C14-C13	3.20	131.90	127.29
24	B	513	CLA	CBD-CHA-C1A	3.20	132.95	128.77
24	B	520	CLA	OBD-CAD-CBD	-3.20	121.11	125.94
24	C	484	CLA	C2D-C1D-ND	3.20	111.83	109.41
27	D	357	PL9	C20-C19-C21	3.20	120.25	115.39
24	C	486	CLA	CBD-CHA-C1A	3.20	132.95	128.77
24	C	480	CLA	C4B-C3B-CAB	3.19	133.64	127.18
24	B	511	CLA	C1-C2-C3	3.19	131.86	126.19
24	A	362	CLA	O2A-CGA-CBA	3.19	121.97	111.94
32	B	532	SQD	C3-C4-C5	-3.19	104.50	110.20
24	B	513	CLA	O2A-CGA-CBA	3.19	121.97	111.94
24	C	482	CLA	OBD-CAD-CBD	-3.19	121.13	125.94
32	A	372	SQD	O48-C23-C24	3.18	121.95	111.94
33	I	220	LMG	O7-C10-C11	3.18	118.52	111.56
24	C	483	CLA	C2A-C3A-C4A	3.18	106.29	101.40
29	K	112	BCR	C16-C17-C18	3.18	131.87	127.29
24	B	526	CLA	CED-O2D-CGD	3.18	123.58	116.02
24	B	512	CLA	CBD-CHA-C1A	3.17	132.91	128.77
24	D	354	CLA	CBA-CAA-C2A	3.17	123.42	114.01
24	C	477	CLA	C2D-C1D-ND	3.16	111.80	109.41
24	B	522	CLA	C6-C5-C3	3.16	120.29	112.78
27	J	59	PL9	C22-C23-C24	-3.15	120.99	127.80
24	D	354	CLA	O2A-CGA-CBA	3.16	121.87	111.94
24	C	484	CLA	C1D-CHD-C4C	3.16	127.49	122.60
24	B	524	CLA	C2D-C1D-ND	3.16	111.79	109.41
24	D	354	CLA	C1D-CHD-C4C	3.15	127.49	122.60
29	A	369	BCR	C29-C30-C25	3.15	115.68	110.44
33	B	531	LMG	O7-C10-C11	3.15	118.46	111.56
24	C	481	CLA	CAA-C2A-C3A	-3.15	105.60	113.04
24	B	526	CLA	CBD-CHA-C1A	3.14	132.88	128.77
24	B	523	CLA	C1D-CHD-C4C	3.14	127.47	122.60
29	D	358	BCR	C2-C1-C6	3.14	115.66	110.44
24	C	478	CLA	O2A-CGA-CBA	3.14	121.81	111.94
24	C	480	CLA	C7-C6-C5	-3.14	103.76	113.01
24	B	520	CLA	CBD-CHA-C1A	3.14	132.87	128.77
27	J	59	PL9	C27-C28-C29	-3.13	121.03	128.63
27	D	357	PL9	C37-C38-C39	-3.13	121.04	127.80
24	B	521	CLA	CBD-CHA-C1A	3.13	132.86	128.77
27	A	367	PL9	C25-C24-C26	3.13	120.14	115.39
29	B	529	BCR	C29-C30-C25	3.11	115.61	110.44
24	C	474	CLA	CBD-CHA-C1A	3.11	132.84	128.77
29	B	527	BCR	C29-C30-C25	3.11	115.61	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	357	PL9	C42-C43-C44	-3.11	121.09	127.80
24	B	521	CLA	C7-C6-C5	-3.11	103.86	113.01
27	D	357	PL9	C25-C24-C26	3.11	120.11	115.39
30	C	491	DGD	O2G-C1B-C2B	3.10	118.36	111.56
25	D	355	PHO	CED-O2D-CGD	3.10	123.40	116.02
29	C	487	BCR	C1-C6-C5	-3.10	118.11	122.60
30	A	370	DGD	O2G-C1B-C2B	3.09	118.34	111.56
24	C	481	CLA	C1D-CHD-C4C	3.09	127.39	122.60
32	A	372	SQD	C44-O6-C1	3.08	119.95	113.81
24	B	526	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
24	B	524	CLA	OBD-CAD-CBD	-3.07	121.30	125.94
29	H	107	BCR	C2-C1-C6	3.07	115.54	110.44
24	D	354	CLA	C2B-C3B-CAB	-3.07	121.05	127.33
24	C	486	CLA	CED-O2D-CGD	3.06	123.31	116.02
33	E	218	LMG	O6-C5-C6	3.06	113.87	106.34
25	D	355	PHO	OBD-CAD-CBD	-3.06	121.32	125.94
33	B	531	LMG	C7-O1-C1	-3.06	107.71	113.81
29	H	107	BCR	C8-C7-C6	3.05	136.33	127.32
33	I	220	LMG	C7-O1-C1	-3.05	107.72	113.81
24	C	474	CLA	O2A-CGA-CBA	3.05	121.53	111.94
29	C	487	BCR	C2-C1-C6	3.05	115.51	110.44
24	B	522	CLA	C1D-CHD-C4C	3.05	127.32	122.60
27	D	357	PL9	C7-C8-C9	-3.04	121.62	126.76
24	B	512	CLA	CED-O2D-CGD	3.04	123.25	116.02
33	B	533	LMG	O7-C10-C11	3.04	118.22	111.56
29	H	107	BCR	C11-C10-C9	3.04	131.67	127.29
33	D	359	LMG	O7-C10-C11	3.04	118.22	111.56
27	D	357	PL9	C15-C14-C16	3.04	120.01	115.39
33	E	218	LMG	O7-C10-C11	3.03	118.21	111.56
26	E	85	HEM	C4A-NA-C1A	3.03	110.76	106.76
32	D	361	SQD	C15-C16-C17	3.03	125.28	113.78
24	B	520	CLA	C1-C2-C3	3.03	131.57	126.19
24	B	519	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
26	V	164	HEM	C4A-NA-C1A	3.02	110.74	106.76
24	B	520	CLA	C1D-CHD-C4C	3.02	127.28	122.60
29	B	527	BCR	C8-C7-C6	3.02	136.23	127.32
24	C	478	CLA	C1D-CHD-C4C	3.02	127.28	122.60
24	B	526	CLA	C2A-C3A-C4A	3.01	106.03	101.40
24	B	519	CLA	CAA-C2A-C3A	-3.01	105.92	113.04
27	A	367	PL9	C10-C9-C11	3.01	119.97	115.39
24	C	477	CLA	CAA-C2A-C3A	-3.01	105.93	113.04
24	B	518	CLA	C1D-CHD-C4C	3.01	127.26	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	518	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
24	B	520	CLA	CAA-C2A-C3A	-3.01	105.93	113.04
24	C	483	CLA	C2D-C1D-ND	3.01	111.68	109.41
24	C	475	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
24	C	485	CLA	C1D-CHD-C4C	3.00	127.25	122.60
33	M	217	LMG	O6-C5-C6	2.99	113.70	106.34
32	D	361	SQD	C18-C17-C16	2.99	121.18	114.46
24	C	485	CLA	C1-C2-C3	2.99	131.50	126.19
29	B	527	BCR	C23-C24-C25	2.99	136.14	127.32
29	B	527	BCR	C30-C25-C26	-2.99	118.28	122.60
27	D	357	PL9	C45-C44-C46	2.99	119.93	115.39
29	B	528	BCR	C24-C23-C22	2.99	130.68	126.22
34	M	226	LMT	C1B-O1B-C4'	-2.99	110.38	117.99
24	C	482	CLA	C1-C2-C3	2.98	131.49	126.19
24	C	486	CLA	C1D-CHD-C4C	2.98	127.22	122.60
24	B	513	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
24	C	481	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
24	B	525	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
24	D	356	CLA	C1D-CHD-C4C	2.98	127.21	122.60
26	E	85	HEM	C1A-CHA-C4D	-2.98	123.56	127.47
24	C	475	CLA	C1D-CHD-C4C	2.97	127.21	122.60
33	C	493	LMG	O6-C5-C6	2.97	113.64	106.34
24	C	475	CLA	CED-O2D-CGD	2.97	123.08	116.02
24	C	486	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
24	C	481	CLA	C2D-C1D-ND	2.97	111.65	109.41
24	B	516	CLA	CBD-CHA-C1A	2.97	132.65	128.77
34	D	363	LMT	C1-O1'-C1'	-2.97	108.61	113.96
24	A	366	CLA	C7-C6-C5	-2.97	104.27	113.01
25	A	365	PHO	OBD-CAD-CBD	-2.97	121.46	125.94
25	A	365	PHO	C1-C2-C3	2.97	131.46	126.19
24	D	354	CLA	CMB-C2B-C1B	-2.97	124.06	128.62
32	F	224	SQD	C3-C4-C5	-2.97	104.91	110.20
29	C	488	BCR	C1-C6-C5	-2.97	118.31	122.60
30	A	375	DGD	O3G-C1D-C2D	2.96	111.95	108.18
24	C	482	CLA	O2A-CGA-CBA	2.96	121.26	111.94
29	H	107	BCR	C16-C17-C18	2.96	131.55	127.29
24	B	512	CLA	C7-C6-C5	-2.95	104.30	113.01
24	B	517	CLA	O2A-CGA-CBA	2.95	121.22	111.94
29	C	487	BCR	C35-C13-C12	2.95	122.86	118.09
29	C	487	BCR	C29-C30-C25	2.95	115.34	110.44
24	C	477	CLA	C1D-CHD-C4C	2.94	127.16	122.60
24	B	515	CLA	C1-C2-C3	2.94	131.41	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	487	BCR	C32-C1-C6	2.93	115.19	110.33
24	C	476	CLA	C1D-CHD-C4C	2.94	127.15	122.60
29	B	528	BCR	C2-C1-C6	2.93	115.31	110.44
24	C	479	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
24	A	362	CLA	CBD-CHA-C1A	2.93	132.60	128.77
24	B	518	CLA	C2D-C1D-ND	2.93	111.62	109.41
24	B	525	CLA	C2D-C1D-ND	2.93	111.62	109.41
24	C	480	CLA	C2A-C1A-NA	-2.93	108.01	111.24
24	B	525	CLA	C1-C2-C3	2.92	131.38	126.19
33	M	217	LMG	O1-C1-C2	2.92	111.90	108.18
24	C	476	CLA	CBD-CHA-C1A	2.92	132.59	128.77
24	C	485	CLA	C2D-C1D-ND	2.92	111.61	109.41
27	A	367	PL9	C15-C14-C16	2.92	119.83	115.39
24	B	521	CLA	CED-O2D-CGD	2.92	122.96	116.02
33	E	218	LMG	O1-C1-C2	2.92	111.89	108.18
29	J	115	BCR	C21-C20-C19	2.92	133.08	123.24
27	A	367	PL9	C20-C19-C21	2.92	119.83	115.39
27	J	59	PL9	C20-C19-C21	2.92	119.82	115.39
30	D	362	DGD	O2G-C1B-C2B	2.92	117.95	111.56
24	D	356	CLA	CBD-CHA-C1A	2.91	132.58	128.77
24	C	483	CLA	O2A-CGA-CBA	2.91	121.10	111.94
24	C	482	CLA	C2A-C3A-C4A	2.91	105.88	101.40
24	C	482	CLA	CED-O2D-CGD	2.91	122.94	116.02
24	C	485	CLA	CAA-C2A-C3A	-2.91	106.17	113.04
29	K	112	BCR	C34-C9-C8	2.91	122.79	118.09
24	B	524	CLA	C1D-CHD-C4C	2.91	127.11	122.60
27	D	357	PL9	C12-C13-C14	-2.90	121.55	127.80
24	C	474	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
33	D	359	LMG	O6-C5-C6	2.89	113.45	106.34
24	C	478	CLA	CED-O2D-CGD	2.89	122.89	116.02
29	B	527	BCR	C2-C1-C6	2.89	115.24	110.44
24	B	512	CLA	O2A-CGA-CBA	2.88	121.01	111.94
24	B	511	CLA	O2A-CGA-CBA	2.88	121.01	111.94
24	D	356	CLA	C2A-C3A-C4A	2.88	105.83	101.40
29	C	487	BCR	C30-C25-C26	-2.88	118.43	122.60
34	M	226	LMT	C1-O1'-C1'	-2.88	108.78	113.96
24	C	482	CLA	CBD-CHA-C1A	2.88	132.53	128.77
24	B	511	CLA	CED-O2D-CGD	2.87	122.86	116.02
24	B	516	CLA	O2A-CGA-CBA	2.87	120.98	111.94
24	B	513	CLA	CED-O2D-CGD	2.87	122.85	116.02
24	B	515	CLA	CED-O2D-CGD	2.87	122.84	116.02
32	A	372	SQD	C32-C31-C30	2.87	130.13	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	357	PL9	C40-C39-C41	2.87	119.75	115.39
24	B	514	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
24	C	480	CLA	C1-C2-C3	2.86	131.28	126.19
24	C	477	CLA	OBD-CAD-CBD	-2.86	121.61	125.94
25	A	365	PHO	CED-O2D-CGD	2.86	122.83	116.02
24	B	519	CLA	C1D-CHD-C4C	2.86	127.04	122.60
24	A	362	CLA	CED-O2D-CGD	2.85	122.81	116.02
24	C	477	CLA	C1-C2-C3	2.85	131.26	126.19
24	A	363	CLA	CBD-CHA-C1A	2.85	132.50	128.77
24	B	515	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
29	B	528	BCR	C23-C24-C25	2.85	135.74	127.32
29	B	530	BCR	C2-C1-C6	2.85	115.17	110.44
24	B	525	CLA	CED-O2D-CGD	2.85	122.79	116.02
24	B	514	CLA	C2D-C1D-ND	2.84	111.56	109.41
29	B	529	BCR	C8-C7-C6	2.84	135.71	127.32
29	B	529	BCR	C23-C24-C25	2.84	135.71	127.32
24	D	364	CLA	CED-O2D-CGD	2.84	122.77	116.02
24	C	484	CLA	CED-O2D-CGD	2.84	122.77	116.02
24	C	480	CLA	C1D-CHD-C4C	2.83	127.00	122.60
24	B	524	CLA	CED-O2D-CGD	2.84	122.76	116.02
32	A	372	SQD	O8-S-O9	-2.83	105.66	111.78
24	D	364	CLA	C1D-CHD-C4C	2.83	126.99	122.60
24	A	366	CLA	C1D-CHD-C4C	2.83	126.99	122.60
24	B	518	CLA	C6-C7-C8	2.83	123.29	115.14
30	C	489	DGD	O2G-C1B-C2B	2.83	117.75	111.56
24	B	515	CLA	CBD-CHA-C1A	2.83	132.47	128.77
30	C	490	DGD	C3G-C2G-C1G	-2.83	105.41	111.86
24	B	514	CLA	C1D-CHD-C4C	2.83	126.99	122.60
29	A	369	BCR	C2-C1-C6	2.83	115.14	110.44
24	D	364	CLA	C2A-C3A-C4A	2.82	105.75	101.40
24	B	516	CLA	C1-C2-C3	2.83	131.21	126.19
24	B	522	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
29	A	369	BCR	C1-C6-C5	-2.82	118.52	122.60
24	A	362	CLA	C6-C5-C3	2.82	119.48	112.78
34	O	274	LMT	C1B-O1B-C4'	-2.82	110.80	117.99
24	D	354	CLA	C4B-C3B-CAB	2.82	132.88	127.18
24	B	513	CLA	C1D-CHD-C4C	2.82	126.97	122.60
24	C	479	CLA	CBD-CHA-C1A	2.82	132.45	128.77
34	B	536	LMT	C1B-O1B-C4'	-2.82	110.81	117.99
24	B	525	CLA	C2A-C3A-C4A	2.82	105.73	101.40
24	B	515	CLA	C2D-C1D-ND	2.81	111.53	109.41
29	B	529	BCR	C2-C1-C6	2.81	115.11	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	483	CLA	C1-C2-C3	2.81	131.19	126.19
29	K	112	BCR	C12-C13-C14	-2.81	114.65	118.97
33	C	492	LMG	O7-C10-C11	2.81	117.71	111.56
24	B	525	CLA	O2A-CGA-CBA	2.81	120.77	111.94
24	B	523	CLA	C2A-C3A-C4A	2.80	105.71	101.40
24	D	356	CLA	CED-O2D-CGD	2.80	122.68	116.02
24	C	474	CLA	C1D-CHD-C4C	2.80	126.94	122.60
24	B	525	CLA	C7-C6-C5	-2.80	104.76	113.01
24	B	524	CLA	CMB-C2B-C1B	-2.80	124.32	128.62
29	D	358	BCR	C37-C22-C23	2.79	122.61	118.09
29	B	529	BCR	C1-C6-C5	-2.79	118.56	122.60
24	B	518	CLA	C6-C5-C3	2.79	119.42	112.78
24	C	478	CLA	C2A-C3A-C4A	2.79	105.69	101.40
24	B	515	CLA	O2A-CGA-CBA	2.79	120.71	111.94
24	B	526	CLA	C7-C6-C5	-2.79	104.80	113.01
34	T	227	LMT	O1B-C1B-C2B	2.78	114.79	108.12
30	C	490	DGD	C1E-O6E-C5E	2.78	119.14	113.73
32	B	532	SQD	C32-C31-C30	2.78	129.66	114.61
24	A	366	CLA	CED-O2D-CGD	2.78	122.63	116.02
32	D	361	SQD	O47-C7-C8	2.78	117.65	111.56
24	C	485	CLA	OBD-CAD-CBD	-2.78	121.75	125.94
29	D	358	BCR	C23-C22-C21	-2.78	114.71	118.97
24	B	524	CLA	CAA-C2A-C3A	-2.78	106.48	113.04
24	C	484	CLA	O2A-CGA-CBA	2.77	120.66	111.94
24	B	512	CLA	CMB-C2B-C1B	-2.77	124.36	128.62
33	B	534	LMG	C7-O1-C1	-2.77	108.28	113.81
24	C	475	CLA	C1-C2-C3	2.77	131.10	126.19
29	D	358	BCR	C12-C13-C14	-2.77	114.72	118.97
24	C	476	CLA	OBD-CAD-CBD	-2.77	121.76	125.94
26	E	85	HEM	C4C-NC-C1C	2.77	108.41	105.53
24	D	354	CLA	CBD-CHA-C1A	2.76	132.38	128.77
24	B	526	CLA	C1-C2-C3	2.76	131.10	126.19
24	C	481	CLA	O2A-CGA-CBA	2.76	120.62	111.94
24	B	514	CLA	O2A-CGA-CBA	2.75	120.61	111.94
32	A	372	SQD	C32-C33-C34	2.75	124.22	113.78
32	A	372	SQD	C3-C4-C5	-2.75	105.28	110.20
24	C	479	CLA	C1D-CHD-C4C	2.75	126.87	122.60
24	C	480	CLA	CED-O2D-CGD	2.75	122.56	116.02
29	J	115	BCR	C3-C4-C5	2.75	117.91	113.74
24	B	518	CLA	CED-O2D-CGD	2.75	122.56	116.02
29	K	112	BCR	C30-C25-C24	2.75	123.31	115.69
27	D	357	PL9	C30-C29-C31	2.75	119.57	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	475	CLA	CBD-CHA-C1A	2.75	132.36	128.77
24	A	362	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
24	B	516	CLA	OBD-CAD-CBD	-2.75	121.80	125.94
24	B	518	CLA	CBD-CHA-C1A	2.74	132.35	128.77
24	C	482	CLA	C6-C5-C3	2.74	119.30	112.78
33	C	492	LMG	O6-C5-C6	2.74	113.08	106.34
24	B	522	CLA	C1-C2-C3	2.74	131.05	126.19
24	B	521	CLA	C1D-CHD-C4C	2.74	126.85	122.60
24	D	356	CLA	O2A-CGA-CBA	2.73	120.52	111.94
24	C	475	CLA	CAA-C2A-C3A	-2.72	106.60	113.04
24	B	526	CLA	O2A-CGA-CBA	2.72	120.50	111.94
24	B	516	CLA	C1D-CHD-C4C	2.72	126.82	122.60
24	B	519	CLA	C7-C6-C5	-2.72	104.99	113.01
25	A	365	PHO	C6-C5-C3	2.72	119.24	112.78
29	B	528	BCR	C1-C6-C5	-2.72	118.66	122.60
24	B	512	CLA	C1D-CHD-C4C	2.72	126.82	122.60
24	C	478	CLA	CBA-CAA-C2A	2.72	122.08	114.01
24	D	354	CLA	CMB-C2B-C3B	2.72	129.25	124.97
27	D	357	PL9	C27-C28-C29	-2.72	121.94	127.80
24	B	521	CLA	C2A-C3A-C4A	2.71	105.57	101.40
24	B	520	CLA	CMB-C2B-C1B	-2.71	124.45	128.62
24	C	483	CLA	CED-O2D-CGD	2.71	122.46	116.02
24	B	522	CLA	O2A-CGA-CBA	2.71	120.45	111.94
29	B	527	BCR	C1-C6-C5	-2.70	118.69	122.60
24	B	511	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
24	A	366	CLA	O2A-CGA-CBA	2.70	120.44	111.94
24	B	522	CLA	C2A-C3A-C4A	2.70	105.56	101.40
24	C	479	CLA	C1-C2-C3	2.70	130.99	126.19
29	A	369	BCR	C23-C24-C25	2.70	135.30	127.32
29	J	115	BCR	C28-C27-C26	2.70	117.83	113.74
24	C	486	CLA	C1-C2-C3	2.70	130.99	126.19
24	B	518	CLA	C2A-C3A-C4A	2.70	105.55	101.40
34	D	363	LMT	C1B-O1B-C4'	-2.70	111.11	117.99
24	B	524	CLA	O2A-CGA-CBA	2.70	120.42	111.94
24	A	366	CLA	CBD-CHA-C1A	2.69	132.29	128.77
24	B	515	CLA	C1D-CHD-C4C	2.69	126.78	122.60
24	B	519	CLA	CBD-CHA-C1A	2.69	132.29	128.77
24	B	523	CLA	CMB-C2B-C1B	-2.69	124.48	128.62
24	B	523	CLA	C7-C6-C5	-2.69	105.08	113.01
24	B	511	CLA	CAA-C2A-C3A	-2.69	106.68	113.04
24	B	520	CLA	CMB-C2B-C3B	2.69	129.21	124.97
24	D	364	CLA	C7-C6-C5	-2.69	105.09	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	514	CLA	C2A-C3A-C4A	2.69	105.53	101.40
24	B	520	CLA	C2A-C3A-C4A	2.68	105.53	101.40
29	D	358	BCR	C23-C24-C25	2.68	135.24	127.32
24	A	362	CLA	C1D-CHD-C4C	2.68	126.76	122.60
24	D	356	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
24	B	519	CLA	C2A-C3A-C4A	2.68	105.52	101.40
32	B	532	SQD	O9-S-C6	-2.68	102.34	107.03
24	C	485	CLA	C7-C6-C5	-2.68	105.12	113.01
24	C	484	CLA	C1-C2-C3	2.68	130.94	126.19
24	B	511	CLA	C2D-C1D-ND	2.68	111.43	109.41
24	B	521	CLA	C6-C5-C3	2.67	119.14	112.78
24	C	483	CLA	C7-C6-C5	-2.67	105.14	113.01
24	C	485	CLA	C2A-C3A-C4A	2.67	105.51	101.40
24	C	474	CLA	CED-O2D-CGD	2.67	122.37	116.02
24	B	524	CLA	C16-C15-C13	2.67	122.83	115.14
30	A	370	DGD	O6D-C5D-C6D	2.67	111.98	106.61
29	C	487	BCR	C23-C24-C25	2.67	135.20	127.32
24	B	517	CLA	C1-C2-C3	2.67	130.93	126.19
24	C	476	CLA	CED-O2D-CGD	2.67	122.37	116.02
24	C	486	CLA	O2A-CGA-CBA	2.67	120.33	111.94
29	B	530	BCR	C1-C6-C5	-2.67	118.74	122.60
24	C	476	CLA	O2A-CGA-CBA	2.67	120.33	111.94
24	B	520	CLA	C2D-C1D-ND	2.66	111.42	109.41
24	D	354	CLA	C2D-C1D-ND	2.66	111.42	109.41
24	B	516	CLA	C2A-C3A-C4A	2.66	105.49	101.40
24	B	523	CLA	CAA-C2A-C3A	-2.65	106.78	113.04
29	C	488	BCR	C16-C17-C18	2.65	131.10	127.29
24	A	363	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
24	B	513	CLA	CMB-C2B-C1B	-2.64	124.56	128.62
24	B	514	CLA	CAA-C2A-C3A	-2.64	106.80	113.04
34	O	274	LMT	C1-O1'-C1'	-2.63	109.22	113.96
30	A	375	DGD	O6D-C5D-C6D	2.63	111.90	106.61
29	K	112	BCR	C35-C13-C12	2.63	122.35	118.09
24	B	523	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
33	I	220	LMG	O6-C5-C6	2.62	112.79	106.34
24	B	522	CLA	CED-O2D-CGD	2.62	122.26	116.02
24	B	513	CLA	C2D-C1D-ND	2.62	111.39	109.41
24	B	521	CLA	CAA-C2A-C3A	-2.62	106.84	113.04
24	C	476	CLA	C2D-C1D-ND	2.62	111.39	109.41
24	C	479	CLA	C7-C6-C5	-2.62	105.28	113.01
26	V	164	HEM	C2A-C1A-NA	-2.62	106.09	109.73
24	B	524	CLA	O2D-CGD-CBD	2.62	116.68	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	372	SQD	O8-S-O7	2.62	117.45	111.78
24	C	480	CLA	C2A-C1A-CHA	2.62	128.37	123.83
24	C	485	CLA	CED-O2D-CGD	2.62	122.25	116.02
29	Z	116	BCR	C1-C6-C5	-2.62	118.81	122.60
24	B	517	CLA	C1D-CHD-C4C	2.62	126.66	122.60
24	C	477	CLA	C2A-C3A-C4A	2.61	105.42	101.40
24	B	515	CLA	C2A-C3A-C4A	2.61	105.42	101.40
30	A	375	DGD	C3G-O3G-C1D	-2.61	108.60	113.81
31	A	374	LHG	O8-C23-C24	2.61	120.17	111.94
24	C	475	CLA	C2A-C3A-C4A	2.61	105.41	101.40
24	D	354	CLA	CED-O2D-CGD	2.61	122.23	116.02
24	B	519	CLA	C2D-C1D-ND	2.61	111.38	109.41
24	B	512	CLA	CMB-C2B-C3B	2.60	129.07	124.97
24	B	511	CLA	C7-C6-C5	-2.60	105.34	113.01
33	A	373	LMG	O7-C10-C11	2.60	117.26	111.56
24	A	366	CLA	C2A-C3A-C4A	2.60	105.40	101.40
24	C	484	CLA	CMB-C2B-C1B	-2.60	124.62	128.62
24	C	484	CLA	C7-C6-C5	-2.60	105.35	113.01
27	D	357	PL9	C35-C34-C36	2.60	119.34	115.39
24	D	356	CLA	C2D-C1D-ND	2.60	111.37	109.41
29	H	107	BCR	C1-C6-C5	-2.60	118.84	122.60
25	D	355	PHO	O2A-CGA-CBA	2.60	120.11	111.94
30	H	208	DGD	O3G-C1D-C2D	2.60	111.48	108.18
24	B	512	CLA	C2A-C3A-C4A	2.59	105.39	101.40
24	B	512	CLA	C2D-C1D-ND	2.59	111.37	109.41
29	B	530	BCR	C7-C8-C9	2.59	130.09	126.22
29	C	488	BCR	C24-C23-C22	2.59	130.09	126.22
24	B	511	CLA	C2A-C3A-C4A	2.59	105.38	101.40
24	C	478	CLA	C7-C6-C5	-2.59	105.38	113.01
25	A	365	PHO	C4A-NA-C1A	2.59	111.83	108.42
24	B	523	CLA	O2A-CGA-CBA	2.59	120.09	111.94
24	A	363	CLA	CMB-C2B-C1B	-2.59	124.64	128.62
29	H	107	BCR	C23-C24-C25	2.59	134.96	127.32
24	C	478	CLA	CMB-C2B-C1B	-2.58	124.65	128.62
25	A	365	PHO	C7-C6-C5	-2.58	105.40	113.01
24	B	521	CLA	O2A-CGA-CBA	2.58	120.06	111.94
24	C	481	CLA	C2A-C3A-C4A	2.58	105.37	101.40
29	A	369	BCR	C37-C22-C23	2.58	122.27	118.09
33	B	533	LMG	O6-C5-C6	2.58	112.69	106.34
29	Z	116	BCR	C8-C7-C6	2.58	134.94	127.32
24	B	520	CLA	O2A-CGA-CBA	2.58	120.06	111.94
29	C	488	BCR	C40-C30-C29	-2.58	98.28	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	59	PL9	C17-C18-C19	-2.58	122.24	127.80
24	C	486	CLA	C2D-C1D-ND	2.58	111.36	109.41
24	B	519	CLA	C1D-C2D-C3D	-2.58	104.68	106.78
24	C	479	CLA	C2A-C3A-C4A	2.58	105.36	101.40
24	B	526	CLA	C6-C5-C3	2.58	118.91	112.78
24	A	363	CLA	C6-C5-C3	2.58	118.91	112.78
24	B	524	CLA	C6-C5-C3	2.58	118.91	112.78
29	H	107	BCR	C35-C13-C12	2.57	122.25	118.09
24	C	477	CLA	C1D-C2D-C3D	-2.57	104.68	106.78
24	B	516	CLA	C2D-C1D-ND	2.57	111.35	109.41
24	C	481	CLA	CED-O2D-CGD	2.57	122.12	116.02
24	C	486	CLA	CMB-C2B-C1B	-2.56	124.68	128.62
24	C	475	CLA	C7-C6-C5	-2.56	105.46	113.01
29	J	115	BCR	C20-C21-C22	-2.56	123.60	127.29
24	B	515	CLA	C7-C6-C5	-2.56	105.46	113.01
32	B	532	SQD	C45-O47-C7	2.56	124.24	117.92
29	B	527	BCR	C35-C13-C12	2.56	122.23	118.09
24	B	523	CLA	CMB-C2B-C3B	2.56	129.00	124.97
24	B	523	CLA	C2D-C1D-ND	2.56	111.34	109.41
29	C	488	BCR	C30-C25-C24	2.56	122.78	115.69
24	A	362	CLA	C16-C15-C13	2.56	122.50	115.14
24	A	366	CLA	C2D-C1D-ND	2.55	111.34	109.41
24	B	513	CLA	C2A-C3A-C4A	2.55	105.33	101.40
32	A	372	SQD	O47-C7-C8	2.55	117.16	111.56
27	D	357	PL9	C10-C9-C11	2.55	119.27	115.39
24	C	477	CLA	CMB-C2B-C1B	-2.55	124.70	128.62
24	B	522	CLA	CMB-C2B-C1B	-2.55	124.70	128.62
24	C	481	CLA	C7-C6-C5	-2.55	105.50	113.01
24	C	475	CLA	C2D-C1D-ND	2.55	111.33	109.41
24	C	477	CLA	O2A-CGA-CBA	2.55	119.95	111.94
29	B	530	BCR	C23-C24-C25	2.55	134.84	127.32
24	B	520	CLA	C6-C5-C3	2.54	118.83	112.78
24	C	475	CLA	O2A-CGA-CBA	2.54	119.94	111.94
32	T	213	SQD	O9-S-C6	-2.54	102.58	107.03
29	Z	116	BCR	C19-C18-C17	-2.54	115.07	118.97
32	T	213	SQD	C44-O6-C1	2.54	118.86	113.81
29	Z	116	BCR	C35-C13-C12	2.54	122.19	118.09
24	C	483	CLA	OBD-CAD-CBD	-2.54	122.11	125.94
29	C	487	BCR	C7-C8-C9	2.53	130.01	126.22
24	B	522	CLA	CAA-C2A-C3A	-2.53	107.05	113.04
24	B	519	CLA	C6-C5-C3	2.53	118.80	112.78
27	D	357	PL9	C22-C23-C24	-2.53	122.33	127.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	484	CLA	C2A-C1A-CHA	2.53	128.22	123.83
24	B	524	CLA	C1D-C2D-C3D	-2.53	104.71	106.78
24	C	474	CLA	C7-C6-C5	-2.53	105.56	113.01
29	B	528	BCR	C23-C22-C21	-2.53	115.08	118.97
29	C	487	BCR	C12-C13-C14	-2.53	115.09	118.97
29	Z	116	BCR	C30-C25-C26	-2.52	118.94	122.60
24	C	479	CLA	O2A-CGA-CBA	2.52	119.88	111.94
24	C	474	CLA	C2A-C3A-C4A	2.52	105.28	101.40
24	B	512	CLA	OBD-CAD-CBD	-2.52	122.14	125.94
33	A	373	LMG	C7-O1-C1	-2.52	108.79	113.81
32	D	361	SQD	C3-C4-C5	-2.52	105.71	110.20
24	A	362	CLA	CMB-C2B-C1B	-2.51	124.75	128.62
29	J	115	BCR	C16-C17-C18	2.51	130.91	127.29
24	B	511	CLA	C1D-CHD-C4C	2.51	126.50	122.60
25	D	355	PHO	CMB-C2B-C3B	2.51	128.93	124.97
24	C	480	CLA	C2A-C3A-C4A	2.51	105.26	101.40
29	D	358	BCR	C15-C14-C13	2.50	130.90	127.29
24	C	486	CLA	C7-C6-C5	-2.50	105.64	113.01
24	B	518	CLA	CMB-C2B-C1B	-2.50	124.78	128.62
24	B	526	CLA	C1D-CHD-C4C	2.50	126.48	122.60
29	B	528	BCR	C8-C9-C10	-2.50	115.13	118.97
26	E	85	HEM	C3A-C4A-NA	-2.50	107.52	109.41
24	B	511	CLA	CMB-C2B-C1B	-2.50	124.78	128.62
24	A	363	CLA	C1D-CHD-C4C	2.50	126.47	122.60
24	C	474	CLA	C2D-C1D-ND	2.50	111.30	109.41
29	C	487	BCR	C23-C22-C21	-2.50	115.14	118.97
29	A	369	BCR	C16-C17-C18	2.50	130.89	127.29
24	B	520	CLA	C16-C15-C13	2.50	122.33	115.14
24	B	516	CLA	C1D-C2D-C3D	-2.49	104.75	106.78
24	B	516	CLA	CED-O2D-CGD	2.49	121.95	116.02
24	D	354	CLA	C1-C2-C3	2.49	130.61	126.19
24	B	524	CLA	CMB-C2B-C3B	2.49	128.89	124.97
29	B	528	BCR	C7-C8-C9	2.48	129.93	126.22
31	A	374	LHG	C5-O7-C7	-2.48	111.79	117.92
24	C	482	CLA	CMB-C2B-C1B	-2.48	124.80	128.62
29	J	115	BCR	C15-C16-C17	-2.48	117.87	123.36
24	B	516	CLA	C7-C6-C5	-2.48	105.71	113.01
24	B	517	CLA	C2A-C3A-C4A	2.47	105.21	101.40
26	V	164	HEM	O2A-CGA-CBA	2.48	122.97	114.22
32	A	372	SQD	C35-C34-C33	2.47	120.02	114.46
24	A	363	CLA	CED-O2D-CGD	2.47	121.90	116.02
24	B	524	CLA	C2A-C3A-C4A	2.47	105.20	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	112	BCR	C32-C1-C2	-2.47	98.74	108.73
24	C	480	CLA	CAA-C2A-C3A	-2.46	107.21	113.04
29	H	107	BCR	C1-C6-C7	2.46	122.52	115.69
24	C	476	CLA	C7-C6-C5	-2.46	105.75	113.01
24	C	485	CLA	C4D-CHA-CBD	-2.46	103.57	109.37
26	V	164	HEM	C4A-C3A-C2A	2.46	108.71	107.00
32	D	361	SQD	O9-S-C6	-2.46	102.72	107.03
24	A	362	CLA	C2A-C3A-C4A	2.46	105.19	101.40
34	O	274	LMT	O1B-C1B-C2B	2.46	114.02	108.12
24	A	362	CLA	C2D-C1D-ND	2.46	111.27	109.41
29	C	488	BCR	C35-C13-C12	2.46	122.07	118.09
24	C	484	CLA	C2A-C3A-C4A	2.45	105.18	101.40
33	E	218	LMG	O7-C8-C7	2.45	117.42	108.40
24	C	481	CLA	CMB-C2B-C1B	-2.45	124.85	128.62
30	D	362	DGD	O6D-C5D-C4D	2.45	114.30	109.76
31	A	371	LHG	O7-C7-C8	2.45	116.93	111.56
24	B	526	CLA	CMB-C2B-C1B	-2.45	124.85	128.62
24	A	363	CLA	O2D-CGD-CBD	2.45	116.32	111.33
29	D	358	BCR	C35-C13-C12	2.45	122.05	118.09
32	T	213	SQD	O47-C7-C8	2.44	116.92	111.56
27	J	59	PL9	C12-C13-C14	-2.45	122.52	127.80
24	C	479	CLA	C2D-C1D-ND	2.44	111.26	109.41
24	B	521	CLA	C1D-C2D-C3D	-2.44	104.79	106.78
24	C	481	CLA	C4D-CHA-CBD	-2.44	103.62	109.37
30	D	362	DGD	O6D-C5D-C6D	2.44	111.52	106.61
24	A	363	CLA	CAA-C2A-C1A	2.44	117.71	111.62
33	C	492	LMG	O1-C1-C2	2.44	111.28	108.18
24	B	525	CLA	CMB-C2B-C1B	-2.44	124.87	128.62
33	M	217	LMG	O8-C9-C8	-2.44	102.44	108.83
24	B	521	CLA	C2D-C1D-ND	2.43	111.25	109.41
24	B	525	CLA	C1D-C2D-C3D	-2.43	104.79	106.78
24	D	356	CLA	CMB-C2B-C1B	-2.43	124.88	128.62
29	B	527	BCR	C12-C13-C14	-2.43	115.23	118.97
32	T	213	SQD	C3-C4-C5	-2.43	105.86	110.20
29	Z	116	BCR	C12-C13-C14	-2.43	115.24	118.97
24	B	514	CLA	C7-C6-C5	-2.43	105.85	113.01
24	C	486	CLA	C2A-C3A-C4A	2.43	105.14	101.40
24	D	354	CLA	C2A-C1A-CHA	2.42	128.03	123.83
24	C	479	CLA	CMB-C2B-C1B	-2.42	124.89	128.62
32	F	224	SQD	C45-O47-C7	2.42	123.88	117.92
29	A	369	BCR	C30-C25-C24	2.42	122.39	115.69
32	F	224	SQD	O9-S-C6	-2.42	102.80	107.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	528	BCR	C30-C25-C24	2.41	122.36	115.69
24	D	356	CLA	O2D-CGD-CBD	2.41	116.23	111.33
24	C	478	CLA	C2D-C1D-ND	2.41	111.23	109.41
24	B	526	CLA	C2D-C1D-ND	2.41	111.23	109.41
24	C	481	CLA	C2A-C1A-NA	-2.41	108.58	111.24
24	C	478	CLA	C2A-C1A-CHA	2.40	127.99	123.83
24	C	481	CLA	O2D-CGD-CBD	2.40	116.22	111.33
34	T	227	LMT	O1B-C4'-C3'	2.40	113.31	107.16
26	E	85	HEM	O2A-CGA-CBA	2.40	122.69	114.22
27	J	59	PL9	C15-C14-C16	2.39	119.02	115.39
29	C	487	BCR	C1-C6-C7	2.39	122.31	115.69
24	B	518	CLA	C7-C6-C5	-2.39	105.97	113.01
32	D	361	SQD	O8-S-O7	2.39	116.95	111.78
24	C	475	CLA	CMB-C2B-C1B	-2.38	124.95	128.62
24	B	514	CLA	C2A-C1A-NA	-2.38	108.61	111.24
24	D	364	CLA	CMB-C2B-C1B	-2.38	124.96	128.62
29	B	528	BCR	C11-C10-C9	2.38	130.72	127.29
24	B	517	CLA	C1D-C2D-C3D	-2.38	104.84	106.78
24	B	514	CLA	C1-C2-C3	2.38	130.41	126.19
24	B	513	CLA	C6-C5-C3	2.38	118.43	112.78
24	C	485	CLA	C1D-C2D-C3D	-2.37	104.84	106.78
30	C	490	DGD	O6D-C5D-C6D	2.37	111.38	106.61
32	A	372	SQD	O9-S-C6	-2.37	102.87	107.03
27	A	367	PL9	C32-C33-C34	-2.37	122.68	127.80
24	B	514	CLA	C4D-CHA-CBD	-2.37	103.78	109.37
25	D	355	PHO	C4A-NA-C1A	2.37	111.54	108.42
24	D	354	CLA	C7-C6-C5	-2.37	106.04	113.01
24	C	484	CLA	C6-C7-C8	2.36	121.95	115.14
29	B	528	BCR	C36-C18-C19	2.36	121.91	118.09
24	A	362	CLA	C7-C6-C5	-2.36	106.04	113.01
24	B	515	CLA	CMB-C2B-C1B	-2.36	124.99	128.62
24	B	512	CLA	C1D-C2D-C3D	-2.36	104.85	106.78
24	C	484	CLA	C4D-CHA-CBD	-2.36	103.82	109.37
29	B	529	BCR	C32-C1-C6	2.36	114.24	110.33
24	C	485	CLA	C2A-C1A-CHA	2.36	127.92	123.83
29	B	528	BCR	C32-C1-C6	2.36	114.23	110.33
33	M	217	LMG	C7-O1-C1	-2.35	109.12	113.81
24	C	484	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
33	B	531	LMG	C9-C8-C7	-2.35	106.51	111.86
27	D	357	PL9	C32-C33-C34	-2.35	122.73	127.80
24	B	522	CLA	O2D-CGD-CBD	2.35	116.11	111.33
24	A	366	CLA	C16-C15-C13	2.35	121.90	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	480	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
24	B	523	CLA	CED-O2D-CGD	2.34	121.59	116.02
29	H	107	BCR	C23-C22-C21	-2.34	115.38	118.97
29	Z	116	BCR	C36-C18-C19	2.34	121.88	118.09
24	B	522	CLA	C2D-C1D-ND	2.34	111.18	109.41
24	C	476	CLA	C2A-C3A-C4A	2.34	105.00	101.40
24	D	364	CLA	O2A-CGA-CBA	2.34	119.29	111.94
29	J	115	BCR	C31-C1-C2	2.34	118.20	108.73
24	C	476	CLA	CMB-C2B-C1B	-2.34	125.03	128.62
24	C	483	CLA	CAA-C2A-C3A	-2.34	107.51	113.04
24	C	479	CLA	C1D-C2D-C3D	-2.34	104.87	106.78
24	B	520	CLA	CED-O2D-CGD	2.34	121.58	116.02
24	B	524	CLA	C6-C7-C8	2.34	121.87	115.14
24	B	516	CLA	CMB-C2B-C1B	-2.33	125.03	128.62
25	A	365	PHO	C6-C7-C8	2.33	121.86	115.14
24	B	511	CLA	C4D-CHA-CBD	-2.32	103.90	109.37
29	A	369	BCR	C35-C13-C12	2.32	121.85	118.09
24	C	482	CLA	C7-C6-C5	-2.32	106.17	113.01
33	C	493	LMG	O8-C28-C29	2.32	119.24	111.94
24	A	362	CLA	CBA-CAA-C2A	2.32	120.90	114.01
29	K	112	BCR	C37-C22-C23	2.32	121.84	118.09
24	C	477	CLA	C7-C6-C5	-2.32	106.17	113.01
25	A	365	PHO	O2D-CGD-CBD	2.32	116.06	111.33
32	A	372	SQD	C15-C14-C13	2.32	127.14	114.61
29	B	528	BCR	C12-C13-C14	-2.31	115.42	118.97
24	B	519	CLA	O2A-CGA-CBA	2.31	119.22	111.94
29	Z	116	BCR	C1-C6-C7	2.31	122.09	115.69
24	B	526	CLA	C4D-CHA-CBD	-2.31	103.93	109.37
24	B	525	CLA	C2A-C1A-CHA	2.31	127.83	123.83
30	D	362	DGD	C2G-O2G-C1B	2.31	123.60	117.92
24	C	484	CLA	CMB-C2B-C3B	2.30	128.60	124.97
29	Z	116	BCR	C28-C27-C26	2.30	117.22	113.74
25	A	365	PHO	C1D-C2D-C3D	-2.30	104.92	106.89
29	B	530	BCR	C8-C7-C6	2.29	134.10	127.32
29	C	487	BCR	C37-C22-C23	2.29	121.80	118.09
24	C	482	CLA	C2D-C1D-ND	2.30	111.14	109.41
24	C	480	CLA	C4D-CHA-CBD	-2.29	103.97	109.37
33	E	218	LMG	C9-C8-C7	-2.29	106.63	111.86
30	A	370	DGD	C3G-C2G-C1G	-2.29	106.64	111.86
24	B	522	CLA	C6-C7-C8	2.29	121.73	115.14
24	B	514	CLA	CMB-C2B-C1B	-2.29	125.10	128.62
24	C	485	CLA	CMB-C2B-C1B	-2.29	125.10	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	482	CLA	CAA-C2A-C3A	-2.29	107.64	113.04
24	B	511	CLA	C2A-C1A-CHA	2.28	127.79	123.83
24	D	364	CLA	CAA-CBA-CGA	2.28	120.62	113.27
24	A	366	CLA	CMB-C2B-C1B	-2.28	125.11	128.62
24	D	364	CLA	CMB-C2B-C3B	2.28	128.56	124.97
24	A	362	CLA	C6-C7-C8	2.28	121.70	115.14
29	C	488	BCR	C12-C13-C14	-2.28	115.47	118.97
29	B	528	BCR	C28-C27-C26	2.28	117.19	113.74
30	C	489	DGD	O3G-C1D-C2D	2.28	111.08	108.18
24	B	526	CLA	C1D-C2D-C3D	-2.28	104.92	106.78
24	A	366	CLA	C1D-C2D-C3D	-2.27	104.92	106.78
24	B	519	CLA	CMB-C2B-C1B	-2.27	125.13	128.62
24	C	486	CLA	CMB-C2B-C3B	2.27	128.55	124.97
24	B	512	CLA	C1-C2-C3	2.27	130.23	126.19
32	B	532	SQD	C36-C35-C34	2.27	126.90	114.61
24	C	480	CLA	C2D-C1D-ND	2.27	111.12	109.41
24	B	517	CLA	C4D-CHA-CBD	-2.27	104.04	109.37
24	B	520	CLA	O2D-CGD-CBD	2.26	115.94	111.33
24	B	520	CLA	C7-C6-C5	-2.26	106.34	113.01
29	C	487	BCR	C30-C25-C24	2.26	121.95	115.69
25	A	365	PHO	O2A-CGA-CBA	2.26	119.05	111.94
29	B	528	BCR	C20-C21-C22	2.26	130.55	127.29
24	B	524	CLA	C2A-C1A-NA	-2.26	108.74	111.24
24	C	478	CLA	C6-C5-C3	2.25	118.14	112.78
24	D	364	CLA	C1-C2-C3	2.25	130.19	126.19
24	C	476	CLA	C1D-C2D-C3D	-2.25	104.94	106.78
24	C	479	CLA	C6-C5-C3	2.25	118.14	112.78
27	A	367	PL9	C53-C6-C1	2.25	119.72	114.80
24	C	484	CLA	CAA-C2A-C3A	-2.25	107.72	113.04
26	V	164	HEM	C4C-NC-C1C	2.25	107.87	105.53
24	B	525	CLA	CMB-C2B-C3B	2.25	128.51	124.97
24	A	366	CLA	OBD-CAD-C3D	2.24	132.09	127.91
24	B	516	CLA	C4D-CHA-CBD	-2.24	104.09	109.37
29	B	528	BCR	C37-C22-C23	2.24	121.72	118.09
24	B	514	CLA	C2A-C1A-CHA	2.24	127.71	123.83
24	B	523	CLA	C6-C7-C8	2.24	121.59	115.14
24	D	354	CLA	C2A-C1A-NA	-2.24	108.77	111.24
24	C	478	CLA	C4D-CHA-CBD	-2.23	104.11	109.37
32	B	532	SQD	O5-C5-C4	2.23	113.90	109.76
24	C	480	CLA	CMB-C2B-C1B	-2.23	125.19	128.62
24	B	513	CLA	CMB-C2B-C3B	2.23	128.48	124.97
24	B	519	CLA	C1-C2-C3	2.23	130.15	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	107	BCR	C37-C22-C23	2.23	121.69	118.09
24	C	477	CLA	C16-C15-C13	2.23	121.55	115.14
29	B	529	BCR	C1-C6-C7	2.22	121.86	115.69
33	B	534	LMG	O6-C5-C6	2.22	111.80	106.34
24	C	474	CLA	O2D-CGD-CBD	2.22	115.85	111.33
29	A	369	BCR	C1-C6-C7	2.22	121.84	115.69
24	C	480	CLA	C1D-C2D-C3D	-2.22	104.97	106.78
24	C	481	CLA	C1D-C2D-C3D	-2.22	104.97	106.78
29	B	530	BCR	C32-C1-C6	2.22	114.00	110.33
29	B	528	BCR	C35-C13-C12	2.22	121.68	118.09
24	C	479	CLA	C4D-CHA-CBD	-2.22	104.15	109.37
24	B	525	CLA	C4D-CHA-CBD	-2.22	104.15	109.37
27	J	59	PL9	C53-C6-C1	2.21	119.64	114.80
29	B	527	BCR	C36-C18-C19	2.21	121.67	118.09
27	J	59	PL9	C10-C9-C8	-2.21	119.14	123.52
30	H	208	DGD	C3G-O3G-C1D	-2.21	109.41	113.81
32	B	532	SQD	C15-C14-C13	2.21	126.55	114.61
24	B	516	CLA	CBA-CAA-C2A	2.21	120.56	114.01
25	D	355	PHO	O2D-CGD-CBD	2.20	115.82	111.33
24	C	480	CLA	CMB-C2B-C3B	2.20	128.44	124.97
24	B	520	CLA	C4D-CHA-CBD	-2.21	104.18	109.37
24	C	474	CLA	C16-C15-C13	2.20	121.48	115.14
24	C	483	CLA	CMB-C2B-C1B	-2.20	125.23	128.62
32	T	213	SQD	C15-C14-C13	2.20	126.52	114.61
29	K	112	BCR	C28-C27-C26	2.20	117.08	113.74
24	B	511	CLA	CMB-C2B-C3B	2.20	128.43	124.97
25	A	365	PHO	CMB-C2B-C3B	2.20	128.43	124.97
29	B	530	BCR	C30-C25-C24	2.19	121.77	115.69
29	B	528	BCR	C40-C30-C29	-2.19	99.85	108.73
24	B	521	CLA	CMB-C2B-C1B	-2.19	125.25	128.62
32	F	224	SQD	O8-S-O9	-2.19	107.04	111.78
24	C	480	CLA	C6-C5-C3	2.19	117.99	112.78
24	B	517	CLA	CMB-C2B-C1B	-2.19	125.25	128.62
29	A	369	BCR	C8-C9-C10	-2.19	115.60	118.97
24	D	354	CLA	C16-C15-C13	2.19	121.44	115.14
29	A	369	BCR	C34-C9-C8	2.19	121.63	118.09
29	H	107	BCR	C32-C1-C6	2.19	113.95	110.33
26	E	85	HEM	C1B-NB-C4B	2.18	107.40	105.16
24	B	515	CLA	C4D-CHA-CBD	-2.18	104.23	109.37
24	C	484	CLA	C2A-C1A-NA	-2.18	108.83	111.24
29	C	488	BCR	C37-C22-C23	2.18	121.62	118.09
24	C	478	CLA	CMB-C2B-C3B	2.18	128.40	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	516	CLA	C2A-C1A-CHA	2.18	127.61	123.83
24	C	476	CLA	C4D-CHA-CBD	-2.18	104.24	109.37
24	B	523	CLA	C6-C5-C3	2.18	117.95	112.78
24	B	518	CLA	CBA-CAA-C2A	2.18	120.47	114.01
24	C	474	CLA	C2A-C1A-CHA	2.17	127.59	123.83
30	A	370	DGD	C3G-O3G-C1D	-2.17	109.48	113.81
24	D	354	CLA	C2A-C3A-C4A	2.17	104.74	101.40
24	B	523	CLA	C4D-CHA-CBD	-2.17	104.26	109.37
24	B	523	CLA	C1D-C2D-C3D	-2.17	105.01	106.78
29	K	112	BCR	C8-C7-C6	2.17	133.72	127.32
24	B	524	CLA	C4D-CHA-CBD	-2.17	104.27	109.37
29	H	107	BCR	C36-C18-C19	2.16	121.59	118.09
24	B	522	CLA	C7-C6-C5	-2.16	106.64	113.01
24	C	486	CLA	C6-C5-C3	2.16	117.92	112.78
29	K	112	BCR	C19-C18-C17	-2.16	115.65	118.97
32	B	532	SQD	C34-C33-C32	2.16	126.30	114.61
24	B	526	CLA	C6-C7-C8	2.16	121.36	115.14
24	C	485	CLA	C2A-C1A-NA	-2.16	108.86	111.24
24	B	525	CLA	O2D-CGD-CBD	2.16	115.73	111.33
29	B	530	BCR	C1-C6-C7	2.16	121.67	115.69
24	D	356	CLA	C1D-C2D-C3D	-2.16	105.02	106.78
24	A	362	CLA	CMB-C2B-C3B	2.16	128.37	124.97
24	C	483	CLA	O2D-CGD-CBD	2.16	115.73	111.33
24	C	479	CLA	CMB-C2B-C3B	2.16	128.37	124.97
24	B	515	CLA	C1D-C2D-C3D	-2.16	105.02	106.78
24	D	356	CLA	C2A-C1A-CHA	2.16	127.57	123.83
24	B	513	CLA	C7-C6-C5	-2.16	106.66	113.01
24	B	519	CLA	C4D-CHA-CBD	-2.16	104.30	109.37
24	B	518	CLA	CMB-C2B-C3B	2.15	128.36	124.97
27	J	59	PL9	C25-C24-C23	-2.15	119.26	123.52
24	B	526	CLA	C2A-C1A-CHA	2.15	127.56	123.83
24	C	478	CLA	OBD-CAD-C3D	2.15	131.91	127.91
24	D	356	CLA	C1-C2-C3	2.15	130.01	126.19
24	C	476	CLA	CAA-C2A-C3A	-2.15	107.96	113.04
24	B	525	CLA	C2A-C1A-NA	-2.15	108.86	111.24
27	A	367	PL9	C30-C29-C28	-2.15	119.27	123.52
24	A	362	CLA	C4D-CHA-CBD	-2.15	104.32	109.37
24	B	524	CLA	C1-O2A-CGA	2.15	122.99	116.98
24	B	526	CLA	CMB-C2B-C3B	2.14	128.35	124.97
24	C	474	CLA	C2A-C1A-NA	-2.14	108.87	111.24
24	C	477	CLA	C4D-CHA-CBD	-2.14	104.33	109.37
32	F	224	SQD	O48-C46-C45	2.14	114.44	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	485	CLA	O2D-CGD-CBD	2.14	115.69	111.33
24	C	481	CLA	C2A-C1A-CHA	2.14	127.54	123.83
24	C	486	CLA	C4D-CHA-CBD	-2.14	104.34	109.37
24	C	480	CLA	O2D-CGD-CBD	2.14	115.68	111.33
24	D	356	CLA	CMB-C2B-C3B	2.14	128.33	124.97
24	C	486	CLA	CAA-C2A-C3A	-2.14	107.99	113.04
24	A	363	CLA	C1D-C2D-C3D	-2.14	105.04	106.78
33	B	533	LMG	O8-C9-C8	-2.13	103.23	108.83
29	B	530	BCR	C16-C17-C18	2.13	130.36	127.29
24	B	518	CLA	OBD-CAD-C3D	2.13	131.87	127.91
24	B	525	CLA	CAA-C2A-C3A	-2.13	108.01	113.04
25	D	355	PHO	C1D-C2D-C3D	-2.13	105.07	106.89
24	B	521	CLA	CHB-C4A-NA	2.13	127.10	124.58
33	C	493	LMG	C7-O1-C1	-2.12	109.58	113.81
24	B	514	CLA	C1D-C2D-C3D	-2.12	105.05	106.78
34	B	535	LMT	C6'-C5'-C4'	-2.12	107.28	113.25
29	B	528	BCR	C16-C17-C18	2.12	130.35	127.29
34	B	535	LMT	C1'-O5'-C5'	-2.12	109.60	113.73
24	B	513	CLA	C4D-CHA-CBD	-2.12	104.39	109.37
24	B	521	CLA	O2D-CGD-CBD	2.11	115.64	111.33
30	C	489	DGD	O3E-C3E-C2E	-2.11	105.62	110.35
24	B	514	CLA	CED-O2D-CGD	2.11	121.05	116.02
32	A	372	SQD	C17-C16-C15	2.11	126.04	114.61
32	F	224	SQD	C15-C14-C13	2.11	126.04	114.61
24	B	524	CLA	C11-C12-C13	2.11	121.22	115.14
31	A	371	LHG	P-O6-C4	-2.11	106.84	122.03
24	C	474	CLA	C1D-C2D-C3D	-2.11	105.06	106.78
33	A	373	LMG	C9-C8-C7	-2.11	107.05	111.86
33	D	360	LMG	O8-C9-C8	-2.11	103.30	108.83
24	B	518	CLA	O2A-C1-C2	2.11	113.12	108.55
24	A	363	CLA	C2A-C1A-CHA	2.11	127.48	123.83
24	B	523	CLA	C2A-C1A-NA	-2.11	108.91	111.24
24	D	356	CLA	C4D-CHA-CBD	-2.10	104.42	109.37
26	V	164	HEM	CMA-C3A-C4A	-2.10	125.39	128.62
29	C	488	BCR	C36-C18-C19	2.10	121.49	118.09
24	D	354	CLA	C1D-C2D-C3D	-2.10	105.07	106.78
24	A	366	CLA	CMB-C2B-C3B	2.10	128.27	124.97
29	B	528	BCR	C34-C9-C8	2.10	121.48	118.09
29	B	528	BCR	C19-C18-C17	-2.10	115.75	118.97
29	C	487	BCR	C40-C30-C25	2.09	113.80	110.33
24	D	354	CLA	C4D-CHA-CBD	-2.09	104.44	109.37
24	C	482	CLA	OBD-CAD-C3D	2.09	131.81	127.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	513	CLA	C2A-C1A-CHA	2.09	127.46	123.83
24	B	512	CLA	C2A-C1A-CHA	2.09	127.46	123.83
24	C	484	CLA	C1D-C2D-C3D	-2.09	105.08	106.78
24	B	517	CLA	OBD-CAD-C3D	2.09	131.79	127.91
24	C	477	CLA	CED-O2D-CGD	2.08	120.97	116.02
24	B	512	CLA	C6-C7-C8	2.08	121.14	115.14
30	A	370	DGD	C6D-C5D-C4D	2.08	116.60	111.87
29	C	487	BCR	C11-C10-C9	2.08	130.29	127.29
24	B	517	CLA	C7-C6-C5	-2.08	106.88	113.01
24	B	513	CLA	C2A-C1A-NA	-2.08	108.95	111.24
24	B	513	CLA	O2D-CGD-CBD	2.07	115.56	111.33
24	B	511	CLA	C1D-C2D-C3D	-2.07	105.09	106.78
30	A	370	DGD	C6D-O5D-C1E	2.07	117.94	113.81
24	C	474	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
24	B	512	CLA	C4D-CHA-CBD	-2.07	104.50	109.37
24	C	475	CLA	C4D-CHA-CBD	-2.06	104.51	109.37
25	A	365	PHO	C3D-C4D-ND	2.06	110.41	106.97
29	K	112	BCR	C40-C30-C25	2.06	113.74	110.33
24	A	366	CLA	C2A-C1A-NA	-2.06	108.97	111.24
34	T	227	LMT	C1B-O1B-C4'	-2.06	112.74	117.99
24	C	483	CLA	CMA-C3A-C2A	-2.06	105.29	114.14
34	B	536	LMT	O1B-C1B-C2B	2.06	113.06	108.12
24	C	480	CLA	C3A-C2A-C1A	2.06	103.99	101.08
24	C	477	CLA	CMB-C2B-C3B	2.05	128.21	124.97
29	B	530	BCR	C12-C13-C14	-2.05	115.81	118.97
24	C	482	CLA	C2A-C1A-CHA	2.05	127.39	123.83
29	Z	116	BCR	C7-C8-C9	2.05	129.29	126.22
24	C	476	CLA	CMB-C2B-C3B	2.05	128.20	124.97
29	K	112	BCR	C36-C18-C19	2.05	121.41	118.09
24	C	475	CLA	CMB-C2B-C3B	2.05	128.19	124.97
25	D	355	PHO	OBD-CAD-C3D	2.05	131.86	127.96
24	B	517	CLA	C2A-C1A-NA	-2.05	108.98	111.24
24	C	483	CLA	C1D-C2D-C3D	-2.05	105.11	106.78
27	A	367	PL9	C15-C14-C13	-2.05	119.47	123.52
29	A	369	BCR	C12-C13-C14	-2.05	115.83	118.97
34	B	536	LMT	C1-O1'-C1'	-2.04	110.28	113.96
24	B	524	CLA	C7-C6-C5	-2.04	106.98	113.01
24	C	486	CLA	CBA-CAA-C2A	2.04	120.08	114.01
24	B	521	CLA	OBD-CAD-C3D	2.04	131.71	127.91
29	D	358	BCR	C16-C17-C18	2.04	130.23	127.29
30	C	490	DGD	C6E-C5E-C4E	-2.04	108.07	113.00
24	C	479	CLA	C2A-C1A-NA	-2.04	108.99	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	355	PHO	C3D-C4D-ND	2.03	110.36	106.97
24	C	481	CLA	CMB-C2B-C3B	2.03	128.17	124.97
24	C	482	CLA	C4D-CHA-CBD	-2.03	104.58	109.37
29	B	529	BCR	C37-C22-C23	2.03	121.38	118.09
29	B	529	BCR	C7-C8-C9	2.03	129.25	126.22
32	F	224	SQD	O47-C7-C8	2.03	116.01	111.56
24	C	475	CLA	OBD-CAD-C3D	2.03	131.69	127.91
29	D	358	BCR	C28-C27-C26	2.03	116.82	113.74
24	B	522	CLA	C4D-CHA-CBD	-2.03	104.59	109.37
24	C	485	CLA	CMB-C2B-C3B	2.03	128.17	124.97
26	V	164	HEM	C3A-C4A-NA	-2.03	107.88	109.41
24	C	481	CLA	C1-C2-C3	2.03	129.79	126.19
24	B	521	CLA	CMB-C2B-C3B	2.03	128.16	124.97
30	C	490	DGD	C6D-C5D-C4D	2.03	116.48	111.87
32	B	532	SQD	O8-S-O7	2.03	116.17	111.78
29	B	527	BCR	C16-C17-C18	2.03	130.21	127.29
24	B	524	CLA	OBD-CAD-C3D	2.03	131.68	127.91
32	T	213	SQD	O3-C3-C2	-2.02	105.82	110.35
24	C	486	CLA	C16-C15-C13	2.02	120.97	115.14
24	B	516	CLA	CMB-C2B-C3B	2.02	128.15	124.97
24	B	520	CLA	C1D-C2D-C3D	-2.02	105.13	106.78
29	D	358	BCR	C36-C18-C19	2.02	121.36	118.09
24	C	482	CLA	O2D-CGD-CBD	2.02	115.45	111.33
24	D	364	CLA	C2D-C1D-ND	2.02	110.94	109.41
24	B	523	CLA	C2A-C1A-CHA	2.02	127.33	123.83
33	M	217	LMG	C37-C36-C35	-2.02	109.93	114.46
24	B	515	CLA	O2D-CGD-CBD	2.02	115.44	111.33
24	B	517	CLA	CMB-C2B-C3B	2.02	128.14	124.97
24	B	519	CLA	CMA-C3A-C2A	-2.01	105.48	114.14
29	A	369	BCR	C36-C18-C19	2.01	121.35	118.09
24	A	363	CLA	C4D-CHA-CBD	-2.01	104.63	109.37
33	I	220	LMG	O6-C1-C2	2.01	114.44	110.31
24	C	474	CLA	CMB-C2B-C1B	-2.01	125.53	128.62
32	D	361	SQD	C15-C14-C13	2.01	125.48	114.61
24	C	474	CLA	C1-C2-C3	2.01	129.75	126.19
29	C	487	BCR	C36-C18-C19	2.01	121.34	118.09
24	C	478	CLA	C2A-C1A-NA	-2.00	109.03	111.24
24	B	526	CLA	CBA-CAA-C2A	2.00	119.95	114.01
24	B	520	CLA	OBD-CAD-C3D	2.00	131.63	127.91
33	B	533	LMG	C9-C8-C7	-2.00	107.30	111.86

All (49) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	C	489	DGD	C2D
30	C	489	DGD	C5D
30	C	489	DGD	C5E
25	D	355	PHO	C2A
25	D	355	PHO	C13
25	D	355	PHO	C8
30	H	208	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
30	A	370	DGD	C2D
30	A	370	DGD	C5D
30	A	370	DGD	C5E
33	I	220	LMG	C2
33	I	220	LMG	C5
33	C	493	LMG	C2
33	C	493	LMG	C5
33	B	531	LMG	C2
33	B	531	LMG	C5
30	D	362	DGD	C2D
30	D	362	DGD	C5D
30	D	362	DGD	C5E
25	A	365	PHO	C2A
25	A	365	PHO	C13
25	A	365	PHO	C8
30	C	491	DGD	C2D
30	C	491	DGD	C5D
30	C	491	DGD	C5E
33	A	373	LMG	C2
33	A	373	LMG	C5
33	D	360	LMG	C2
33	D	360	LMG	C5
30	A	375	DGD	C2D
30	A	375	DGD	C5D
30	A	375	DGD	C5E
30	C	490	DGD	C2D
30	C	490	DGD	C5D
30	C	490	DGD	C5E
33	M	217	LMG	C2
33	M	217	LMG	C5
33	C	492	LMG	C2
33	C	492	LMG	C5
33	E	218	LMG	C2
33	E	218	LMG	C5

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Mol	Chain	Res	Type	Atom
33	D	359	LMG	C2
33	D	359	LMG	C5
33	B	534	LMG	C2
33	B	534	LMG	C5
33	B	533	LMG	C2
33	B	533	LMG	C5

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	D	361	SQD	C45-O47-C7-C8
32	D	361	SQD	C45-O47-C7-O49
33	M	217	LMG	C8-O7-C10-C11
24	C	475	CLA	C1-C2-C3-C4
33	D	360	LMG	C7-O1-C1-O6
24	C	482	CLA	C1-C2-C3-C4
24	A	363	CLA	C1-C2-C3-C4
24	B	512	CLA	C1-C2-C3-C4
24	B	516	CLA	C1-C2-C3-C4
25	A	365	PHO	C1-C2-C3-C4
24	C	483	CLA	C1-C2-C3-C4
24	C	486	CLA	C1-C2-C3-C4
24	B	521	CLA	C1-C2-C3-C4

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.