



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:34 am GMT

PDB ID : 2EIM  
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state  
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2007-03-13  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

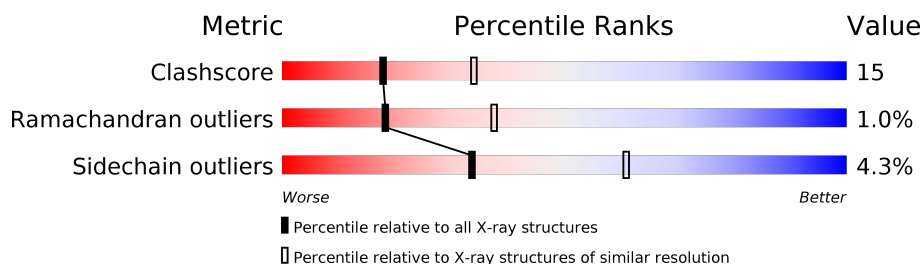
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)















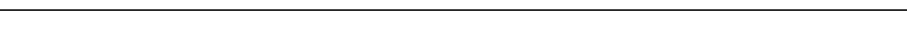




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	

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Mol	Chain	Length	Quality of chain
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
20	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CHD	J	60	X	-	-	-
20	CHD	W	1060	X	-	-	-
20	CHD	W	1271	X	-	-	-
22	TGL	L	522	-	-	X	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 31961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

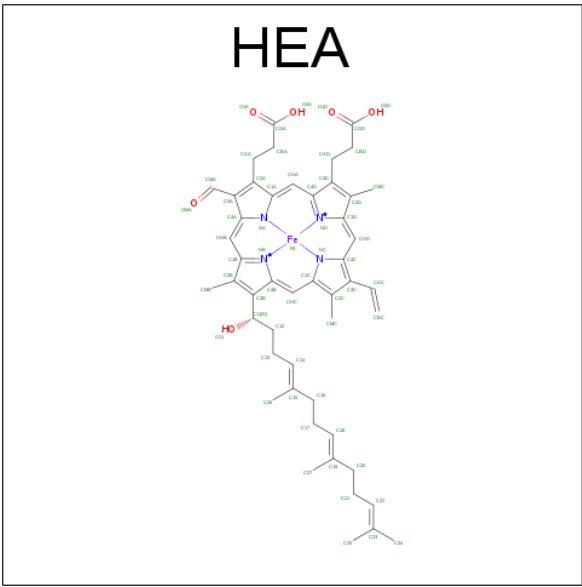
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	A	1	Total	Zn	0	0
			1	1		
17	N	1	Total	Zn	0	0
			1	1		
17	S	1	Total	Zn	0	0
			1	1		
17	F	1	Total	Zn	0	0
			1	1		

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

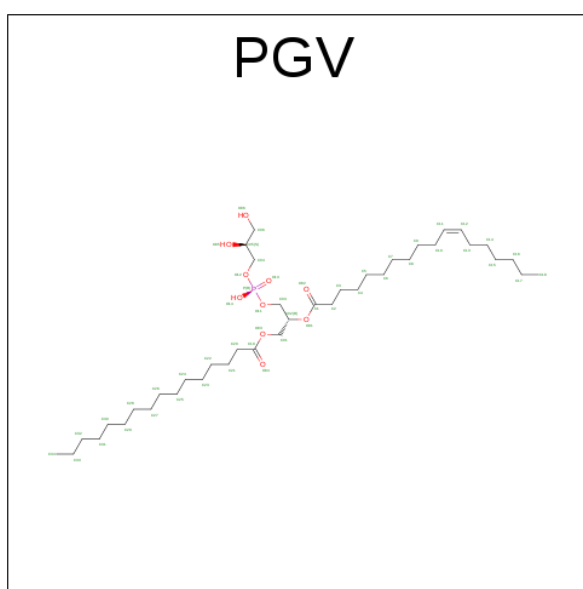
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



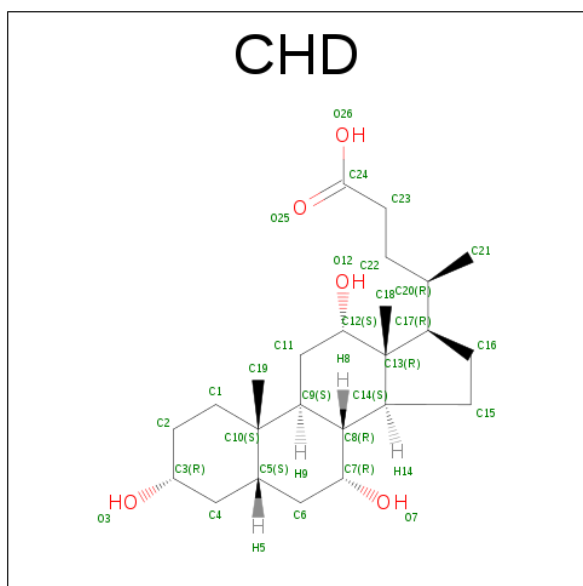
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	N	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
			51	40	10	1	0	0

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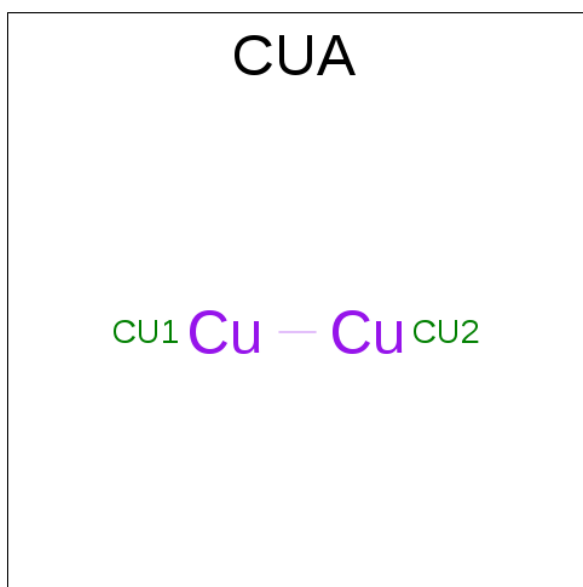
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



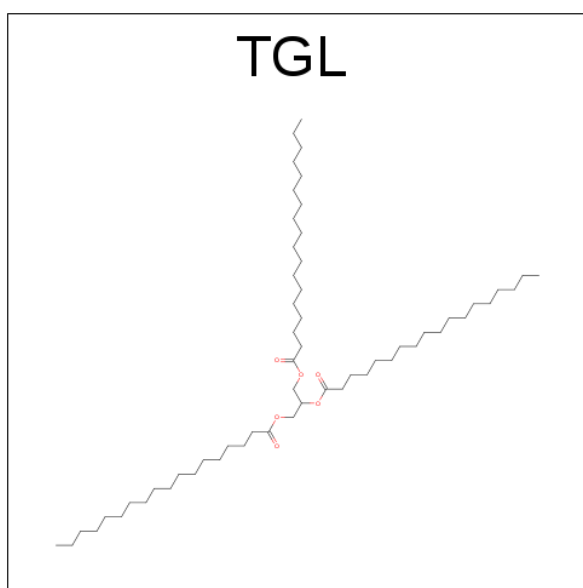
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			29	24	5		
20	B	1	Total	C	O	0	0
			29	24	5		
20	C	1	Total	C	O	0	0
			29	24	5		
20	J	1	Total	C	O	0	0
			29	24	5		
20	N	1	Total	C	O	0	0
			29	24	5		
20	P	1	Total	C	O	0	0
			29	24	5		
20	W	1	Total	C	O	0	0
			29	24	5		
20	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



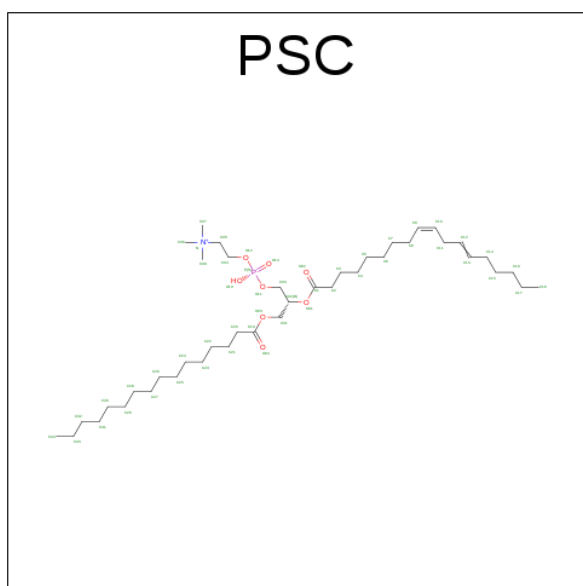
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		

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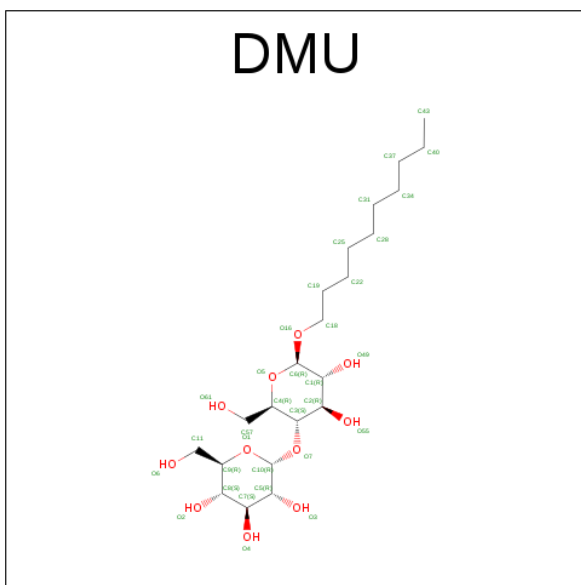
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).



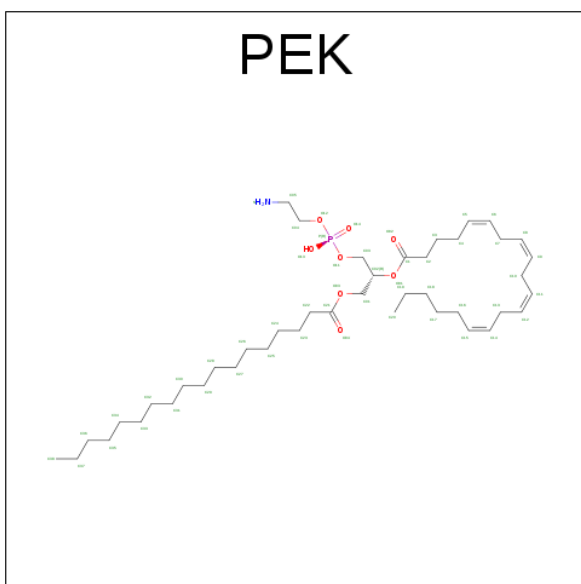
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



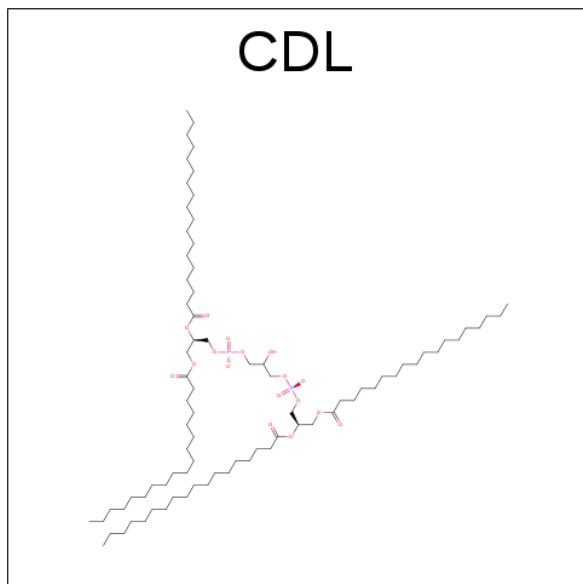
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total 33	C 22	O 11	0	0
24	M	1	Total 33	C 22	O 11	0	0
24	P	1	Total 33	C 22	O 11	0	0
24	Z	1	Total 33	C 22	O 11	0	0

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	182	Total O 182 182	0	0
27	B	96	Total O 96 96	0	0
27	C	82	Total O 82 82	0	0
27	D	61	Total O 61 61	0	0
27	E	43	Total O 43 43	0	0
27	F	52	Total O 52 52	0	0
27	G	37	Total O 37 37	0	0
27	H	35	Total O 35 35	0	0
27	I	22	Total O 22 22	0	0
27	J	12	Total O 12 12	0	0
27	K	12	Total O 12 12	0	0
27	L	13	Total O 13 13	0	0
27	M	13	Total O 13 13	0	0
27	N	171	Total O 171 171	0	0
27	O	79	Total O 79 79	0	0
27	P	73	Total O 73 73	0	0
27	Q	42	Total O 42 42	0	0
27	R	30	Total O 30 30	0	0
27	S	42	Total O 42 42	0	0
27	T	30	Total O 30 30	0	0
27	U	30	Total O 30 30	0	0
27	V	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	W	8	Total 8	O 8	0	0
27	X	18	Total 18	O 18	0	0
27	Y	14	Total 14	O 14	0	0
27	Z	11	Total 11	O 11	0	0

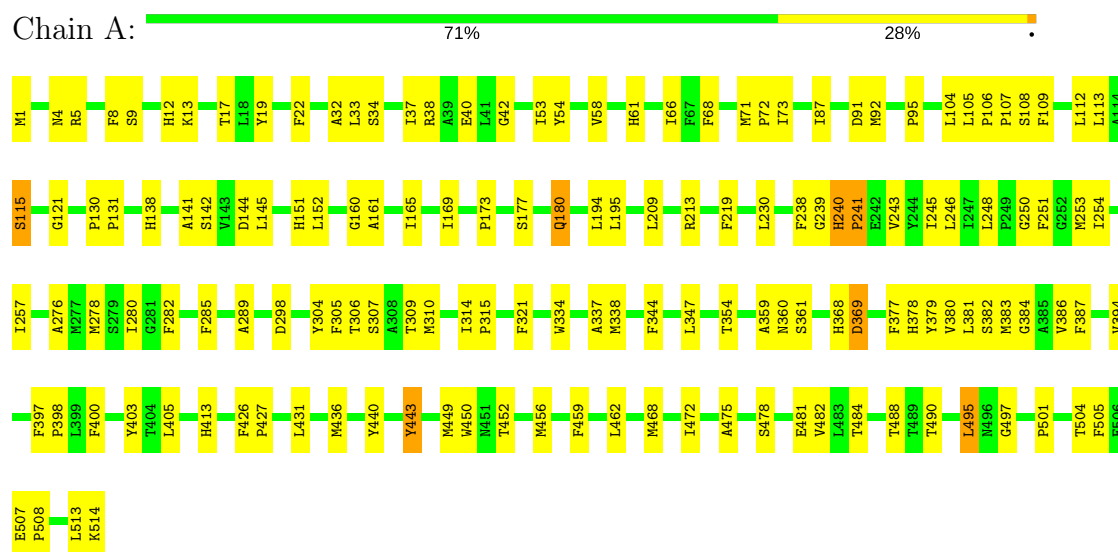


### 3 Residue-property plots

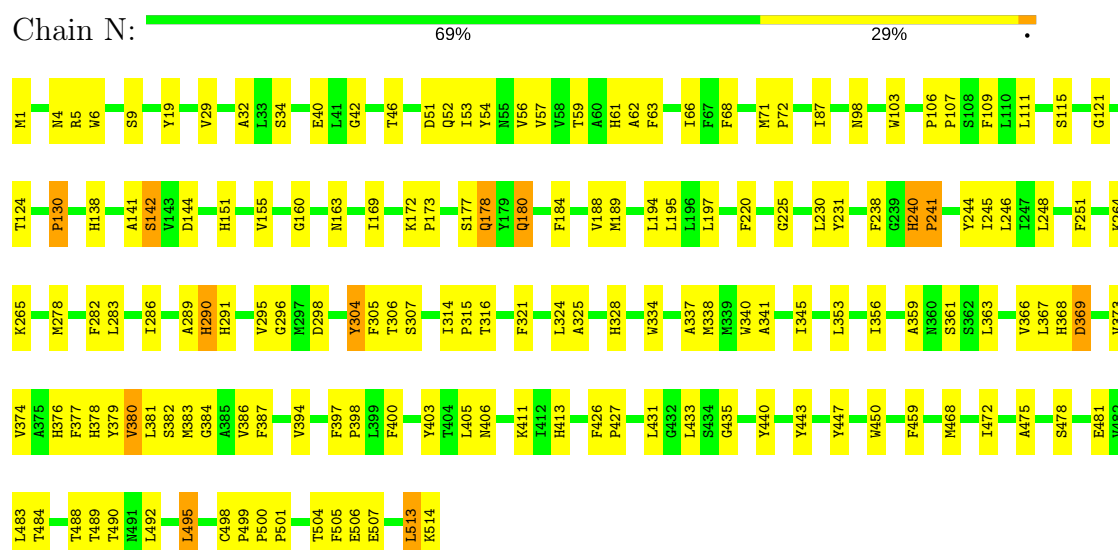
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

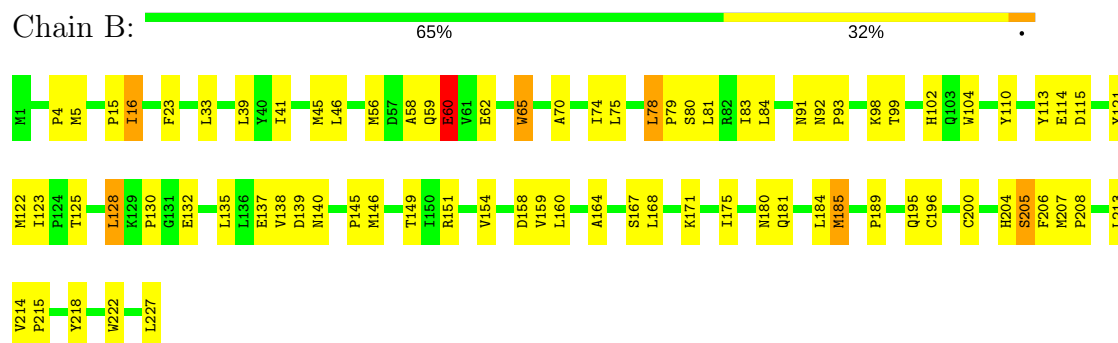
#### • Molecule 1: Cytochrome c oxidase subunit 1



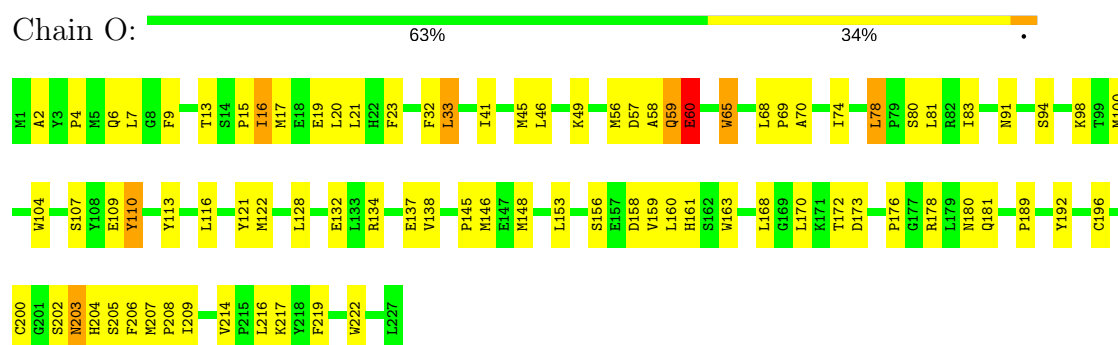
#### • Molecule 1: Cytochrome c oxidase subunit 1



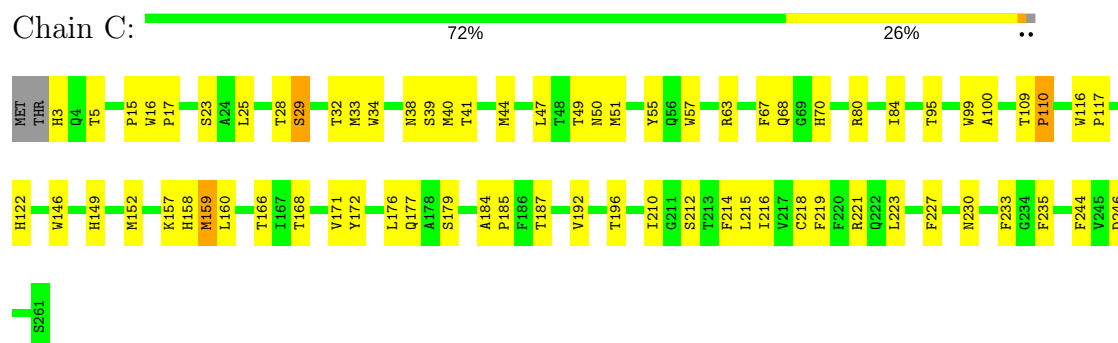
- Molecule 2: Cytochrome c oxidase subunit 2



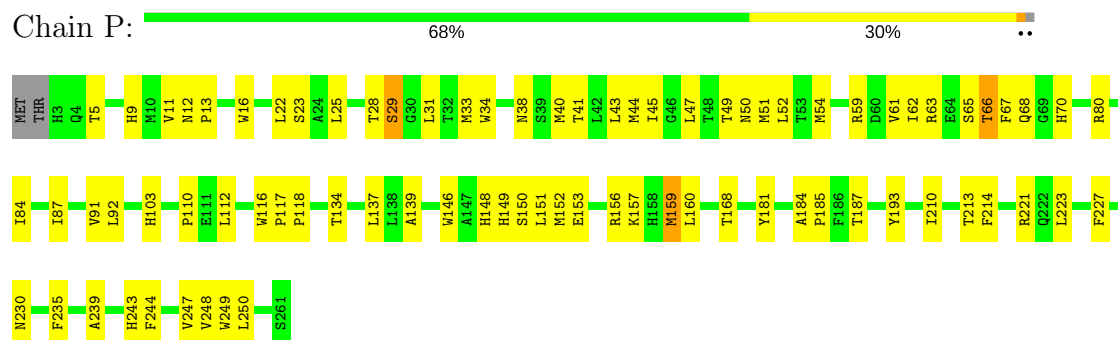
- Molecule 2: Cytochrome c oxidase subunit 2



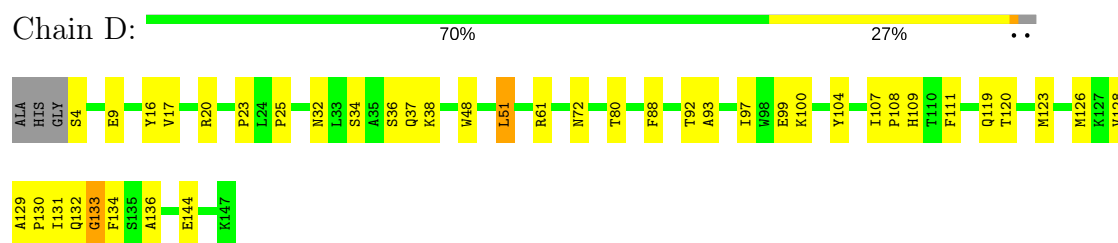
- Molecule 3: Cytochrome c oxidase subunit 3



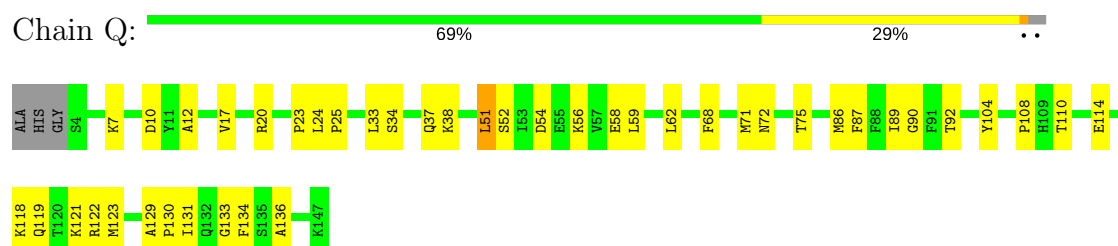
- Molecule 3: Cytochrome c oxidase subunit 3



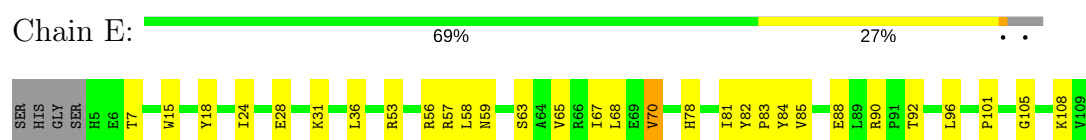
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



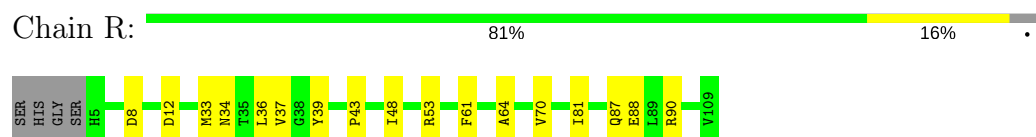
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



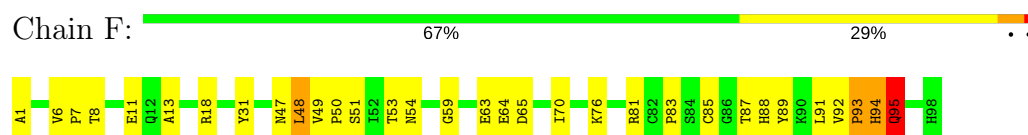
- Molecule 5: Cytochrome c oxidase polypeptide Va



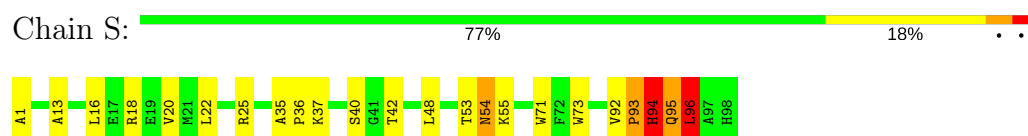
- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 6: Cytochrome c oxidase polypeptide Vb

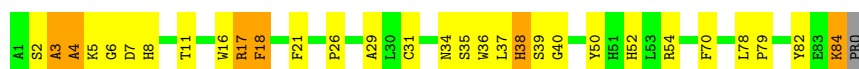


- Molecule 6: Cytochrome c oxidase polypeptide Vb



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

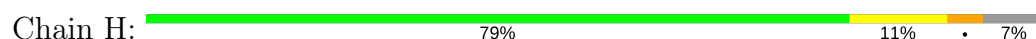




- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



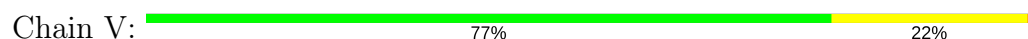
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



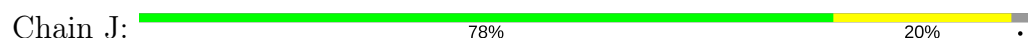
- Molecule 9: Cytochrome c oxidase polypeptide VIc



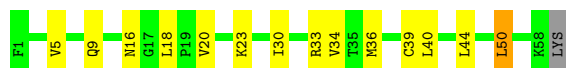
- Molecule 9: Cytochrome c oxidase polypeptide VIc



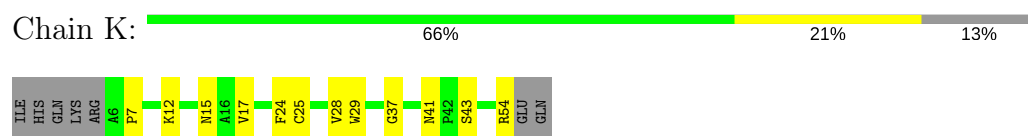
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



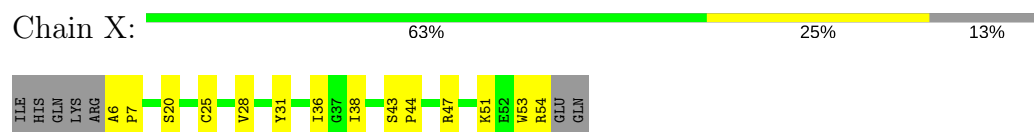
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



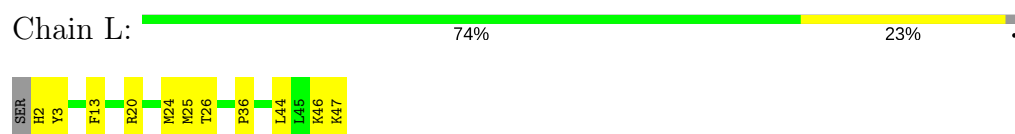
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



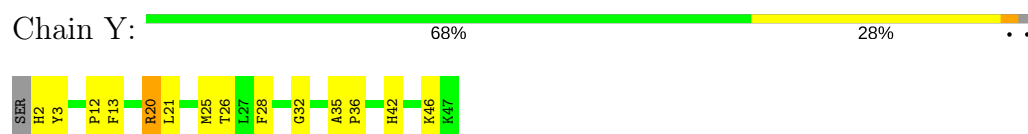
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



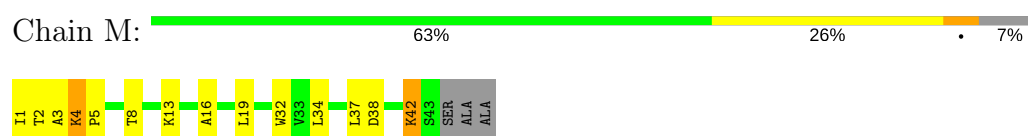
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



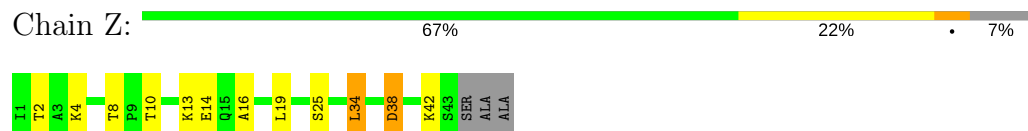
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.91Å 206.72Å 178.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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	0.70	0/4156	0.78	1/5678 (0.0%)
1	N	0.64	0/4156	0.76	2/5678 (0.0%)
2	B	0.60	0/1860	0.83	1/2534 (0.0%)
2	O	0.59	0/1860	0.83	0/2534
3	C	0.68	0/2197	0.70	0/3005
3	P	0.63	0/2197	0.72	0/3005
4	D	0.60	0/1229	0.73	1/1658 (0.1%)
4	Q	0.64	0/1229	0.71	0/1658
5	E	0.62	0/871	0.73	0/1182
5	R	0.61	0/871	0.75	0/1182
6	F	0.60	0/765	0.86	2/1038 (0.2%)
6	S	0.59	0/765	0.86	2/1038 (0.2%)
7	G	0.61	0/690	0.77	1/937 (0.1%)
7	T	0.63	0/690	0.81	2/937 (0.2%)
8	H	0.64	0/682	0.71	0/921
8	U	0.57	0/682	0.72	0/921
9	I	0.62	0/605	0.70	0/802
9	V	0.60	0/605	0.68	0/802
10	J	0.59	0/471	0.74	0/636
10	W	0.59	0/471	0.73	0/636
11	K	0.71	0/398	0.75	0/546
11	X	0.59	0/398	0.74	0/546
12	L	0.63	0/393	0.69	0/526
12	Y	0.62	0/393	0.67	0/526
13	M	0.57	0/345	0.70	0/470
13	Z	0.60	0/345	0.70	0/470
All	All	0.63	0/29324	0.76	12/39866 (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	3
1	N	0	5
2	B	0	1
2	O	0	1
All	All	0	10

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.74	129.20	111.00
6	F	94	HIS	N-CA-C	6.46	128.43	111.00
2	B	128	LEU	CA-CB-CG	6.03	129.16	115.30
6	S	93	PRO	N-CA-C	5.74	127.02	112.10
7	T	33	LEU	CA-CB-CG	5.72	128.47	115.30
6	F	93	PRO	N-CA-C	5.72	126.98	112.10
7	T	6	GLY	N-CA-C	5.29	126.32	113.10
1	A	130	PRO	N-CA-C	-5.24	98.48	112.10
7	G	6	GLY	N-CA-C	5.12	125.89	113.10
4	D	133	GLY	N-CA-C	5.05	125.72	113.10
1	N	435	GLY	N-CA-C	5.03	125.68	113.10
1	N	130	PRO	N-CA-C	-5.00	99.09	112.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	443	TYR	Sidechain
2	B	218	TYR	Sidechain
1	N	19	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	244	TYR	Sidechain
1	N	304	TYR	Sidechain
1	N	379	TYR	Sidechain
2	O	192	TYR	Sidechain



## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	130	0
1	N	4027	0	4001	145	0
2	B	1824	0	1833	66	0
2	O	1824	0	1833	85	0
3	C	2110	0	2027	66	0
3	P	2110	0	2027	76	0
4	D	1195	0	1183	34	0
4	Q	1195	0	1183	37	0
5	E	852	0	845	23	0
5	R	852	0	845	11	0
6	F	748	0	728	24	0
6	S	748	0	728	16	0
7	G	675	0	644	35	0
7	T	675	0	644	40	0
8	H	662	0	623	8	0
8	U	662	0	623	14	0
9	I	601	0	613	14	0
9	V	601	0	613	16	0
10	J	460	0	459	12	0
10	W	460	0	459	11	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	380	0	380	21	0
12	Y	380	0	380	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	F	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	1	0	0	0	0
18	A	120	0	108	9	0
18	N	120	0	108	12	0
19	A	51	0	76	7	0
19	C	153	0	228	12	0
19	N	51	0	76	10	0
19	P	153	0	228	11	0
20	A	29	0	39	1	0
20	B	29	0	39	1	0
20	C	29	0	39	2	0
20	J	29	0	37	5	0
20	N	29	0	39	2	0
20	P	29	0	39	2	0
20	W	58	0	76	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	6	0
22	D	63	0	110	5	0
22	L	63	0	110	27	0
22	N	126	0	220	22	0
22	O	63	0	110	8	0
23	B	52	0	80	19	0
23	O	52	0	80	18	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	17	0
25	G	53	0	77	9	0
25	P	106	0	154	18	0
25	T	53	0	77	14	0
26	C	100	0	156	19	0
26	G	100	0	156	22	0
26	P	100	0	156	13	0
26	T	100	0	156	23	0
27	A	182	0	0	9	0
27	B	96	0	0	2	0
27	C	82	0	0	5	0
27	D	61	0	0	7	0
27	E	43	0	0	4	0
27	F	52	0	0	5	0
27	G	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	H	35	0	0	1	0
27	I	22	0	0	2	0
27	J	12	0	0	1	0
27	K	12	0	0	2	0
27	L	13	0	0	0	0
27	M	13	0	0	2	0
27	N	171	0	0	14	0
27	O	79	0	0	4	0
27	P	73	0	0	0	0
27	Q	42	0	0	1	0
27	R	30	0	0	2	0
27	S	42	0	0	0	0
27	T	30	0	0	3	0
27	U	30	0	0	0	0
27	V	19	0	0	3	0
27	W	8	0	0	0	0
27	X	18	0	0	1	0
27	Y	14	0	0	0	0
27	Z	11	0	0	2	0
All	All	31961	0	31295	945	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	20:W:1060:CHD:H152	1.29	1.14
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.19	1.07
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.97
23:O:1230:PSC:H142	23:O:1230:PSC:H343	1.46	0.97
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.49	0.95
23:B:230:PSC:H142	23:B:230:PSC:H343	1.51	0.93
4:D:34:SER:H	4:D:37:GLN:HE21	1.04	0.93
7:G:84:LYS:HD2	7:G:84:LYS:H	1.33	0.93
7:T:84:LYS:HD2	7:T:84:LYS:H	1.34	0.92
7:G:31:CYS:SG	26:G:269:CDL:H532	2.10	0.92
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.90
12:L:20:ARG:HH12	22:L:522:TGL:HC61	1.34	0.90
26:T:1269:CDL:H231	26:T:1269:CDL:H541	1.54	0.90
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:522:TGL:HC62	22:L:522:TGL:HC22	1.55	0.88
25:C:264:PEK:H161	25:C:264:PEK:H102	1.54	0.88
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.09	0.88
23:O:1230:PSC:H071	9:V:10:ARG:HE	1.39	0.88
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.57	0.87
10:J:33:ARG:HG2	20:J:60:CHD:H152	1.56	0.85
22:N:1522:TGL:HC62	22:N:1522:TGL:HC22	1.60	0.84
22:L:522:TGL:H242	22:L:522:TGL:H202	1.60	0.83
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.60	0.83
4:D:34:SER:H	4:D:37:GLN:NE2	1.77	0.82
1:N:151:HIS:HD2	25:P:1264:PEK:H382	1.44	0.82
1:N:472:ILE:HG21	22:N:1522:TGL:HA92	1.59	0.82
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.62	0.81
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.61	0.81
4:D:120:THR:HA	27:D:4164:HOH:O	1.78	0.81
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.64	0.80
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.21	0.80
22:N:1522:TGL:H242	22:N:1522:TGL:H202	1.63	0.79
12:L:13:PHE:HA	22:L:522:TGL:HC31	1.63	0.79
2:O:41:ILE:HD13	23:O:1230:PSC:H342	1.63	0.79
2:O:15:PRO:HD2	27:O:3142:HOH:O	1.83	0.79
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.62	0.79
1:A:472:ILE:HG21	22:L:522:TGL:HA92	1.64	0.79
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.64	0.79
23:O:1230:PSC:H222	23:O:1230:PSC:H21	1.64	0.78
3:C:80:ARG:NH1	25:T:263:PEK:H032	1.99	0.78
22:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.64	0.78
12:L:24:MET:SD	22:L:522:TGL:H162	2.24	0.78
22:N:1522:TGL:H361	22:N:1522:TGL:HB91	1.66	0.78
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.32	0.78
23:B:230:PSC:H222	23:B:230:PSC:H21	1.66	0.77
3:C:80:ARG:HH11	25:T:263:PEK:H032	1.48	0.77
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.65	0.77
22:B:521:TGL:H281	22:B:521:TGL:H102	1.67	0.76
3:C:160:LEU:HD13	20:C:271:CHD:H181	1.68	0.76
22:B:521:TGL:C28	22:B:521:TGL:H102	2.15	0.76
12:L:20:ARG:NH1	22:L:522:TGL:HC61	2.00	0.76
22:O:1521:TGL:H102	22:O:1521:TGL:C28	2.15	0.76
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.67	0.76
7:T:47:PHE:CD2	7:T:81:GLY:HA2	2.22	0.75
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.21	0.74
22:O:1521:TGL:H102	22:O:1521:TGL:H281	1.67	0.74
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.70	0.74
26:C:270:CDL:H642	26:C:270:CDL:H191	1.67	0.74
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.70	0.74
3:C:168:THR:HG22	25:C:265:PEK:H14	1.70	0.74
1:N:1:FME:HCN	1:N:4:ASN:H	1.53	0.73
27:A:4014:HOH:O	12:L:3:TYR:HB3	1.88	0.73
22:B:521:TGL:H201	22:B:521:TGL:H241	1.71	0.73
26:G:269:CDL:H541	26:G:269:CDL:C23	2.20	0.72
1:A:1:FME:HCN	1:A:4:ASN:H	1.54	0.72
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.72	0.72
2:B:41:ILE:HD13	23:B:230:PSC:H342	1.71	0.71
3:P:168:THR:HG21	25:P:1265:PEK:H12	1.71	0.71
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.72	0.71
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.05	0.70
1:A:278:MET:SD	7:T:5:LYS:HB3	2.31	0.70
22:O:1521:TGL:H201	22:O:1521:TGL:H241	1.73	0.70
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.74	0.70
1:A:160:GLY:HA3	27:A:2064:HOH:O	1.91	0.70
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.27	0.69
3:P:47:LEU:O	3:P:51:MET:HG2	1.92	0.69
12:L:20:ARG:HH22	22:L:522:TGL:HC61	1.55	0.69
1:A:87:ILE:O	1:A:173:PRO:HD3	1.91	0.69
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.75	0.69
3:C:149:HIS:HA	3:C:152:MET:HE2	1.74	0.69
7:G:5:LYS:HB3	1:N:278:MET:SD	2.33	0.69
1:A:484:THR:HB	13:M:2:THR:OG1	1.92	0.68
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.93	0.68
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.68
10:J:12:PHE:O	10:J:23:LYS:HE2	1.94	0.68
26:G:269:CDL:H522	26:G:269:CDL:H202	1.76	0.68
1:N:472:ILE:HG21	22:N:1522:TGL:CA9	2.22	0.68
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.28	0.68
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.76	0.68
5:E:68:LEU:HD12	5:E:101:PRO:HD3	1.76	0.68
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.75	0.67
3:P:160:LEU:HD13	20:W:1271:CHD:H181	1.76	0.67
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.77	0.67
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.29	0.67
1:N:177:SER:H	1:N:180:GLN:HE21	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:CD1	23:O:1230:PSC:H342	2.24	0.67
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.59	0.67
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.59	0.67
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.24	0.67
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.67
26:C:270:CDL:H431	27:J:4266:HOH:O	1.95	0.67
3:P:148:HIS:CE1	3:P:152:MET:SD	2.87	0.66
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.30	0.66
1:N:514:LYS:HE3	27:N:3395:HOH:O	1.94	0.66
1:N:328:HIS:O	2:O:56:MET:HE1	1.95	0.66
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.77	0.66
7:T:47:PHE:CE2	7:T:81:GLY:HA2	2.31	0.66
1:A:219:PHE:HE2	3:C:196:THR:HG22	1.60	0.66
3:C:168:THR:CG2	25:C:265:PEK:H14	2.25	0.66
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.61	0.66
4:D:34:SER:N	4:D:37:GLN:HE21	1.87	0.65
2:B:98:LYS:HD3	8:H:63:LEU:O	1.95	0.65
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.11	0.65
9:V:58:LYS:O	9:V:62:GLU:HG3	1.96	0.65
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.78	0.65
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	1.79	0.65
2:O:160:LEU:HD23	2:O:176:PRO:HD2	1.78	0.65
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.61	0.65
3:P:80:ARG:O	3:P:84:ILE:HD12	1.96	0.65
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.78	0.65
1:A:73:ILE:HD11	18:A:515:HEA:H22	1.79	0.65
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.15	0.65
6:S:94:HIS:CD2	6:S:95:GLN:N	2.62	0.65
7:G:2:SER:OG	25:G:1263:PEK:H301	1.96	0.64
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.79	0.64
19:N:1524:PGV:H062	27:Z:3160:HOH:O	1.96	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.64
1:N:334:TRP:CZ3	22:N:1523:TGL:HA51	2.33	0.64
22:L:522:TGL:HB91	22:L:522:TGL:H361	1.80	0.64
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.61	0.64
19:A:524:PGV:H062	27:M:2160:HOH:O	1.98	0.64
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.63	0.64
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.79	0.64
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.78	0.63
12:L:20:ARG:NH2	22:L:522:TGL:HC32	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.80	0.63
5:E:57:ARG:HH11	5:E:57:ARG:HG3	1.63	0.63
1:N:381:LEU:HD13	18:N:516:HEA:HBC2	1.81	0.63
6:F:1:ALA:HB2	27:N:4346:HOH:O	1.99	0.63
5:R:87:GLN:HG2	5:R:88:GLU:N	2.13	0.63
2:B:184:LEU:HD23	2:B:185:MET:N	2.14	0.63
1:N:376:HIS:O	1:N:380:VAL:HG22	1.98	0.63
22:O:1521:TGL:HC92	27:O:4117:HOH:O	1.99	0.63
4:Q:130:PRO:O	4:Q:136:ALA:HB2	1.99	0.62
1:N:341:ALA:O	1:N:345:ILE:HG13	2.00	0.62
23:O:1230:PSC:H142	23:O:1230:PSC:C34	2.27	0.62
12:L:20:ARG:NH2	22:L:522:TGL:HC61	2.14	0.62
23:O:1230:PSC:C07	9:V:10:ARG:HE	2.09	0.62
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.30	0.62
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.82	0.62
23:B:230:PSC:H072	9:I:10:ARG:HH21	1.65	0.62
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.81	0.62
1:A:354:THR:HG21	27:A:2228:HOH:O	1.99	0.62
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.34	0.62
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.13	0.62
1:A:452:THR:O	1:A:456:MET:HG3	1.99	0.62
26:G:269:CDL:H511	26:G:269:CDL:H172	1.81	0.62
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.80	0.62
3:P:25:LEU:O	3:P:29:SER:HB2	2.01	0.61
1:N:321:PHE:CD2	23:O:1230:PSC:H341	2.36	0.61
1:A:472:ILE:HG21	22:L:522:TGL:CA9	2.30	0.61
1:N:87:ILE:O	1:N:173:PRO:HD3	2.00	0.61
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.61
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.82	0.61
6:S:22:LEU:O	6:S:25:ARG:HB3	2.00	0.61
1:A:306:THR:HG23	1:A:359:ALA:O	2.01	0.61
19:A:524:PGV:H311	13:M:16:ALA:HA	1.82	0.61
3:C:25:LEU:O	3:C:29:SER:HB2	2.01	0.61
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.83	0.61
1:N:160:GLY:HA3	27:N:3064:HOH:O	2.00	0.61
12:L:20:ARG:HH22	22:L:522:TGL:HC32	1.65	0.61
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.15	0.61
2:B:99:THR:HG23	2:B:154:VAL:HG13	1.83	0.60
22:N:1523:TGL:H271	2:O:46:LEU:HD12	1.83	0.60
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.31	0.60
8:H:60:TYR:C	8:H:60:TYR:CD1	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.31	0.60
1:A:253:MET:O	1:A:257:ILE:HG13	2.01	0.60
7:G:84:LYS:H	7:G:84:LYS:CD	2.07	0.60
2:O:32:PHE:HE2	22:O:1521:TGL:HB91	1.66	0.60
12:Y:20:ARG:NH1	12:Y:20:ARG:HB3	2.15	0.60
3:C:47:LEU:O	3:C:51:MET:HG2	2.00	0.60
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.84	0.60
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.37	0.60
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.01	0.60
2:B:123:ILE:HG22	2:B:128:LEU:HD23	1.84	0.60
6:S:16:LEU:O	6:S:20:VAL:HG23	2.01	0.60
3:C:28:THR:HG22	19:C:266:PGV:H182	1.84	0.59
2:B:65:TRP:CZ3	23:B:230:PSC:H331	2.37	0.59
23:B:230:PSC:H032	27:E:2129:HOH:O	2.02	0.59
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.84	0.59
1:N:5:ARG:O	1:N:9:SER:HB2	2.01	0.59
2:O:116:LEU:HD21	2:O:222:TRP:CH2	2.37	0.59
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.37	0.59
4:D:20:ARG:HG2	4:D:72:ASN:HD21	1.68	0.59
4:D:9:GLU:CD	4:D:9:GLU:H	2.05	0.59
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.59
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.84	0.59
1:A:488:THR:HB	1:A:495:LEU:HD13	1.84	0.59
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.37	0.59
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.03	0.59
3:C:40:MET:O	3:C:44:MET:HG2	2.01	0.59
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.00	0.59
2:B:145:PRO:HA	2:B:214:VAL:O	2.03	0.58
3:C:122:HIS:HB3	27:C:4324:HOH:O	2.02	0.58
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.37	0.58
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.85	0.58
22:B:521:TGL:HC22	27:I:2383:HOH:O	2.02	0.58
10:W:16:ASN:ND2	10:W:18:LEU:HD12	2.19	0.58
2:B:15:PRO:HB2	27:B:4350:HOH:O	2.04	0.58
1:N:378:HIS:O	1:N:382:SER:HB2	2.02	0.58
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.34	0.58
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.04	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.04	0.58
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.58
2:B:122:MET:SD	2:B:206:PHE:HB3	2.43	0.58
6:F:51:SER:CB	6:F:91:LEU:HD11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:CD2	12:L:36:PRO:HB3	2.34	0.58
1:A:361:SER:OG	2:B:84:LEU:HD13	2.04	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.57
1:N:377:PHE:HA	1:N:380:VAL:CG2	2.34	0.57
3:P:40:MET:O	3:P:44:MET:HG2	2.03	0.57
7:G:17:ARG:HD2	27:N:2309:HOH:O	2.04	0.57
2:O:134:ARG:HD3	4:Q:110:THR:OG1	2.04	0.57
2:O:7:LEU:HD11	22:O:1521:TGL:H161	1.86	0.57
27:B:4027:HOH:O	25:P:1265:PEK:H292	2.03	0.57
1:N:6:TRP:CD2	12:Y:12:PRO:HB3	2.39	0.57
3:P:41:THR:O	3:P:45:ILE:HG13	2.04	0.57
2:B:164:ALA:HB2	2:B:171:LYS:HG3	1.85	0.57
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.88	0.57
7:T:8:HIS:HE1	27:T:4411:HOH:O	1.86	0.57
19:C:267:PGV:H172	26:C:270:CDL:H662	1.86	0.57
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.87	0.57
12:L:20:ARG:HH22	22:L:522:TGL:CC6	2.17	0.57
22:N:1522:TGL:C24	22:N:1522:TGL:H202	2.34	0.57
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.40	0.57
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.04	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.57
22:B:521:TGL:H222	22:B:521:TGL:HA82	1.87	0.56
2:O:146:MET:SD	2:O:189:PRO:HB3	2.45	0.56
11:K:24:PHE:O	11:K:28:VAL:HG12	2.04	0.56
12:Y:21:LEU:O	12:Y:25:MET:HG3	2.05	0.56
22:D:523:TGL:HC61	27:D:4382:HOH:O	2.05	0.56
26:G:269:CDL:C54	26:G:269:CDL:H231	2.33	0.56
22:L:522:TGL:C24	22:L:522:TGL:H202	2.34	0.56
6:S:54:ASN:HD22	6:S:54:ASN:C	2.08	0.56
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.56
22:O:1521:TGL:HA82	22:O:1521:TGL:H222	1.87	0.56
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.05	0.56
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.86	0.56
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.41	0.56
2:B:56:MET:HG2	23:B:230:PSC:H211	1.87	0.56
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.88	0.56
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.40	0.56
10:J:40:LEU:HD12	20:J:60:CHD:H183	1.87	0.56
1:N:406:ASN:HD21	19:N:1524:PGV:H22	1.70	0.56
2:B:135:LEU:HD22	2:B:206:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:265:PEK:H371	26:G:269:CDL:H261	1.88	0.55
12:L:20:ARG:HH12	22:L:522:TGL:CC6	2.14	0.55
2:B:74:ILE:O	2:B:78:LEU:HD22	2.06	0.55
3:P:244:PHE:O	3:P:248:VAL:HG23	2.07	0.55
6:S:40:SER:OG	6:S:42:THR:HG23	2.06	0.55
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.88	0.55
1:N:483:LEU:HD21	13:Z:4:LYS:HG2	1.88	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
22:N:1523:TGL:HC21	22:N:1523:TGL:HG11	1.89	0.55
1:A:66:ILE:HG23	1:A:246:LEU:HD21	1.87	0.55
25:C:264:PEK:C16	25:C:264:PEK:H102	2.33	0.55
3:P:87:ILE:O	3:P:91:VAL:HG23	2.06	0.55
1:A:379:TYR:O	1:A:383:MET:HB2	2.07	0.55
2:B:214:VAL:HB	2:B:215:PRO:CD	2.36	0.55
2:O:146:MET:CE	9:V:56:SER:HB2	2.37	0.55
1:A:306:THR:O	1:A:310:MET:HG3	2.07	0.55
5:E:24:ILE:O	5:E:58:LEU:HD21	2.05	0.55
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.88	0.55
6:S:94:HIS:CG	6:S:95:GLN:H	2.13	0.55
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.21	0.55
1:N:459:PHE:HB3	4:Q:92:THR:CG2	2.37	0.55
26:C:270:CDL:C19	26:C:270:CDL:H642	2.37	0.55
12:L:20:ARG:CZ	22:L:522:TGL:HC61	2.37	0.55
6:S:13:ALA:O	6:S:18:ARG:HD2	2.07	0.55
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.89	0.54
6:F:18:ARG:HB3	27:F:4412:HOH:O	2.08	0.54
4:D:130:PRO:O	4:D:136:ALA:HB2	2.06	0.54
1:A:334:TRP:CZ3	22:D:523:TGL:HA51	2.42	0.54
23:B:230:PSC:H142	23:B:230:PSC:C34	2.31	0.54
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.42	0.54
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.54
1:N:440:TYR:HE2	2:O:204:HIS:NE2	2.05	0.54
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.37	0.54
23:B:230:PSC:C07	9:I:10:ARG:HH21	2.20	0.54
1:A:161:ALA:O	1:A:165:ILE:HG13	2.07	0.54
12:L:25:MET:HG2	22:L:522:TGL:HA62	1.90	0.54
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.90	0.54
9:V:36:LYS:HA	9:V:40:ALA:HB3	1.88	0.54
1:A:243:VAL:HA	1:A:246:LEU:HD12	1.89	0.54
5:E:57:ARG:NH1	5:E:57:ARG:HG3	2.23	0.54
1:A:115:SER:HA	1:A:145:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:GLU:HG3	27:F:4360:HOH:O	2.07	0.54
2:O:100:MET:HB2	2:O:107:SER:OG	2.08	0.54
1:A:282:PHE:HA	7:T:4:ALA:CB	2.38	0.54
1:N:380:VAL:O	1:N:384:GLY:HA3	2.07	0.54
1:A:377:PHE:O	1:A:381:LEU:HB3	2.08	0.53
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.53
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.90	0.53
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.43	0.53
1:A:12:HIS:CD2	1:A:91:ASP:HA	2.43	0.53
1:N:197:LEU:O	3:P:92:LEU:HD12	2.08	0.53
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.90	0.53
22:L:522:TGL:H272	22:L:522:TGL:H231	1.91	0.53
2:O:56:MET:HA	23:O:1230:PSC:H202	1.91	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.91	0.53
3:P:66:THR:HG23	19:P:1267:PGV:O05	2.09	0.53
1:A:472:ILE:HD13	22:L:522:TGL:HA91	1.91	0.53
1:N:169:ILE:HD11	1:N:189:MET:SD	2.48	0.53
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.44	0.53
2:O:203:ASN:HD22	2:O:203:ASN:N	2.05	0.53
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.23	0.53
1:N:459:PHE:HB3	4:Q:92:THR:HG23	1.90	0.53
11:K:25:CYS:O	11:K:29:TRP:HD1	1.92	0.53
22:N:1522:TGL:HC21	22:N:1522:TGL:OA1	2.08	0.53
3:C:168:THR:HG21	25:C:265:PEK:H12	1.89	0.53
1:N:314:ILE:HB	1:N:315:PRO:CD	2.39	0.53
1:N:400:PHE:HB3	22:N:1522:TGL:H283	1.91	0.53
3:P:250:LEU:HD22	26:T:1269:CDL:H673	1.90	0.53
3:C:80:ARG:HH11	25:T:263:PEK:C03	2.18	0.53
5:E:53:ARG:NH2	5:E:92:THR:HG23	2.23	0.53
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.38	0.52
1:A:240:HIS:O	1:A:243:VAL:HG22	2.09	0.52
1:A:347:LEU:HD13	1:A:383:MET:SD	2.49	0.52
3:C:51:MET:SD	26:C:270:CDL:H622	2.49	0.52
2:O:122:MET:SD	2:O:206:PHE:HB3	2.49	0.52
2:O:74:ILE:O	2:O:78:LEU:HD22	2.10	0.52
2:O:146:MET:HE3	9:V:56:SER:HB2	1.91	0.52
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.25	0.52
1:A:165:ILE:O	1:A:169:ILE:HG12	2.08	0.52
4:Q:134:PHE:HE1	11:X:44:PRO:HD2	1.74	0.52
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.44	0.52
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CG	2:B:205:SER:HB3	2.45	0.52
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.10	0.52
10:J:12:PHE:HD2	10:J:23:LYS:HG2	1.75	0.52
1:N:468:MET:HG2	1:N:468:MET:O	2.09	0.52
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.90	0.52
11:X:31:TYR:HB2	27:X:4091:HOH:O	2.08	0.52
1:N:52:GLN:O	1:N:56:VAL:HG23	2.10	0.52
2:O:121:TYR:O	2:O:138:VAL:HA	2.09	0.52
1:A:33:LEU:HB3	1:A:61:HIS:HB2	1.91	0.52
4:D:144:GLU:HB2	27:D:4097:HOH:O	2.10	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.92	0.52
1:A:248:LEU:O	1:A:251:PHE:HB2	2.10	0.52
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.45	0.52
11:K:7:PRO:O	11:K:12:LYS:HE3	2.10	0.52
22:L:522:TGL:OA1	22:L:522:TGL:HC21	2.10	0.52
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.51
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.92	0.51
7:G:34:ASN:O	7:G:37:LEU:HB3	2.09	0.51
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.76	0.51
1:A:482:VAL:HG22	13:M:1:ILE:HD11	1.92	0.51
2:O:163:TRP:CD1	2:O:209:ILE:HG12	2.46	0.51
2:O:4:PRO:HB2	11:X:43:SER:HA	1.91	0.51
25:C:265:PEK:H22	27:C:4087:HOH:O	2.09	0.51
4:D:80:THR:HA	11:K:17:VAL:HG11	1.93	0.51
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.51
3:C:51:MET:SD	26:C:270:CDL:C62	2.99	0.51
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.93	0.51
3:P:28:THR:HG22	19:P:1266:PGV:H182	1.91	0.51
1:A:314:ILE:HB	1:A:315:PRO:CD	2.41	0.51
22:D:523:TGL:HC21	22:D:523:TGL:HG11	1.92	0.51
5:E:84:TYR:O	5:E:88:GLU:HG2	2.10	0.51
26:G:269:CDL:H182	1:N:307:SER:CB	2.39	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.93	0.51
1:A:1:FME:HA	1:A:1:FME:CE	2.41	0.51
2:B:123:ILE:CG2	2:B:128:LEU:HD23	2.40	0.51
2:B:200:CYS:SG	2:B:204:HIS:HA	2.50	0.51
4:Q:52:SER:O	4:Q:56:LYS:HG3	2.10	0.51
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.92	0.51
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.93	0.51
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.91	0.51
3:P:62:ILE:HG23	3:P:221:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG22	1:A:309:THR:O	2.10	0.51
1:A:459:PHE:O	1:A:462:LEU:HB3	2.11	0.51
7:G:31:CYS:HG	26:G:269:CDL:H532	1.74	0.51
1:N:151:HIS:O	1:N:155:VAL:HG23	2.11	0.51
1:N:411:LYS:HD3	22:N:1523:TGL:HB21	1.93	0.51
6:S:94:HIS:HD2	6:S:95:GLN:N	2.09	0.51
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.46	0.50
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.46	0.50
1:A:398:PRO:HA	1:A:403:TYR:O	2.12	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.50
2:O:59:GLN:O	2:O:59:GLN:HG3	2.11	0.50
2:O:20:LEU:HD21	2:O:83:ILE:HG21	1.93	0.50
2:B:39:LEU:HD22	22:B:521:TGL:H141	1.92	0.50
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.46	0.50
1:N:115:SER:O	1:N:121:GLY:HA2	2.11	0.50
18:N:516:HEA:HMD1	18:N:516:HEA:HBD2	1.94	0.50
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.93	0.50
19:A:524:PGV:H321	19:A:524:PGV:H152	1.93	0.50
4:D:93:ALA:O	4:D:97:ILE:HG13	2.11	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
26:G:269:CDL:H182	1:N:307:SER:HB3	1.93	0.50
2:O:57:ASP:H	23:O:1230:PSC:H201	1.76	0.50
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.11	0.50
1:A:382:SER:O	1:A:386:VAL:HB	2.12	0.50
3:P:65:SER:HB2	19:P:1267:PGV:H041	1.94	0.50
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.41	0.50
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.93	0.50
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.50
2:B:4:PRO:HB2	11:K:43:SER:HA	1.94	0.50
6:F:81:ARG:HG2	6:F:88:HIS:CD2	2.46	0.50
4:Q:75:THR:HG22	27:Q:4352:HOH:O	2.11	0.50
1:N:29:VAL:HG22	12:Y:32:GLY:O	2.12	0.50
19:A:524:PGV:P	19:A:524:PGV:H061	2.52	0.49
1:A:37:ILE:HD11	1:A:58:VAL:HA	1.93	0.49
1:N:298:ASP:HB3	27:N:3389:HOH:O	2.12	0.49
3:C:212:SER:O	3:C:216:ILE:HG13	2.11	0.49
4:D:34:SER:O	4:D:38:LYS:HG3	2.12	0.49
7:G:18:PHE:O	7:G:18:PHE:HD2	1.95	0.49
1:N:440:TYR:CE2	2:O:204:HIS:NE2	2.80	0.49
4:Q:90:GLY:O	11:X:28:VAL:HG11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:267:PGV:H161	19:C:267:PGV:H12	1.94	0.49
6:S:92:VAL:HG23	6:S:92:VAL:O	2.12	0.49
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.11	0.49
3:P:239:ALA:O	3:P:243:HIS:CD2	2.65	0.49
1:A:131:PRO:HG3	27:A:4333:HOH:O	2.13	0.49
1:A:5:ARG:O	1:A:9:SER:HB2	2.12	0.49
23:B:230:PSC:O01	23:B:230:PSC:H212	2.12	0.49
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.47	0.49
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.48	0.49
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.78	0.49
2:O:56:MET:HA	23:O:1230:PSC:C20	2.42	0.49
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.77	0.49
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.49
2:B:214:VAL:HB	2:B:215:PRO:HD2	1.95	0.49
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.93	0.49
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.95	0.49
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.43	0.49
1:N:377:PHE:HA	1:N:380:VAL:HG23	1.93	0.49
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.11	0.49
25:C:265:PEK:C38	26:G:269:CDL:H273	2.43	0.49
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.93	0.49
9:I:23:GLY:O	9:I:27:VAL:HG23	2.13	0.49
19:N:1524:PGV:H012	27:N:4191:HOH:O	2.11	0.49
1:N:381:LEU:CD1	18:N:516:HEA:HBC2	2.42	0.49
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.94	0.49
3:P:50:ASN:O	3:P:54:MET:HG3	2.13	0.49
1:A:383:MET:O	1:A:387:PHE:HB2	2.12	0.48
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.95	0.48
1:N:398:PRO:HA	1:N:403:TYR:O	2.12	0.48
2:O:172:THR:HG21	2:O:180:ASN:HB3	1.94	0.48
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.28	0.48
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.13	0.48
1:A:380:VAL:O	1:A:384:GLY:HA3	2.13	0.48
2:B:93:PRO:HA	2:B:149:THR:HG22	1.94	0.48
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.42	0.48
1:N:115:SER:HB2	1:N:142:SER:O	2.13	0.48
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.94	0.48
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.95	0.48
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.48
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.66	0.48
23:O:1230:PSC:O01	23:O:1230:PSC:H212	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
4:Q:129:ALA:HB3	4:Q:134:PHE:H	1.77	0.48
2:B:135:LEU:HD22	2:B:206:PHE:HD2	1.77	0.48
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.96	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.13	0.48
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.26	0.48
2:O:156:SER:HB3	2:O:176:PRO:HD3	1.96	0.48
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.95	0.48
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.49	0.48
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.94	0.48
1:A:104:LEU:C	1:A:107:PRO:HD2	2.34	0.48
1:A:115:SER:HB2	1:A:142:SER:O	2.14	0.48
2:B:41:ILE:CD1	23:B:230:PSC:H342	2.41	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
1:N:68:PHE:C	1:N:72:PRO:HG2	2.34	0.48
6:F:95:GLN:HG3	27:F:4316:HOH:O	2.13	0.48
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.94	0.48
7:T:3:ALA:O	7:T:4:ALA:HB2	2.14	0.48
1:A:497:GLY:HA3	27:A:2398:HOH:O	2.14	0.48
3:C:57:TRP:CZ2	19:C:266:PGV:H21	2.49	0.48
4:D:129:ALA:HB1	4:D:133:GLY:HA3	1.96	0.48
22:N:1522:TGL:H231	22:N:1522:TGL:H272	1.95	0.48
1:N:380:VAL:HG23	1:N:381:LEU:H	1.78	0.48
1:N:492:LEU:HD12	1:N:492:LEU:O	2.14	0.48
2:O:122:MET:HE2	27:O:4368:HOH:O	2.13	0.48
1:A:501:PRO:HG2	1:A:504:THR:HG22	1.94	0.47
1:N:103:TRP:O	1:N:106:PRO:HD2	2.14	0.47
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.47
1:N:316:THR:HG21	18:N:516:HEA:H14	1.95	0.47
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.47
1:A:400:PHE:HB3	22:L:522:TGL:H283	1.96	0.47
1:A:61:HIS:CE1	18:A:515:HEA:NB	2.82	0.47
22:L:522:TGL:HC62	22:L:522:TGL:CC2	2.30	0.47
1:N:130:PRO:HD2	1:N:231:TYR:CD1	2.49	0.47
1:N:184:PHE:O	1:N:188:VAL:HG23	2.15	0.47
1:N:306:THR:HG23	1:N:359:ALA:O	2.14	0.47
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.36	0.47
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.97	0.47
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.97	0.47
10:W:16:ASN:CG	10:W:18:LEU:HD12	2.35	0.47
1:A:436:MET:HE3	1:A:443:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:MET:HB3	27:A:4144:HOH:O	2.13	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.47
3:P:61:VAL:HG22	19:P:1266:PGV:H061	1.96	0.47
3:P:43:LEU:O	3:P:47:LEU:HG	2.13	0.47
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.79	0.47
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.80	0.47
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.18	0.47
2:B:114:GLU:HB3	2:B:227:LEU:HD21	1.96	0.47
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.15	0.47
19:C:267:PGV:H182	26:C:270:CDL:C67	2.43	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.47
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.96	0.47
1:A:33:LEU:HD12	1:A:61:HIS:HA	1.97	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.47
6:F:49:VAL:O	6:F:91:LEU:HD12	2.15	0.47
7:T:2:SER:O	25:T:263:PEK:H322	2.14	0.47
7:T:6:GLY:O	25:T:263:PEK:H311	2.15	0.47
1:A:195:LEU:HG	1:A:245:ILE:HD13	1.97	0.47
4:D:109:HIS:HD2	27:D:2159:HOH:O	1.97	0.47
13:M:4:LYS:HE3	27:M:4199:HOH:O	2.15	0.47
1:N:124:THR:HB	27:N:4378:HOH:O	2.14	0.47
9:V:64:ARG:HG3	9:V:72:ALA:O	2.15	0.47
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.47
1:N:151:HIS:HD2	25:P:1264:PEK:C38	2.22	0.47
2:O:20:LEU:CD2	2:O:83:ILE:HG21	2.45	0.47
25:P:1265:PEK:H041	6:S:1:ALA:N	2.30	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.12	0.46
4:D:129:ALA:HB3	4:D:134:PHE:H	1.79	0.46
23:O:1230:PSC:H032	27:R:3129:HOH:O	2.15	0.46
22:O:1521:TGL:HC22	27:V:3383:HOH:O	2.15	0.46
1:N:230:LEU:HD13	3:P:103:HIS:CG	2.50	0.46
3:P:9:HIS:CE1	3:P:11:VAL:HG22	2.50	0.46
1:A:17:THR:OG1	22:L:522:TGL:H281	2.15	0.46
2:B:79:PRO:O	2:B:83:ILE:HG13	2.14	0.46
2:O:110:TYR:CD2	2:O:110:TYR:N	2.83	0.46
3:P:221:ARG:NH1	3:P:227:PHE:HE1	2.13	0.46
18:A:516:HEA:HMD1	18:A:516:HEA:HBD2	1.97	0.46
1:N:304:TYR:HD2	1:N:305:PHE:CD2	2.33	0.46
1:A:426:PHE:N	1:A:427:PRO:CD	2.79	0.46
3:C:109:THR:HB	3:C:110:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:MET:C	3:C:159:MET:SD	2.94	0.46
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
1:N:59:THR:HG22	1:N:63:PHE:CE2	2.50	0.46
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.46
1:A:194:LEU:CB	1:A:245:ILE:HD11	2.46	0.46
1:N:472:ILE:HD13	22:N:1522:TGL:HA91	1.97	0.46
26:T:1269:CDL:H601	26:T:1269:CDL:H571	1.45	0.46
1:A:115:SER:O	1:A:121:GLY:HA2	2.15	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.96	0.46
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.80	0.46
22:D:523:TGL:HG31	27:D:4040:HOH:O	2.16	0.46
5:E:105:GLY:O	5:E:108:LYS:HG2	2.16	0.46
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.98	0.46
3:P:139:ALA:CB	7:T:24:ALA:HB1	2.45	0.46
1:N:398:PRO:HG3	27:N:4079:HOH:O	2.15	0.46
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.50	0.46
20:W:1060:CHD:H161	20:W:1060:CHD:H212	1.76	0.46
4:D:131:ILE:HG22	4:D:132:GLN:HG3	1.98	0.46
4:D:23:PRO:HB3	5:E:70:VAL:HG21	1.97	0.46
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.97	0.46
1:A:239:GLY:O	1:A:243:VAL:HG13	2.16	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
23:B:230:PSC:H212	23:B:230:PSC:C02	2.47	0.45
19:N:1524:PGV:P	19:N:1524:PGV:H061	2.56	0.45
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.16	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.45
5:E:65:VAL:HG13	5:E:101:PRO:HG3	1.98	0.45
1:N:325:ALA:HA	23:O:1230:PSC:H291	1.98	0.45
3:P:187:THR:CB	7:T:68:THR:HG21	2.46	0.45
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.16	0.45
3:C:184:ALA:HA	3:C:185:PRO:HD2	1.88	0.45
26:C:270:CDL:H641	26:C:270:CDL:H672	1.80	0.45
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.80	0.45
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.98	0.45
2:O:170:LEU:HD23	27:O:4107:HOH:O	2.15	0.45
1:N:295:VAL:HG12	2:O:173:ASP:OD2	2.16	0.45
2:O:200:CYS:SG	2:O:204:HIS:HA	2.56	0.45
2:O:65:TRP:CZ3	23:O:1230:PSC:H331	2.51	0.45
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.97	0.45
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.17	0.45
1:A:481:GLU:O	13:M:3:ALA:HB1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD21	3:C:100:ALA:HA	1.98	0.45
3:C:55:TYR:CD1	26:C:270:CDL:H532	2.52	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
2:O:113:TYR:HE1	8:U:11:TYR:O	2.00	0.45
2:O:145:PRO:HA	2:O:214:VAL:O	2.16	0.45
3:P:134:THR:OG1	3:P:249:TRP:NE1	2.41	0.45
3:P:50:ASN:ND2	3:P:54:MET:CE	2.80	0.45
3:P:68:GLN:HE21	3:P:70:HIS:CD2	2.34	0.45
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.32	0.45
10:W:5:VAL:O	10:W:9:GLN:HG3	2.16	0.45
1:A:321:PHE:CD2	23:B:230:PSC:H341	2.51	0.45
3:C:246:ASP:HB2	27:C:4141:HOH:O	2.15	0.45
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.51	0.45
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.98	0.45
2:O:98:LYS:HD3	8:U:63:LEU:O	2.17	0.45
20:W:1271:CHD:H112	20:W:1271:CHD:H12A	1.61	0.45
1:A:194:LEU:HD12	1:A:245:ILE:HG13	1.99	0.45
3:C:171:VAL:HA	27:C:4409:HOH:O	2.16	0.45
5:E:56:ARG:HG2	5:E:96:LEU:HD22	1.99	0.45
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.99	0.45
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.46	0.45
7:T:47:PHE:CD2	7:T:77:PRO:HB2	2.52	0.45
1:A:276:ALA:O	1:A:280:ILE:HG13	2.17	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.37	0.45
2:O:58:ALA:O	2:O:60:GLU:N	2.48	0.45
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.98	0.45
4:Q:24:LEU:HD12	5:R:33:MET:HB2	1.99	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
1:A:306:THR:HG23	1:A:360:ASN:HA	1.99	0.45
2:B:146:MET:SD	2:B:189:PRO:HB3	2.57	0.45
3:C:166:THR:HG22	3:C:215:LEU:HD13	1.99	0.45
3:C:158:HIS:NE2	25:C:265:PEK:H051	2.32	0.45
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.32	0.45
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.31	0.45
9:I:15:ARG:HD3	9:I:16:ARG:N	2.32	0.45
3:P:243:HIS:O	3:P:247:VAL:HG23	2.16	0.45
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.98	0.45
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.99	0.45
2:B:184:LEU:HD23	2:B:184:LEU:C	2.37	0.44
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.52	0.44
3:C:187:THR:HG22	25:C:264:PEK:H052	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:HIS:CD2	9:I:12:LEU:HD13	2.53	0.44
6:F:64:GLU:O	6:F:65:ASP:HB2	2.17	0.44
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.16	0.44
3:C:63:ARG:NH1	10:J:20:VAL:O	2.49	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.18	0.44
4:Q:119:GLN:O	4:Q:123:MET:HG3	2.17	0.44
1:A:505:PHE:HB3	27:A:2194:HOH:O	2.18	0.44
1:A:321:PHE:HB3	2:B:65:TRP:CZ3	2.52	0.44
3:C:51:MET:HB3	26:C:270:CDL:H622	1.98	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44
22:N:1523:TGL:H311	4:Q:89:ILE:HD13	2.00	0.44
7:T:2:SER:O	7:T:3:ALA:HB3	2.18	0.44
7:T:79:PRO:HD2	27:T:3136:HOH:O	2.17	0.44
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.04	0.44
2:B:160:LEU:O	2:B:200:CYS:HB3	2.15	0.44
23:B:230:PSC:H221	23:B:230:PSC:H251	1.71	0.44
2:B:58:ALA:O	2:B:60:GLU:N	2.49	0.44
9:I:35:TYR:C	9:I:37:PHE:H	2.21	0.44
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.85	0.44
8:H:46:LYS:CB	8:U:52:VAL:HG12	2.48	0.44
11:X:36:ILE:HG13	11:X:38:ILE:HG13	1.99	0.44
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.44
4:D:99:GLU:HB3	27:D:4113:HOH:O	2.17	0.44
5:E:63:SER:O	5:E:67:ILE:HG13	2.18	0.44
6:F:13:ALA:O	6:F:18:ARG:HD2	2.17	0.44
11:K:15:ASN:HB2	27:K:2386:HOH:O	2.16	0.44
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.00	0.44
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.47	0.44
3:P:187:THR:HB	7:T:68:THR:HG21	2.00	0.44
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.17	0.44
20:A:525:CHD:H112	20:A:525:CHD:H12A	1.78	0.44
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.83	0.44
18:N:516:HEA:HMB1	18:N:516:HEA:H11	1.94	0.44
1:N:66:ILE:O	1:N:71:MET:HG3	2.17	0.44
3:P:156:ARG:HH22	3:P:223:LEU:HA	1.81	0.44
3:P:193:TYR:CD2	3:P:193:TYR:C	2.90	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.53	0.44
20:B:1086:CHD:H212	20:B:1086:CHD:H12	1.99	0.44
1:N:383:MET:O	1:N:387:PHE:HB2	2.18	0.44
2:O:203:ASN:ND2	2:O:203:ASN:N	2.66	0.44
10:W:36:MET:HB3	20:W:1060:CHD:H181	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:CD2	2:B:213:LEU:N	2.81	0.44
3:C:68:GLN:HB3	27:C:2153:HOH:O	2.18	0.44
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.98	0.44
6:F:95:GLN:NE2	27:F:4185:HOH:O	2.49	0.44
27:N:3090:HOH:O	3:P:13:PRO:HG3	2.17	0.44
1:A:145:LEU:HD21	3:C:32:THR:HG21	2.00	0.44
3:C:221:ARG:NH1	3:C:227:PHE:CE1	2.86	0.44
3:C:63:ARG:O	3:C:68:GLN:HG3	2.17	0.44
5:E:28:GLU:HG2	27:E:4385:HOH:O	2.17	0.44
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.49	0.44
1:A:53:ILE:CD1	12:L:44:LEU:HD23	2.48	0.44
1:N:40:GLU:OE1	1:N:46:THR:HA	2.18	0.44
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.00	0.44
1:N:68:PHE:O	1:N:72:PRO:HG2	2.18	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
1:A:307:SER:CB	26:T:1269:CDL:H182	2.48	0.44
7:T:5:LYS:HD2	25:T:263:PEK:H371	2.00	0.44
1:A:92:MET:O	1:A:95:PRO:HD3	2.18	0.44
3:C:233:PHE:N	19:C:267:PGV:O14	2.47	0.44
4:D:23:PRO:HB3	5:E:70:VAL:CG2	2.48	0.44
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.53	0.44
1:N:506:GLU:HB2	27:N:4072:HOH:O	2.18	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.44
7:T:78:LEU:HB3	7:T:79:PRO:CD	2.48	0.44
23:B:230:PSC:H12	23:B:230:PSC:H322	2.01	0.43
2:B:65:TRP:HZ3	23:B:230:PSC:H331	1.81	0.43
8:H:27:ARG:NH1	27:H:2303:HOH:O	2.48	0.43
1:N:382:SER:O	1:N:386:VAL:HB	2.18	0.43
18:A:516:HEA:H11	18:A:516:HEA:HMB1	1.89	0.43
4:D:126:MET:HG3	4:D:128:VAL:HG23	1.99	0.43
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.17	0.43
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.83	0.43
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.88	0.43
1:N:366:VAL:HG12	27:N:3400:HOH:O	2.18	0.43
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.34	0.43
4:Q:51:LEU:HD21	4:Q:59:LEU:HD11	1.99	0.43
7:T:49:PRO:HD2	8:U:80:THR:HG22	2.00	0.43
10:W:50:LEU:HD22	10:W:50:LEU:O	2.19	0.43
26:C:270:CDL:H171	26:C:270:CDL:H202	1.79	0.43
20:N:1604:CHD:H12	20:N:1604:CHD:H212	2.00	0.43
3:P:63:ARG:NH1	10:W:20:VAL:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ARG:NE	2:B:181:GLN:NE2	2.66	0.43
3:C:218:CYS:SG	3:C:235:PHE:HA	2.59	0.43
10:J:36:MET:HG2	20:J:60:CHD:H222	1.99	0.43
4:Q:129:ALA:CB	4:Q:134:PHE:H	2.31	0.43
1:A:68:PHE:HA	1:A:72:PRO:HG2	1.99	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
2:B:175:ILE:HD12	2:B:180:ASN:HD21	1.82	0.43
3:C:16:TRP:HA	3:C:16:TRP:HE3	1.83	0.43
4:D:119:GLN:O	4:D:123:MET:HG3	2.18	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.19	0.43
1:N:321:PHE:CZ	23:O:1230:PSC:H171	2.54	0.43
23:O:1230:PSC:C02	23:O:1230:PSC:H212	2.48	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.43
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.08	0.43
1:A:141:ALA:O	1:A:144:ASP:N	2.51	0.43
11:K:41:ASN:ND2	27:K:2283:HOH:O	2.48	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.85	0.43
3:P:149:HIS:O	3:P:153:GLU:HG3	2.18	0.43
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.82	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
19:A:524:PGV:H301	19:A:524:PGV:H152	2.01	0.43
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.06	0.43
1:N:443:TYR:HB2	1:N:447:TYR:HD2	1.83	0.43
1:N:53:ILE:O	1:N:57:VAL:HG23	2.19	0.43
1:A:108:SER:HB2	1:A:152:LEU:HB2	2.01	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.54	0.43
2:O:160:LEU:O	2:O:200:CYS:HB3	2.19	0.43
3:P:139:ALA:HB1	7:T:24:ALA:HB1	2.00	0.43
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.84	0.43
7:T:3:ALA:CB	25:T:263:PEK:H382	2.43	0.43
1:A:309:THR:CG2	18:A:516:HEA:HMB2	2.49	0.43
20:P:1525:CHD:H12A	20:P:1525:CHD:H112	1.82	0.43
6:S:54:ASN:ND2	6:S:55:LYS:HG2	2.34	0.43
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.19	0.43
2:B:189:PRO:HG2	9:I:63:MET:HE3	2.01	0.43
5:E:84:TYR:HE1	27:E:4265:HOH:O	2.01	0.43
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
7:T:30:LEU:HA	7:T:30:LEU:HD23	1.87	0.43
8:U:78:GLU:O	8:U:78:GLU:HG2	2.19	0.43
22:N:1522:TGL:HB62	12:Y:28:PHE:CZ	2.53	0.43
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLU:HA	3:C:5:THR:OG1	2.19	0.42
10:J:45:TYR:O	10:J:48:TYR:HB3	2.19	0.42
1:N:505:PHE:HB3	27:N:3194:HOH:O	2.19	0.42
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.02	0.42
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.00	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
2:B:121:TYR:O	2:B:138:VAL:HA	2.19	0.42
7:G:26:PRO:O	7:G:29:ALA:HB3	2.19	0.42
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.49	0.42
1:N:501:PRO:HG2	1:N:504:THR:HG22	2.01	0.42
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.42
25:G:1263:PEK:H132	3:P:247:VAL:CG1	2.49	0.42
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.73	0.42
6:F:6:VAL:HA	6:F:7:PRO:HD2	1.92	0.42
8:H:57:ARG:O	8:H:61:LYS:HB2	2.19	0.42
7:T:58:LYS:HA	7:T:59:PRO:HD2	1.92	0.42
1:A:106:PRO:N	1:A:107:PRO:CD	2.83	0.42
4:D:61:ARG:HA	4:D:61:ARG:HD3	1.83	0.42
4:D:100:LYS:HE2	11:K:37:GLY:O	2.19	0.42
1:N:106:PRO:N	1:N:107:PRO:CD	2.83	0.42
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.54	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
6:S:35:ALA:HA	6:S:36:PRO:HD2	1.94	0.42
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	2.02	0.42
23:B:230:PSC:H042	27:E:2401:HOH:O	2.20	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.61	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.19	0.42
13:Z:38:ASP:HB2	27:Z:4321:HOH:O	2.20	0.42
1:A:289:ALA:HB3	1:A:305:PHE:CG	2.55	0.42
3:C:158:HIS:CE1	25:C:265:PEK:H051	2.55	0.42
6:F:48:LEU:O	6:F:50:PRO:HD3	2.19	0.42
1:A:478:SER:HA	13:M:8:THR:O	2.19	0.42
1:N:111:LEU:HA	1:N:111:LEU:HD23	1.78	0.42
4:Q:68:PHE:HA	4:Q:71:MET:HG2	2.02	0.42
5:E:81:ILE:O	5:E:85:VAL:HG23	2.20	0.42
7:G:5:LYS:CB	25:G:1263:PEK:H362	2.40	0.42
1:N:353:LEU:O	1:N:356:ILE:HB	2.20	0.42
2:O:20:LEU:HD23	2:O:83:ILE:HD13	2.02	0.42
2:O:68:LEU:CB	2:O:69:PRO:CD	2.98	0.42
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.79	0.42
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
6:S:95:GLN:O	6:S:96:LEU:HB3	2.18	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.19	0.42
3:C:216:ILE:O	3:C:219:PHE:HB3	2.20	0.42
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.83	0.42
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.18	0.42
1:N:194:LEU:HD12	1:N:245:ILE:HG13	2.01	0.42
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.42
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.42
3:P:156:ARG:HG3	3:P:156:ARG:HH11	1.84	0.42
10:W:40:LEU:O	10:W:44:LEU:HG	2.19	0.42
1:A:8:PHE:CE2	3:C:15:PRO:HB3	2.55	0.42
2:B:56:MET:HA	23:B:230:PSC:H202	2.02	0.42
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.09	0.42
5:E:15:TRP:O	5:E:18:TYR:HB3	2.19	0.42
5:E:56:ARG:NH2	5:E:59:ASN:OD1	2.48	0.42
22:N:1523:TGL:HG11	22:N:1523:TGL:CC2	2.50	0.42
1:N:426:PHE:N	1:N:427:PRO:CD	2.82	0.42
2:O:100:MET:HB2	2:O:107:SER:HG	1.83	0.42
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.85	0.42
13:Z:34:LEU:HA	13:Z:34:LEU:HD12	1.89	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.41
19:A:524:PGV:H011	19:A:524:PGV:H202	1.94	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.20	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
1:A:459:PHE:HB3	4:D:92:THR:CG2	2.50	0.41
5:E:15:TRP:CD2	5:E:36:LEU:HD13	2.55	0.41
5:E:31:LYS:HE3	6:F:83:PRO:O	2.19	0.41
1:N:472:ILE:CG2	22:N:1522:TGL:HA92	2.42	0.41
1:N:246:LEU:HD13	1:N:381:LEU:HD21	2.02	0.41
1:A:13:LYS:NZ	27:A:2081:HOH:O	2.53	0.41
12:L:24:MET:SD	22:L:522:TGL:C16	3.04	0.41
1:N:283:LEU:HD23	1:N:286:ILE:HD11	2.02	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
1:N:53:ILE:HG12	27:N:3076:HOH:O	2.18	0.41
2:B:125:THR:HA	2:B:128:LEU:HG	2.02	0.41
23:B:230:PSC:C07	9:I:10:ARG:HE	2.33	0.41
8:H:33:TYR:HE1	8:H:69:VAL:HG13	1.85	0.41
13:M:42:LYS:CE	13:M:42:LYS:HA	2.36	0.41
7:G:2:SER:HB3	1:N:197:LEU:HD11	2.01	0.41
2:O:110:TYR:HD2	2:O:110:TYR:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:440:TYR:CZ	2:O:205:SER:HA	2.55	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.87	0.41
5:R:53:ARG:HD2	27:R:4076:HOH:O	2.20	0.41
9:V:31:PHE:HA	27:V:4259:HOH:O	2.20	0.41
1:A:33:LEU:HD13	1:A:61:HIS:N	2.35	0.41
4:D:17:VAL:HA	27:D:4085:HOH:O	2.21	0.41
4:D:32:ASN:HA	4:D:32:ASN:HD22	1.70	0.41
22:N:1523:TGL:H271	2:O:46:LEU:CD1	2.49	0.41
8:U:50:VAL:HG12	8:U:50:VAL:O	2.20	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.41
4:Q:114:GLU:HG3	11:X:51:LYS:HZ2	1.85	0.41
24:C:272:DMU:H25	25:C:264:PEK:H341	2.03	0.41
5:E:57:ARG:CG	5:E:57:ARG:HH11	2.33	0.41
6:F:59:GLY:HA2	6:F:70:ILE:O	2.20	0.41
1:A:113:LEU:CD1	22:L:522:TGL:H292	2.50	0.41
1:N:381:LEU:HD13	18:N:516:HEA:CBC	2.49	0.41
2:O:153:LEU:HD23	2:O:181:GLN:HA	2.02	0.41
2:O:59:GLN:O	2:O:59:GLN:CG	2.68	0.41
2:O:98:LYS:HE3	2:O:98:LYS:HB2	1.90	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.89	0.41
3:P:146:TRP:CE2	7:T:17:ARG:HG3	2.56	0.41
1:A:309:THR:HG22	18:A:516:HEA:HMB2	2.02	0.41
3:C:23:SER:HB2	3:C:49:THR:OG1	2.21	0.41
3:C:3:HIS:HE1	6:F:31:TYR:OH	2.04	0.41
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.80	0.41
3:P:137:LEU:HA	3:P:137:LEU:HD23	1.81	0.41
1:A:209:LEU:O	1:A:213:ARG:HG3	2.21	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.78	0.41
2:B:146:MET:CE	9:I:56:SER:HB2	2.50	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
3:C:172:TYR:O	3:C:176:LEU:HG	2.21	0.41
7:G:38:HIS:NE2	26:G:269:CDL:H111	2.36	0.41
26:G:269:CDL:H601	26:G:269:CDL:H571	1.51	0.41
3:C:41:THR:HG21	10:J:45:TYR:CE2	2.56	0.41
20:N:1604:CHD:H112	20:N:1604:CHD:H12A	1.90	0.41
2:O:158:ASP:O	2:O:176:PRO:HG3	2.21	0.41
3:P:134:THR:HG22	26:T:1269:CDL:H591	2.02	0.41
19:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.55	0.41
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.51	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.93	0.41
20:J:60:CHD:H161	20:J:60:CHD:H212	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:248:LEU:O	1:N:251:PHE:HB2	2.20	0.41
1:N:340:TRP:HZ2	1:N:413:HIS:ND1	2.18	0.41
3:P:181:TYR:O	25:P:1264:PEK:C04	2.69	0.41
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.49	0.41
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.20	0.41
5:R:61:PHE:O	5:R:64:ALA:HB3	2.20	0.41
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.92	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
1:A:219:PHE:CE2	3:C:196:THR:HG22	2.48	0.41
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.56	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
1:N:500:PRO:HB3	27:N:3186:HOH:O	2.19	0.41
7:T:15:THR:O	7:T:18:PHE:HB3	2.21	0.41
1:A:22:PHE:CZ	1:A:105:LEU:HB3	2.55	0.41
1:A:53:ILE:HD12	12:L:44:LEU:HD23	2.03	0.41
25:G:1263:PEK:H102	3:P:247:VAL:HG11	2.02	0.41
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.84	0.41
2:O:16:ILE:HG22	2:O:17:MET:N	2.35	0.41
5:R:36:LEU:O	5:R:39:TYR:HD2	2.04	0.41
12:Y:2:HIS:HB3	12:Y:3:TYR:H	1.66	0.41
1:A:501:PRO:HG2	1:A:504:THR:CG2	2.50	0.41
2:B:151:ARG:NE	2:B:181:GLN:HE21	2.18	0.41
2:B:213:LEU:N	2:B:213:LEU:HD22	2.36	0.41
7:G:2:SER:O	7:G:3:ALA:HB3	2.21	0.41
2:B:222:TRP:HB2	9:I:71:SER:HB2	2.02	0.41
1:N:400:PHE:HB3	22:N:1522:TGL:C28	2.51	0.41
20:P:1525:CHD:H182	20:P:1525:CHD:H111	1.74	0.41
3:P:49:THR:HB	10:W:39:CYS:SG	2.61	0.41
4:Q:86:MET:O	11:X:25:CYS:HB2	2.21	0.41
26:C:270:CDL:H242	26:C:270:CDL:H661	2.03	0.40
10:J:50:LEU:HD22	10:J:50:LEU:O	2.21	0.40
2:O:19:GLU:OE2	2:O:19:GLU:HA	2.21	0.40
26:P:1270:CDL:H641	26:P:1270:CDL:H672	1.77	0.40
7:T:47:PHE:CE2	7:T:77:PRO:HB2	2.56	0.40
1:A:298:ASP:HB3	27:A:2389:HOH:O	2.21	0.40
19:A:524:PGV:O14	19:A:524:PGV:H02	2.21	0.40
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.90	0.40
25:C:265:PEK:H041	6:F:1:ALA:N	2.36	0.40
3:C:50:ASN:OD1	19:C:266:PGV:H91	2.21	0.40
23:O:1230:PSC:H221	23:O:1230:PSC:H251	1.70	0.40
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:18:PHE:HD2	7:T:18:PHE:O	2.03	0.40
26:C:270:CDL:H602	26:C:270:CDL:H632	1.78	0.40
19:C:267:PGV:H181	26:C:270:CDL:H812	2.04	0.40
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.61	0.40
20:C:271:CHD:H12A	20:C:271:CHD:H112	1.60	0.40
3:C:84:ILE:HG12	25:T:263:PEK:H32	2.03	0.40
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.94	0.40
12:L:20:ARG:HH22	22:L:522:TGL:CC3	2.32	0.40
13:M:32:TRP:N	24:M:526:DMU:H1	2.36	0.40
1:N:141:ALA:O	1:N:144:ASP:N	2.54	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.40
3:P:12:ASN:O	3:P:13:PRO:C	2.59	0.40
3:P:49:THR:HA	3:P:52:LEU:HD12	2.04	0.40
22:N:1522:TGL:HB62	12:Y:28:PHE:HZ	1.86	0.40
1:A:34:SER:HB2	18:A:515:HEA:C2B	2.51	0.40
1:A:459:PHE:HB3	4:D:92:THR:HG23	2.02	0.40
10:J:36:MET:HB3	20:J:60:CHD:H181	2.03	0.40
1:N:296:GLY:O	2:O:178:ARG:NH2	2.53	0.40
1:N:478:SER:HA	13:Z:8:THR:O	2.21	0.40
1:N:61:HIS:CE1	18:N:515:HEA:NB	2.87	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.03	0.40
3:P:148:HIS:CD2	3:P:235:PHE:HE2	2.40	0.40
22:D:523:TGL:H242	22:D:523:TGL:H212	1.86	0.40
2:B:146:MET:HE1	9:I:56:SER:HB2	2.03	0.40
9:I:67:GLY:HA2	27:I:2310:HOH:O	2.22	0.40
10:J:11:LEU:HD12	10:J:11:LEU:O	2.21	0.40
1:N:373:VAL:HG13	18:N:516:HEA:HBA1	2.04	0.40
2:O:70:ALA:O	2:O:74:ILE:HG13	2.22	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	512/514 (100%)	488 (95%)	24 (5%)	0	100	100
1	N	512/514 (100%)	484 (94%)	27 (5%)	1 (0%)	51	76
2	B	225/227 (99%)	210 (93%)	10 (4%)	5 (2%)	8	14
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	14	29
3	C	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	38	63
3	P	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	38	63
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100	100
6	F	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	5	8
6	S	96/98 (98%)	85 (88%)	7 (7%)	4 (4%)	3	4
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	1
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	1
8	H	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	14	29
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	14	29
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	13	26
9	V	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	13	26
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	10	19
10	W	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3279 (94%)	189 (5%)	36 (1%)	18	37

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP

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Mol	Chain	Res	Type
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	39	SER
2	B	59	GLN
6	F	95	GLN
7	G	3	ALA
7	G	8	HIS
7	G	40	GLY
8	H	8	ILE
10	J	15	ASP
2	O	59	GLN
7	T	3	ALA
7	T	8	HIS
7	T	40	GLY
2	B	60	GLU
2	O	60	GLU
3	P	38	ASN
8	U	8	ILE
7	G	82	TYR
9	V	36	LYS
3	C	38	ASN
9	I	36	LYS
1	N	142	SER
6	S	96	LEU
2	B	158	ASP
6	S	93	PRO
2	B	159	VAL
2	O	159	VAL
2	B	92	ASN
6	F	93	PRO

### 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	426/426 (100%)	413 (97%)	13 (3%)	45	73
1	N	426/426 (100%)	411 (96%)	15 (4%)	41	68
2	B	210/210 (100%)	196 (93%)	14 (7%)	19	38
2	O	210/210 (100%)	200 (95%)	10 (5%)	30	55
3	C	224/226 (99%)	213 (95%)	11 (5%)	29	54
3	P	224/226 (99%)	216 (96%)	8 (4%)	40	68
4	D	128/129 (99%)	125 (98%)	3 (2%)	56	81
4	Q	128/129 (99%)	124 (97%)	4 (3%)	45	73
5	E	92/95 (97%)	89 (97%)	3 (3%)	43	70
5	R	92/95 (97%)	91 (99%)	1 (1%)	78	92
6	F	81/81 (100%)	78 (96%)	3 (4%)	39	66
6	S	81/81 (100%)	75 (93%)	6 (7%)	16	32
7	G	67/68 (98%)	60 (90%)	7 (10%)	8	15
7	T	67/68 (98%)	62 (92%)	5 (8%)	16	31
8	H	71/75 (95%)	67 (94%)	4 (6%)	25	48
8	U	71/75 (95%)	70 (99%)	1 (1%)	71	89
9	I	57/57 (100%)	55 (96%)	2 (4%)	41	68
9	V	57/57 (100%)	56 (98%)	1 (2%)	64	85
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	60	83
11	K	39/46 (85%)	38 (97%)	1 (3%)	51	78
11	X	39/46 (85%)	36 (92%)	3 (8%)	15	29
12	L	39/40 (98%)	37 (95%)	2 (5%)	28	52
12	Y	39/40 (98%)	38 (97%)	1 (3%)	51	78
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	14
All	All	3040/3082 (99%)	2910 (96%)	130 (4%)	33	61

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	490	THR
1	A	495	LEU
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	113	TYR
2	B	115	ASP
2	B	130	PRO
2	B	167	SER
2	B	185	MET
2	B	205	SER
3	C	17	PRO
3	C	29	SER
3	C	33	MET
3	C	39	SER
3	C	95	THR
3	C	110	PRO
3	C	159	MET
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	36	SER
4	D	51	LEU
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU

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Mol	Chain	Res	Type
6	F	53	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	35	SER
7	G	36	TRP
7	G	38	HIS
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	27	ARG
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
11	K	54	ARG
12	L	2	HIS
12	L	26	THR
13	M	4	LYS
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	38	ASP
13	M	42	LYS
1	N	109	PHE
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	264	LYS
1	N	290	HIS
1	N	338	MET
1	N	361	SER
1	N	369	ASP
1	N	380	VAL
1	N	484	THR
1	N	495	LEU
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU

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Mol	Chain	Res	Type
2	O	60	GLU
2	O	65	TRP
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	203	ASN
2	O	217	LYS
3	P	23	SER
3	P	29	SER
3	P	33	MET
3	P	66	THR
3	P	150	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
4	Q	54	ASP
4	Q	108	PRO
4	Q	121	LYS
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	94	HIS
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	35	SER
7	T	43	GLU
7	T	54	ARG
8	U	29	CYS
9	V	8	GLN
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP

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Mol	Chain	Res	Type
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	413	HIS
2	B	10	GLN
2	B	91	ASN
2	B	102	HIS
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	9	HIS
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	34	ASN
7	G	71	HIS
8	H	31	GLN
11	K	35	GLN
11	K	41	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	203	ASN
3	P	3	HIS
3	P	12	ASN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN

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Mol	Chain	Res	Type
3	P	243	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
6	S	54	ASN
6	S	94	HIS
7	T	34	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	FME	A	1	1	9,9,10	0.90	0	7,9,11	1.21	2 (28%)
2	FME	B	1	2	9,9,10	1.10	0	7,9,11	1.52	1 (14%)
7	TPO	G	11	7	9,10,11	2.09	2 (22%)	10,14,16	1.02	0
9	SAC	I	1	9	8,8,9	2.58	3 (37%)	6,9,11	1.73	1 (16%)
1	FME	N	1	1	9,9,10	0.94	0	7,9,11	1.33	2 (28%)
2	FME	O	1	2	9,9,10	0.83	0	7,9,11	1.69	2 (28%)
7	TPO	T	11	7	9,10,11	1.72	2 (22%)	10,14,16	1.05	0
9	SAC	V	1	9	8,8,9	3.11	3 (37%)	6,9,11	1.97	3 (50%)

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
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.28	1.58	1.50
7	T	11	TPO	CA-C	3.36	1.54	1.50
9	I	1	SAC	CA-C	3.44	1.54	1.50
7	G	11	TPO	CA-C	3.46	1.54	1.50
9	I	1	SAC	CA-N	3.72	1.51	1.46
7	G	11	TPO	CB-CA	3.90	1.60	1.53
9	V	1	SAC	CA-N	4.35	1.52	1.46
9	V	1	SAC	CA-C	4.94	1.56	1.50
9	I	1	SAC	OAC-C1A	5.01	1.35	1.23
9	V	1	SAC	OAC-C1A	5.25	1.35	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-3.50	117.45	122.82
2	B	1	FME	CA-N-CN	-2.80	118.51	122.82
1	N	1	FME	CA-N-CN	-2.51	118.97	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.47	117.57	122.06
2	O	1	FME	CB-CA-C	-2.31	107.84	111.65
1	N	1	FME	O-C-CA	-2.14	120.15	125.15
1	A	1	FME	CA-N-CN	-2.12	119.57	122.82
1	A	1	FME	O-C-CA	-2.05	120.36	125.15
9	V	1	SAC	CB-CA-N	2.22	115.79	110.60
9	V	1	SAC	C2A-C1A-N	2.79	121.15	116.11
9	I	1	SAC	CB-CA-N	3.05	117.71	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
7	G	11	TPO	1	0
1	N	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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	$\# Z  > 2$
18	HEA	A	515	1	44,67,67	1.54	8 (18%)	37,103,103	1.77	10 (27%)
18	HEA	A	516	1	44,67,67	1.52	7 (15%)	37,103,103	1.36	6 (16%)
19	PGV	A	524	-	50,50,50	1.27	5 (10%)	51,56,56	0.82	1 (1%)
20	CHD	A	525	-	29,32,32	0.93	0	47,51,51	2.53	18 (38%)
20	CHD	B	1086	-	29,32,32	0.80	0	47,51,51	2.52	20 (42%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	PSC	B	230	-	51,51,51	1.42	7 (13%)	56,59,59	1.09	1 (1%)
22	TGL	B	521	-	62,62,62	1.08	4 (6%)	65,65,65	1.53	10 (15%)
25	PEK	C	264	-	52,52,52	1.51	6 (11%)	54,57,57	1.30	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PEK	C	265	-	52,52,52	1.81	11 (21%)	54,57,57	1.26	7 (12%)
19	PGV	C	266	-	50,50,50	1.19	5 (10%)	51,56,56	0.99	2 (3%)
19	PGV	C	267	-	50,50,50	1.03	3 (6%)	51,56,56	1.08	6 (11%)
19	PGV	C	268	-	50,50,50	1.45	7 (14%)	51,56,56	0.90	1 (1%)
26	CDL	C	270	-	99,99,99	1.07	8 (8%)	101,111,111	1.06	8 (7%)
20	CHD	C	271	-	29,32,32	1.35	3 (10%)	47,51,51	3.70	24 (51%)
24	DMU	C	272	-	34,34,34	2.67	16 (47%)	45,45,45	4.18	19 (42%)
22	TGL	D	523	-	62,62,62	1.00	3 (4%)	65,65,65	1.36	7 (10%)
25	PEK	G	1263	-	52,52,52	2.15	11 (21%)	54,57,57	1.30	4 (7%)
26	CDL	G	269	-	99,99,99	1.25	9 (9%)	101,111,111	1.00	7 (6%)
20	CHD	J	60	-	29,32,32	1.91	9 (31%)	47,51,51	4.08	28 (59%)
22	TGL	L	522	-	62,62,62	1.36	5 (8%)	65,65,65	1.67	12 (18%)
24	DMU	M	526	-	34,34,34	3.44	8 (23%)	45,45,45	4.16	22 (48%)
22	TGL	N	1522	-	62,62,62	1.50	6 (9%)	65,65,65	1.63	10 (15%)
22	TGL	N	1523	-	62,62,62	0.96	3 (4%)	65,65,65	1.31	7 (10%)
19	PGV	N	1524	-	50,50,50	1.24	5 (10%)	51,56,56	0.89	1 (1%)
20	CHD	N	1604	-	29,32,32	0.95	1 (3%)	47,51,51	2.47	17 (36%)
18	HEA	N	515	1	44,67,67	1.48	8 (18%)	37,103,103	1.91	13 (35%)
18	HEA	N	516	1	44,67,67	1.46	7 (15%)	37,103,103	1.40	6 (16%)
23	PSC	O	1230	-	51,51,51	1.54	6 (11%)	56,59,59	1.06	2 (3%)
22	TGL	O	1521	-	62,62,62	1.12	5 (8%)	65,65,65	1.54	8 (12%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
25	PEK	P	1264	-	52,52,52	1.70	8 (15%)	54,57,57	1.45	8 (14%)
25	PEK	P	1265	-	52,52,52	1.84	11 (21%)	54,57,57	1.25	7 (12%)
19	PGV	P	1266	-	50,50,50	1.38	6 (12%)	51,56,56	1.11	4 (7%)
19	PGV	P	1267	-	50,50,50	0.98	3 (6%)	51,56,56	1.05	4 (7%)
19	PGV	P	1268	-	50,50,50	1.42	6 (12%)	51,56,56	0.88	2 (3%)
26	CDL	P	1270	-	99,99,99	1.21	9 (9%)	101,111,111	1.06	4 (3%)
24	DMU	P	1272	-	34,34,34	2.72	15 (44%)	45,45,45	4.11	19 (42%)
20	CHD	P	1525	-	29,32,32	0.96	2 (6%)	47,51,51	2.65	21 (44%)
26	CDL	T	1269	-	99,99,99	1.25	11 (11%)	101,111,111	1.00	7 (6%)
25	PEK	T	263	-	52,52,52	2.19	12 (23%)	54,57,57	1.32	4 (7%)
20	CHD	W	1060	-	29,32,32	2.04	8 (27%)	47,51,51	4.13	27 (57%)
20	CHD	W	1271	-	29,32,32	1.28	4 (13%)	47,51,51	3.61	24 (51%)
24	DMU	Z	1526	-	34,34,34	3.32	8 (23%)	45,45,45	4.16	21 (46%)

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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0
20	CHD	A	525	-	-	0/7/74/74	0/4/4/4
20	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
23	PSC	B	230	-	-	0/55/55/55	0/0/0/0
22	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	266	-	-	0/55/55/55	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
20	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	TGL	D	523	-	-	0/65/65/65	0/0/0/0
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
20	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
22	TGL	L	522	-	-	0/65/65/65	0/0/0/0
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
22	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
22	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
20	CHD	N	1604	-	-	0/7/74/74	0/4/4/4
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
23	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
22	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1266	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
20	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
20	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
20	CHD	W	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (279) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-9.21	1.21	1.43
24	Z	1526	DMU	O7-C3	-8.35	1.23	1.43
24	M	526	DMU	O16-C6	-7.71	1.26	1.40
24	Z	1526	DMU	O1-C9	-7.50	1.26	1.44
24	M	526	DMU	O1-C9	-7.48	1.26	1.44
24	Z	1526	DMU	O16-C6	-7.22	1.27	1.40
24	M	526	DMU	O7-C10	-7.03	1.23	1.41
24	Z	1526	DMU	O16-C18	-6.88	1.24	1.43
24	Z	1526	DMU	O7-C10	-6.64	1.24	1.41
24	M	526	DMU	O5-C4	-6.59	1.28	1.44
24	M	526	DMU	O16-C18	-6.40	1.25	1.43
24	Z	1526	DMU	O5-C4	-6.22	1.29	1.44
24	P	1272	DMU	O16-C18	-6.16	1.26	1.43
24	C	272	DMU	O16-C18	-5.90	1.27	1.43
24	M	526	DMU	O1-C10	-5.80	1.27	1.41
24	Z	1526	DMU	O1-C10	-5.38	1.28	1.41
24	P	1272	DMU	O16-C6	-5.07	1.31	1.40
24	C	272	DMU	O7-C3	-5.05	1.31	1.43
24	P	1272	DMU	O7-C3	-4.98	1.31	1.43
24	C	272	DMU	O1-C9	-4.94	1.32	1.44
24	C	272	DMU	O16-C6	-4.73	1.31	1.40
24	C	272	DMU	O5-C4	-4.69	1.32	1.44
24	P	1272	DMU	O1-C9	-4.60	1.33	1.44
24	Z	1526	DMU	O5-C6	-4.60	1.30	1.41
24	M	526	DMU	O5-C6	-4.55	1.30	1.41
18	A	515	HEA	C1D-ND	-4.55	1.31	1.36
18	A	516	HEA	C3A-C2A	-3.97	1.35	1.40
18	A	515	HEA	C3A-CMA	-3.82	1.37	1.46
24	P	1272	DMU	O5-C4	-3.56	1.35	1.44
24	P	1272	DMU	O7-C10	-3.50	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	O7-C10	-3.49	1.32	1.41
24	C	272	DMU	O1-C10	-3.44	1.33	1.41
18	N	516	HEA	C3A-CMA	-3.15	1.39	1.46
24	C	272	DMU	O5-C6	-3.02	1.34	1.41
18	N	515	HEA	C3A-CMA	-2.90	1.39	1.46
18	A	516	HEA	C3A-CMA	-2.85	1.39	1.46
24	P	1272	DMU	O5-C6	-2.73	1.35	1.41
18	N	516	HEA	C3A-C2A	-2.65	1.36	1.40
24	P	1272	DMU	O1-C10	-2.47	1.35	1.41
20	N	1604	CHD	C13-C12	-2.36	1.50	1.54
18	N	515	HEA	C3A-C2A	-2.32	1.37	1.40
18	N	516	HEA	C1B-CHB	-2.31	1.34	1.40
25	C	264	PEK	O03-C01	-2.24	1.40	1.45
18	N	516	HEA	C3C-C2C	-2.22	1.37	1.40
18	N	515	HEA	C1D-ND	-2.22	1.34	1.36
18	N	515	HEA	C1C-CHC	-2.00	1.34	1.40
22	B	521	TGL	CA2-CA1	2.01	1.56	1.50
20	W	1271	CHD	C1-C10	2.01	1.57	1.54
18	A	516	HEA	C4A-NA	2.02	1.39	1.36
18	A	516	HEA	C20-C19	2.03	1.55	1.51
25	C	264	PEK	C4-C5	2.05	1.61	1.50
23	B	230	PSC	P-O11	2.05	1.67	1.59
20	P	1525	CHD	C8-C9	2.06	1.57	1.53
19	P	1268	PGV	C06-C05	2.07	1.59	1.52
19	C	268	PGV	P-O11	2.07	1.68	1.59
20	J	60	CHD	C10-C9	2.08	1.60	1.56
19	C	268	PGV	C20-C19	2.09	1.56	1.50
25	P	1264	PEK	C22-C21	2.10	1.56	1.50
26	G	269	CDL	C71-CB7	2.11	1.56	1.50
23	B	230	PSC	C01-C02	2.12	1.56	1.50
19	A	524	PGV	C06-C05	2.12	1.60	1.52
26	C	270	CDL	C11-CA5	2.13	1.56	1.50
25	T	263	PEK	P-O12	2.13	1.68	1.59
22	O	1521	TGL	CA2-CA1	2.13	1.56	1.50
23	B	230	PSC	P-O12	2.14	1.68	1.59
19	P	1268	PGV	C03-C02	2.15	1.56	1.50
24	C	272	DMU	C2-C3	2.17	1.58	1.52
22	D	523	TGL	OG3-CC1	2.20	1.39	1.33
18	A	515	HEA	C1C-NC	2.20	1.40	1.36
20	J	60	CHD	C1-C10	2.20	1.58	1.54
25	C	265	PEK	P-O12	2.21	1.68	1.59
24	C	272	DMU	C2-C1	2.21	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	516	HEA	C17-C18	2.21	1.57	1.50
26	T	1269	CDL	C51-CB5	2.21	1.57	1.50
20	J	60	CHD	C20-C17	2.22	1.58	1.54
26	C	270	CDL	PB2-OB2	2.23	1.68	1.59
18	N	515	HEA	C1A-NA	2.24	1.39	1.36
26	T	1269	CDL	OB6-CB5	2.25	1.40	1.34
20	P	1525	CHD	C13-C14	2.25	1.59	1.55
23	O	1230	PSC	C3-C2	2.25	1.60	1.52
19	N	1524	PGV	C20-C19	2.26	1.57	1.50
19	C	266	PGV	C20-C19	2.27	1.57	1.50
19	N	1524	PGV	O01-C1	2.27	1.40	1.34
26	C	270	CDL	PA1-OA5	2.28	1.68	1.59
22	N	1523	TGL	OG3-CC1	2.28	1.40	1.33
25	T	263	PEK	C2-C1	2.28	1.57	1.50
18	A	515	HEA	C26-C15	2.30	1.56	1.50
19	A	524	PGV	C20-C19	2.31	1.57	1.50
18	A	516	HEA	C16-C15	2.32	1.56	1.51
22	L	522	TGL	CB2-CB1	2.32	1.57	1.50
22	N	1523	TGL	CG3-CG2	2.32	1.57	1.50
23	O	1230	PSC	C01-C02	2.34	1.57	1.50
25	P	1265	PEK	P-O12	2.36	1.69	1.59
25	G	1263	PEK	C22-C21	2.36	1.57	1.50
22	O	1521	TGL	OG3-CC1	2.36	1.40	1.33
25	C	265	PEK	O01-C1	2.38	1.41	1.34
26	P	1270	CDL	PB2-OB2	2.40	1.69	1.59
25	C	265	PEK	C22-C21	2.41	1.57	1.50
20	J	60	CHD	C8-C14	2.42	1.58	1.53
19	C	268	PGV	C06-C05	2.45	1.61	1.52
26	T	1269	CDL	C71-CB7	2.47	1.57	1.50
19	C	266	PGV	O01-C1	2.47	1.41	1.34
26	T	1269	CDL	C31-CA7	2.48	1.57	1.50
18	A	515	HEA	C4A-NA	2.51	1.39	1.36
24	P	1272	DMU	C2-C1	2.52	1.58	1.52
26	C	270	CDL	OA8-CA7	2.52	1.40	1.33
23	O	1230	PSC	P-O12	2.52	1.69	1.59
19	P	1266	PGV	O01-C1	2.53	1.41	1.34
24	C	272	DMU	C10-C5	2.56	1.59	1.52
26	T	1269	CDL	CA6-CA4	2.56	1.58	1.50
26	G	269	CDL	CB2-C1	2.57	1.61	1.51
25	P	1265	PEK	O01-C1	2.58	1.41	1.34
22	N	1522	TGL	CB2-CB1	2.58	1.58	1.50
25	G	1263	PEK	P-O12	2.59	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	1267	PGV	O03-C19	2.60	1.41	1.33
19	A	524	PGV	C03-C02	2.63	1.58	1.50
20	W	1271	CHD	C13-C14	2.63	1.60	1.55
25	T	263	PEK	C22-C21	2.64	1.58	1.50
20	J	60	CHD	C13-C12	2.64	1.58	1.54
20	W	1060	CHD	C10-C9	2.64	1.61	1.56
26	P	1270	CDL	OB6-CB5	2.64	1.42	1.34
18	A	515	HEA	C4D-ND	2.65	1.41	1.36
19	N	1524	PGV	O03-C19	2.65	1.41	1.33
19	P	1266	PGV	C20-C19	2.65	1.58	1.50
26	P	1270	CDL	C11-CA5	2.66	1.58	1.50
20	W	1060	CHD	C8-C9	2.66	1.59	1.53
26	C	270	CDL	C31-CA7	2.66	1.58	1.50
22	D	523	TGL	CB2-CB1	2.66	1.58	1.50
24	C	272	DMU	C8-C9	2.68	1.58	1.53
20	W	1060	CHD	C8-C14	2.71	1.59	1.53
25	T	263	PEK	O03-C01	2.71	1.51	1.45
25	P	1264	PEK	C2-C1	2.72	1.58	1.50
25	P	1265	PEK	C22-C21	2.73	1.58	1.50
25	C	265	PEK	P-O11	2.74	1.70	1.59
25	P	1265	PEK	P-O11	2.74	1.70	1.59
19	P	1268	PGV	P-O12	2.74	1.70	1.59
26	T	1269	CDL	CB2-C1	2.74	1.61	1.51
19	P	1266	PGV	C03-C02	2.76	1.58	1.50
25	G	1263	PEK	O03-C01	2.77	1.51	1.45
26	G	269	CDL	OB6-CB5	2.78	1.42	1.34
24	C	272	DMU	C8-C7	2.78	1.59	1.52
19	C	268	PGV	P-O12	2.78	1.71	1.59
26	T	1269	CDL	PB2-OB2	2.79	1.71	1.59
26	G	269	CDL	CA6-CA4	2.80	1.58	1.50
22	B	521	TGL	CB2-CB1	2.82	1.58	1.50
19	P	1267	PGV	C01-C02	2.82	1.58	1.50
24	P	1272	DMU	C8-C9	2.82	1.59	1.53
26	G	269	CDL	PB2-OB2	2.83	1.71	1.59
18	A	515	HEA	C4B-NB	2.83	1.40	1.36
26	C	270	CDL	CA3-CA4	2.86	1.58	1.50
20	W	1271	CHD	C13-C12	2.87	1.59	1.54
20	W	1060	CHD	C13-C12	2.95	1.59	1.54
25	C	265	PEK	C01-C02	2.96	1.59	1.50
25	P	1264	PEK	O01-C1	2.96	1.42	1.34
24	C	272	DMU	C5-C7	2.97	1.59	1.52
20	J	60	CHD	C8-C9	2.98	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	C5-C7	2.98	1.60	1.52
22	N	1523	TGL	OG2-CB1	2.99	1.43	1.34
20	C	271	CHD	C13-C17	3.00	1.60	1.55
23	B	230	PSC	O01-C1	3.00	1.43	1.34
24	P	1272	DMU	C10-C5	3.01	1.61	1.52
19	C	267	PGV	O03-C19	3.02	1.42	1.33
22	N	1522	TGL	CA2-CA1	3.04	1.59	1.50
19	P	1268	PGV	C04-C05	3.05	1.62	1.51
25	T	263	PEK	P-O11	3.06	1.72	1.59
19	C	268	PGV	C04-C05	3.07	1.63	1.51
19	N	1524	PGV	C03-C02	3.08	1.59	1.50
20	W	1271	CHD	C13-C17	3.13	1.61	1.55
20	C	271	CHD	C13-C12	3.13	1.59	1.54
22	O	1521	TGL	CG3-CG2	3.16	1.59	1.50
25	P	1265	PEK	C01-C02	3.17	1.59	1.50
22	B	521	TGL	CG3-CG2	3.19	1.59	1.50
26	C	270	CDL	C71-CB7	3.19	1.59	1.50
22	N	1522	TGL	CG3-CG2	3.19	1.59	1.50
20	J	60	CHD	C10-C5	3.20	1.60	1.55
19	C	267	PGV	C12-C11	3.21	1.49	1.31
26	G	269	CDL	CB3-CB4	3.21	1.59	1.50
20	J	60	CHD	C8-C7	3.21	1.59	1.53
20	W	1060	CHD	C10-C5	3.22	1.60	1.55
25	P	1264	PEK	O03-C21	3.24	1.42	1.33
26	T	1269	CDL	CB3-CB4	3.24	1.59	1.50
22	O	1521	TGL	OG2-CB1	3.24	1.43	1.34
25	P	1265	PEK	O03-C21	3.24	1.42	1.33
25	G	1263	PEK	P-O11	3.25	1.73	1.59
19	C	267	PGV	O01-C1	3.26	1.43	1.34
25	P	1265	PEK	C03-C02	3.27	1.60	1.50
25	C	265	PEK	O03-C21	3.27	1.43	1.33
20	C	271	CHD	C13-C14	3.29	1.61	1.55
26	P	1270	CDL	C71-CB7	3.29	1.60	1.50
18	A	516	HEA	C3C-CAC	3.31	1.54	1.47
19	P	1267	PGV	C12-C11	3.32	1.50	1.31
19	C	266	PGV	C03-C02	3.33	1.60	1.50
26	P	1270	CDL	PA1-OA5	3.37	1.73	1.59
26	C	270	CDL	CA6-CA4	3.38	1.60	1.50
22	L	522	TGL	CG3-CG2	3.40	1.60	1.50
23	B	230	PSC	C2-C1	3.41	1.60	1.50
26	P	1270	CDL	C31-CA7	3.43	1.60	1.50
26	P	1270	CDL	OA8-CA7	3.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	265	PEK	C03-C02	3.44	1.60	1.50
22	O	1521	TGL	CB2-CB1	3.44	1.60	1.50
26	P	1270	CDL	CA6-CA4	3.45	1.60	1.50
20	W	1060	CHD	C20-C17	3.46	1.60	1.54
18	N	515	HEA	C4B-NB	3.49	1.40	1.36
26	T	1269	CDL	C11-CA5	3.49	1.60	1.50
24	C	272	DMU	C3-C4	3.51	1.62	1.52
22	N	1522	TGL	CG1-CG2	3.53	1.60	1.50
18	N	515	HEA	C4A-NA	3.54	1.40	1.36
18	N	515	HEA	C1C-NC	3.54	1.43	1.36
20	W	1060	CHD	C8-C7	3.55	1.59	1.53
26	P	1270	CDL	CA3-CA4	3.56	1.60	1.50
19	C	268	PGV	O01-C1	3.69	1.45	1.34
22	L	522	TGL	CG1-CG2	3.70	1.61	1.50
22	B	521	TGL	OG2-CB1	3.71	1.45	1.34
26	G	269	CDL	CB6-CB4	3.71	1.61	1.50
18	A	516	HEA	C4B-NB	3.75	1.41	1.36
23	O	1230	PSC	C13-C12	3.78	1.52	1.31
19	P	1266	PGV	C01-C02	3.81	1.61	1.50
26	G	269	CDL	C11-CA5	3.90	1.62	1.50
18	N	516	HEA	C4B-NB	3.90	1.41	1.36
22	D	523	TGL	OG2-CB1	3.91	1.45	1.34
23	B	230	PSC	C13-C12	3.91	1.53	1.31
18	N	516	HEA	C1A-NA	4.00	1.41	1.36
24	C	272	DMU	C6-C1	4.00	1.64	1.52
19	C	266	PGV	C12-C11	4.01	1.54	1.31
19	P	1268	PGV	O01-C1	4.01	1.45	1.34
25	C	265	PEK	C6-C5	4.01	1.54	1.31
18	A	515	HEA	C1A-NA	4.02	1.41	1.36
24	P	1272	DMU	C3-C4	4.03	1.63	1.52
26	T	1269	CDL	CB6-CB4	4.07	1.62	1.50
19	P	1266	PGV	C12-C11	4.09	1.54	1.31
26	T	1269	CDL	OA6-CA5	4.12	1.46	1.34
19	A	524	PGV	O03-C19	4.14	1.45	1.33
25	P	1265	PEK	C6-C5	4.21	1.55	1.31
26	G	269	CDL	OA6-CA5	4.30	1.46	1.34
25	C	264	PEK	C9-C8	4.30	1.55	1.31
19	A	524	PGV	C12-C11	4.34	1.56	1.31
19	C	266	PGV	O03-C19	4.40	1.46	1.33
24	P	1272	DMU	C8-C7	4.47	1.63	1.52
25	G	1263	PEK	C15-C14	4.47	1.56	1.31
25	P	1265	PEK	C15-C14	4.48	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1264	PEK	C9-C8	4.49	1.56	1.31
25	P	1264	PEK	C15-C14	4.51	1.57	1.31
25	T	263	PEK	C15-C14	4.51	1.57	1.31
19	N	1524	PGV	C12-C11	4.52	1.57	1.31
25	C	265	PEK	C9-C8	4.56	1.57	1.31
24	P	1272	DMU	C6-C1	4.56	1.65	1.52
25	C	265	PEK	C15-C14	4.58	1.57	1.31
25	C	265	PEK	C12-C11	4.61	1.57	1.31
25	P	1264	PEK	C12-C11	4.62	1.57	1.31
22	L	522	TGL	OG1-CA1	4.65	1.47	1.33
25	P	1265	PEK	C9-C8	4.67	1.57	1.31
22	N	1522	TGL	OG2-CB1	4.70	1.47	1.34
25	P	1264	PEK	C6-C5	4.73	1.58	1.31
22	L	522	TGL	OG2-CB1	4.74	1.48	1.34
25	T	263	PEK	C9-C8	4.74	1.58	1.31
25	P	1265	PEK	C12-C11	4.74	1.58	1.31
25	C	264	PEK	C6-C5	4.75	1.58	1.31
25	T	263	PEK	C03-C02	4.75	1.64	1.50
25	G	1263	PEK	C6-C5	4.76	1.58	1.31
25	C	264	PEK	C12-C11	4.77	1.58	1.31
25	T	263	PEK	C6-C5	4.77	1.58	1.31
23	B	230	PSC	C10-C9	4.78	1.58	1.31
25	G	1263	PEK	C03-C02	4.83	1.64	1.50
25	G	1263	PEK	C9-C8	4.88	1.59	1.31
19	P	1268	PGV	C12-C11	4.89	1.59	1.31
23	O	1230	PSC	C10-C9	4.91	1.59	1.31
25	C	264	PEK	C15-C14	5.02	1.59	1.31
25	G	1263	PEK	C12-C11	5.03	1.60	1.31
19	C	268	PGV	C12-C11	5.10	1.60	1.31
25	T	263	PEK	C12-C11	5.28	1.61	1.31
25	G	1263	PEK	O03-C21	5.37	1.49	1.33
19	P	1266	PGV	O03-C19	5.46	1.49	1.33
25	T	263	PEK	C01-C02	5.53	1.66	1.50
23	O	1230	PSC	C2-C1	5.56	1.66	1.50
25	G	1263	PEK	C01-C02	5.58	1.66	1.50
20	J	60	CHD	C13-C17	5.59	1.65	1.55
20	W	1060	CHD	C13-C17	5.90	1.65	1.55
25	T	263	PEK	O03-C21	5.93	1.50	1.33
22	N	1522	TGL	OG1-CA1	6.28	1.51	1.33

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1086	CHD	C18-C13-C12	-9.58	99.33	109.08
20	N	1604	CHD	C18-C13-C12	-8.20	100.73	109.08
20	W	1271	CHD	C19-C10-C9	-8.17	99.47	111.16
20	C	271	CHD	C19-C10-C9	-7.92	99.82	111.16
20	W	1271	CHD	C17-C13-C12	-7.68	110.61	117.67
20	C	271	CHD	C17-C13-C12	-7.24	111.02	117.67
20	W	1060	CHD	C18-C13-C14	-6.14	101.52	111.23
20	P	1525	CHD	C11-C12-C13	-6.10	104.91	111.22
24	Z	1526	DMU	C8-C7-C5	-5.81	100.59	110.84
24	M	526	DMU	C8-C7-C5	-5.43	101.26	110.84
20	J	60	CHD	C18-C13-C14	-5.28	102.89	111.23
20	W	1271	CHD	C15-C14-C8	-5.09	111.13	118.32
22	N	1522	TGL	C12-C11-C10	-5.03	88.52	114.45
20	W	1060	CHD	C15-C14-C8	-4.99	111.26	118.32
20	C	271	CHD	C15-C14-C8	-4.95	111.33	118.32
20	C	271	CHD	C18-C13-C12	-4.90	104.09	109.08
20	J	60	CHD	C15-C14-C8	-4.87	111.43	118.32
22	O	1521	TGL	CG1-OG1-CA1	-4.87	102.48	117.13
20	W	1060	CHD	C19-C10-C1	-4.82	100.31	108.24
22	L	522	TGL	C12-C11-C10	-4.82	89.60	114.45
20	J	60	CHD	C19-C10-C1	-4.74	100.45	108.24
23	B	230	PSC	C01-O03-C19	-4.69	103.01	117.13
26	C	270	CDL	CB6-OB8-CB7	-4.49	103.62	117.13
20	A	525	CHD	C11-C12-C13	-4.48	106.59	111.22
23	O	1230	PSC	C01-O03-C19	-4.45	103.74	117.13
22	N	1522	TGL	CB9-CB8-CB7	-4.42	91.70	114.45
19	P	1266	PGV	O01-C1-C2	-4.40	102.42	111.55
22	B	521	TGL	CG1-OG1-CA1	-4.35	104.05	117.13
26	P	1270	CDL	CB6-OB8-CB7	-4.35	104.06	117.13
19	C	266	PGV	O01-C1-C2	-4.22	102.80	111.55
22	L	522	TGL	CB9-CB8-CB7	-4.11	93.26	114.45
20	J	60	CHD	C18-C13-C12	-4.09	104.92	109.08
18	N	515	HEA	C12-C13-C14	-4.06	101.67	112.33
20	C	271	CHD	C19-C10-C1	-4.04	101.60	108.24
25	P	1264	PEK	O03-C21-C22	-3.95	100.40	111.90
20	N	1604	CHD	C15-C14-C13	-3.93	99.65	103.57
19	C	267	PGV	O01-C1-C2	-3.87	103.52	111.55
20	P	1525	CHD	C15-C14-C8	-3.87	112.85	118.32
22	D	523	TGL	CG1-OG1-CA1	-3.81	105.67	117.13
22	N	1523	TGL	CG1-OG1-CA1	-3.79	105.73	117.13
20	N	1604	CHD	C16-C17-C13	-3.74	99.84	103.57
26	P	1270	CDL	OB6-CB5-C51	-3.74	103.78	111.55
19	P	1267	PGV	O01-C1-C2	-3.69	103.90	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	W	1271	CHD	C18-C13-C12	-3.68	105.34	109.08
20	A	525	CHD	C15-C14-C8	-3.60	113.23	118.32
20	N	1604	CHD	C15-C14-C8	-3.56	113.28	118.32
20	B	1086	CHD	C16-C17-C13	-3.48	100.11	103.57
25	P	1264	PEK	C3-C2-C1	-3.47	100.92	113.58
24	Z	1526	DMU	C2-C3-C4	-3.43	103.59	110.88
20	B	1086	CHD	C15-C14-C8	-3.41	113.49	118.32
26	C	270	CDL	OB6-CB5-C51	-3.30	104.70	111.55
18	A	515	HEA	C12-C13-C14	-3.29	103.69	112.33
25	C	264	PEK	C3-C2-C1	-3.27	101.66	113.58
20	W	1271	CHD	C18-C13-C14	-3.25	106.09	111.23
24	M	526	DMU	C2-C3-C4	-3.24	104.01	110.88
20	W	1060	CHD	C18-C13-C12	-3.22	105.80	109.08
18	N	515	HEA	C17-C18-C19	-3.19	119.68	127.68
20	P	1525	CHD	C14-C13-C12	-3.13	104.42	107.39
20	W	1271	CHD	C19-C10-C1	-3.09	103.17	108.24
25	P	1264	PEK	C23-C22-C21	-3.04	102.47	113.58
25	C	264	PEK	O03-C21-C22	-2.99	103.21	111.90
20	A	525	CHD	C14-C13-C12	-2.94	104.60	107.39
20	A	525	CHD	C18-C13-C17	-2.92	106.61	111.23
18	N	515	HEA	C1B-C2B-C3B	-2.92	104.97	107.00
18	A	516	HEA	C1B-C2B-C3B	-2.90	104.98	107.00
26	T	1269	CDL	OB8-CB7-C71	-2.86	103.57	111.90
20	B	1086	CHD	C15-C14-C13	-2.78	100.80	103.57
20	C	271	CHD	C18-C13-C14	-2.75	106.88	111.23
20	B	1086	CHD	O7-C7-C6	-2.75	103.37	110.02
18	N	515	HEA	C16-C15-C14	-2.70	115.57	121.10
26	G	269	CDL	OB8-CB7-C71	-2.70	104.04	111.90
20	B	1086	CHD	O12-C12-C13	-2.63	106.73	111.12
18	N	516	HEA	CMC-C2C-C1C	-2.63	124.42	128.46
22	B	521	TGL	CA8-CA7-CA6	-2.59	101.13	114.45
18	A	515	HEA	C16-C15-C14	-2.58	115.82	121.10
20	N	1604	CHD	O12-C12-C13	-2.55	106.86	111.12
19	P	1266	PGV	C02-O01-C1	-2.50	111.97	117.88
22	O	1521	TGL	CA8-CA7-CA6	-2.49	101.61	114.45
20	N	1604	CHD	C19-C10-C1	-2.49	104.15	108.24
24	C	272	DMU	C2-C3-C4	-2.49	105.59	110.88
25	C	265	PEK	C23-C22-C21	-2.42	104.76	113.58
26	C	270	CDL	C52-C51-CB5	-2.40	104.82	113.58
18	A	515	HEA	C1B-C2B-C3B	-2.40	105.33	107.00
19	P	1266	PGV	C01-O03-C19	-2.37	109.99	117.13
18	A	515	HEA	C17-C18-C19	-2.35	121.78	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C26-C15-C14	-2.34	117.44	123.69
22	O	1521	TGL	CB7-CB6-CB5	-2.32	102.50	114.45
25	P	1264	PEK	C24-C23-C22	-2.32	104.75	113.24
20	A	525	CHD	C15-C14-C13	-2.26	101.32	103.57
22	O	1521	TGL	OG3-CC1-CC2	-2.26	105.33	111.90
18	N	515	HEA	CMC-C2C-C1C	-2.25	125.00	128.46
20	B	1086	CHD	C14-C8-C9	-2.24	106.58	109.64
20	P	1525	CHD	C19-C10-C9	-2.24	107.96	111.16
25	C	264	PEK	O03-C01-C02	-2.23	103.06	108.66
20	P	1525	CHD	C16-C17-C13	-2.20	101.37	103.57
20	P	1525	CHD	C18-C13-C17	-2.20	107.74	111.23
25	P	1265	PEK	C23-C22-C21	-2.20	105.56	113.58
25	P	1264	PEK	C02-O01-C1	-2.19	112.71	117.88
26	C	270	CDL	CB6-CB4-CB3	-2.16	106.98	111.86
20	P	1525	CHD	C15-C14-C13	-2.16	101.42	103.57
19	C	267	PGV	C9-C10-C11	-2.15	100.77	112.50
22	D	523	TGL	CC3-CC2-CC1	-2.15	105.72	113.58
20	B	1086	CHD	C19-C10-C1	-2.14	104.72	108.24
24	M	526	DMU	C6-C1-C2	-2.12	106.03	109.98
18	A	515	HEA	CMC-C2C-C1C	-2.08	125.26	128.46
22	B	521	TGL	CB7-CB6-CB5	-2.06	103.82	114.45
19	C	267	PGV	C3-C2-C1	-2.06	106.05	113.58
18	A	516	HEA	CMC-C2C-C1C	-2.06	125.30	128.46
18	N	515	HEA	CMB-C2B-C1B	-2.06	125.31	128.46
23	O	1230	PSC	O01-C1-C2	-2.04	107.31	111.55
19	P	1268	PGV	C01-O03-C19	-2.04	111.00	117.13
19	P	1267	PGV	C3-C2-C1	-2.03	106.16	113.58
24	P	1272	DMU	C2-C3-C4	-2.02	106.59	110.88
19	C	267	PGV	C8-C9-C10	-2.01	106.01	113.74
25	P	1264	PEK	C25-C24-C23	-2.00	104.15	114.45
26	C	270	CDL	C80-C79-C78	2.01	124.79	114.45
26	G	269	CDL	O1-C1-CB2	2.01	116.75	109.34
24	Z	1526	DMU	C10-O1-C9	2.01	117.50	113.72
19	P	1267	PGV	O01-C1-O02	2.01	128.70	123.68
26	C	270	CDL	C79-C78-C77	2.02	124.86	114.45
26	T	1269	CDL	C83-C82-C81	2.02	124.86	114.45
22	N	1522	TGL	CC3-CC2-CC1	2.04	121.03	113.58
18	N	515	HEA	C4B-C3B-C2B	2.04	108.29	106.87
25	T	263	PEK	P-O12-C04	2.04	132.29	121.60
24	P	1272	DMU	O55-C2-C3	2.04	114.52	109.87
18	N	515	HEA	C3C-C4C-NC	2.05	111.86	109.21
20	W	1060	CHD	C1-C10-C9	2.06	114.68	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	521	TGL	OG3-CG3-CG2	2.08	113.88	108.66
22	B	521	TGL	C33-C19-C18	2.08	125.19	114.45
19	C	267	PGV	O03-C19-O04	2.08	128.73	123.55
18	N	516	HEA	CMC-C2C-C3C	2.10	128.79	124.89
22	O	1521	TGL	C10-CB9-CB8	2.11	125.32	114.45
25	P	1265	PEK	O03-C01-C02	2.11	113.96	108.66
22	N	1523	TGL	OG2-CG2-CG1	2.11	116.12	108.44
26	G	269	CDL	C20-C19-C18	2.12	125.38	114.45
22	L	522	TGL	CC7-CC6-CC5	2.12	125.40	114.45
20	P	1525	CHD	O3-C3-C4	2.12	114.11	109.87
22	B	521	TGL	C10-CB9-CB8	2.14	125.46	114.45
24	C	272	DMU	O55-C2-C3	2.15	114.76	109.87
25	G	1263	PEK	P-O12-C04	2.15	132.87	121.60
20	B	1086	CHD	C18-C13-C14	2.16	114.64	111.23
20	N	1604	CHD	C9-C11-C12	2.18	117.20	114.32
20	P	1525	CHD	O3-C3-C2	2.19	115.41	110.10
22	B	521	TGL	OG1-CG1-CG2	2.19	114.17	108.66
26	T	1269	CDL	C19-C18-C17	2.20	125.77	114.45
19	C	268	PGV	O03-C01-C02	2.20	114.18	108.66
25	P	1265	PEK	C03-C02-C01	2.20	116.82	111.86
19	A	524	PGV	O01-C02-C03	2.21	116.45	108.44
18	A	515	HEA	C27-C19-C20	2.21	119.13	115.29
25	C	265	PEK	O03-C01-C02	2.22	114.23	108.66
26	T	1269	CDL	C20-C19-C18	2.23	125.95	114.45
26	G	269	CDL	C19-C18-C17	2.24	126.00	114.45
25	P	1264	PEK	C11-C10-C9	2.24	119.47	111.84
24	P	1272	DMU	O55-C2-C1	2.27	115.29	110.36
25	C	265	PEK	C2-C3-C4	2.31	117.42	113.29
18	A	516	HEA	C27-C19-C20	2.33	119.33	115.29
18	A	515	HEA	C4B-C3B-C2B	2.36	108.52	106.87
25	P	1265	PEK	P-O12-C04	2.40	134.15	121.60
22	L	522	TGL	C20-CA9-CA8	2.40	126.82	114.45
19	N	1524	PGV	O01-C02-C03	2.42	117.24	108.44
22	L	522	TGL	CC3-CC2-CC1	2.43	122.46	113.58
20	A	525	CHD	C2-C1-C10	2.45	117.06	112.80
25	P	1265	PEK	C2-C3-C4	2.45	117.66	113.29
25	C	265	PEK	P-O12-C04	2.45	134.41	121.60
24	Z	1526	DMU	O7-C10-C5	2.45	113.64	108.11
25	C	265	PEK	C03-C02-C01	2.47	117.42	111.86
20	C	271	CHD	C1-C10-C9	2.47	115.33	111.39
22	L	522	TGL	CG2-OG2-CB1	2.47	123.72	117.88
19	P	1267	PGV	O03-C19-O04	2.48	129.71	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	525	CHD	C1-C2-C3	2.48	113.58	110.42
22	N	1522	TGL	C20-CA9-CA8	2.48	127.25	114.45
20	C	271	CHD	C2-C1-C10	2.50	117.15	112.80
18	N	515	HEA	CMB-C2B-C3B	2.50	129.71	124.92
19	P	1268	PGV	O03-C01-C02	2.51	114.97	108.66
22	N	1523	TGL	CB3-CB2-CB1	2.52	122.77	113.58
22	N	1523	TGL	OG1-CG1-CG2	2.52	115.00	108.66
22	N	1522	TGL	CC4-CC3-CC2	2.52	122.49	113.24
25	C	265	PEK	C24-C23-C22	2.53	122.53	113.24
20	N	1604	CHD	C18-C13-C14	2.54	115.25	111.23
20	J	60	CHD	C6-C5-C4	2.55	114.02	111.13
20	B	1086	CHD	C4-C3-C2	2.55	113.72	110.55
25	C	264	PEK	O03-C21-O04	2.56	129.91	123.55
26	C	270	CDL	OA8-CA6-CA4	2.56	115.09	108.66
20	J	60	CHD	C17-C13-C12	2.57	120.03	117.67
18	N	515	HEA	C27-C19-C20	2.57	119.75	115.29
18	N	516	HEA	C26-C15-C16	2.58	119.76	115.29
18	N	516	HEA	C12-C11-C3B	2.58	118.95	112.65
24	M	526	DMU	O1-C10-C5	2.58	115.28	110.30
19	C	266	PGV	O03-C01-C02	2.59	115.17	108.66
25	P	1265	PEK	C24-C23-C22	2.63	122.86	113.24
19	C	267	PGV	O01-C1-O02	2.63	130.25	123.68
26	C	270	CDL	OB6-CB5-OB7	2.64	130.25	123.68
20	W	1271	CHD	C15-C16-C17	2.64	110.39	105.12
18	A	516	HEA	C12-C11-C3B	2.64	119.11	112.65
22	D	523	TGL	OG2-CG2-CG3	2.66	118.09	108.44
20	W	1060	CHD	O7-C7-C6	2.66	116.45	110.02
20	W	1271	CHD	C16-C15-C14	2.67	110.44	105.12
20	W	1060	CHD	C6-C5-C4	2.67	114.17	111.13
20	C	271	CHD	C16-C15-C14	2.68	110.47	105.12
20	B	1086	CHD	C9-C11-C12	2.68	117.86	114.32
20	W	1271	CHD	C1-C10-C9	2.68	115.67	111.39
26	G	269	CDL	C23-C22-C21	2.68	128.27	114.45
20	B	1086	CHD	C5-C4-C3	2.71	116.84	112.87
26	P	1270	CDL	OA8-CA6-CA4	2.71	115.47	108.66
20	N	1604	CHD	C6-C5-C10	2.71	115.62	112.66
22	N	1522	TGL	OG1-CG1-CG2	2.72	115.48	108.66
26	G	269	CDL	OB8-CB6-CB4	2.72	115.48	108.66
25	T	263	PEK	C8-C7-C6	2.73	121.12	111.84
20	N	1604	CHD	C4-C3-C2	2.74	113.95	110.55
20	W	1271	CHD	C11-C12-C13	2.74	114.06	111.22
18	N	515	HEA	C25-C23-C24	2.75	121.01	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	60	CHD	C9-C11-C12	2.77	117.98	114.32
24	Z	1526	DMU	C10-O7-C3	2.79	124.78	118.00
20	W	1060	CHD	C15-C16-C17	2.79	110.69	105.12
20	J	60	CHD	C16-C15-C14	2.81	110.74	105.12
24	C	272	DMU	C10-O7-C3	2.82	124.87	118.00
20	W	1271	CHD	C1-C2-C3	2.83	114.03	110.42
20	A	525	CHD	C17-C13-C12	2.84	120.28	117.67
22	L	522	TGL	CC4-CC3-CC2	2.85	123.67	113.24
26	T	1269	CDL	OB8-CB6-CB4	2.87	115.86	108.66
20	C	271	CHD	C15-C16-C17	2.87	110.85	105.12
20	P	1525	CHD	C17-C13-C12	2.88	120.32	117.67
20	J	60	CHD	C1-C10-C9	2.88	115.99	111.39
26	T	1269	CDL	C22-C21-C20	2.88	129.31	114.45
20	N	1604	CHD	C5-C6-C7	2.89	117.64	114.44
26	T	1269	CDL	C23-C22-C21	2.89	129.35	114.45
22	N	1523	TGL	OG2-CG2-CG3	2.90	118.97	108.44
18	N	516	HEA	C3C-C4C-NC	2.90	112.96	109.21
25	P	1264	PEK	O03-C21-O04	2.92	130.81	123.55
25	G	1263	PEK	C8-C7-C6	2.93	121.80	111.84
26	G	269	CDL	C22-C21-C20	2.93	129.56	114.45
20	B	1086	CHD	C5-C6-C7	2.93	117.68	114.44
20	J	60	CHD	C15-C16-C17	2.94	110.99	105.12
20	N	1604	CHD	C17-C13-C14	2.94	103.08	100.08
22	D	523	TGL	OG1-CG1-CG2	2.95	116.07	108.66
20	J	60	CHD	O7-C7-C6	2.96	117.18	110.02
22	N	1523	TGL	CG2-OG2-CB1	2.96	124.87	117.88
20	B	1086	CHD	C9-C8-C7	2.98	115.43	111.92
20	C	271	CHD	C5-C4-C3	2.99	117.27	112.87
22	D	523	TGL	CB3-CB2-CB1	3.02	124.61	113.58
20	C	271	CHD	C11-C12-C13	3.03	114.36	111.22
22	N	1523	TGL	CG3-OG3-CC1	3.04	126.26	117.13
26	P	1270	CDL	OB6-CB5-OB7	3.04	131.26	123.68
20	W	1060	CHD	C16-C15-C14	3.06	111.24	105.12
20	W	1060	CHD	C5-C4-C3	3.07	117.38	112.87
20	W	1271	CHD	C2-C1-C10	3.08	118.16	112.80
22	L	522	TGL	C13-C12-C11	3.09	130.40	114.45
20	W	1060	CHD	C9-C11-C12	3.10	118.41	114.32
24	Z	1526	DMU	O1-C10-C5	3.11	116.30	110.30
20	B	1086	CHD	C14-C13-C12	3.12	110.35	107.39
20	A	525	CHD	C4-C5-C10	3.15	116.10	112.66
22	L	522	TGL	OG1-CG1-CG2	3.16	116.58	108.66
24	C	272	DMU	O1-C10-C5	3.16	116.39	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	271	CHD	C5-C6-C7	3.17	117.94	114.44
20	W	1271	CHD	C6-C5-C10	3.19	116.14	112.66
20	A	525	CHD	C6-C5-C10	3.19	116.15	112.66
22	O	1521	TGL	CG3-OG3-CC1	3.20	126.77	117.13
18	A	515	HEA	CMC-C2C-C3C	3.21	130.84	124.89
20	P	1525	CHD	C5-C4-C3	3.21	117.58	112.87
20	C	271	CHD	C1-C2-C3	3.21	114.51	110.42
18	A	516	HEA	C26-C15-C16	3.23	120.89	115.29
22	B	521	TGL	CG3-OG3-CC1	3.24	126.87	117.13
20	P	1525	CHD	C4-C5-C10	3.26	116.22	112.66
20	A	525	CHD	C9-C8-C7	3.29	115.79	111.92
18	N	515	HEA	CMC-C2C-C3C	3.30	131.01	124.89
20	N	1604	CHD	C5-C4-C3	3.30	117.72	112.87
18	N	516	HEA	C27-C19-C20	3.30	121.02	115.29
18	A	515	HEA	C25-C23-C24	3.31	122.31	114.60
24	M	526	DMU	O7-C10-C5	3.31	115.58	108.11
22	D	523	TGL	CG2-OG2-CB1	3.32	125.72	117.88
22	D	523	TGL	CG3-OG3-CC1	3.33	127.14	117.13
20	A	525	CHD	C18-C13-C14	3.33	116.48	111.23
20	W	1271	CHD	C5-C6-C7	3.35	118.15	114.44
20	B	1086	CHD	C17-C13-C12	3.37	120.77	117.67
22	N	1522	TGL	C13-C12-C11	3.37	131.84	114.45
24	M	526	DMU	C10-O1-C9	3.38	120.08	113.72
20	W	1271	CHD	C9-C11-C12	3.44	118.85	114.32
20	P	1525	CHD	C1-C2-C3	3.44	114.80	110.42
24	M	526	DMU	C10-O7-C3	3.44	126.38	118.00
19	P	1266	PGV	O03-C01-C02	3.45	117.33	108.66
20	C	271	CHD	O12-C12-C13	3.49	116.94	111.12
22	O	1521	TGL	CG3-CG2-CG1	3.50	119.76	111.86
22	B	521	TGL	CG3-CG2-CG1	3.51	119.77	111.86
20	W	1060	CHD	C1-C2-C3	3.53	114.91	110.42
20	J	60	CHD	C5-C4-C3	3.54	118.06	112.87
20	W	1271	CHD	C5-C4-C3	3.54	118.06	112.87
20	P	1525	CHD	C18-C13-C14	3.54	116.82	111.23
20	J	60	CHD	C14-C8-C7	3.55	116.61	111.80
20	B	1086	CHD	C6-C5-C10	3.56	116.54	112.66
20	A	525	CHD	C5-C4-C3	3.56	118.09	112.87
24	P	1272	DMU	C10-O1-C9	3.60	120.49	113.72
20	N	1604	CHD	C1-C2-C3	3.60	115.00	110.42
20	B	1086	CHD	C1-C2-C3	3.61	115.02	110.42
24	M	526	DMU	O7-C10-O1	3.67	119.61	110.70
22	N	1522	TGL	C11-C10-CB9	3.68	133.41	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	1522	TGL	C16-C15-CC9	3.68	133.44	114.45
24	M	526	DMU	C18-O16-C6	3.71	120.24	113.87
22	L	522	TGL	C16-C15-CC9	3.74	133.75	114.45
25	G	1263	PEK	C02-O01-C1	3.75	126.74	117.88
22	L	522	TGL	C15-CC9-CC8	3.78	133.93	114.45
20	P	1525	CHD	C6-C5-C10	3.79	116.80	112.66
20	B	1086	CHD	C10-C9-C8	3.82	115.99	111.87
20	A	525	CHD	C1-C10-C5	3.83	113.72	107.79
22	N	1522	TGL	C15-CC9-CC8	3.85	134.31	114.45
20	P	1525	CHD	C4-C3-C2	3.87	115.36	110.55
24	P	1272	DMU	O7-C10-O1	3.87	120.10	110.70
20	W	1271	CHD	O12-C12-C13	3.89	117.61	111.12
20	J	60	CHD	C1-C10-C5	3.90	113.83	107.79
20	J	60	CHD	C1-C2-C3	3.91	115.40	110.42
24	Z	1526	DMU	C18-O16-C6	3.98	120.69	113.87
20	W	1060	CHD	C14-C8-C7	3.98	117.20	111.80
22	L	522	TGL	C11-C10-CB9	4.00	135.06	114.45
20	P	1525	CHD	C9-C8-C7	4.03	116.66	111.92
20	C	271	CHD	C9-C11-C12	4.04	119.65	114.32
20	C	271	CHD	C6-C5-C10	4.08	117.12	112.66
24	C	272	DMU	O7-C10-O1	4.28	121.08	110.70
20	W	1060	CHD	C1-C10-C5	4.28	114.42	107.79
25	T	263	PEK	C02-O01-C1	4.28	127.99	117.88
20	W	1271	CHD	C4-C5-C10	4.30	117.36	112.66
24	M	526	DMU	O16-C6-C1	4.33	115.30	108.23
24	P	1272	DMU	O1-C10-C5	4.33	118.66	110.30
20	N	1604	CHD	C17-C13-C12	4.35	121.67	117.67
20	P	1525	CHD	C1-C10-C5	4.36	114.55	107.79
20	W	1060	CHD	C2-C1-C10	4.39	120.45	112.80
20	J	60	CHD	C2-C1-C10	4.43	120.52	112.80
20	N	1604	CHD	C1-C10-C5	4.43	114.66	107.79
24	M	526	DMU	O7-C3-C4	4.49	120.39	109.34
20	P	1525	CHD	C13-C17-C20	4.52	124.97	119.49
20	W	1060	CHD	C13-C14-C8	4.52	120.59	114.77
20	C	271	CHD	C4-C5-C10	4.57	117.65	112.66
24	Z	1526	DMU	O7-C10-O1	4.59	121.85	110.70
24	Z	1526	DMU	O16-C6-C1	4.65	115.81	108.23
18	N	515	HEA	C26-C15-C16	4.68	123.41	115.29
20	W	1060	CHD	C9-C8-C7	4.68	117.42	111.92
24	C	272	DMU	C10-O1-C9	4.68	122.54	113.72
20	W	1271	CHD	C1-C10-C5	4.73	115.12	107.79
20	J	60	CHD	C13-C14-C8	4.77	120.92	114.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1086	CHD	C1-C10-C5	4.81	115.24	107.79
18	A	515	HEA	C26-C15-C16	4.81	123.64	115.29
20	J	60	CHD	C9-C8-C7	4.86	117.64	111.92
24	C	272	DMU	O1-C9-C8	4.89	118.66	109.66
24	Z	1526	DMU	O7-C3-C4	4.91	121.41	109.34
20	A	525	CHD	C4-C3-C2	4.92	116.66	110.55
20	A	525	CHD	C13-C17-C20	4.94	125.49	119.49
25	P	1265	PEK	C11-C10-C9	5.00	128.83	111.84
25	C	265	PEK	C11-C10-C9	5.05	129.03	111.84
24	M	526	DMU	O5-C6-O16	5.08	122.08	110.02
20	A	525	CHD	C5-C6-C7	5.14	120.12	114.44
24	Z	1526	DMU	O7-C3-C2	5.14	119.57	107.19
24	Z	1526	DMU	O5-C6-O16	5.18	122.33	110.02
20	P	1525	CHD	C5-C6-C7	5.21	120.21	114.44
24	M	526	DMU	O7-C3-C2	5.22	119.76	107.19
20	N	1604	CHD	C10-C9-C8	5.26	117.55	111.87
20	J	60	CHD	C14-C8-C9	5.29	116.83	109.64
24	P	1272	DMU	O7-C10-C5	5.32	120.09	108.11
25	G	1263	PEK	O03-C01-C02	5.35	122.09	108.66
20	C	271	CHD	C1-C10-C5	5.42	116.19	107.79
24	P	1272	DMU	C8-C7-C5	5.43	120.41	110.84
25	T	263	PEK	O03-C01-C02	5.43	122.31	108.66
24	P	1272	DMU	O5-C4-C57	5.56	119.74	106.41
24	C	272	DMU	C8-C7-C5	5.58	120.67	110.84
22	O	1521	TGL	CG2-OG2-CB1	5.60	131.10	117.88
24	C	272	DMU	O5-C4-C57	5.65	119.96	106.41
24	P	1272	DMU	C18-O16-C6	5.66	123.58	113.87
20	W	1060	CHD	C14-C8-C9	5.69	117.38	109.64
24	C	272	DMU	O5-C6-C1	5.70	121.28	110.30
20	W	1271	CHD	C4-C3-C2	5.73	117.66	110.55
20	C	271	CHD	C4-C3-C2	5.74	117.67	110.55
24	C	272	DMU	C18-O16-C6	5.78	123.78	113.87
24	P	1272	DMU	O7-C3-C2	5.79	121.13	107.19
22	B	521	TGL	CG2-OG2-CB1	5.82	131.63	117.88
24	Z	1526	DMU	O5-C6-C1	5.85	121.58	110.30
24	C	272	DMU	O7-C10-C5	5.93	121.47	108.11
20	J	60	CHD	C11-C9-C10	5.94	120.03	113.74
24	P	1272	DMU	O1-C9-C8	5.98	120.68	109.66
20	J	60	CHD	C4-C3-C2	6.11	118.14	110.55
20	W	1271	CHD	C9-C8-C7	6.15	119.15	111.92
20	C	271	CHD	C9-C8-C7	6.16	119.16	111.92
24	C	272	DMU	O7-C3-C2	6.19	122.08	107.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	C6-O5-C4	6.20	125.39	113.72
24	Z	1526	DMU	O1-C9-C8	6.24	121.16	109.66
24	M	526	DMU	O5-C6-C1	6.27	122.39	110.30
24	M	526	DMU	O1-C9-C8	6.32	121.30	109.66
24	P	1272	DMU	O5-C6-C1	6.37	122.59	110.30
20	W	1060	CHD	C11-C12-C13	6.40	117.85	111.22
20	A	525	CHD	C10-C9-C8	6.50	118.87	111.87
20	P	1525	CHD	C10-C9-C8	6.51	118.88	111.87
20	W	1060	CHD	C5-C6-C7	6.54	121.68	114.44
20	C	271	CHD	C14-C13-C12	6.57	113.63	107.39
20	W	1271	CHD	C14-C13-C12	6.66	113.71	107.39
20	W	1060	CHD	C11-C9-C10	6.67	120.81	113.74
20	W	1060	CHD	C4-C3-C2	6.91	119.14	110.55
24	Z	1526	DMU	O5-C4-C57	7.04	123.28	106.41
20	J	60	CHD	C5-C6-C7	7.06	122.25	114.44
20	J	60	CHD	C11-C12-C13	7.07	118.54	111.22
20	J	60	CHD	C13-C17-C20	7.09	128.09	119.49
24	M	526	DMU	O5-C4-C3	7.17	124.43	109.75
24	Z	1526	DMU	C6-O5-C4	7.18	127.24	113.72
24	M	526	DMU	O5-C4-C57	7.20	123.65	106.41
20	J	60	CHD	C17-C13-C14	7.21	107.42	100.08
20	J	60	CHD	C6-C5-C10	7.25	120.57	112.66
20	W	1060	CHD	C17-C13-C14	7.25	107.47	100.08
20	W	1060	CHD	C13-C17-C20	7.37	128.43	119.49
24	M	526	DMU	C6-O5-C4	7.40	127.65	113.72
24	M	526	DMU	C7-C8-C9	7.42	123.30	110.22
24	Z	1526	DMU	O5-C4-C3	7.47	125.03	109.75
24	C	272	DMU	O5-C4-C3	7.52	125.13	109.75
20	W	1060	CHD	C6-C5-C10	7.57	120.93	112.66
20	J	60	CHD	O12-C12-C13	7.73	124.01	111.12
24	C	272	DMU	O7-C3-C4	7.78	128.48	109.34
24	C	272	DMU	C6-O5-C4	7.86	128.52	113.72
20	W	1271	CHD	C17-C13-C14	7.94	108.17	100.08
24	Z	1526	DMU	C7-C8-C9	8.03	124.37	110.22
24	P	1272	DMU	O5-C4-C3	8.16	126.44	109.75
24	Z	1526	DMU	C10-C5-C7	8.17	125.16	109.98
24	Z	1526	DMU	O1-C9-C11	8.17	125.98	106.41
20	W	1060	CHD	O12-C12-C13	8.22	124.83	111.12
24	M	526	DMU	O1-C9-C11	8.26	126.19	106.41
24	P	1272	DMU	O7-C3-C4	8.29	129.74	109.34
24	P	1272	DMU	O1-C9-C11	8.33	126.37	106.41
20	C	271	CHD	C17-C13-C14	8.46	108.70	100.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	C10-C5-C7	8.48	125.75	109.98
24	P	1272	DMU	C1-C2-C3	8.78	127.81	109.61
20	W	1271	CHD	C10-C9-C8	9.04	121.62	111.87
24	C	272	DMU	O1-C9-C11	9.05	128.09	106.41
20	J	60	CHD	C10-C9-C8	9.05	121.63	111.87
20	W	1060	CHD	C10-C9-C8	9.24	121.82	111.87
20	C	271	CHD	C10-C9-C8	9.59	122.21	111.87
24	C	272	DMU	C1-C2-C3	9.80	129.92	109.61
24	C	272	DMU	O16-C6-C1	10.30	125.04	108.23
24	Z	1526	DMU	C1-C2-C3	10.78	131.95	109.61
24	M	526	DMU	C1-C2-C3	10.89	132.19	109.61
24	P	1272	DMU	O16-C6-C1	11.39	126.82	108.23

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	J	60	CHD	C12
20	J	60	CHD	C8
20	J	60	CHD	C9
20	J	60	CHD	C14
20	J	60	CHD	C17
20	W	1060	CHD	C12
20	W	1060	CHD	C8
20	W	1060	CHD	C9
20	W	1060	CHD	C14
20	W	1060	CHD	C17
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	P	1272	DMU	C10
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
24	Z	1526	DMU	C4
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6
24	Z	1526	DMU	C2

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Mol	Chain	Res	Type	Atom
24	Z	1526	DMU	C9
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
24	M	526	DMU	C4
24	M	526	DMU	C5
24	M	526	DMU	C6
24	M	526	DMU	C2
24	M	526	DMU	C9
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C10
20	C	271	CHD	C12
20	C	271	CHD	C8
20	C	271	CHD	C3
20	C	271	CHD	C9
20	C	271	CHD	C14
20	W	1271	CHD	C12
20	W	1271	CHD	C8
20	W	1271	CHD	C3
20	W	1271	CHD	C9
20	W	1271	CHD	C14

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	P-O11-C03-C02
19	N	1524	PGV	P-O11-C03-C02

There are no ring outliers.

41 monomers are involved in 312 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	4	0
18	A	516	HEA	5	0
19	A	524	PGV	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	525	CHD	1	0
20	B	1086	CHD	1	0
23	B	230	PSC	19	0
22	B	521	TGL	6	0
25	C	264	PEK	6	0
25	C	265	PEK	11	0
19	C	266	PGV	3	0
19	C	267	PGV	7	0
19	C	268	PGV	2	0
26	C	270	CDL	19	0
20	C	271	CHD	2	0
24	C	272	DMU	3	0
22	D	523	TGL	5	0
25	G	1263	PEK	9	0
26	G	269	CDL	22	0
20	J	60	CHD	5	0
22	L	522	TGL	27	0
24	M	526	DMU	1	0
22	N	1522	TGL	15	0
22	N	1523	TGL	7	0
19	N	1524	PGV	10	0
20	N	1604	CHD	2	0
18	N	515	HEA	4	0
18	N	516	HEA	8	0
23	O	1230	PSC	18	0
22	O	1521	TGL	8	0
25	P	1264	PEK	9	0
25	P	1265	PEK	9	0
19	P	1266	PGV	2	0
19	P	1267	PGV	8	0
19	P	1268	PGV	1	0
26	P	1270	CDL	13	0
24	P	1272	DMU	4	0
20	P	1525	CHD	2	0
26	T	1269	CDL	23	0
25	T	263	PEK	14	0
20	W	1060	CHD	3	0
20	W	1271	CHD	2	0

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.