



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:54 AM GMT

PDB ID : 2EIN
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized 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 : 2.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

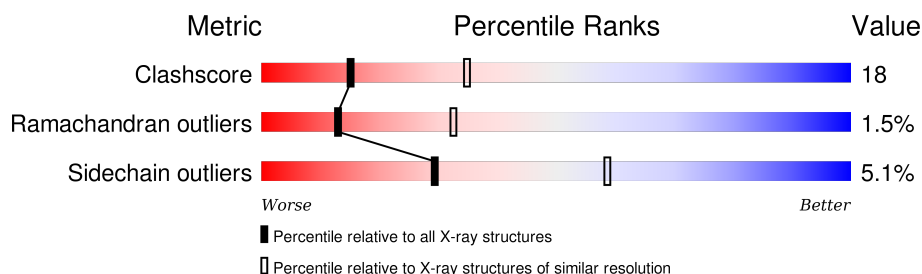
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)









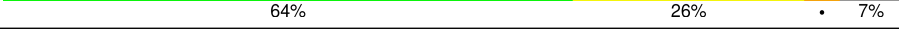


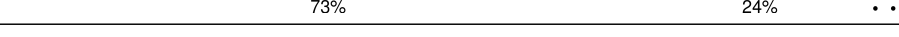

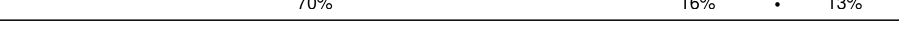


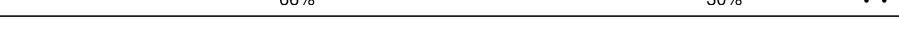

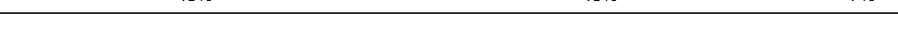
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	 68% 31% .
1	N	514	 66% 33% .
2	B	227	 56% 39% .
2	O	227	 51% 45% .
3	C	261	 70% 28% ..
3	P	261	 67% 32% .
4	D	147	 69% 27% ..

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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
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	PSC	B	230	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	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 31815 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	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- 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		

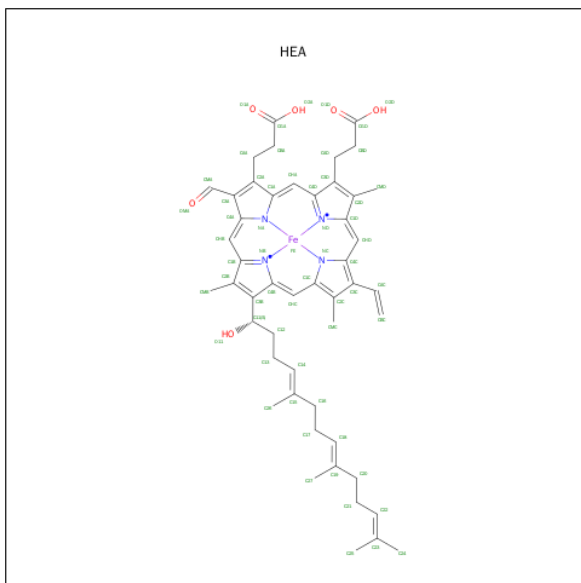
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

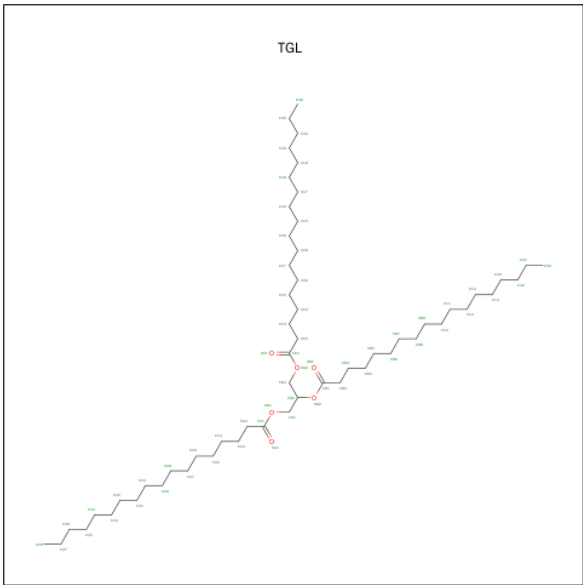
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



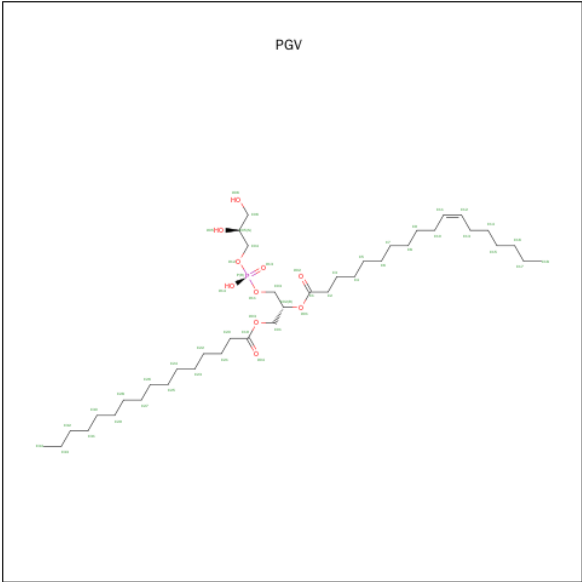
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	O	1	Total	C	O	0	0
			63	57	6		
18	Y	1	Total	C	O	0	0
			63	57	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: C₄₀H₇₇O₁₀P).



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

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

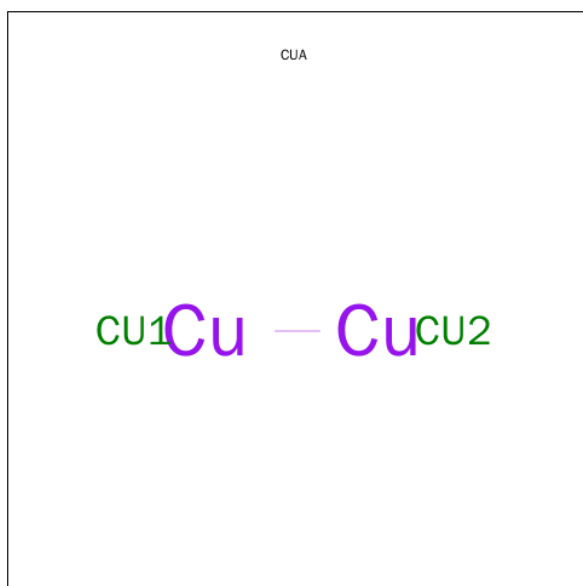
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	P	2	Total	Zn	0	0
			2	2		
20	G	1	Total	Zn	0	0
			1	1		
20	D	1	Total	Zn	0	0
			1	1		
20	B	1	Total	Zn	0	0
			1	1		

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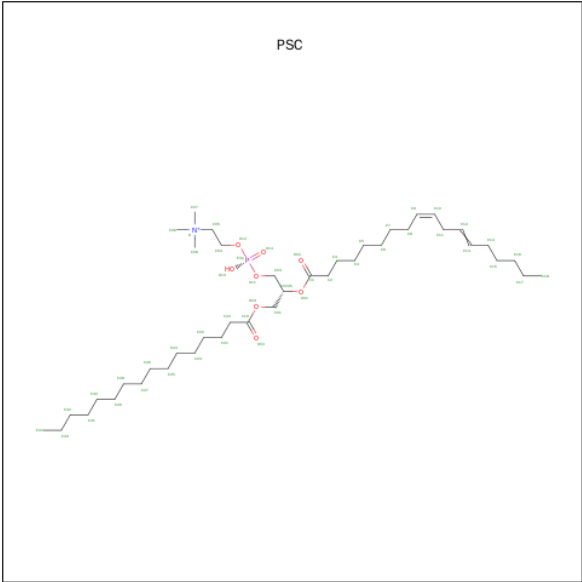
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	1	Total 1	Zn 1	0	0
20	T	1	Total 1	Zn 1	0	0
20	N	2	Total 2	Zn 2	0	0
20	O	1	Total 1	Zn 1	0	0
20	L	1	Total 1	Zn 1	0	0
20	S	1	Total 1	Zn 1	0	0
20	F	2	Total 2	Zn 2	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



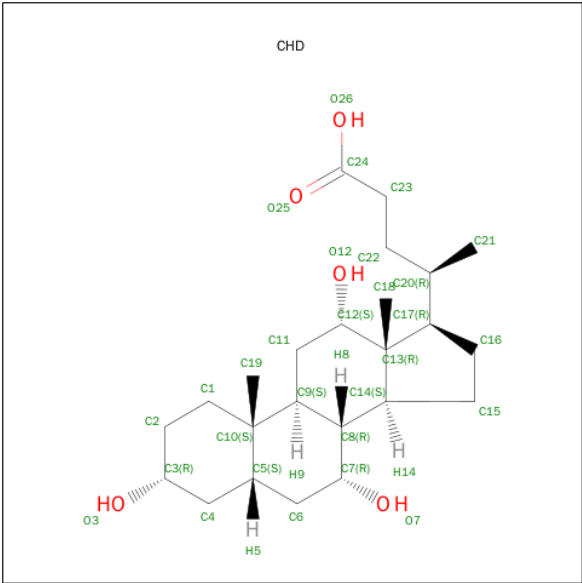
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total 2	Cu 2	0	0
21	O	1	Total 2	Cu 2	0	0

- Molecule 22 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: C₄₂H₈₁NO₈P).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



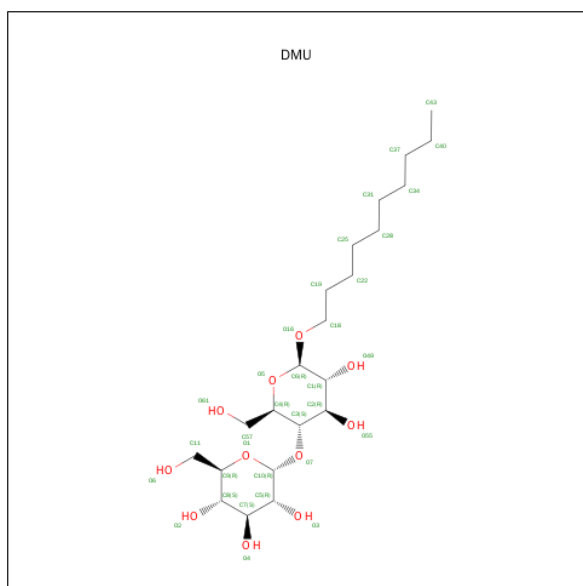
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0
			29	24	5		

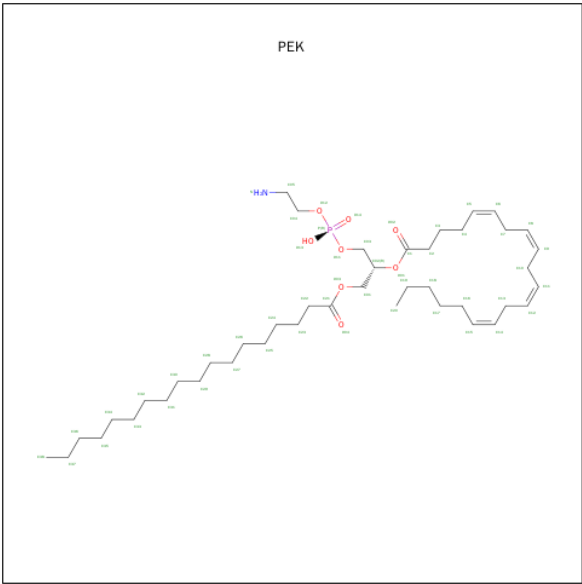
- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

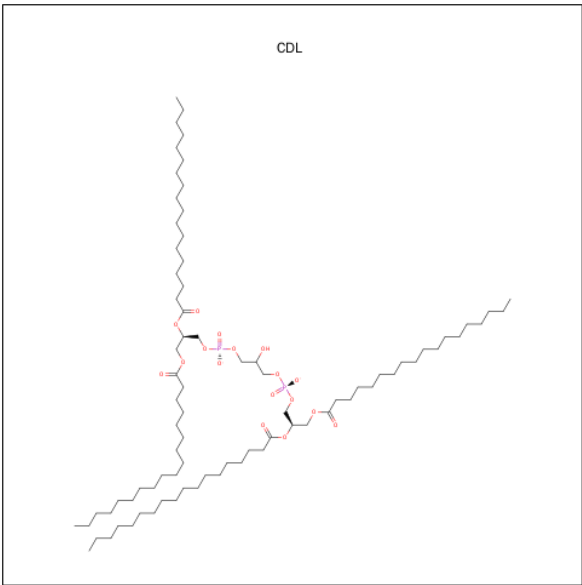
- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

EAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE
(three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



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	T	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: C₈₁H₁₅₆O₁₇P₂).



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	160	Total	O	0	0
			160	160		
27	B	86	Total	O	0	0
			86	86		
27	C	73	Total	O	0	0
			73	73		
27	D	38	Total	O	0	0
			38	38		
27	E	23	Total	O	0	0
			23	23		
27	F	37	Total	O	0	0
			37	37		
27	G	29	Total	O	0	0
			29	29		
27	H	31	Total	O	0	0
			31	31		

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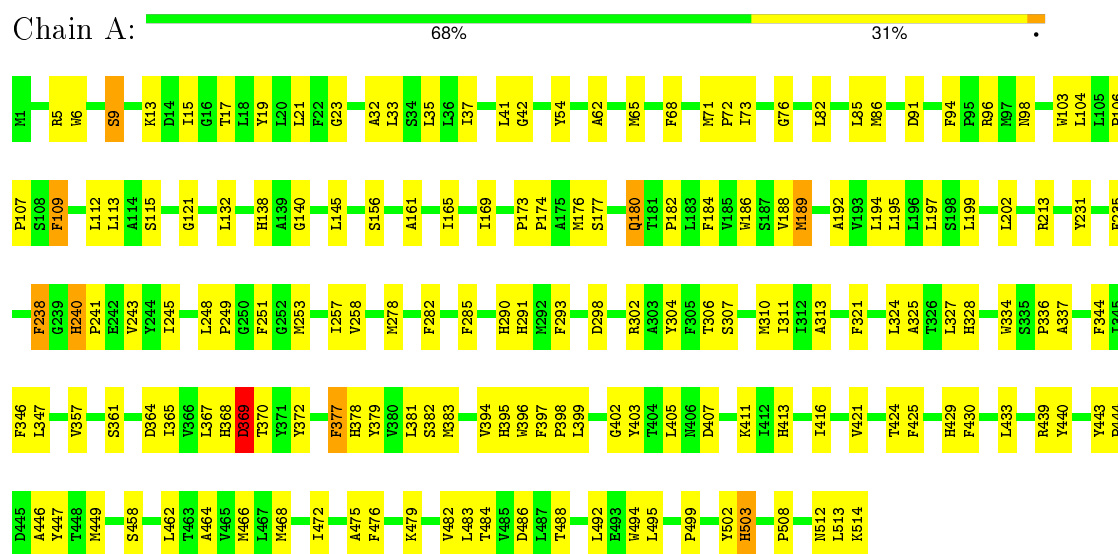
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	18	Total 18	O 18	0	0
27	J	9	Total 9	O 9	0	0
27	K	20	Total 20	O 20	0	0
27	L	12	Total 12	O 12	0	0
27	M	11	Total 11	O 11	0	0
27	N	161	Total 161	O 161	0	0
27	O	77	Total 77	O 77	0	0
27	P	72	Total 72	O 72	0	0
27	Q	42	Total 42	O 42	0	0
27	R	22	Total 22	O 22	0	0
27	S	39	Total 39	O 39	0	0
27	T	26	Total 26	O 26	0	0
27	U	28	Total 28	O 28	0	0
27	V	17	Total 17	O 17	0	0
27	W	13	Total 13	O 13	0	0
27	X	13	Total 13	O 13	0	0
27	Y	11	Total 11	O 11	0	0
27	Z	5	Total 5	O 5	0	0

3 Residue-property plots

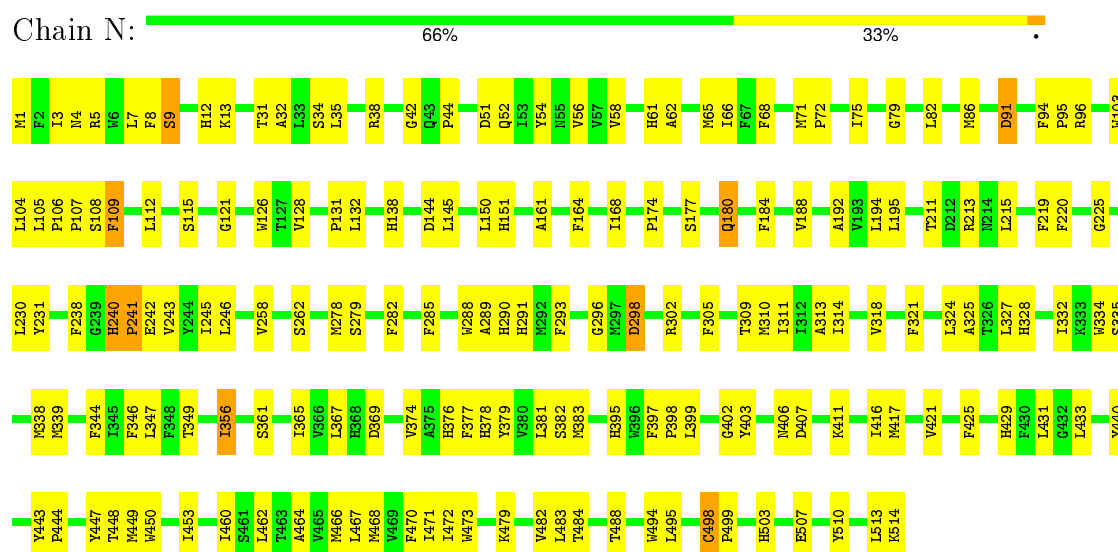
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

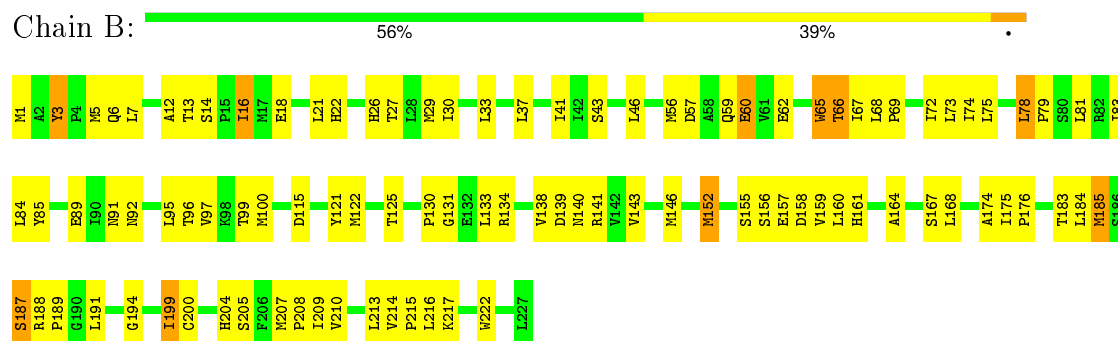
• Molecule 1: Cytochrome c oxidase subunit 1



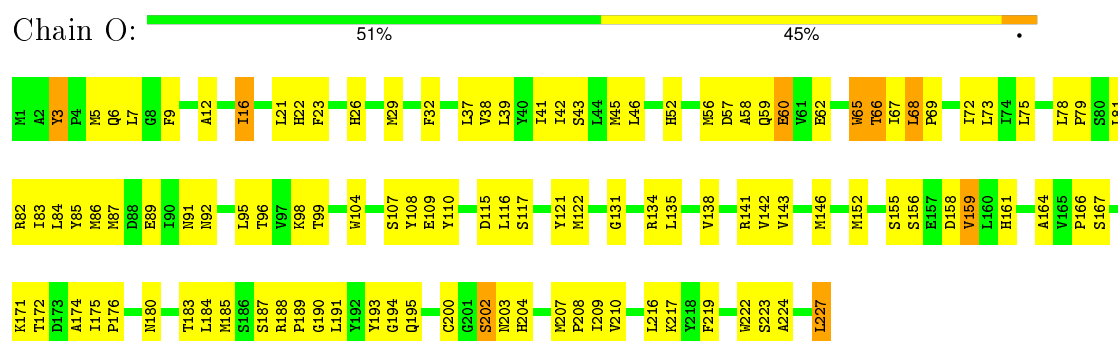
• Molecule 1: Cytochrome c oxidase subunit 1



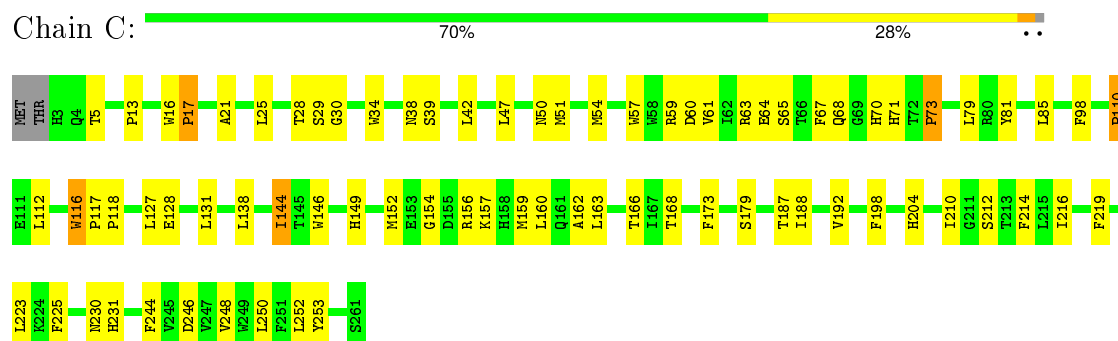
- Molecule 2: Cytochrome c oxidase subunit 2



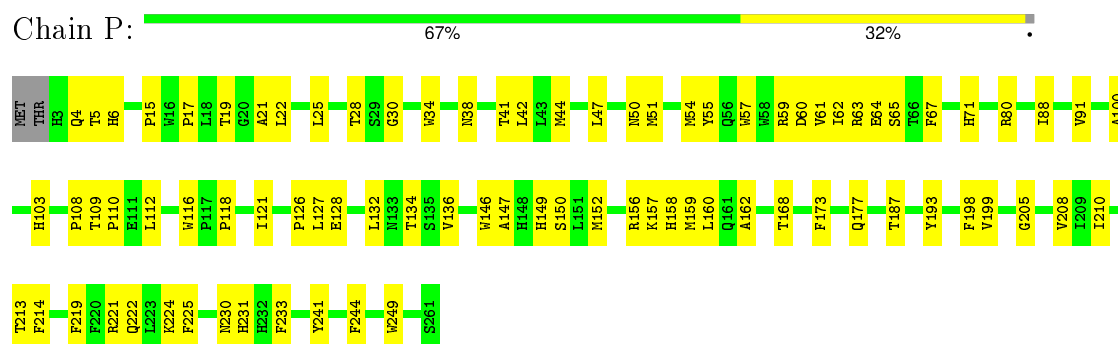
- Molecule 2: Cytochrome c oxidase subunit 2



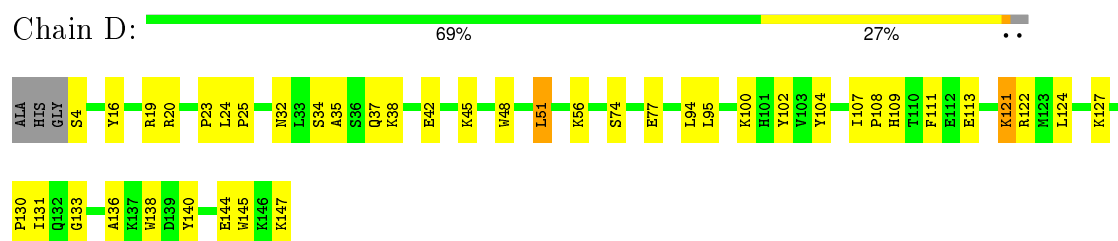
- Molecule 3: Cytochrome c oxidase subunit 3



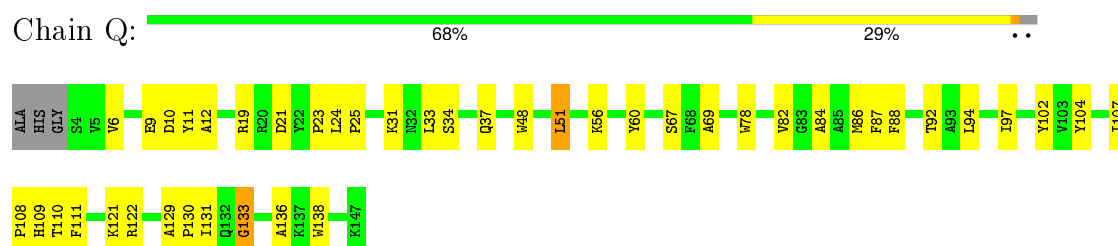
- Molecule 3: Cytochrome c oxidase subunit 3



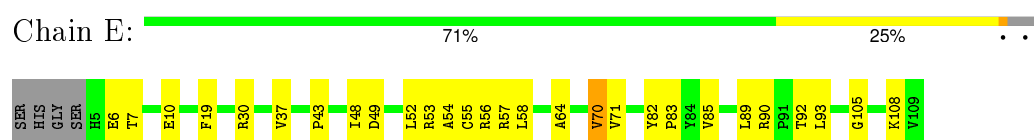
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



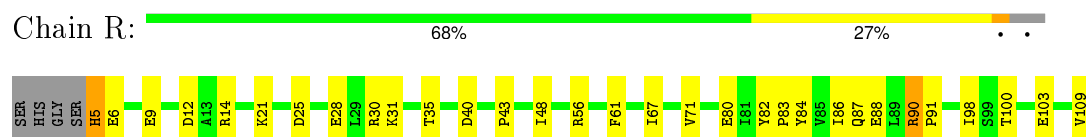
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



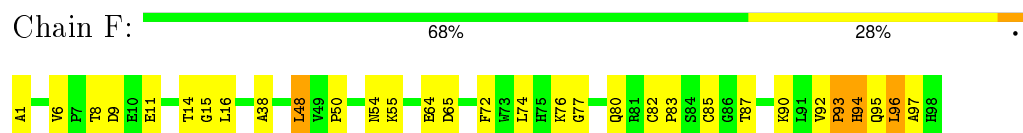
- Molecule 5: Cytochrome c oxidase polypeptide Va



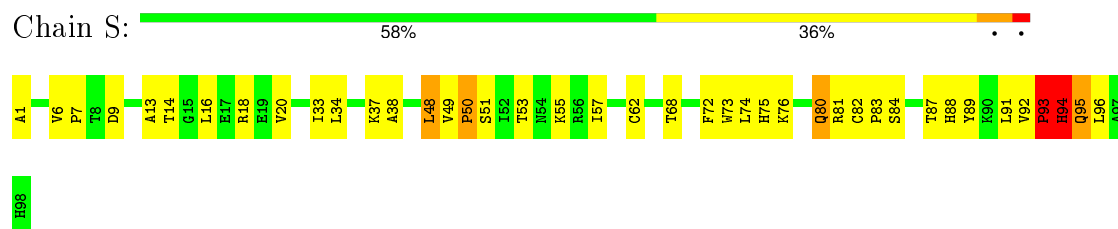
- Molecule 5: Cytochrome c oxidase polypeptide Va



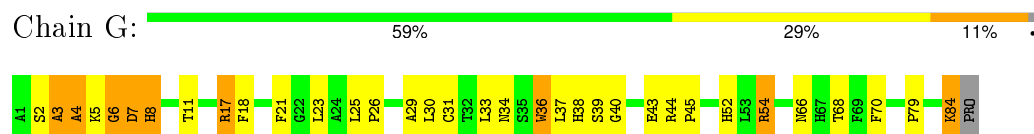
- Molecule 6: Cytochrome c oxidase polypeptide Vb



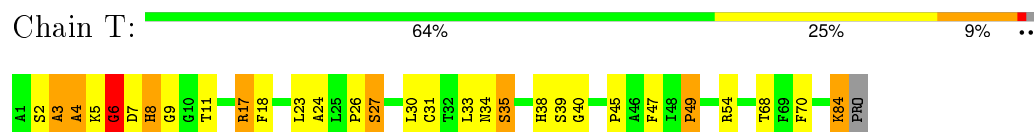
- Molecule 6: Cytochrome c oxidase polypeptide Vb



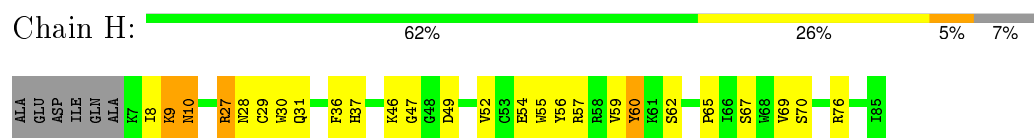
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



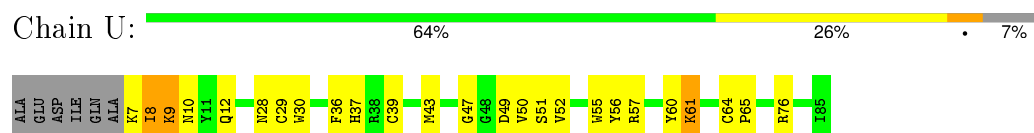
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



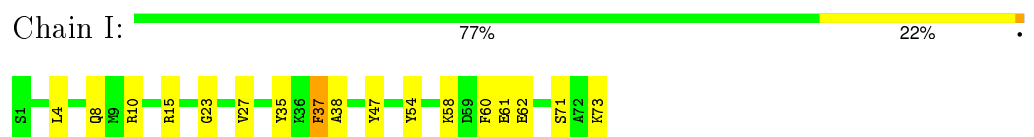
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



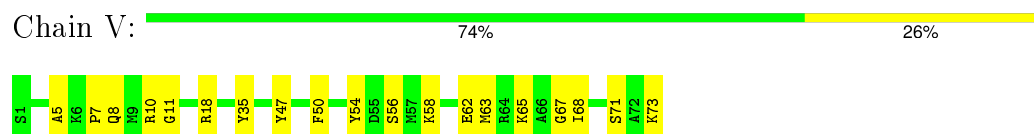
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



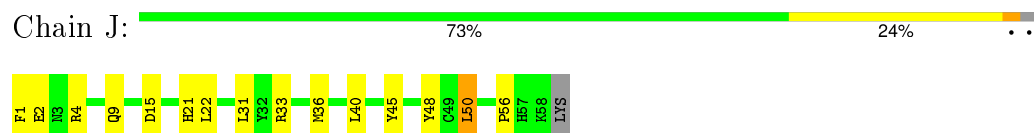
- Molecule 9: Cytochrome c oxidase polypeptide VIc



- 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

Chain K: 70% 16% 13%



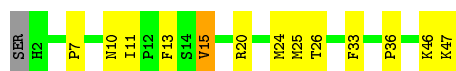
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X: 66% 20% 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L: 70% 26% 4%



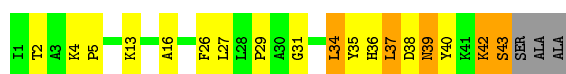
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y: 66% 30% 4%



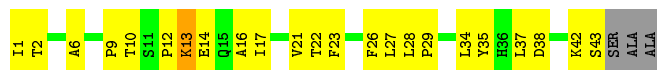
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M: 54% 28% 11% 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z: 43% 48% 7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 203.58Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.208 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31815	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.69	0/4156	0.79	0/5678
1	N	0.58	0/4156	0.73	0/5678
2	B	0.68	0/1860	0.87	0/2534
2	O	0.66	0/1860	0.84	1/2534 (0.0%)
3	C	0.69	1/2197 (0.0%)	0.69	0/3005
3	P	0.62	0/2197	0.69	0/3005
4	D	0.63	0/1229	0.74	1/1658 (0.1%)
4	Q	0.66	0/1229	0.71	1/1658 (0.1%)
5	E	0.62	0/871	0.71	0/1182
5	R	0.52	0/871	0.68	0/1182
6	F	0.70	0/765	0.94	3/1038 (0.3%)
6	S	0.67	0/765	0.89	3/1038 (0.3%)
7	G	0.67	1/690 (0.1%)	0.80	1/937 (0.1%)
7	T	0.71	0/690	0.78	1/937 (0.1%)
8	H	0.65	0/682	0.72	0/921
8	U	0.62	0/682	0.74	0/921
9	I	0.69	0/605	0.69	0/802
9	V	0.63	0/605	0.64	0/802
10	J	0.60	0/471	0.71	0/636
10	W	0.62	0/471	0.74	0/636
11	K	0.63	0/398	0.75	0/546
11	X	0.61	0/398	0.76	0/546
12	L	0.80	0/393	0.72	0/526
12	Y	0.64	0/393	0.68	0/526
13	M	0.64	0/345	0.76	0/470
13	Z	0.60	0/345	0.76	0/470
All	All	0.65	2/29324 (0.0%)	0.76	11/39866 (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	1
2	B	0	1
2	O	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	116	TRP	CB-CG	5.36	1.59	1.50
7	G	36	TRP	CB-CG	5.02	1.59	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.42	128.32	111.00
6	S	9	ASP	CB-CG-OD2	6.35	124.02	118.30
6	F	94	HIS	N-CA-C	6.19	127.72	111.00
6	F	9	ASP	CB-CG-OD2	6.15	123.84	118.30
7	G	6	GLY	N-CA-C	5.79	127.59	113.10
2	O	227	LEU	CA-CB-CG	5.63	128.25	115.30
4	D	133	GLY	N-CA-C	5.46	126.74	113.10
4	Q	133	GLY	N-CA-C	5.38	126.55	113.10
6	F	93	PRO	N-CA-C	5.25	125.75	112.10
6	S	93	PRO	N-CA-C	5.22	125.67	112.10
7	T	6	GLY	N-CA-C	5.12	125.90	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	372	TYR	Sidechain
1	A	502	TYR	Sidechain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
2	O	85	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	162	0
1	N	4027	0	4001	165	0
2	B	1824	0	1833	91	0
2	O	1824	0	1833	101	0
3	C	2110	0	2027	79	0
3	P	2110	0	2027	83	0
4	D	1195	0	1183	38	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	16	0
5	R	852	0	845	22	0
6	F	748	0	728	18	0
6	S	748	0	728	26	0
7	G	675	0	643	38	0
7	T	675	0	643	46	0
8	H	662	0	623	18	0
8	U	662	0	623	15	0
9	I	601	0	613	15	0
9	V	601	0	613	20	0
10	J	460	0	459	11	0
10	W	460	0	459	11	0
11	K	384	0	366	11	0
11	X	384	0	366	13	0
12	L	380	0	380	17	0
12	Y	380	0	380	17	0
13	M	335	0	352	17	0
13	Z	335	0	352	12	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	120	0	108	15	0
17	N	120	0	108	18	0
18	A	126	0	220	11	0
18	L	63	0	110	20	0
18	N	63	0	110	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	63	0	110	8	0
18	Y	63	0	110	16	0
19	A	102	0	152	9	0
19	C	102	0	152	7	0
19	N	102	0	152	9	0
19	P	102	0	152	11	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	2	0	0	0	0
20	G	1	0	0	0	0
20	L	1	0	0	0	0
20	N	2	0	0	0	0
20	O	1	0	0	0	0
20	P	2	0	0	0	0
20	S	1	0	0	0	0
20	T	1	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	21	0
22	O	52	0	80	20	0
23	B	29	0	39	5	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	6	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	38	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	20	0
25	G	53	0	77	10	0
25	P	53	0	77	10	0
25	T	106	0	154	23	0
26	C	100	0	156	17	0
26	G	100	0	156	23	0
26	P	100	0	156	17	0
26	T	100	0	156	32	0
27	A	160	0	0	8	0
27	B	86	0	0	3	0
27	C	73	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D	38	0	0	3	0
27	E	23	0	0	2	0
27	F	37	0	0	1	0
27	G	29	0	0	5	0
27	H	31	0	0	2	0
27	I	18	0	0	1	0
27	J	9	0	0	0	0
27	K	20	0	0	0	0
27	L	12	0	0	0	0
27	M	11	0	0	1	0
27	N	161	0	0	9	0
27	O	77	0	0	5	0
27	P	72	0	0	7	0
27	Q	42	0	0	2	0
27	R	22	0	0	1	0
27	S	39	0	0	1	0
27	T	26	0	0	3	0
27	U	28	0	0	1	0
27	V	17	0	0	3	0
27	W	13	0	0	1	0
27	X	13	0	0	1	0
27	Y	11	0	0	2	0
27	Z	5	0	0	1	0
All	All	31815	0	31298	1087	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 18.

All (1087) 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)
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.12	1.11
25:C:264:PEK:H161	25:C:264:PEK:H102	1.38	1.04
7:T:31:CYS:SG	26:T:1269:CDL:H532	1.98	1.04
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.08	1.01
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.45	0.99
26:G:269:CDL:H541	26:G:269:CDL:H231	1.46	0.97
22:B:230:PSC:H142	22:B:230:PSC:H343	1.43	0.97
25:T:1264:PEK:H161	25:T:1264:PEK:H102	1.48	0.96
26:T:1269:CDL:H231	26:T:1269:CDL:H541	1.47	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:1521:TGL:H102	18:O:1521:TGL:H281	1.50	0.94
1:A:503:HIS:CD2	1:A:503:HIS:H	1.82	0.92
12:L:20:ARG:HH12	18:L:522:TGL:HC61	1.34	0.91
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.52	0.90
26:C:270:CDL:H642	26:C:270:CDL:H191	1.54	0.89
12:Y:13:PHE:HA	18:Y:1522:TGL:HC31	1.54	0.89
18:A:521:TGL:H102	18:A:521:TGL:H281	1.51	0.89
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.53	0.89
18:L:522:TGL:HC62	18:L:522:TGL:HC22	1.56	0.87
1:A:278:MET:SD	7:T:5:LYS:HB3	2.15	0.87
26:G:269:CDL:H522	26:G:269:CDL:H202	1.57	0.86
3:C:187:THR:HB	7:G:68:THR:HG21	1.59	0.85
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.59	0.84
18:O:1521:TGL:H102	18:O:1521:TGL:C28	2.06	0.84
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.57	0.84
18:A:521:TGL:H102	18:A:521:TGL:C28	2.07	0.84
18:Y:1522:TGL:HC22	18:Y:1522:TGL:HC62	1.60	0.83
7:G:5:LYS:HB3	1:N:278:MET:SD	2.20	0.82
7:T:84:LYS:HD2	7:T:84:LYS:H	1.42	0.82
1:A:42:GLY:HA3	4:D:104:TYR:OH	1.78	0.82
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.15	0.82
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.44	0.82
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.60	0.82
1:N:488:THR:HB	1:N:495:LEU:HD13	1.62	0.81
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.60	0.80
1:N:42:GLY:HA3	4:Q:104:TYR:OH	1.82	0.79
2:O:57:ASP:H	22:O:1230:PSC:H201	1.45	0.79
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.64	0.78
3:C:54:MET:HE3	26:C:270:CDL:H612	1.64	0.78
18:A:523:TGL:HG11	18:A:523:TGL:HC21	1.66	0.78
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.66	0.77
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.67	0.77
26:G:269:CDL:H541	26:G:269:CDL:C23	2.15	0.77
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.66	0.77
1:A:472:ILE:HD13	18:L:522:TGL:HA91	1.65	0.77
1:N:177:SER:H	1:N:180:GLN:HE21	1.34	0.76
1:A:381:LEU:HB3	17:A:515:HEA:HBC1	1.66	0.76
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.15	0.76
1:N:472:ILE:HG21	18:Y:1522:TGL:CA9	2.16	0.75
7:T:34:ASN:HD22	26:T:1269:CDL:H151	1.52	0.75
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:1523:TGL:HG11	18:N:1523:TGL:HC21	1.68	0.75
1:N:82:LEU:O	1:N:86:MET:HG3	1.86	0.75
3:C:63:ARG:NE	26:C:270:CDL:HA22	1.97	0.74
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.67	0.74
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.52	0.74
3:P:187:THR:HB	7:T:68:THR:HG21	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.68	0.73
1:N:472:ILE:HG21	18:Y:1522:TGL:HA92	1.67	0.73
6:F:54:ASN:OD1	6:F:76:LYS:HD2	1.89	0.73
2:O:65:TRP:CZ3	22:O:1230:PSC:H331	2.23	0.73
7:T:27:SER:OG	26:T:1269:CDL:H792	1.89	0.73
18:A:521:TGL:H201	18:A:521:TGL:H241	1.71	0.72
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.52	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.37	0.72
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.54	0.72
7:G:45:PRO:HD2	27:G:2152:HOH:O	1.90	0.72
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.24	0.72
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.72	0.71
17:N:516:HEA:H241	2:O:72:ILE:CG2	2.21	0.71
3:P:62:ILE:HD11	3:P:221:ARG:HD2	1.72	0.71
6:S:75:HIS:H	6:S:80:GLN:HE22	1.38	0.71
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.72	0.71
27:Y:4268:HOH:O	13:Z:22:THR:HA	1.91	0.71
2:O:22:HIS:CE1	2:O:26:HIS:HE1	2.09	0.71
4:D:127:LYS:O	4:D:130:PRO:HD3	1.91	0.71
18:Y:1522:TGL:H242	18:Y:1522:TGL:H202	1.73	0.70
7:G:7:ASP:HB2	27:N:4030:HOH:O	1.90	0.70
1:N:195:LEU:HG	1:N:245:ILE:HD13	1.72	0.70
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.22	0.70
2:O:224:ALA:O	2:O:227:LEU:HG	1.91	0.70
3:C:54:MET:HE3	26:C:270:CDL:C61	2.22	0.70
2:O:22:HIS:NE2	2:O:26:HIS:CE1	2.60	0.70
2:B:22:HIS:CE1	2:B:26:HIS:HE1	2.10	0.70
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.73	0.70
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.27	0.70
2:B:156:SER:HB3	2:B:176:PRO:HD3	1.72	0.70
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.73	0.69
12:L:20:ARG:NH1	18:L:522:TGL:HC61	2.07	0.69
1:N:298:ASP:HB3	27:N:3389:HOH:O	1.91	0.69
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.06	0.69
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:N	4:Q:37:GLN:HE21	1.88	0.69
22:B:230:PSC:H222	22:B:230:PSC:H21	1.74	0.69
6:S:51:SER:HB2	6:S:91:LEU:HD11	1.74	0.69
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.74	0.69
2:B:56:MET:HG2	22:B:230:PSC:H211	1.75	0.69
1:N:402:GLY:O	1:N:482:VAL:HG23	1.93	0.69
8:U:7:LYS:O	8:U:8:ILE:HG22	1.94	0.68
3:P:59:ARG:O	3:P:63:ARG:HG3	1.93	0.68
1:N:177:SER:H	1:N:180:GLN:NE2	1.91	0.68
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.27	0.68
2:B:143:VAL:HB	2:B:222:TRP:CE3	2.29	0.68
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.29	0.68
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.75	0.68
18:L:522:TGL:H242	18:L:522:TGL:H202	1.75	0.68
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.76	0.68
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.06	0.68
1:A:65:MET:HE3	17:A:515:HEA:HMC3	1.76	0.68
3:C:187:THR:CB	7:G:68:THR:HG21	2.25	0.67
27:A:4207:HOH:O	7:T:9:GLY:HA3	1.94	0.67
1:A:365:ILE:HD11	27:A:4150:HOH:O	1.94	0.67
26:G:269:CDL:H511	26:G:269:CDL:H172	1.77	0.67
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.77	0.67
1:N:381:LEU:HB3	17:N:515:HEA:HBC1	1.76	0.67
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.76	0.67
2:B:22:HIS:NE2	2:B:26:HIS:CE1	2.63	0.66
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.78	0.66
7:T:30:LEU:HD12	26:T:1269:CDL:H252	1.77	0.66
2:B:68:LEU:O	2:B:72:ILE:HD12	1.95	0.66
7:G:31:CYS:SG	26:G:269:CDL:H532	2.36	0.66
1:N:503:HIS:HB2	27:Y:3093:HOH:O	1.94	0.66
2:O:56:MET:HA	22:O:1230:PSC:C20	2.26	0.66
26:P:1270:CDL:H431	27:W:4131:HOH:O	1.95	0.66
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.30	0.66
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.31	0.66
6:S:94:HIS:CD2	6:S:95:GLN:H	2.14	0.66
7:T:70:PHE:HB2	25:T:1264:PEK:H041	1.78	0.65
1:N:479:LYS:HD3	27:N:4148:HOH:O	1.96	0.65
2:O:7:LEU:HD11	18:O:1521:TGL:H161	1.78	0.65
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	1.79	0.65
18:O:1521:TGL:H201	18:O:1521:TGL:H241	1.78	0.65
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383:MET:HB2	1.95	0.65
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.01	0.65
2:B:22:HIS:CE1	2:B:26:HIS:CE1	2.84	0.65
1:A:165:ILE:O	1:A:169:ILE:HG12	1.97	0.65
1:N:240:HIS:O	1:N:243:VAL:HG22	1.97	0.65
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.79	0.65
25:C:264:PEK:C16	25:C:264:PEK:H102	2.21	0.64
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.12	0.64
18:A:521:TGL:H161	2:B:7:LEU:HD11	1.79	0.64
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.79	0.64
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.77	0.64
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.79	0.64
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.09	0.64
2:O:209:ILE:HA	27:O:3158:HOH:O	1.98	0.64
1:A:377:PHE:CE2	1:A:378:HIS:CE1	2.86	0.64
1:A:382:SER:HA	17:A:515:HEA:HMC2	1.79	0.64
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.32	0.64
2:O:57:ASP:N	22:O:1230:PSC:H201	2.11	0.64
1:A:298:ASP:HB3	27:A:2389:HOH:O	1.98	0.64
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.63	0.64
10:W:45:TYR:O	10:W:48:TYR:HB3	1.98	0.64
3:C:246:ASP:HB2	27:C:4064:HOH:O	1.97	0.64
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.79	0.63
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.63
1:A:488:THR:HB	1:A:495:LEU:HD13	1.81	0.63
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.12	0.63
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.80	0.63
11:X:24:PHE:O	11:X:28:VAL:HG12	1.99	0.63
7:G:4:ALA:CB	1:N:282:PHE:HA	2.29	0.63
2:O:22:HIS:CE1	2:O:26:HIS:CE1	2.86	0.63
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.62	0.63
6:S:94:HIS:CG	6:S:95:GLN:H	2.17	0.63
1:A:466:MET:HG2	13:M:26:PHE:CD2	2.34	0.63
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.81	0.63
19:C:267:PGV:H172	26:C:270:CDL:H662	1.81	0.62
26:P:1270:CDL:H112	27:P:4194:HOH:O	1.98	0.62
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.35	0.62
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.34	0.62
1:A:347:LEU:HD13	1:A:383:MET:SD	2.38	0.62
1:N:324:LEU:HD13	2:O:41:ILE:HG21	1.82	0.62
2:O:161:HIS:CE1	2:O:200:CYS:SG	2.92	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:O	1:A:411:LYS:HG3	2.00	0.62
2:B:1:FME:SD	2:B:133:LEU:HD11	2.40	0.62
1:N:347:LEU:HD13	1:N:383:MET:SD	2.39	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.62
27:P:4092:HOH:O	6:S:1:ALA:HB2	2.00	0.62
2:O:42:ILE:O	2:O:46:LEU:HG	2.00	0.61
2:O:82:ARG:HG2	2:O:86:MET:HE1	1.82	0.61
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.81	0.61
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.00	0.61
2:B:62:GLU:O	2:B:66:THR:HB	2.00	0.61
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.15	0.61
1:N:416:ILE:HG22	1:N:464:ALA:HB2	1.82	0.61
3:P:112:LEU:HB3	3:P:118:PRO:HB3	1.82	0.61
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.82	0.61
10:W:30:ILE:O	10:W:34:VAL:HG23	2.00	0.61
3:P:47:LEU:O	3:P:51:MET:HG2	2.01	0.61
1:A:367:LEU:HD21	1:A:433:LEU:HD23	1.82	0.61
1:N:103:TRP:O	3:P:21:ALA:HB1	2.01	0.61
3:C:204:HIS:HD2	3:C:248:VAL:HG12	1.65	0.61
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.65	0.61
19:N:1524:PGV:H062	27:Z:3160:HOH:O	2.01	0.61
3:C:212:SER:O	3:C:216:ILE:HG13	2.01	0.60
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.83	0.60
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.82	0.60
1:A:112:LEU:HG	27:A:2073:HOH:O	2.00	0.60
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.36	0.60
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.82	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.82	0.60
19:A:524:PGV:H062	27:M:2160:HOH:O	2.01	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
1:N:128:VAL:HG12	1:N:128:VAL:O	2.02	0.60
3:P:157:LYS:HE2	27:P:3156:HOH:O	2.01	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.37	0.60
8:H:60:TYR:C	8:H:60:TYR:CD1	2.75	0.60
1:N:54:TYR:HB2	27:N:3113:HOH:O	2.02	0.60
3:C:168:THR:HG22	25:C:265:PEK:H14	1.84	0.59
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.84	0.59
6:F:85:CYS:SG	6:F:87:THR:HG23	2.42	0.59
3:C:204:HIS:HD2	3:C:248:VAL:CG1	2.16	0.59
10:J:40:LEU:HD12	23:J:60:CHD:H183	1.85	0.59
7:G:17:ARG:HD2	27:G:2309:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:HIS:CD2	10:J:22:LEU:HG	2.37	0.59
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.83	0.59
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.03	0.59
6:S:14:THR:HB	10:W:9:GLN:NE2	2.18	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.59
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.17	0.59
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.67	0.59
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.85	0.59
25:C:264:PEK:H041	7:G:70:PHE:HB2	1.85	0.59
4:D:102:TYR:HD1	13:M:35:TYR:HE1	1.51	0.58
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.91	0.58
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
1:A:240:HIS:O	1:A:243:VAL:HG22	2.03	0.58
13:Z:17:ILE:O	13:Z:21:VAL:HG23	2.02	0.58
1:N:115:SER:O	1:N:121:GLY:HA2	2.02	0.58
2:B:146:MET:HA	2:B:213:LEU:HD12	1.85	0.58
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.66	0.58
3:C:168:THR:CG2	25:C:265:PEK:H14	2.34	0.58
4:D:131:ILE:HD12	4:D:131:ILE:H	1.68	0.58
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.85	0.58
18:O:1521:TGL:H222	18:O:1521:TGL:HA82	1.85	0.58
2:B:157:GLU:HA	27:B:4023:HOH:O	2.02	0.58
1:A:311:ILE:HD12	26:T:1269:CDL:H212	1.86	0.58
3:P:63:ARG:NH1	10:W:20:VAL:O	2.34	0.58
1:A:449:MET:SD	2:B:5:MET:HG2	2.44	0.58
18:L:522:TGL:C24	18:L:522:TGL:H202	2.34	0.58
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.58
3:P:30:GLY:HA2	3:P:42:LEU:HB3	1.85	0.58
25:T:1264:PEK:H71	25:T:1264:PEK:H32	1.85	0.58
1:A:514:LYS:NZ	27:A:2395:HOH:O	2.37	0.58
1:N:335:SER:O	1:N:339:MET:HG3	2.03	0.57
1:A:94:PHE:HE1	3:C:79:LEU:HD23	1.69	0.57
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.86	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C53	2.86	0.57
2:B:66:THR:HG22	2:B:67:ILE:N	2.17	0.57
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.86	0.57
3:P:15:PRO:O	3:P:19:THR:HG23	2.04	0.57
1:N:290:HIS:CD2	1:N:291:HIS:NE2	2.73	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
2:B:1:FME:SD	2:B:133:LEU:CD1	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:HG22	2:B:27:THR:HG21	1.86	0.57
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.85	0.57
3:P:126:PRO:HG2	3:P:127:LEU:HD22	1.86	0.57
7:T:47:PHE:HE1	7:T:49:PRO:HG3	1.70	0.57
3:C:51:MET:SD	26:C:270:CDL:H622	2.44	0.57
3:C:204:HIS:CD2	3:C:248:VAL:HG12	2.39	0.57
1:A:13:LYS:HE3	1:A:85:LEU:HD21	1.86	0.57
1:A:41:LEU:HD11	1:A:54:TYR:OH	2.05	0.57
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.57
18:A:521:TGL:HC22	27:I:2383:HOH:O	2.05	0.57
1:N:382:SER:HA	17:N:515:HEA:HMC2	1.86	0.57
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.87	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.39	0.57
2:B:56:MET:HA	22:B:230:PSC:C20	2.35	0.57
1:A:112:LEU:C	1:A:112:LEU:HD23	2.26	0.57
2:B:99:THR:HG22	2:B:152:MET:CE	2.35	0.57
1:A:253:MET:O	1:A:257:ILE:HG13	2.04	0.57
2:O:56:MET:HA	22:O:1230:PSC:H202	1.87	0.56
18:A:521:TGL:HA82	18:A:521:TGL:H222	1.86	0.56
3:P:187:THR:CB	7:T:68:THR:HG21	2.34	0.56
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.05	0.56
1:A:416:ILE:HG22	1:A:464:ALA:HB2	1.87	0.56
1:A:492:LEU:O	1:A:492:LEU:HD12	2.04	0.56
1:A:115:SER:O	1:A:121:GLY:HA2	2.06	0.56
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.39	0.56
2:O:82:ARG:HG2	2:O:86:MET:CE	2.36	0.56
25:C:265:PEK:H371	26:G:269:CDL:H261	1.87	0.56
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.06	0.56
25:C:265:PEK:C38	26:G:269:CDL:H273	2.35	0.56
5:R:67:ILE:O	5:R:71:VAL:HG23	2.06	0.56
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.87	0.56
6:S:48:LEU:O	6:S:50:PRO:HD3	2.06	0.56
23:B:1086:CHD:H14	27:B:2112:HOH:O	2.05	0.56
1:A:103:TRP:O	3:C:21:ALA:HB1	2.05	0.56
1:A:484:THR:HB	13:M:2:THR:OG1	2.06	0.56
1:N:31:THR:HG23	17:N:515:HEA:H14	1.87	0.56
4:Q:69:ALA:O	5:R:109:VAL:HG12	2.05	0.56
1:N:52:GLN:O	1:N:56:VAL:HG23	2.06	0.56
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.28	0.56
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.87	0.56
6:S:16:LEU:O	6:S:20:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:TYR:CD1	13:M:35:TYR:HE1	2.24	0.55
1:A:104:LEU:O	1:A:107:PRO:HD2	2.06	0.55
1:N:310:MET:O	2:O:73:LEU:HD13	2.06	0.55
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.87	0.55
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.21	0.55
1:A:399:LEU:HB2	1:A:494:TRP:CE3	2.41	0.55
2:O:23:PHE:CE2	2:O:79:PRO:HG2	2.42	0.55
6:F:16:LEU:O	6:F:16:LEU:HD12	2.06	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.07	0.55
18:Y:1522:TGL:H272	18:Y:1522:TGL:H231	1.87	0.55
1:A:381:LEU:HB3	17:A:515:HEA:CBC	2.35	0.55
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.89	0.55
2:B:57:ASP:H	22:B:230:PSC:H201	1.71	0.55
1:A:173:PRO:HD2	1:A:176:MET:SD	2.45	0.55
12:Y:40:VAL:O	12:Y:44:LEU:HG	2.07	0.55
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.87	0.55
3:C:57:TRP:O	3:C:61:VAL:HG23	2.07	0.55
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.42	0.55
1:A:324:LEU:HD13	2:B:41:ILE:HG21	1.89	0.55
1:A:113:LEU:HD12	18:L:522:TGL:H292	1.89	0.55
1:A:398:PRO:HA	1:A:403:TYR:O	2.07	0.55
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.72	0.55
3:P:213:THR:CG2	19:P:1267:PGV:H11	2.36	0.55
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.88	0.55
7:G:66:ASN:HD21	7:G:79:PRO:HD2	1.72	0.55
1:N:184:PHE:O	1:N:188:VAL:HG23	2.07	0.54
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.54
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.89	0.54
1:N:144:ASP:CG	1:N:213:ARG:HH21	2.11	0.54
2:B:158:ASP:O	2:B:176:PRO:HG3	2.06	0.54
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.89	0.54
19:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.89	0.54
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.89	0.54
25:C:265:PEK:H22	27:G:4145:HOH:O	2.07	0.54
7:T:45:PRO:HD2	27:T:3152:HOH:O	2.07	0.54
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.43	0.54
18:O:1521:TGL:HC22	27:V:3383:HOH:O	2.08	0.54
6:F:77:GLY:O	6:F:90:LYS:HE2	2.07	0.54
9:I:23:GLY:O	9:I:27:VAL:HG23	2.08	0.54
8:H:46:LYS:NZ	8:U:55:TRP:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.90	0.54
7:T:2:SER:O	25:T:263:PEK:H322	2.07	0.54
13:M:39:ASN:O	13:M:43:SER:HB2	2.08	0.54
27:G:4051:HOH:O	2:O:67:ILE:HD11	2.07	0.54
1:N:104:LEU:O	1:N:107:PRO:HD2	2.08	0.54
2:O:155:SER:O	2:O:174:ALA:HB1	2.08	0.54
1:N:132:LEU:O	1:N:132:LEU:HD12	2.08	0.54
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.89	0.54
2:B:99:THR:HG22	2:B:152:MET:HE2	1.90	0.54
2:B:138:VAL:HG22	2:B:210:VAL:CG2	2.38	0.54
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.73	0.54
2:O:216:LEU:O	2:O:219:PHE:HB3	2.08	0.54
1:A:5:ARG:O	1:A:9:SER:HB2	2.08	0.54
1:N:65:MET:HB3	17:N:515:HEA:HAC	1.90	0.53
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.89	0.53
24:P:1272:DMU:H25	25:T:1264:PEK:H341	1.90	0.53
2:O:121:TYR:O	2:O:138:VAL:HA	2.08	0.53
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.07	0.53
18:Y:1522:TGL:C24	18:Y:1522:TGL:H202	2.37	0.53
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.43	0.53
1:A:443:TYR:HD1	1:A:447:TYR:HB2	1.72	0.53
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.74	0.53
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.22	0.53
9:V:5:ALA:O	9:V:7:PRO:HD3	2.09	0.53
2:B:69:PRO:HG3	22:B:230:PSC:H183	1.91	0.53
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.22	0.53
4:D:100:LYS:HE2	11:K:37:GLY:O	2.07	0.53
3:P:225:PHE:HA	27:P:3236:HOH:O	2.09	0.53
6:S:62:CYS:SG	6:S:84:SER:HB3	2.49	0.53
4:D:94:LEU:HD23	11:K:28:VAL:HG21	1.89	0.53
1:A:503:HIS:CD2	1:A:503:HIS:N	2.58	0.53
1:N:399:LEU:HA	1:N:498:CYS:HB3	1.90	0.53
3:C:98:PHE:CZ	3:C:252:LEU:HD23	2.44	0.53
1:A:86:MET:HB3	1:A:182:PRO:HG2	1.91	0.53
1:N:466:MET:HG2	13:Z:26:PHE:CD2	2.44	0.53
1:N:35:LEU:HD11	1:N:462:LEU:HD13	1.91	0.53
1:N:344:PHE:C	1:N:344:PHE:CD1	2.81	0.53
24:C:272:DMU:H25	25:C:264:PEK:H341	1.90	0.53
18:Y:1522:TGL:H211	18:Y:1522:TGL:HA72	1.91	0.53
3:P:118:PRO:HD2	3:P:121:ILE:HG13	1.91	0.53
4:D:102:TYR:HD1	13:M:35:TYR:CE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.90	0.53
1:A:499:PRO:HD2	12:L:7:PRO:HD3	1.91	0.53
1:A:306:THR:O	1:A:310:MET:HG3	2.09	0.53
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.91	0.53
1:N:472:ILE:HD13	18:Y:1522:TGL:HA91	1.91	0.52
6:S:51:SER:CB	6:S:91:LEU:HD11	2.39	0.52
2:O:141:ARG:NH1	2:O:191:LEU:HD11	2.24	0.52
2:B:216:LEU:O	2:B:216:LEU:HD12	2.09	0.52
19:C:267:PGV:H161	19:C:267:PGV:H12	1.90	0.52
2:O:68:LEU:HB3	22:O:1230:PSC:H182	1.91	0.52
3:C:29:SER:HB3	3:C:42:LEU:CD1	2.40	0.52
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.44	0.52
4:Q:97:ILE:HG13	11:X:32:MET:HG3	1.92	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.09	0.52
26:T:1269:CDL:H342	26:T:1269:CDL:OA7	2.10	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.92	0.52
2:O:108:TYR:CE1	2:O:142:VAL:HG21	2.45	0.52
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.75	0.52
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.73	0.52
25:T:1264:PEK:C16	25:T:1264:PEK:H102	2.32	0.52
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.91	0.52
27:O:4075:HOH:O	4:Q:108:PRO:HG3	2.08	0.52
26:C:270:CDL:H112	27:C:4234:HOH:O	2.09	0.52
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.45	0.52
3:C:73:PRO:HB2	27:C:4140:HOH:O	2.10	0.52
9:V:58:LYS:O	9:V:62:GLU:HG3	2.09	0.52
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.91	0.52
19:A:524:PGV:H301	19:A:524:PGV:H152	1.91	0.52
13:M:31:GLY:HA3	24:M:526:DMU:H9	1.91	0.52
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.45	0.52
1:N:443:TYR:HE1	1:N:448:THR:HA	1.73	0.52
2:B:209:ILE:HA	27:B:2158:HOH:O	2.09	0.52
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.10	0.51
23:B:1086:CHD:H20	7:T:18:PHE:HD2	1.75	0.51
4:D:107:ILE:CD1	11:K:39:GLU:HB2	2.40	0.51
3:C:127:LEU:HD12	3:C:131:LEU:HD22	1.92	0.51
2:B:29:MET:HE2	2:B:30:ILE:HG13	1.92	0.51
1:N:243:VAL:HB	17:N:516:HEA:HAC	1.92	0.51
12:Y:11:ILE:HG13	12:Y:13:PHE:O	2.10	0.51
7:T:6:GLY:O	25:T:263:PEK:H311	2.11	0.51
2:B:222:TRP:HB2	9:I:71:SER:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
3:P:156:ARG:HE	23:P:1271:CHD:H232	1.76	0.51
3:C:68:GLN:HE21	3:C:70:HIS:CD2	2.29	0.51
11:X:19:ALA:HA	27:X:4125:HOH:O	2.10	0.51
12:L:20:ARG:HH22	18:L:522:TGL:HC32	1.75	0.51
3:C:60:ASP:O	3:C:64:GLU:HG3	2.10	0.51
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.93	0.51
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.92	0.51
27:N:3198:HOH:O	3:P:17:PRO:HG2	2.11	0.51
25:C:265:PEK:H371	26:G:269:CDL:C26	2.41	0.51
1:N:472:ILE:CG2	18:Y:1522:TGL:HA92	2.36	0.51
6:S:94:HIS:CD2	6:S:95:GLN:N	2.79	0.51
6:S:55:LYS:HA	6:S:74:LEU:O	2.11	0.51
1:N:219:PHE:HZ	3:P:199:VAL:HG21	1.76	0.51
1:N:398:PRO:HA	1:N:403:TYR:O	2.10	0.51
3:P:198:PHE:CD2	25:T:1264:PEK:H032	2.46	0.51
3:P:67:PHE:HA	10:W:9:GLN:HG2	1.92	0.51
3:P:80:ARG:HG2	3:P:233:PHE:CE2	2.46	0.51
26:G:269:CDL:C54	26:G:269:CDL:H231	2.29	0.51
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.93	0.51
2:B:141:ARG:HH11	2:B:191:LEU:HD21	1.75	0.51
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.51
18:A:523:TGL:HG11	18:A:523:TGL:CC2	2.39	0.51
7:T:23:LEU:C	7:T:26:PRO:HD2	2.31	0.51
3:P:116:TRP:CZ2	3:P:193:TYR:HD1	2.29	0.51
19:C:267:PGV:H182	26:C:270:CDL:C67	2.41	0.51
1:A:37:ILE:HG21	17:A:515:HEA:HMA	1.93	0.51
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.93	0.51
3:P:80:ARG:HG2	3:P:233:PHE:HE2	1.76	0.51
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.46	0.51
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.10	0.51
1:A:243:VAL:HB	17:A:516:HEA:HAC	1.93	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.46	0.51
1:N:349:THR:HG21	2:O:38:VAL:HG21	1.93	0.51
6:F:55:LYS:HA	6:F:74:LEU:O	2.10	0.51
1:N:346:PHE:CE1	2:O:39:LEU:HB2	2.46	0.51
1:N:1:FME:HCN	1:N:4:ASN:H	1.76	0.51
2:B:3:TYR:N	2:B:3:TYR:CD2	2.79	0.51
1:A:82:LEU:O	1:A:86:MET:HG3	2.10	0.50
4:D:113:GLU:HG3	27:D:2281:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:LEU:HD22	10:J:50:LEU:O	2.10	0.50
1:A:429:HIS:HB3	18:A:521:TGL:HB41	1.93	0.50
26:P:1270:CDL:C19	26:P:1270:CDL:H642	2.34	0.50
6:F:72:PHE:CE2	6:F:82:CYS:HA	2.47	0.50
1:A:379:TYR:O	1:A:383:MET:HB2	2.11	0.50
1:N:406:ASN:HD21	19:N:1524:PGV:H032	1.75	0.50
1:A:94:PHE:CE1	3:C:79:LEU:HD23	2.46	0.50
23:B:1086:CHD:H162	7:T:18:PHE:CE2	2.46	0.50
1:N:219:PHE:CZ	3:P:199:VAL:HG21	2.47	0.50
1:N:443:TYR:HD1	1:N:447:TYR:HB2	1.77	0.50
6:F:48:LEU:O	6:F:50:PRO:HD3	2.11	0.50
2:B:184:LEU:HD23	2:B:185:MET:N	2.27	0.50
4:D:35:ALA:HB3	27:D:4135:HOH:O	2.12	0.50
1:N:302:ARG:NH1	2:O:84:LEU:HD11	2.26	0.50
25:C:264:PEK:H71	25:C:264:PEK:H32	1.94	0.50
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.12	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.10	0.50
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50
3:C:47:LEU:O	3:C:51:MET:HG2	2.12	0.50
1:N:472:ILE:HG21	18:Y:1522:TGL:HA91	1.91	0.50
2:O:22:HIS:CD2	2:O:26:HIS:CE1	2.99	0.50
2:B:146:MET:SD	2:B:189:PRO:HB3	2.52	0.50
8:H:46:LYS:HZ3	8:U:55:TRP:HB2	1.75	0.50
2:B:79:PRO:O	2:B:83:ILE:HG13	2.10	0.50
2:O:65:TRP:HZ3	22:O:1230:PSC:H331	1.72	0.50
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.93	0.50
1:A:472:ILE:HG21	18:L:522:TGL:CA9	2.41	0.50
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.50
4:Q:78:TRP:O	4:Q:82:VAL:HG23	2.12	0.50
6:S:81:ARG:HG2	6:S:88:HIS:CD2	2.47	0.50
4:D:51:LEU:HB3	4:D:56:LYS:HG3	1.93	0.49
13:Z:23:PHE:O	13:Z:27:LEU:HG	2.12	0.49
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.47	0.49
27:E:2292:HOH:O	9:I:4:LEU:HD13	2.11	0.49
2:B:207:MET:O	2:B:207:MET:HG3	2.12	0.49
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.11	0.49
1:N:309:THR:HG22	17:N:516:HEA:HMB2	1.92	0.49
22:B:230:PSC:H12	22:B:230:PSC:H322	1.94	0.49
23:B:1086:CHD:H212	23:B:1086:CHD:H12	1.94	0.49
23:B:1086:CHD:H20	7:T:18:PHE:CD2	2.47	0.49
5:E:52:LEU:O	5:E:55:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:GLU:HB2	5:E:10:GLU:OE1	2.12	0.49
6:F:64:GLU:O	6:F:65:ASP:HB2	2.12	0.49
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.94	0.49
7:T:38:HIS:CE1	26:T:1269:CDL:H111	2.47	0.49
1:N:35:LEU:CD1	1:N:462:LEU:HD13	2.42	0.49
3:P:157:LYS:HZ2	25:P:1265:PEK:H052	1.77	0.49
8:H:36:PHE:HB2	8:H:56:TYR:HB2	1.94	0.49
1:A:15:ILE:HG21	1:A:98:ASN:ND2	2.27	0.49
7:G:8:HIS:HD2	25:G:1263:PEK:H232	1.78	0.49
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.12	0.49
2:O:134:ARG:HG2	2:O:135:LEU:HG	1.94	0.49
19:N:1524:PGV:H152	19:N:1524:PGV:H301	1.94	0.49
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.42	0.49
2:B:33:LEU:O	2:B:37:LEU:HB2	2.13	0.49
1:N:293:PHE:CE1	1:N:361:SER:HB3	2.48	0.49
1:N:5:ARG:O	1:N:9:SER:HB2	2.12	0.49
3:P:57:TRP:O	3:P:57:TRP:HD1	1.96	0.49
1:A:17:THR:OG1	18:L:522:TGL:H281	2.11	0.49
18:Y:1522:TGL:OA1	18:Y:1522:TGL:HC21	2.12	0.49
1:N:115:SER:HB3	1:N:145:LEU:HB2	1.94	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.13	0.49
6:S:33:ILE:HG22	6:S:34:LEU:HD23	1.95	0.49
3:P:134:THR:HA	3:P:249:TRP:HE1	1.77	0.49
10:W:8:LYS:O	10:W:12:PHE:HD1	1.96	0.49
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.28	0.49
22:O:1230:PSC:H12	22:O:1230:PSC:H322	1.95	0.49
1:N:514:LYS:NZ	27:N:3395:HOH:O	2.43	0.49
12:L:20:ARG:HH22	18:L:522:TGL:HC61	1.78	0.49
1:A:68:PHE:CE2	1:A:109:PHE:HA	2.47	0.49
2:B:125:THR:HG23	2:B:134:ARG:HG3	1.93	0.49
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.93	0.49
10:W:56:PRO:HD3	12:Y:46:LYS:HE3	1.93	0.49
3:P:219:PHE:O	3:P:222:GLN:HB3	2.13	0.49
2:O:95:LEU:HG	2:O:96:THR:N	2.28	0.49
17:N:516:HEA:H241	2:O:72:ILE:HG22	1.94	0.48
1:N:339:MET:HE1	18:N:1523:TGL:HB62	1.95	0.48
3:P:225:PHE:N	3:P:225:PHE:CD1	2.81	0.48
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.47	0.48
3:P:128:GLU:OE1	7:T:38:HIS:HB3	2.14	0.48
12:L:24:MET:SD	18:L:522:TGL:H162	2.53	0.48
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.96	0.48
2:B:56:MET:HA	22:B:230:PSC:H202	1.94	0.48
1:N:443:TYR:CD1	1:N:447:TYR:HB2	2.49	0.48
4:D:121:LYS:HG2	11:K:53:TRP:CD1	2.48	0.48
1:N:65:MET:HB3	17:N:515:HEA:CAC	2.42	0.48
1:A:248:LEU:HB2	1:A:249:PRO:HD3	1.94	0.48
3:C:225:PHE:HA	27:C:2236:HOH:O	2.13	0.48
7:T:31:CYS:SG	26:T:1269:CDL:H552	2.53	0.48
1:N:5:ARG:HB2	12:Y:3:TYR:CE1	2.49	0.48
9:I:37:PHE:CD1	9:I:38:ALA:N	2.82	0.48
2:O:57:ASP:H	22:O:1230:PSC:C20	2.19	0.48
2:O:69:PRO:HA	2:O:72:ILE:HD12	1.95	0.48
22:O:1230:PSC:H072	9:V:10:ARG:HE	1.77	0.48
22:B:230:PSC:H142	22:B:230:PSC:C34	2.31	0.48
7:T:84:LYS:CD	7:T:84:LYS:H	2.19	0.48
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.95	0.48
1:N:510:TYR:CG	6:S:49:VAL:HG13	2.48	0.48
1:A:476:PHE:CD2	12:L:15:VAL:HG11	2.49	0.48
2:B:155:SER:OG	2:B:156:SER:N	2.46	0.48
2:B:143:VAL:HB	2:B:222:TRP:CZ3	2.49	0.48
2:B:100:MET:CE	2:B:157:GLU:HG3	2.44	0.48
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.67	0.48
2:B:95:LEU:HD12	2:B:96:THR:H	1.79	0.48
5:R:14:ARG:HB3	5:R:14:ARG:HH11	1.79	0.48
3:C:187:THR:HG22	25:C:264:PEK:H052	1.96	0.48
1:N:66:ILE:HG23	1:N:246:LEU:HD21	1.96	0.48
23:C:271:CHD:H222	23:C:271:CHD:H162	1.53	0.48
1:A:361:SER:O	1:A:365:ILE:HG12	2.13	0.48
1:A:383:MET:HE2	1:A:421:VAL:HB	1.96	0.48
2:B:188:ARG:HB3	2:B:189:PRO:HD2	1.96	0.48
1:N:94:PHE:HB3	19:N:1266:PGV:O11	2.14	0.48
2:O:66:THR:HG22	2:O:67:ILE:N	2.28	0.48
3:C:144:ILE:HG13	3:C:166:THR:HG21	1.96	0.48
3:P:149:HIS:HA	3:P:152:MET:HE2	1.96	0.48
18:N:1523:TGL:HG32	27:Q:4216:HOH:O	2.12	0.48
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.13	0.48
2:O:52:HIS:ND1	5:R:40:ASP:HB2	2.28	0.48
1:A:161:ALA:HB1	1:A:192:ALA:O	2.14	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.96	0.48
7:T:8:HIS:HD2	25:T:263:PEK:H232	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:TYR:O	2:B:138:VAL:HA	2.14	0.47
1:N:513:LEU:O	1:N:514:LYS:HB2	2.13	0.47
7:G:26:PRO:O	7:G:29:ALA:HB3	2.14	0.47
3:P:4:GLN:NE2	3:P:6:HIS:O	2.43	0.47
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.97	0.47
3:P:88:ILE:O	3:P:91:VAL:HB	2.14	0.47
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.95	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
3:C:198:PHE:O	25:C:264:PEK:H22	2.15	0.47
1:N:468:MET:O	1:N:472:ILE:HG13	2.14	0.47
1:N:44:PRO:HB3	2:O:134:ARG:NH2	2.29	0.47
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.25	0.47
19:A:524:PGV:H321	19:A:524:PGV:H152	1.96	0.47
3:C:131:LEU:HD13	3:C:253:TYR:OH	2.14	0.47
8:H:49:ASP:O	8:H:52:VAL:HG22	2.14	0.47
18:L:522:TGL:H272	18:L:522:TGL:H231	1.96	0.47
19:A:524:PGV:C15	19:A:524:PGV:H321	2.45	0.47
1:A:310:MET:O	2:B:73:LEU:HD13	2.14	0.47
3:C:149:HIS:HA	3:C:152:MET:HE2	1.95	0.47
6:F:96:LEU:HD23	6:F:97:ALA:N	2.29	0.47
18:L:522:TGL:OA1	18:L:522:TGL:HC21	2.15	0.47
17:A:515:HEA:H11	17:A:515:HEA:HMB1	1.70	0.47
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.49	0.47
13:M:35:TYR:HD2	13:M:36:HIS:ND1	2.12	0.47
1:A:357:VAL:HG22	2:B:27:THR:CG2	2.44	0.47
5:R:21:LYS:HE3	27:R:3128:HOH:O	2.13	0.47
11:X:47:ARG:HG3	11:X:48:VAL:N	2.29	0.47
8:U:49:ASP:O	8:U:52:VAL:HG22	2.14	0.47
2:O:65:TRP:CE3	22:O:1230:PSC:H331	2.50	0.47
7:G:84:LYS:HD2	7:G:84:LYS:N	2.16	0.47
18:L:522:TGL:HA72	18:L:522:TGL:H211	1.97	0.47
1:A:104:LEU:HB2	1:A:156:SER:HB2	1.97	0.47
6:F:74:LEU:HD12	6:F:80:GLN:OE1	2.14	0.47
26:C:270:CDL:C19	26:C:270:CDL:H642	2.35	0.47
5:R:43:PRO:HB2	5:R:48:ILE:CD1	2.42	0.47
19:N:1524:PGV:C15	19:N:1524:PGV:H321	2.44	0.47
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.50	0.47
8:H:55:TRP:O	8:H:59:VAL:HG23	2.14	0.47
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.78	0.47
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.47
1:A:132:LEU:HD12	1:A:132:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.74	0.47
3:P:50:ASN:O	3:P:54:MET:HG3	2.14	0.47
3:C:67:PHE:N	3:C:67:PHE:CD2	2.82	0.47
25:T:1264:PEK:H71	25:T:1264:PEK:C3	2.45	0.47
4:Q:131:ILE:HG23	9:V:50:PHE:HB2	1.97	0.47
1:N:164:PHE:O	1:N:168:ILE:HG13	2.15	0.47
1:N:376:HIS:HA	27:N:3228:HOH:O	2.14	0.47
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.45	0.47
7:G:3:ALA:HB3	25:G:1263:PEK:H361	1.97	0.47
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.50	0.47
1:N:3:ILE:HG23	1:N:7:LEU:HD22	1.97	0.47
13:M:42:LYS:CE	13:M:42:LYS:HA	2.41	0.46
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.50	0.46
3:C:173:PHE:C	3:C:173:PHE:CD2	2.89	0.46
1:N:429:HIS:HB3	18:O:1521:TGL:HB41	1.96	0.46
1:A:382:SER:CA	17:A:515:HEA:HMC2	2.43	0.46
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.71	0.46
2:B:185:MET:SD	2:B:185:MET:C	2.93	0.46
1:N:12:HIS:CE1	1:N:13:LYS:HG2	2.51	0.46
8:U:28:ASN:ND2	27:U:3134:HOH:O	2.40	0.46
1:A:378:HIS:CG	1:A:425:PHE:CE2	3.03	0.46
6:S:13:ALA:O	6:S:18:ARG:HD2	2.15	0.46
8:U:36:PHE:HB2	8:U:56:TYR:HB2	1.98	0.46
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.97	0.46
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.67	0.46
13:M:26:PHE:O	13:M:29:PRO:HD2	2.15	0.46
6:S:72:PHE:CE2	6:S:83:PRO:HD3	2.49	0.46
3:C:51:MET:SD	26:C:270:CDL:C62	3.04	0.46
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.16	0.46
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.96	0.46
1:A:413:HIS:HE2	1:A:468:MET:HB2	1.79	0.46
3:P:147:ALA:HB2	3:P:162:ALA:CB	2.46	0.46
1:A:235:PHE:C	1:A:235:PHE:CD2	2.88	0.46
7:G:2:SER:OG	25:G:1263:PEK:H301	2.16	0.46
19:P:1267:PGV:H181	26:P:1270:CDL:H812	1.96	0.46
1:A:140:GLY:O	1:A:213:ARG:NH2	2.49	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.46
7:T:70:PHE:O	25:T:1264:PEK:N	2.48	0.46
12:L:11:ILE:HG13	12:L:13:PHE:O	2.16	0.46
1:A:346:PHE:CD2	1:A:347:LEU:HD23	2.50	0.46
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:46:LYS:HE2	27:H:4276:HOH:O	2.16	0.46
1:N:417:MET:O	1:N:421:VAL:HG22	2.16	0.46
27:C:4266:HOH:O	25:T:263:PEK:H042	2.15	0.46
17:A:515:HEA:H261	17:A:515:HEA:H171	1.72	0.46
19:A:525:PGV:H21	3:C:57:TRP:CZ2	2.51	0.46
7:T:11:TPO:O	7:T:11:TPO:CG2	2.64	0.46
3:C:112:LEU:HA	7:G:52:HIS:CD2	2.50	0.46
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.98	0.45
12:Y:24:MET:HE1	18:Y:1522:TGL:HC82	1.99	0.45
18:N:1523:TGL:H271	2:O:46:LEU:HD12	1.97	0.45
3:C:156:ARG:HE	23:C:271:CHD:H232	1.80	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
1:A:395:HIS:HD2	1:A:396:TRP:CD2	2.34	0.45
2:B:217:LYS:HD3	2:B:217:LYS:HA	1.79	0.45
2:O:72:ILE:HG13	27:O:4128:HOH:O	2.15	0.45
25:C:265:PEK:H041	6:F:1:ALA:N	2.32	0.45
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.16	0.45
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.84	0.45
1:A:377:PHE:HE2	1:A:378:HIS:CE1	2.34	0.45
3:P:173:PHE:CD2	3:P:173:PHE:C	2.88	0.45
1:A:21:LEU:HD23	18:L:522:TGL:H221	1.98	0.45
2:B:22:HIS:NE2	2:B:26:HIS:NE2	2.64	0.45
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.97	0.45
19:A:525:PGV:H251	19:A:525:PGV:H42	1.98	0.45
1:N:230:LEU:HD21	3:P:100:ALA:HA	1.97	0.45
26:T:1269:CDL:C52	26:T:1269:CDL:H202	2.40	0.45
2:B:22:HIS:CD2	2:B:26:HIS:CE1	3.04	0.45
1:N:367:LEU:CD2	1:N:433:LEU:HD23	2.46	0.45
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.97	0.45
23:G:86:CHD:H12	23:G:86:CHD:H212	1.97	0.45
13:M:34:LEU:HA	13:M:34:LEU:HD12	1.68	0.45
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.32	0.45
1:N:309:THR:CG2	17:N:516:HEA:HMB2	2.47	0.45
2:O:69:PRO:HG3	22:O:1230:PSC:H183	1.98	0.45
25:C:265:PEK:H371	26:G:269:CDL:H273	1.99	0.45
1:N:450:TRP:CE3	1:N:453:ILE:HD12	2.52	0.45
1:A:115:SER:HA	1:A:145:LEU:HD12	1.99	0.45
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.45
1:A:248:LEU:O	1:A:251:PHE:HB2	2.15	0.45
1:N:313:ALA:CB	17:N:516:HEA:H262	2.46	0.45
7:T:70:PHE:HD1	25:T:1264:PEK:O11	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:ARG:HA	7:G:45:PRO:HD2	1.83	0.45
1:N:195:LEU:HG	1:N:245:ILE:CD1	2.42	0.45
1:A:513:LEU:O	1:A:514:LYS:HB2	2.17	0.45
1:A:443:TYR:CD1	1:A:447:TYR:HB2	2.50	0.45
1:N:397:PHE:N	1:N:398:PRO:CD	2.78	0.45
2:B:131:GLY:O	4:D:122:ARG:HD3	2.16	0.45
2:B:161:HIS:CE1	2:B:200:CYS:HB2	2.52	0.45
2:B:215:PRO:HD3	9:I:60:PHE:CD2	2.52	0.45
2:B:78:LEU:HD12	26:T:1269:CDL:C35	2.47	0.45
26:T:1269:CDL:H222	26:T:1269:CDL:H251	1.84	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H342	2.47	0.45
23:J:60:CHD:H161	23:J:60:CHD:H212	1.79	0.45
2:B:97:VAL:O	2:B:152:MET:HE3	2.17	0.45
3:P:160:LEU:HD21	3:P:222:GLN:HG3	1.99	0.45
1:A:443:TYR:N	1:A:443:TYR:CD2	2.85	0.45
3:C:112:LEU:HB3	3:C:118:PRO:HB3	1.98	0.45
4:D:145:TRP:CZ3	11:K:45:VAL:HG22	2.52	0.45
2:B:14:SER:O	2:B:18:GLU:HG3	2.16	0.45
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.74	0.45
26:G:269:CDL:H222	26:G:269:CDL:H251	1.86	0.45
2:O:32:PHE:HE2	18:O:1521:TGL:HB91	1.80	0.45
4:D:95:LEU:HD21	13:M:27:LEU:CD1	2.47	0.45
3:C:163:LEU:HD23	3:C:219:PHE:HA	1.99	0.45
3:C:16:TRP:HB2	3:C:17:PRO:HD3	1.98	0.45
1:N:460:ILE:HA	4:Q:92:THR:HG21	1.98	0.45
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.45
1:N:8:PHE:N	1:N:8:PHE:CD1	2.85	0.45
8:U:37:HIS:CD2	8:U:76:ARG:CZ	2.99	0.45
26:G:269:CDL:H271	1:N:282:PHE:HE2	1.81	0.45
2:B:68:LEU:HB3	22:B:230:PSC:H182	1.99	0.45
18:N:1523:TGL:HG11	18:N:1523:TGL:CC2	2.41	0.45
2:O:22:HIS:NE2	2:O:26:HIS:HE1	2.06	0.45
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.69	0.45
12:L:33:PHE:O	12:L:36:PRO:HD2	2.16	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
1:A:302:ARG:NH1	27:A:4150:HOH:O	2.49	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.45
1:N:91:ASP:OD1	1:N:95:PRO:HB3	2.15	0.45
1:N:467:LEU:O	1:N:470:PHE:HB3	2.17	0.45
26:C:270:CDL:H171	26:C:270:CDL:H202	1.77	0.44
1:N:151:HIS:CD2	25:T:1264:PEK:H382	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:6:VAL:HA	6:S:7:PRO:HD2	1.87	0.44
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.99	0.44
1:N:507:GLU:OE1	6:S:51:SER:HA	2.18	0.44
2:O:161:HIS:CE1	2:O:200:CYS:CB	3.01	0.44
12:Y:36:PRO:O	12:Y:40:VAL:HG23	2.17	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.44
1:N:381:LEU:HB3	17:N:515:HEA:CBC	2.46	0.44
1:A:449:MET:SD	2:B:5:MET:CG	3.05	0.44
3:C:81:TYR:O	3:C:85:LEU:HG	2.18	0.44
2:B:12:ALA:HB3	9:I:47:TYR:CE2	2.53	0.44
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.83	0.44
18:Y:1522:TGL:C23	18:Y:1522:TGL:H272	2.47	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.44
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.53	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.72	0.44
22:O:1230:PSC:C34	22:O:1230:PSC:H142	2.32	0.44
1:A:439:ARG:HH21	17:A:515:HEA:CGD	2.30	0.44
3:P:156:ARG:HE	23:P:1271:CHD:C23	2.30	0.44
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.53	0.44
1:N:12:HIS:CD2	1:N:91:ASP:HA	2.53	0.44
1:A:424:THR:OG1	1:A:458:SER:N	2.51	0.44
2:O:12:ALA:HB3	9:V:47:TYR:CE2	2.53	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.62	0.44
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.17	0.44
1:A:96:ARG:NH2	3:C:61:VAL:HG22	2.32	0.44
1:A:397:PHE:N	1:A:398:PRO:CD	2.80	0.44
1:A:35:LEU:CD1	1:A:462:LEU:HD13	2.48	0.44
1:A:6:TRP:HH2	12:L:10:ASN:O	2.01	0.44
1:N:473:TRP:NE1	12:Y:22:LEU:HB2	2.32	0.44
4:D:32:ASN:HA	4:D:32:ASN:HD22	1.64	0.44
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.86	0.44
1:N:314:ILE:O	1:N:318:VAL:HG23	2.18	0.44
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.99	0.44
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.44
18:N:1523:TGL:HC22	18:N:1523:TGL:HC51	1.78	0.44
1:A:397:PHE:HD1	1:A:405:LEU:HG	1.83	0.44
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.17	0.44
4:Q:11:TYR:CD1	4:Q:12:ALA:N	2.86	0.44
2:O:131:GLY:O	4:Q:122:ARG:HD3	2.18	0.44
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.74	0.44
7:G:11:TPO:CG2	7:G:11:TPO:O	2.66	0.44
26:G:269:CDL:H601	26:G:269:CDL:H571	1.48	0.44
22:B:230:PSC:H032	27:E:2129:HOH:O	2.17	0.44
22:B:230:PSC:H241	22:B:230:PSC:H62	2.00	0.44
4:Q:131:ILE:HG23	9:V:50:PHE:CB	2.48	0.44
1:A:98:ASN:HA	27:A:2052:HOH:O	2.17	0.44
1:N:361:SER:O	1:N:365:ILE:HG12	2.17	0.44
2:B:159:VAL:HG23	2:B:160:LEU:N	2.32	0.44
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.98	0.44
8:U:39:CYS:O	8:U:43:MET:HG2	2.17	0.44
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.83	0.44
1:A:397:PHE:CD1	1:A:405:LEU:HG	2.53	0.44
1:N:395:HIS:O	1:N:398:PRO:HD2	2.18	0.44
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.53	0.44
5:E:19:PHE:O	5:E:57:ARG:NH2	2.51	0.44
8:H:37:HIS:CD2	8:H:76:ARG:CZ	3.01	0.44
26:P:1270:CDL:H632	26:P:1270:CDL:H602	1.76	0.43
4:D:23:PRO:O	4:D:25:PRO:HD3	2.18	0.43
4:D:48:TRP:O	4:D:51:LEU:HB2	2.18	0.43
8:H:9:LYS:O	8:H:10:ASN:CB	2.66	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.43
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.99	0.43
1:N:499:PRO:HD2	12:Y:7:PRO:HD3	1.99	0.43
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.18	0.43
8:U:49:ASP:OD1	8:U:51:SER:HB3	2.18	0.43
5:R:100:THR:OG1	5:R:103:GLU:HG3	2.17	0.43
8:H:28:ASN:ND2	27:H:2134:HOH:O	2.50	0.43
4:D:20:ARG:HG3	4:D:20:ARG:H	1.66	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.87	0.43
18:A:523:TGL:H242	18:A:523:TGL:H212	1.78	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.53	0.43
2:O:23:PHE:HE2	2:O:79:PRO:HG2	1.82	0.43
1:A:368:HIS:O	1:A:370:THR:HG23	2.18	0.43
1:N:9:SER:HB3	27:N:4019:HOH:O	2.18	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.74	0.43
8:U:57:ARG:O	8:U:61:LYS:HB2	2.18	0.43
4:D:42:GLU:OE2	4:D:45:LYS:HE2	2.18	0.43
22:O:1230:PSC:H221	22:O:1230:PSC:H251	1.77	0.43
3:P:198:PHE:O	25:T:1264:PEK:H22	2.19	0.43
1:A:377:PHE:HB2	17:A:516:HEA:HMD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.18	0.43
1:A:440:TYR:HE2	2:B:204:HIS:CE1	2.37	0.43
2:O:29:MET:HB2	9:V:35:TYR:CE2	2.53	0.43
2:O:184:LEU:HD23	2:O:185:MET:N	2.33	0.43
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.19	0.43
26:C:270:CDL:H602	26:C:270:CDL:H632	1.81	0.43
25:G:1263:PEK:C9	3:P:244:PHE:HA	2.47	0.43
1:A:325:ALA:HA	22:B:230:PSC:H291	1.99	0.43
17:N:515:HEA:H122	17:N:515:HEA:HHC	2.00	0.43
1:N:109:PHE:CE2	1:N:112:LEU:HD22	2.53	0.43
9:V:47:TYR:HB2	27:V:4249:HOH:O	2.19	0.43
5:E:105:GLY:O	5:E:108:LYS:HE2	2.17	0.43
1:A:186:TRP:O	1:A:189:MET:N	2.52	0.43
7:T:31:CYS:SG	26:T:1269:CDL:C55	3.07	0.43
1:A:302:ARG:NH1	2:B:84:LEU:HD11	2.34	0.43
1:A:440:TYR:CE2	2:B:205:SER:HA	2.53	0.43
10:W:50:LEU:HD22	10:W:50:LEU:O	2.18	0.43
1:N:131:PRO:HG2	2:O:159:VAL:HA	2.00	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.74	0.43
1:N:450:TRP:HE3	1:N:453:ILE:HD12	1.83	0.43
1:A:104:LEU:C	1:A:107:PRO:HD2	2.39	0.43
5:R:14:ARG:HB3	5:R:14:ARG:NH1	2.33	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43
5:R:40:ASP:CG	9:V:11:GLY:HA2	2.39	0.43
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.78	0.43
4:Q:60:TYR:OH	4:Q:67:SER:HA	2.19	0.43
1:N:51:ASP:HB2	2:O:202:SER:O	2.19	0.43
26:T:1269:CDL:H141	27:T:4142:HOH:O	2.17	0.43
1:A:35:LEU:HD11	1:A:462:LEU:HD13	2.01	0.43
2:O:3:TYR:CE1	2:O:6:GLN:HG3	2.54	0.43
2:O:190:GLY:HA3	27:O:4222:HOH:O	2.18	0.43
6:F:14:THR:OG1	6:F:15:GLY:N	2.51	0.43
25:C:265:PEK:H382	1:N:279:SER:OG	2.19	0.43
1:A:65:MET:HB3	17:A:515:HEA:HAC	2.00	0.43
1:A:293:PHE:HB2	1:A:364:ASP:OD1	2.19	0.43
25:P:1265:PEK:H21	27:P:4191:HOH:O	2.19	0.42
1:N:243:VAL:HA	1:N:246:LEU:HD12	1.99	0.42
7:G:23:LEU:C	7:G:26:PRO:HD2	2.39	0.42
2:B:12:ALA:HB3	9:I:47:TYR:HE2	1.84	0.42
6:S:87:THR:HG22	27:S:3350:HOH:O	2.18	0.42
4:Q:102:TYR:HD1	13:Z:35:TYR:HE1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:188:ARG:HB3	2:O:189:PRO:HD2	2.01	0.42
1:N:75:ILE:O	1:N:79:GLY:HA3	2.18	0.42
1:A:344:PHE:C	1:A:344:PHE:CD1	2.92	0.42
2:B:59:GLN:NE2	25:P:1265:PEK:O04	2.52	0.42
17:N:516:HEA:H241	2:O:72:ILE:HG21	1.98	0.42
1:A:324:LEU:HD13	2:B:41:ILE:CG2	2.48	0.42
1:A:278:MET:HB3	7:T:5:LYS:HD3	2.02	0.42
1:A:176:MET:HG3	1:A:180:GLN:HB3	2.00	0.42
4:Q:109:HIS:C	4:Q:111:PHE:H	2.22	0.42
2:B:13:THR:O	2:B:187:SER:HB2	2.19	0.42
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.49	0.42
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.83	0.42
3:P:241:TYR:O	3:P:244:PHE:HB3	2.19	0.42
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.76	0.42
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.59	0.42
2:O:22:HIS:CD2	2:O:26:HIS:HE1	2.38	0.42
2:O:216:LEU:HB3	27:O:4168:HOH:O	2.18	0.42
2:O:108:TYR:CE1	2:O:142:VAL:CG2	3.02	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.52	0.42
8:H:65:PRO:O	8:H:69:VAL:HG23	2.19	0.42
3:P:198:PHE:CD2	25:T:1264:PEK:C03	3.02	0.42
4:D:102:TYR:CD1	13:M:35:TYR:CE1	3.04	0.42
23:P:1271:CHD:H222	23:P:1271:CHD:H162	1.54	0.42
3:P:57:TRP:O	3:P:61:VAL:HG23	2.19	0.42
1:A:35:LEU:HD11	1:A:462:LEU:HB2	2.01	0.42
4:D:124:LEU:O	4:D:140:TYR:OH	2.30	0.42
7:T:38:HIS:NE2	26:T:1269:CDL:HA21	2.34	0.42
7:G:30:LEU:CD1	26:G:269:CDL:H252	2.49	0.42
2:B:41:ILE:HD13	22:B:230:PSC:H342	2.01	0.42
1:N:416:ILE:CG2	1:N:464:ALA:HB2	2.49	0.42
1:A:484:THR:HG22	27:A:4238:HOH:O	2.18	0.42
6:S:74:LEU:HD11	6:S:89:TYR:O	2.19	0.42
1:N:325:ALA:O	1:N:328:HIS:HB3	2.20	0.42
2:O:99:THR:HG22	2:O:152:MET:CE	2.49	0.42
2:O:146:MET:CE	9:V:56:SER:HB2	2.49	0.42
5:R:5:HIS:HB3	5:R:6:GLU:H	1.67	0.42
27:N:4241:HOH:O	2:O:58:ALA:HB3	2.20	0.42
5:R:61:PHE:HE1	5:R:98:ILE:HA	1.83	0.42
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.94	0.42
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.59	0.42
12:L:25:MET:HG2	18:L:522:TGL:HA62	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:PHE:HA	25:T:263:PEK:H9	2.01	0.42
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.00	0.42
2:B:66:THR:CG2	2:B:67:ILE:N	2.80	0.42
2:B:138:VAL:HG22	2:B:210:VAL:HG21	2.02	0.42
4:D:109:HIS:C	4:D:111:PHE:H	2.22	0.42
6:S:76:LYS:HE2	6:S:93:PRO:HG3	1.99	0.42
2:O:37:LEU:HD12	2:O:37:LEU:HA	1.89	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.42
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.54	0.42
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.88	0.42
7:T:2:SER:O	7:T:3:ALA:HB3	2.20	0.42
4:Q:130:PRO:HG2	4:Q:131:ILE:CD1	2.49	0.42
1:N:62:ALA:HB3	1:N:126:TRP:HB3	2.01	0.42
4:D:94:LEU:HD23	11:K:28:VAL:CG2	2.50	0.42
2:B:3:TYR:CE1	2:B:6:GLN:HG3	2.54	0.42
5:E:52:LEU:HA	5:E:52:LEU:HD23	1.87	0.42
6:S:57:ILE:HG13	6:S:73:TRP:CZ3	2.55	0.42
1:A:231:TYR:C	1:A:231:TYR:CD1	2.92	0.42
1:A:258:VAL:HG13	1:A:327:LEU:CD2	2.50	0.42
3:C:187:THR:HA	25:C:264:PEK:O12	2.20	0.42
17:N:516:HEA:HMB1	17:N:516:HEA:H11	1.86	0.42
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.19	0.42
10:J:36:MET:O	10:J:40:LEU:HG	2.20	0.42
2:B:155:SER:O	2:B:174:ALA:HB1	2.19	0.42
3:C:30:GLY:HA2	3:C:42:LEU:HB3	2.02	0.42
1:A:104:LEU:HD23	3:C:21:ALA:HA	2.02	0.42
2:O:143:VAL:HG12	2:O:219:PHE:HD1	1.84	0.42
2:O:84:LEU:HD12	2:O:87:MET:HE2	2.00	0.42
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.67	0.42
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.85	0.42
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.51	0.42
1:A:446:ALA:HB1	2:B:3:TYR:C	2.41	0.42
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.54	0.42
13:Z:6:ALA:O	13:Z:9:PRO:HD3	2.20	0.42
7:T:24:ALA:O	7:T:27:SER:HB2	2.19	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
25:C:265:PEK:H371	26:G:269:CDL:C27	2.50	0.42
1:A:325:ALA:O	1:A:328:HIS:HB3	2.20	0.42
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.55	0.42
3:P:132:LEU:O	3:P:136:VAL:HG23	2.20	0.42
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:84:TYR:CZ	5:R:88:GLU:HG3	2.54	0.42
3:P:60:ASP:HA	3:P:63:ARG:HD2	2.02	0.41
4:Q:130:PRO:O	4:Q:136:ALA:HB2	2.20	0.41
2:O:224:ALA:O	2:O:227:LEU:CG	2.65	0.41
2:O:135:LEU:O	2:O:208:PRO:HG3	2.19	0.41
3:C:68:GLN:HB2	3:C:70:HIS:CD2	2.55	0.41
8:U:43:MET:HE3	8:U:43:MET:HB3	1.88	0.41
5:E:49:ASP:OD2	5:E:92:THR:HG21	2.20	0.41
3:C:128:GLU:OE1	7:G:38:HIS:HB3	2.20	0.41
4:Q:84:ALA:O	4:Q:88:PHE:HD1	2.03	0.41
5:E:89:LEU:O	5:E:93:LEU:HG	2.20	0.41
11:K:32:MET:HE2	11:K:32:MET:HB3	2.01	0.41
7:G:25:LEU:HA	7:G:25:LEU:HD23	1.76	0.41
4:D:24:LEU:HD12	5:E:30:ARG:HA	2.02	0.41
3:C:67:PHE:HA	10:J:9:GLN:HG2	2.03	0.41
12:L:46:LYS:O	12:L:47:LYS:HB2	2.20	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.91	0.41
3:P:41:THR:O	3:P:44:MET:HB2	2.20	0.41
4:Q:34:SER:OG	4:Q:37:GLN:HG3	2.20	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.41
4:D:77:GLU:HA	11:K:10:HIS:CD2	2.55	0.41
1:N:258:VAL:HG13	1:N:327:LEU:CD2	2.51	0.41
3:C:231:HIS:CG	19:C:267:PGV:H061	2.55	0.41
1:A:243:VAL:HB	17:A:516:HEA:CAC	2.50	0.41
18:N:1523:TGL:H212	18:N:1523:TGL:H242	1.79	0.41
8:H:27:ARG:O	8:H:31:GLN:N	2.44	0.41
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.81	0.41
10:J:45:TYR:O	10:J:48:TYR:HB3	2.20	0.41
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.02	0.41
3:P:231:HIS:CG	19:P:1267:PGV:H061	2.56	0.41
1:A:425:PHE:HZ	17:A:515:HEA:C2B	2.34	0.41
1:A:197:LEU:HB2	1:A:285:PHE:CZ	2.56	0.41
3:C:146:TRP:CE3	3:C:162:ALA:HB2	2.56	0.41
3:P:30:GLY:CA	3:P:42:LEU:HB3	2.49	0.41
2:O:79:PRO:O	2:O:83:ILE:HG13	2.20	0.41
1:A:512:ASN:HB3	6:F:38:ALA:HB2	2.01	0.41
2:O:175:ILE:HA	2:O:176:PRO:HD2	1.82	0.41
8:U:50:VAL:HG12	8:U:50:VAL:O	2.20	0.41
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.95	0.41
5:R:9:GLU:CD	5:R:9:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:87:PHE:C	4:Q:87:PHE:CD2	2.94	0.41
7:T:31:CYS:O	7:T:35:SER:HB2	2.21	0.41
3:P:42:LEU:HA	3:P:42:LEU:HD23	1.83	0.41
12:Y:20:ARG:NH1	12:Y:20:ARG:HB3	2.36	0.41
3:P:108:PRO:HA	27:P:3207:HOH:O	2.20	0.41
2:O:207:MET:HG3	2:O:207:MET:O	2.21	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
2:B:146:MET:HG2	2:B:214:VAL:O	2.21	0.41
19:A:525:PGV:H182	3:C:28:THR:HG22	2.02	0.41
3:P:224:LYS:C	3:P:225:PHE:HD1	2.24	0.41
1:N:443:TYR:N	1:N:443:TYR:CD2	2.88	0.41
1:N:440:TYR:HE1	2:O:195:GLN:NE2	2.17	0.41
1:A:184:PHE:O	1:A:188:VAL:HG23	2.21	0.41
1:N:105:LEU:HA	1:N:108:SER:HB3	2.02	0.41
7:G:3:ALA:CB	25:G:1263:PEK:H382	2.40	0.41
1:A:94:PHE:HB3	19:A:525:PGV:O11	2.21	0.41
3:P:205:GLY:O	3:P:208:VAL:HB	2.21	0.41
8:H:67:SER:HA	8:H:70:SER:HB3	2.03	0.41
1:N:161:ALA:HB1	1:N:192:ALA:O	2.20	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.56	0.41
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.02	0.41
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.83	0.41
3:C:138:LEU:HA	3:C:138:LEU:HD23	1.93	0.41
7:G:33:LEU:HD22	7:G:33:LEU:HA	1.88	0.41
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.24	0.41
3:P:103:HIS:HA	19:P:1268:PGV:O04	2.21	0.41
12:Y:11:ILE:HG22	18:Y:1522:TGL:H271	2.02	0.41
12:Y:13:PHE:CA	18:Y:1522:TGL:HC31	2.38	0.41
3:P:60:ASP:O	3:P:64:GLU:HG3	2.21	0.41
1:N:381:LEU:HD23	1:N:381:LEU:HA	1.92	0.41
6:F:72:PHE:CE2	6:F:83:PRO:HD3	2.56	0.41
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.39	0.41
6:S:82:CYS:HA	6:S:83:PRO:HD3	1.93	0.41
2:O:12:ALA:HB3	9:V:47:TYR:HE2	1.84	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.41
4:D:38:LYS:HE2	27:D:4155:HOH:O	2.21	0.41
4:Q:31:LYS:HB3	27:Q:4171:HOH:O	2.20	0.41
1:N:262:SER:HA	1:N:332:ILE:HD13	2.03	0.41
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.96	0.41
4:D:130:PRO:O	4:D:136:ALA:HB2	2.20	0.41
4:Q:94:LEU:CD2	11:X:28:VAL:HG21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:TYR:CD1	1:A:479:LYS:HA	2.56	0.41
5:E:53:ARG:O	5:E:57:ARG:HG3	2.21	0.41
1:N:150:LEU:HD23	1:N:150:LEU:HA	1.81	0.41
3:C:188:ILE:HG22	25:C:264:PEK:O13	2.21	0.40
22:B:230:PSC:H072	9:I:10:ARG:NH2	2.30	0.40
3:C:248:VAL:HG22	25:T:263:PEK:H15	2.02	0.40
23:J:60:CHD:H112	23:J:60:CHD:H12A	1.88	0.40
1:A:378:HIS:CD2	1:A:425:PHE:CE2	3.08	0.40
1:N:58:VAL:HG13	17:N:515:HEA:HBA1	2.02	0.40
1:A:313:ALA:HB3	2:B:73:LEU:HD11	2.02	0.40
1:A:189:MET:HB3	1:A:189:MET:HE3	1.98	0.40
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	2.03	0.40
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.40
1:A:402:GLY:O	1:A:482:VAL:HG23	2.21	0.40
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.84	0.40
1:A:202:LEU:HB2	1:A:238:PHE:CG	2.56	0.40
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.56	0.40
1:N:96:ARG:NH2	3:P:61:VAL:HG22	2.35	0.40
1:A:132:LEU:HD23	2:B:199:ILE:HG23	2.03	0.40
1:N:467:LEU:O	1:N:471:ILE:HG13	2.21	0.40
1:A:19:TYR:CG	1:A:76:GLY:HA3	2.55	0.40
5:E:54:ALA:O	5:E:58:LEU:HD12	2.20	0.40
10:W:32:TYR:CD2	10:W:32:TYR:C	2.94	0.40
3:C:250:LEU:HA	3:C:250:LEU:HD23	1.66	0.40
3:C:59:ARG:O	3:C:63:ARG:HG3	2.21	0.40
7:G:8:HIS:HA	7:G:11:TPO:O1P	2.21	0.40
26:G:269:CDL:C27	1:N:282:PHE:HE2	2.35	0.40
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	2.03	0.40
2:O:191:LEU:HD23	2:O:191:LEU:HA	1.96	0.40
2:O:95:LEU:HD12	2:O:96:THR:H	1.86	0.40
2:B:14:SER:HB3	2:B:168:LEU:HD22	2.04	0.40
11:X:43:SER:HA	11:X:44:PRO:HD3	1.91	0.40
5:E:37:VAL:HG11	5:E:70:VAL:HG21	2.03	0.40
13:M:37:LEU:O	13:M:40:TYR:HB2	2.21	0.40
3:C:157:LYS:HB3	3:C:157:LYS:HE2	1.93	0.40
3:P:158:HIS:CE1	25:P:1265:PEK:H051	2.56	0.40
1:N:243:VAL:HB	17:N:516:HEA:CAC	2.51	0.40
26:G:269:CDL:H421	1:N:311:ILE:HG13	2.04	0.40
10:W:40:LEU:HD12	23:W:1060:CHD:H183	2.04	0.40
2:B:175:ILE:HA	2:B:176:PRO:HD2	1.85	0.40
1:N:288:TRP:O	1:N:291:HIS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:LEU:HD22	5:E:64:ALA:HB1	2.03	0.40
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.21	0.40
2:O:32:PHE:HD2	2:O:32:PHE:HA	1.79	0.40
1:N:42:GLY:HA3	4:Q:104:TYR:HH	1.82	0.40
3:P:62:ILE:CD1	3:P:221:ARG:HD2	2.45	0.40
3:C:57:TRP:O	3:C:57:TRP:HD1	2.04	0.40
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.57	0.40
1:N:365:ILE:O	2:O:171:LYS:NZ	2.47	0.40
3:P:109:THR:HA	27:P:4232:HOH:O	2.20	0.40
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.40
12:Y:9:LYS:HA	12:Y:9:LYS:HD3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	466 (91%)	42 (8%)	4 (1%)	24	51
1	N	512/514 (100%)	469 (92%)	40 (8%)	3 (1%)	30	59
2	B	225/227 (99%)	202 (90%)	20 (9%)	3 (1%)	15	37
2	O	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	6	16
3	C	257/261 (98%)	247 (96%)	9 (4%)	1 (0%)	39	69
3	P	257/261 (98%)	246 (96%)	10 (4%)	1 (0%)	39	69
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	80 (83%)	12 (12%)	4 (4%)	3	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	96/98 (98%)	83 (86%)	9 (9%)	4 (4%)	3	7
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	1	0
7	T	81/85 (95%)	61 (75%)	12 (15%)	8 (10%)	1	0
8	H	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	4	8
8	U	77/85 (91%)	66 (86%)	8 (10%)	3 (4%)	4	8
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	11	27
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	11	27
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	1 (2%)	1 (2%)	8	20
13	M	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
13	Z	41/46 (89%)	36 (88%)	5 (12%)	0	100	100
All	All	3504/3614 (97%)	3204 (91%)	249 (7%)	51 (2%)	13	32

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	93	PRO
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
2	O	60	GLU
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	89	GLU

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Mol	Chain	Res	Type
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	10	ASN
1	N	9	SER
2	O	89	GLU
7	T	3	ALA
8	U	8	ILE
8	U	10	ASN
6	F	96	LEU
6	S	96	LEU
7	T	40	GLY
1	A	9	SER
7	G	54	ARG
1	N	91	ASP
3	P	38	ASN
10	W	15	ASP
1	A	91	ASP
1	A	369	ASP
3	C	38	ASN
10	J	15	ASP
2	O	59	GLN
2	O	202	SER
2	B	92	ASN
2	O	92	ASN
7	T	6	GLY
12	Y	28	PHE
7	G	6	GLY
1	A	174	PRO
8	H	47	GLY
7	T	49	PRO
8	U	47	GLY
1	N	296	GLY
2	O	159	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	54	83
1	N	426/426 (100%)	412 (97%)	14 (3%)	45	76
2	B	210/210 (100%)	192 (91%)	18 (9%)	13	29
2	O	210/210 (100%)	190 (90%)	20 (10%)	11	24
3	C	224/226 (99%)	213 (95%)	11 (5%)	31	61
3	P	224/226 (99%)	220 (98%)	4 (2%)	66	89
4	D	128/129 (99%)	123 (96%)	5 (4%)	39	70
4	Q	128/129 (99%)	123 (96%)	5 (4%)	39	70
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	76
5	R	92/95 (97%)	88 (96%)	4 (4%)	35	66
6	F	81/81 (100%)	80 (99%)	1 (1%)	78	93
6	S	81/81 (100%)	74 (91%)	7 (9%)	13	29
7	G	67/68 (98%)	61 (91%)	6 (9%)	12	27
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	27
8	H	71/75 (95%)	66 (93%)	5 (7%)	19	42
8	U	71/75 (95%)	66 (93%)	5 (7%)	19	42
9	I	57/57 (100%)	53 (93%)	4 (7%)	19	42
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	74
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	87
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	87
11	K	39/46 (85%)	37 (95%)	2 (5%)	29	59
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	59
12	L	39/40 (98%)	37 (95%)	2 (5%)	29	59
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	59
13	M	37/38 (97%)	29 (78%)	8 (22%)	1	3
13	Z	37/38 (97%)	30 (81%)	7 (19%)	2	5
All	All	3040/3082 (99%)	2884 (95%)	156 (5%)	29	59

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	189	MET
1	A	238	PHE
1	A	241	PRO
1	A	336	PRO
1	A	369	ASP
1	A	377	PHE
1	A	444	PRO
1	A	503	HIS
2	B	3	TYR
2	B	16	ILE
2	B	21	LEU
2	B	43	SER
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	130	PRO
2	B	152	MET
2	B	167	SER
2	B	183	THR
2	B	185	MET
2	B	187	SER
2	B	199	ILE
3	C	13	PRO
3	C	17	PRO
3	C	39	SER
3	C	73	PRO
3	C	110	PRO
3	C	144	ILE
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	51	LEU
4	D	74	SER
4	D	108	PRO
4	D	121	LYS

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Mol	Chain	Res	Type
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	27	ARG
8	H	29	CYS
8	H	60	TYR
8	H	62	SER
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	32	MET
11	K	54	ARG
12	L	15	VAL
12	L	26	THR
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	174	PRO
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	298	ASP
1	N	338	MET
1	N	356	ILE

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Mol	Chain	Res	Type
1	N	369	ASP
1	N	444	PRO
1	N	484	THR
1	N	498	CYS
2	O	3	TYR
2	O	16	ILE
2	O	43	SER
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	107	SER
2	O	110	TYR
2	O	115	ASP
2	O	156	SER
2	O	158	ASP
2	O	166	PRO
2	O	167	SER
2	O	183	THR
2	O	187	SER
2	O	223	SER
3	P	150	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	10	ASP
4	Q	51	LEU
4	Q	110	THR
4	Q	121	LYS
5	R	5	HIS
5	R	80	GLU
5	R	87	GLN
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	50	PRO
6	S	53	THR
6	S	68	THR

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Mol	Chain	Res	Type
6	S	80	GLN
6	S	94	HIS
7	T	17	ARG
7	T	27	SER
7	T	33	LEU
7	T	35	SER
7	T	54	ARG
7	T	84	LYS
8	U	9	LYS
8	U	12	GLN
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	18	ARG
10	W	50	LEU
11	X	38	ILE
11	X	54	ARG
12	Y	11	ILE
12	Y	26	THR
13	Z	12	PRO
13	Z	13	LYS
13	Z	34	LEU
13	Z	37	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	151	HIS
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN

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Mol	Chain	Res	Type
3	C	204	HIS
4	D	32	ASN
4	D	37	GLN
5	E	94	ASN
7	G	8	HIS
7	G	66	ASN
7	G	71	HIS
9	I	20	HIS
10	J	21	HIS
11	K	35	GLN
11	K	41	ASN
1	N	55	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	491	ASN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
7	T	34	ASN
7	T	66	ASN
9	V	8	GLN
10	W	9	GLN
10	W	29	ASN
11	X	35	GLN
11	X	41	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	8,9,10	0.66	0	6,9,11	1.22	0
2	FME	B	1	2	8,9,10	0.68	0	6,9,11	1.57	1 (16%)
7	TPO	G	11	7	8,10,11	1.85	2 (25%)	7,14,16	1.01	0
9	SAC	I	1	9	7,8,9	2.76	2 (28%)	7,9,11	1.96	3 (42%)
1	FME	N	1	1	8,9,10	0.91	0	6,9,11	1.00	0
2	FME	O	1	2	8,9,10	0.55	0	6,9,11	1.16	1 (16%)
7	TPO	T	11	7	8,10,11	1.80	3 (37%)	7,14,16	0.97	0
9	SAC	V	1	9	7,8,9	3.04	2 (28%)	7,9,11	2.21	4 (57%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.45	1.59	1.51
7	G	11	TPO	CG2-CB	2.74	1.58	1.51
7	T	11	TPO	CG2-CB	2.75	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.91	1.59	1.54
7	G	11	TPO	CB-CA	3.67	1.60	1.54
9	I	1	SAC	CA-N	4.56	1.52	1.46
9	V	1	SAC	OAC-C1A	5.26	1.35	1.23
9	I	1	SAC	OAC-C1A	5.30	1.35	1.23
9	V	1	SAC	CA-N	5.46	1.54	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-3.26	117.80	122.82
9	V	1	SAC	CA-N-C1A	-3.10	110.85	121.37
9	I	1	SAC	CA-N-C1A	-3.04	111.06	121.37
9	V	1	SAC	OAC-C1A-C2A	-2.47	117.52	122.06
2	O	1	FME	CA-N-CN	-2.35	119.21	122.82
9	I	1	SAC	C2A-C1A-N	2.24	120.39	116.11
9	I	1	SAC	CB-CA-N	2.49	116.05	110.60
9	V	1	SAC	C2A-C1A-N	2.66	121.19	116.11
9	V	1	SAC	CB-CA-N	2.69	116.50	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 20 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$
17	HEA	A	515	1	40,67,67	1.38	5 (12%)	41,103,103	2.15	12 (29%)
17	HEA	A	516	1	40,67,67	1.54	9 (22%)	41,103,103	1.70	8 (19%)
18	TGL	A	521	-	62,62,62	0.97	3 (4%)	65,65,65	1.56	10 (15%)
18	TGL	A	523	-	62,62,62	1.11	5 (8%)	65,65,65	1.49	10 (15%)
19	PGV	A	524	-	50,50,50	1.49	8 (16%)	51,56,56	1.08	4 (7%)
19	PGV	A	525	-	50,50,50	1.12	5 (10%)	51,56,56	0.99	2 (3%)
23	CHD	B	1086	-	29,32,32	0.86	0	48,51,51	2.47	20 (41%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.56	11 (21%)	55,59,59	1.15	4 (7%)
25	PEK	C	264	-	51,52,52	2.05	13 (25%)	52,57,57	1.65	12 (23%)
25	PEK	C	265	-	51,52,52	1.90	12 (23%)	52,57,57	1.14	4 (7%)
19	PGV	C	267	-	50,50,50	1.05	3 (6%)	51,56,56	1.07	5 (9%)
19	PGV	C	268	-	50,50,50	1.56	9 (18%)	51,56,56	0.92	2 (3%)
26	CDL	C	270	-	99,99,99	1.20	10 (10%)	101,111,111	0.99	6 (5%)
23	CHD	C	271	-	29,32,32	1.25	4 (13%)	48,51,51	3.76	23 (47%)
24	DMU	C	272	-	34,34,34	2.68	14 (41%)	45,45,45	4.10	18 (40%)
23	CHD	C	525	-	29,32,32	1.22	2 (6%)	48,51,51	2.12	15 (31%)
25	PEK	G	1263	-	51,52,52	2.38	15 (29%)	52,57,57	1.36	7 (13%)
26	CDL	G	269	-	99,99,99	1.50	14 (14%)	101,111,111	1.02	9 (8%)
23	CHD	G	86	-	29,32,32	1.13	3 (10%)	48,51,51	2.61	21 (43%)
23	CHD	J	60	-	29,32,32	1.49	3 (10%)	48,51,51	3.74	25 (52%)
18	TGL	L	522	-	62,62,62	1.32	5 (8%)	65,65,65	1.71	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	M	526	-	34,34,34	3.30	9 (26%)	45,45,45	3.57	21 (46%)
19	PGV	N	1266	-	50,50,50	1.24	6 (12%)	51,56,56	0.93	2 (3%)
18	TGL	N	1523	-	62,62,62	1.12	4 (6%)	65,65,65	1.51	9 (13%)
19	PGV	N	1524	-	50,50,50	1.50	8 (16%)	51,56,56	1.04	5 (9%)
17	HEA	N	515	1	40,67,67	1.55	7 (17%)	41,103,103	2.15	14 (34%)
17	HEA	N	516	1	40,67,67	1.35	8 (20%)	41,103,103	1.71	8 (19%)
22	PSC	O	1230	-	51,51,51	1.62	12 (23%)	55,59,59	1.10	4 (7%)
18	TGL	O	1521	-	62,62,62	1.02	5 (8%)	65,65,65	1.58	10 (15%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
25	PEK	P	1265	-	51,52,52	1.86	12 (23%)	52,57,57	1.13	4 (7%)
19	PGV	P	1267	-	50,50,50	1.10	4 (8%)	51,56,56	0.89	1 (1%)
19	PGV	P	1268	-	50,50,50	1.58	9 (18%)	51,56,56	0.90	2 (3%)
26	CDL	P	1270	-	99,99,99	1.24	12 (12%)	101,111,111	1.03	6 (5%)
23	CHD	P	1271	-	29,32,32	1.30	6 (20%)	48,51,51	3.83	25 (52%)
24	DMU	P	1272	-	34,34,34	2.75	14 (41%)	45,45,45	3.96	20 (44%)
23	CHD	P	1525	-	29,32,32	1.44	4 (13%)	48,51,51	2.05	14 (29%)
25	PEK	T	1264	-	51,52,52	2.15	13 (25%)	52,57,57	1.62	10 (19%)
26	CDL	T	1269	-	99,99,99	1.41	14 (14%)	101,111,111	1.02	8 (7%)
25	PEK	T	263	-	51,52,52	2.40	15 (29%)	52,57,57	1.33	8 (15%)
23	CHD	W	1060	-	29,32,32	1.77	5 (17%)	48,51,51	3.67	25 (52%)
18	TGL	Y	1522	-	62,62,62	1.37	5 (8%)	65,65,65	1.65	9 (13%)
24	DMU	Z	1526	-	34,34,34	3.29	8 (23%)	45,45,45	3.49	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
17	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
18	TGL	A	521	-	-	0/65/65/65	0/0/0/0
18	TGL	A	523	-	-	0/65/65/65	0/0/0/0
19	PGV	A	524	-	-	2/55/55/55	0/0/0/0
19	PGV	A	525	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSC	B	230	-	-	0/55/55/55	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	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
23	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
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	G	86	-	-	0/7/74/74	0/4/4/4
23	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
18	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
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
17	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
18	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	1265	-	-	0/56/56/56	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
23	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
25	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
18	TGL	Y	1522	-	-	0/65/65/65	0/0/0/0
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.02	1.23	1.43
24	Z	1526	DMU	O16-C6	-7.92	1.25	1.40
24	Z	1526	DMU	O7-C3	-7.75	1.24	1.43
24	M	526	DMU	O16-C6	-7.68	1.26	1.40
24	Z	1526	DMU	O5-C4	-7.24	1.26	1.44
24	M	526	DMU	O1-C9	-7.05	1.26	1.44
24	Z	1526	DMU	O1-C9	-6.92	1.27	1.44
24	M	526	DMU	O5-C4	-6.91	1.27	1.44
24	Z	1526	DMU	O16-C18	-6.76	1.24	1.42
24	M	526	DMU	O16-C18	-6.74	1.24	1.42
24	M	526	DMU	O7-C10	-6.08	1.25	1.41
24	Z	1526	DMU	O7-C10	-5.94	1.25	1.41
24	P	1272	DMU	O16-C18	-5.69	1.27	1.42
24	C	272	DMU	O16-C18	-5.56	1.27	1.42
24	M	526	DMU	O1-C10	-5.48	1.27	1.41
24	P	1272	DMU	O7-C3	-5.04	1.31	1.43
24	Z	1526	DMU	O1-C10	-4.98	1.29	1.41
24	Z	1526	DMU	O5-C6	-4.75	1.29	1.41
24	M	526	DMU	O5-C6	-4.31	1.30	1.41
23	P	1525	CHD	C10-C9	-4.17	1.47	1.56
17	N	515	HEA	C3C-C2C	-4.12	1.34	1.40
24	P	1272	DMU	O16-C6	-3.98	1.32	1.40
24	C	272	DMU	O5-C4	-3.90	1.34	1.44
17	N	515	HEA	C3A-C2A	-3.86	1.35	1.40
17	A	515	HEA	C3A-CMA	-3.78	1.37	1.46
23	C	525	CHD	C10-C9	-3.74	1.48	1.56
23	P	1525	CHD	C13-C12	-3.70	1.48	1.54
24	C	272	DMU	O7-C3	-3.68	1.34	1.43
24	C	272	DMU	O1-C9	-3.53	1.35	1.44
17	A	516	HEA	C3C-C2C	-3.53	1.35	1.40
17	N	515	HEA	C3A-CMA	-3.50	1.38	1.46
24	C	272	DMU	O16-C6	-3.44	1.33	1.40
23	G	86	CHD	C1-C10	-3.38	1.47	1.54
17	A	516	HEA	C4C-CHD	-3.30	1.30	1.39
24	P	1272	DMU	O5-C4	-3.08	1.36	1.44
17	N	515	HEA	C3B-C2B	-3.05	1.30	1.41
17	A	515	HEA	C3A-C2A	-3.04	1.36	1.40
17	N	516	HEA	C4C-CHD	-3.02	1.31	1.39
17	A	515	HEA	C3C-C2C	-2.86	1.36	1.40
17	A	516	HEA	C3A-C2A	-2.75	1.36	1.40
23	C	525	CHD	C13-C12	-2.69	1.50	1.54
17	N	516	HEA	C3C-C2C	-2.56	1.36	1.40
17	A	516	HEA	C1B-CHB	-2.53	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	1525	CHD	C18-C13	-2.46	1.50	1.54
17	A	516	HEA	C3A-CMA	-2.45	1.40	1.46
17	A	515	HEA	C3B-C2B	-2.39	1.32	1.41
17	N	516	HEA	C3A-CMA	-2.39	1.40	1.46
23	P	1525	CHD	C10-C5	-2.36	1.51	1.55
24	C	272	DMU	O7-C10	-2.34	1.35	1.41
17	A	516	HEA	C1D-ND	-2.34	1.33	1.36
24	P	1272	DMU	O7-C10	-2.33	1.35	1.41
24	P	1272	DMU	O1-C9	-2.33	1.38	1.44
17	N	516	HEA	C3A-C2A	-2.26	1.37	1.40
17	N	516	HEA	C3B-C2B	-2.17	1.33	1.41
23	G	86	CHD	C10-C5	-2.17	1.51	1.55
17	A	515	HEA	CMD-C2D	-2.02	1.47	1.51
17	N	515	HEA	C16-C15	2.00	1.55	1.51
23	C	271	CHD	C8-C14	2.01	1.57	1.53
25	P	1265	PEK	C2-C1	2.02	1.56	1.50
19	N	1524	PGV	C06-C05	2.02	1.60	1.52
19	C	267	PGV	C03-C02	2.03	1.56	1.50
22	O	1230	PSC	C05-C04	2.05	1.58	1.51
26	P	1270	CDL	CB2-C1	2.05	1.59	1.51
19	N	1524	PGV	P-O12	2.06	1.68	1.59
18	O	1521	TGL	CC2-CC1	2.06	1.56	1.50
22	B	230	PSC	C8-C9	2.07	1.59	1.50
19	P	1268	PGV	P-O11	2.08	1.68	1.59
19	C	268	PGV	C10-C11	2.08	1.59	1.50
25	C	264	PEK	P-O14	2.09	1.58	1.51
23	P	1271	CHD	C8-C7	2.10	1.56	1.53
22	O	1230	PSC	C20-C19	2.11	1.56	1.50
26	G	269	CDL	PA1-OA2	2.11	1.68	1.59
26	T	1269	CDL	PA1-OA2	2.11	1.68	1.59
22	B	230	PSC	P-O11	2.11	1.68	1.59
25	G	1263	PEK	C23-C22	2.12	1.60	1.52
19	C	268	PGV	C04-C05	2.12	1.59	1.51
25	C	264	PEK	C03-C02	2.13	1.56	1.50
26	T	1269	CDL	PA1-OA5	2.15	1.68	1.59
26	P	1270	CDL	PB2-OB5	2.15	1.68	1.59
24	M	526	DMU	C8-C9	2.16	1.57	1.53
26	C	270	CDL	OA6-CA5	2.16	1.40	1.34
25	T	263	PEK	C13-C14	2.16	1.62	1.51
19	A	525	PGV	C20-C19	2.17	1.57	1.50
19	P	1267	PGV	C20-C19	2.18	1.57	1.50
26	T	1269	CDL	C85-C84	2.18	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	PA1-OA5	2.19	1.69	1.59
25	T	1264	PEK	O03-C21	2.19	1.39	1.33
19	C	268	PGV	C06-C05	2.19	1.60	1.52
26	T	1269	CDL	OA8-CA7	2.20	1.39	1.33
18	A	523	TGL	CA2-CA1	2.20	1.57	1.50
22	O	1230	PSC	C03-C02	2.21	1.57	1.50
26	P	1270	CDL	OA6-CA5	2.21	1.40	1.34
17	N	516	HEA	C4B-NB	2.24	1.39	1.36
23	W	1060	CHD	C8-C14	2.24	1.58	1.53
22	O	1230	PSC	P-O11	2.26	1.69	1.59
19	A	524	PGV	P-O11	2.27	1.69	1.59
19	A	524	PGV	C06-C05	2.27	1.61	1.52
19	A	524	PGV	O01-C1	2.27	1.41	1.34
26	G	269	CDL	C11-CA5	2.27	1.57	1.50
23	P	1271	CHD	C13-C12	2.28	1.58	1.54
25	C	265	PEK	C01-C02	2.29	1.57	1.50
25	T	263	PEK	C4-C5	2.30	1.60	1.50
17	N	516	HEA	C22-C23	2.30	1.39	1.32
25	C	264	PEK	P-O11	2.30	1.69	1.59
26	C	270	CDL	OB6-CB5	2.31	1.41	1.34
25	T	1264	PEK	C01-C02	2.31	1.57	1.50
25	C	265	PEK	C2-C1	2.32	1.57	1.50
23	J	60	CHD	C8-C7	2.32	1.57	1.53
18	Y	1522	TGL	CC2-CC1	2.32	1.57	1.50
18	A	521	TGL	CA2-CA1	2.33	1.57	1.50
23	P	1271	CHD	C10-C5	2.33	1.59	1.55
18	L	522	TGL	OG1-CA1	2.34	1.40	1.33
19	P	1267	PGV	C01-C02	2.34	1.57	1.50
25	G	1263	PEK	O01-C1	2.36	1.41	1.34
26	C	270	CDL	C11-CA5	2.36	1.57	1.50
25	C	264	PEK	C16-C15	2.36	1.60	1.50
26	G	269	CDL	OB8-CB7	2.37	1.40	1.33
18	A	521	TGL	OG2-CB1	2.37	1.41	1.34
25	C	264	PEK	C22-C21	2.38	1.57	1.50
23	P	1271	CHD	C8-C9	2.38	1.58	1.53
22	O	1230	PSC	C8-C9	2.39	1.60	1.50
22	B	230	PSC	C01-C02	2.39	1.57	1.50
19	P	1268	PGV	P-O12	2.40	1.70	1.59
19	C	268	PGV	P-O12	2.40	1.70	1.59
19	N	1266	PGV	C20-C19	2.41	1.57	1.50
22	B	230	PSC	O03-C19	2.41	1.40	1.33
26	C	270	CDL	OA8-CA7	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	C31-CA7	2.42	1.57	1.50
26	P	1270	CDL	C31-CA7	2.43	1.57	1.50
17	A	516	HEA	C14-C15	2.43	1.37	1.33
19	N	1266	PGV	C03-C02	2.44	1.57	1.50
17	N	515	HEA	C20-C19	2.44	1.56	1.51
23	C	271	CHD	C13-C12	2.44	1.58	1.54
19	P	1268	PGV	C04-C05	2.44	1.61	1.51
19	P	1268	PGV	C06-C05	2.44	1.61	1.52
19	C	268	PGV	P-O11	2.46	1.70	1.59
23	C	271	CHD	C13-C14	2.47	1.59	1.55
19	A	524	PGV	P-O12	2.48	1.70	1.59
25	T	263	PEK	P-O12	2.49	1.70	1.59
22	B	230	PSC	C05-C04	2.49	1.59	1.51
18	O	1521	TGL	CA2-CA1	2.51	1.58	1.50
23	G	86	CHD	C8-C9	2.52	1.58	1.53
19	N	1524	PGV	O01-C1	2.52	1.41	1.34
26	P	1270	CDL	CA6-CA4	2.53	1.57	1.50
19	A	524	PGV	C03-C02	2.53	1.57	1.50
23	P	1271	CHD	C13-C17	2.54	1.60	1.55
19	N	1266	PGV	C01-C02	2.55	1.57	1.50
18	O	1521	TGL	OG3-CC1	2.56	1.41	1.33
23	W	1060	CHD	C8-C7	2.56	1.57	1.53
25	C	265	PEK	C03-C02	2.57	1.58	1.50
22	B	230	PSC	C03-C02	2.58	1.58	1.50
25	T	1264	PEK	C4-C5	2.58	1.61	1.50
22	O	1230	PSC	C01-C02	2.60	1.58	1.50
19	P	1268	PGV	C20-C19	2.61	1.58	1.50
25	C	264	PEK	C2-C1	2.62	1.58	1.50
25	P	1265	PEK	P-O12	2.63	1.71	1.59
19	A	525	PGV	O01-C1	2.64	1.42	1.34
25	G	1263	PEK	C4-C5	2.64	1.61	1.50
19	N	1524	PGV	C03-C02	2.65	1.58	1.50
22	O	1230	PSC	O03-C19	2.66	1.41	1.33
26	P	1270	CDL	CA3-CA4	2.67	1.58	1.50
19	N	1524	PGV	P-O11	2.68	1.71	1.59
18	A	523	TGL	OG3-CC1	2.70	1.41	1.33
19	A	525	PGV	O03-C19	2.71	1.41	1.33
26	C	270	CDL	C31-CA7	2.71	1.58	1.50
22	B	230	PSC	C2-C1	2.72	1.58	1.50
23	J	60	CHD	C20-C17	2.73	1.59	1.54
23	P	1271	CHD	C13-C14	2.73	1.60	1.55
25	G	1263	PEK	P-O12	2.75	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	1230	PSC	O01-C1	2.75	1.42	1.34
18	L	522	TGL	CG1-CG2	2.77	1.58	1.50
25	G	1263	PEK	C2-C1	2.78	1.59	1.50
25	P	1265	PEK	C01-C02	2.79	1.58	1.50
26	P	1270	CDL	C11-CA5	2.80	1.59	1.50
25	T	263	PEK	O03-C01	2.82	1.51	1.45
25	P	1265	PEK	C03-C02	2.83	1.58	1.50
17	A	516	HEA	C4B-NB	2.83	1.40	1.36
26	T	1269	CDL	C11-CA5	2.85	1.59	1.50
25	C	264	PEK	P-O12	2.85	1.72	1.59
23	W	1060	CHD	C13-C12	2.86	1.59	1.54
17	N	515	HEA	C1D-ND	2.87	1.40	1.36
25	P	1265	PEK	O01-C1	2.87	1.42	1.34
22	B	230	PSC	O01-C1	2.87	1.42	1.34
24	P	1272	DMU	C2-C3	2.88	1.60	1.52
18	N	1523	TGL	OG3-CC1	2.88	1.42	1.33
18	N	1523	TGL	CB2-CB1	2.89	1.59	1.50
18	Y	1522	TGL	CG1-CG2	2.90	1.58	1.50
26	G	269	CDL	CB3-CB4	2.90	1.58	1.50
25	T	1264	PEK	P-O12	2.91	1.72	1.59
26	T	1269	CDL	CB2-C1	2.91	1.63	1.51
18	Y	1522	TGL	OG1-CA1	2.92	1.42	1.33
26	P	1270	CDL	OB6-CB5	2.92	1.43	1.34
17	N	516	HEA	C21-C22	2.92	1.58	1.50
25	P	1265	PEK	P-O11	2.93	1.72	1.59
18	N	1523	TGL	CA2-CA1	2.93	1.59	1.50
25	C	264	PEK	O03-C21	2.93	1.42	1.33
18	A	523	TGL	OG1-CA1	2.93	1.42	1.33
19	P	1267	PGV	O03-C19	2.95	1.42	1.33
25	G	1263	PEK	O03-C01	2.95	1.51	1.45
18	O	1521	TGL	CG3-CG2	2.96	1.59	1.50
25	T	1264	PEK	C16-C15	2.97	1.63	1.50
26	T	1269	CDL	OB8-CB7	2.97	1.42	1.33
26	T	1269	CDL	OA6-CA5	3.01	1.43	1.34
19	C	267	PGV	C01-C02	3.02	1.59	1.50
19	A	525	PGV	C03-C02	3.03	1.59	1.50
26	G	269	CDL	OA8-CA7	3.04	1.42	1.33
25	C	265	PEK	P-O12	3.05	1.73	1.59
26	T	1269	CDL	CB3-CB4	3.06	1.59	1.50
18	L	522	TGL	CC2-CC1	3.06	1.59	1.50
23	C	271	CHD	C13-C17	3.07	1.61	1.55
18	A	523	TGL	OG2-CB1	3.07	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	CA6-CA4	3.07	1.59	1.50
22	O	1230	PSC	P-O12	3.08	1.73	1.59
24	C	272	DMU	C2-C1	3.08	1.60	1.52
19	P	1268	PGV	C2-C1	3.10	1.59	1.50
26	P	1270	CDL	C71-CB7	3.10	1.59	1.50
25	T	263	PEK	O01-C1	3.15	1.43	1.34
19	N	1266	PGV	C2-C1	3.15	1.60	1.50
26	G	269	CDL	CB2-C1	3.17	1.64	1.51
26	C	270	CDL	PB2-OB2	3.21	1.73	1.59
25	T	263	PEK	P-O11	3.21	1.73	1.59
26	C	270	CDL	CA3-CA4	3.22	1.59	1.50
18	O	1521	TGL	OG2-CB1	3.23	1.44	1.34
25	G	1263	PEK	C22-C21	3.25	1.60	1.50
19	N	1524	PGV	C20-C19	3.25	1.60	1.50
26	T	1269	CDL	CA6-CA4	3.26	1.59	1.50
19	C	268	PGV	C2-C1	3.28	1.60	1.50
25	C	265	PEK	C22-C21	3.29	1.60	1.50
19	C	268	PGV	O03-C19	3.29	1.43	1.33
26	C	270	CDL	C71-CB7	3.33	1.60	1.50
25	P	1265	PEK	C22-C21	3.36	1.60	1.50
25	G	1263	PEK	P-O11	3.36	1.74	1.59
25	T	1264	PEK	C22-C21	3.37	1.60	1.50
22	B	230	PSC	P-O12	3.39	1.74	1.59
17	A	516	HEA	C21-C22	3.39	1.60	1.50
26	P	1270	CDL	PB2-OB2	3.39	1.74	1.59
25	C	265	PEK	P-O11	3.41	1.74	1.59
18	A	523	TGL	CB2-CB1	3.42	1.60	1.50
24	P	1272	DMU	C2-C1	3.44	1.61	1.52
19	A	524	PGV	C20-C19	3.46	1.61	1.50
23	W	1060	CHD	C20-C17	3.46	1.60	1.54
26	P	1270	CDL	OB8-CB7	3.46	1.43	1.33
19	P	1268	PGV	O03-C19	3.47	1.43	1.33
25	P	1265	PEK	O03-C21	3.47	1.43	1.33
18	A	521	TGL	CG3-CG2	3.47	1.60	1.50
22	O	1230	PSC	C2-C1	3.49	1.61	1.50
26	C	270	CDL	OB8-CB7	3.51	1.43	1.33
18	N	1523	TGL	OG1-CA1	3.56	1.44	1.33
24	C	272	DMU	C10-C5	3.57	1.63	1.52
19	C	267	PGV	C12-C11	3.59	1.52	1.31
25	C	265	PEK	O03-C21	3.60	1.44	1.33
26	T	1269	CDL	CB6-CB4	3.62	1.60	1.50
19	P	1267	PGV	C12-C11	3.65	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	263	PEK	C2-C1	3.66	1.61	1.50
26	P	1270	CDL	OA8-CA7	3.67	1.44	1.33
24	C	272	DMU	C2-C3	3.67	1.62	1.52
19	N	1266	PGV	O03-C19	3.73	1.44	1.33
25	T	1264	PEK	P-O11	3.74	1.76	1.59
25	T	263	PEK	C22-C21	3.80	1.62	1.50
19	A	525	PGV	C12-C11	3.81	1.53	1.31
26	G	269	CDL	CB6-CB4	3.87	1.61	1.50
25	C	265	PEK	O01-C1	3.87	1.45	1.34
26	G	269	CDL	CA6-CA4	3.88	1.61	1.50
26	G	269	CDL	C71-CB7	3.88	1.62	1.50
25	C	265	PEK	C6-C5	3.88	1.54	1.31
18	L	522	TGL	CB2-CB1	3.89	1.62	1.50
26	T	1269	CDL	C51-CB5	3.90	1.62	1.50
19	N	1266	PGV	C12-C11	3.92	1.54	1.31
26	T	1269	CDL	OB6-CB5	3.93	1.46	1.34
18	Y	1522	TGL	CB2-CB1	3.93	1.62	1.50
26	T	1269	CDL	C71-CB7	3.97	1.62	1.50
25	P	1265	PEK	C6-C5	4.01	1.54	1.31
24	C	272	DMU	C8-C7	4.02	1.62	1.52
24	P	1272	DMU	C10-C5	4.09	1.64	1.52
26	G	269	CDL	C51-CB5	4.11	1.62	1.50
24	C	272	DMU	C5-C7	4.12	1.63	1.52
25	C	265	PEK	C9-C8	4.17	1.55	1.31
26	G	269	CDL	OA6-CA5	4.22	1.46	1.34
25	T	1264	PEK	C12-C11	4.27	1.56	1.31
24	P	1272	DMU	C5-C7	4.30	1.63	1.52
22	B	230	PSC	C13-C12	4.31	1.56	1.31
19	N	1524	PGV	C12-C11	4.33	1.56	1.31
22	O	1230	PSC	C13-C12	4.33	1.56	1.31
25	C	264	PEK	C9-C8	4.33	1.56	1.31
25	P	1265	PEK	C9-C8	4.34	1.56	1.31
24	P	1272	DMU	C3-C4	4.39	1.65	1.52
25	G	1263	PEK	C9-C8	4.43	1.57	1.31
19	A	524	PGV	C12-C11	4.43	1.57	1.31
19	P	1268	PGV	O01-C1	4.45	1.47	1.34
25	T	1264	PEK	C2-C1	4.46	1.64	1.50
25	P	1265	PEK	C15-C14	4.46	1.57	1.31
25	T	263	PEK	C9-C8	4.48	1.57	1.31
25	C	265	PEK	C15-C14	4.52	1.57	1.31
22	B	230	PSC	C10-C9	4.58	1.58	1.31
26	G	269	CDL	OB6-CB5	4.59	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	264	PEK	C6-C5	4.60	1.58	1.31
24	C	272	DMU	C6-C1	4.62	1.66	1.52
24	C	272	DMU	C3-C4	4.63	1.65	1.52
24	P	1272	DMU	C6-C1	4.66	1.66	1.52
19	P	1268	PGV	C12-C11	4.66	1.58	1.31
25	T	1264	PEK	C9-C8	4.67	1.58	1.31
25	G	1263	PEK	C12-C11	4.68	1.58	1.31
24	P	1272	DMU	C8-C7	4.69	1.64	1.52
25	T	1264	PEK	C6-C5	4.75	1.59	1.31
19	C	268	PGV	C12-C11	4.76	1.59	1.31
25	C	265	PEK	C12-C11	4.76	1.59	1.31
24	C	272	DMU	C8-C9	4.80	1.63	1.53
25	P	1265	PEK	C12-C11	4.80	1.59	1.31
22	O	1230	PSC	C10-C9	4.83	1.59	1.31
19	C	268	PGV	O01-C1	4.85	1.48	1.34
25	T	263	PEK	C12-C11	4.90	1.60	1.31
25	T	263	PEK	C6-C5	4.91	1.60	1.31
25	G	1263	PEK	C15-C14	4.97	1.60	1.31
25	G	1263	PEK	C01-C02	4.98	1.64	1.50
25	T	263	PEK	C15-C14	5.00	1.60	1.31
25	T	263	PEK	C03-C02	5.04	1.65	1.50
25	C	264	PEK	C12-C11	5.05	1.60	1.31
24	P	1272	DMU	C8-C9	5.09	1.63	1.53
25	C	264	PEK	C15-C14	5.12	1.61	1.31
25	G	1263	PEK	C6-C5	5.15	1.61	1.31
19	A	524	PGV	O03-C19	5.15	1.48	1.33
25	T	263	PEK	C01-C02	5.21	1.65	1.50
19	N	1524	PGV	O03-C19	5.26	1.49	1.33
25	G	1263	PEK	C03-C02	5.53	1.66	1.50
25	T	1264	PEK	C15-C14	5.62	1.64	1.31
18	L	522	TGL	OG2-CB1	5.65	1.51	1.34
25	T	1264	PEK	O01-C1	5.82	1.51	1.34
23	J	60	CHD	C13-C17	6.03	1.66	1.55
25	C	264	PEK	O01-C1	6.26	1.53	1.34
23	W	1060	CHD	C13-C17	6.30	1.66	1.55
25	T	263	PEK	O03-C21	6.56	1.53	1.33
18	Y	1522	TGL	OG2-CB1	6.57	1.54	1.34
25	G	1263	PEK	O03-C21	6.77	1.53	1.33

All (455) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C17-C13-C12	-7.70	110.86	117.68
23	C	271	CHD	C19-C10-C9	-7.10	100.53	111.18
23	P	1271	CHD	C19-C10-C9	-6.97	100.74	111.18
23	J	60	CHD	C18-C13-C14	-6.72	100.61	111.22
23	W	1060	CHD	C18-C13-C14	-6.56	100.86	111.22
23	G	86	CHD	C9-C8-C7	-6.53	104.21	111.92
23	C	271	CHD	C17-C13-C12	-6.39	112.02	117.68
23	C	271	CHD	C19-C10-C1	-6.35	97.53	108.20
23	B	1086	CHD	C9-C8-C7	-6.00	104.83	111.92
18	A	521	TGL	CG1-OG1-CA1	-5.92	100.30	116.85
23	P	1271	CHD	C19-C10-C1	-5.73	98.57	108.20
18	O	1521	TGL	CG1-OG1-CA1	-5.69	100.94	116.85
23	B	1086	CHD	C16-C17-C13	-5.63	97.99	103.60
23	G	86	CHD	C16-C17-C13	-5.40	98.23	103.60
23	C	525	CHD	C14-C8-C9	-5.14	102.55	109.62
18	L	522	TGL	C12-C11-C10	-5.13	88.04	114.53
23	P	1271	CHD	C15-C14-C8	-4.96	111.12	118.32
18	Y	1522	TGL	C12-C11-C10	-4.93	89.08	114.53
23	J	60	CHD	C15-C14-C8	-4.92	111.18	118.32
23	G	86	CHD	C15-C14-C13	-4.81	98.81	103.60
25	C	264	PEK	C01-O03-C21	-4.77	103.50	116.85
17	N	515	HEA	C27-C19-C18	-4.75	114.17	123.50
17	A	515	HEA	C27-C19-C18	-4.59	114.50	123.50
22	B	230	PSC	C01-O03-C19	-4.56	104.09	116.85
23	W	1060	CHD	C15-C14-C8	-4.52	111.75	118.32
26	P	1270	CDL	CB6-OB8-CB7	-4.43	104.47	116.85
18	L	522	TGL	CB9-CB8-CB7	-4.39	91.88	114.53
23	C	271	CHD	C15-C14-C8	-4.35	112.00	118.32
25	T	1264	PEK	C01-O03-C21	-4.35	104.69	116.85
18	Y	1522	TGL	CB9-CB8-CB7	-4.34	92.13	114.53
18	N	1523	TGL	CG1-OG1-CA1	-4.25	104.97	116.85
19	A	525	PGV	O01-C1-C2	-4.09	102.63	111.53
23	P	1525	CHD	C14-C8-C9	-4.03	104.08	109.62
26	C	270	CDL	CB6-OB8-CB7	-4.00	105.67	116.85
23	C	271	CHD	C18-C13-C12	-3.92	105.26	109.09
23	B	1086	CHD	C15-C14-C13	-3.92	99.70	103.60
22	O	1230	PSC	C01-O03-C19	-3.85	106.08	116.85
17	A	516	HEA	C3C-CAC-CBC	-3.81	118.52	126.32
25	T	1264	PEK	C02-O01-C1	-3.76	108.88	117.89
18	A	523	TGL	CG1-OG1-CA1	-3.74	106.39	116.85
23	P	1525	CHD	C15-C14-C8	-3.70	112.94	118.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	264	PEK	C2-C3-C4	-3.69	105.94	113.30
23	B	1086	CHD	C15-C14-C8	-3.69	112.96	118.32
23	C	525	CHD	C15-C14-C8	-3.68	112.98	118.32
23	B	1086	CHD	C11-C12-C13	-3.65	107.49	111.20
17	N	515	HEA	C26-C15-C14	-3.64	116.35	123.50
17	N	516	HEA	C20-C19-C18	-3.62	114.19	121.05
23	G	86	CHD	C15-C14-C8	-3.56	113.15	118.32
23	P	1271	CHD	C18-C13-C12	-3.54	105.64	109.09
23	G	86	CHD	O3-C3-C4	-3.53	102.85	109.86
18	N	1523	TGL	OG2-CB1-CB2	-3.51	103.91	111.53
17	N	515	HEA	C1A-C2A-C3A	-3.41	103.66	107.07
17	N	516	HEA	C3C-CAC-CBC	-3.26	119.65	126.32
17	A	515	HEA	CAD-C3D-C4D	-3.20	123.53	127.01
23	B	1086	CHD	C14-C8-C9	-3.19	105.24	109.62
23	W	1060	CHD	C18-C13-C12	-3.18	105.99	109.09
19	A	524	PGV	C3-C2-C1	-3.07	101.52	113.59
19	N	1266	PGV	O01-C1-C2	-3.06	104.87	111.53
23	P	1525	CHD	C11-C9-C10	-3.06	110.61	113.79
19	C	268	PGV	C02-O01-C1	-3.03	110.62	117.89
18	A	523	TGL	OG3-CG3-CG2	-3.03	100.54	108.69
25	C	264	PEK	O01-C1-C2	-3.00	105.01	111.53
17	A	516	HEA	C20-C19-C18	-2.98	115.41	121.05
17	N	515	HEA	OMA-CMA-C3A	-2.97	119.12	125.11
23	G	86	CHD	C19-C10-C5	-2.95	105.03	110.25
23	G	86	CHD	C11-C12-C13	-2.94	108.21	111.20
26	P	1270	CDL	OB6-CB5-C51	-2.93	105.17	111.53
25	C	264	PEK	C02-O01-C1	-2.92	110.89	117.89
18	A	523	TGL	OG2-CB1-CB2	-2.90	105.23	111.53
23	W	1060	CHD	C19-C10-C5	-2.86	105.20	110.25
17	A	516	HEA	CMC-C2C-C1C	-2.84	123.67	128.36
17	A	515	HEA	C26-C15-C14	-2.84	117.93	123.50
17	A	515	HEA	C3C-CAC-CBC	-2.83	120.53	126.32
17	N	516	HEA	CAA-C2A-C1A	-2.83	123.94	127.01
25	T	1264	PEK	C23-C22-C21	-2.82	102.53	113.59
25	C	264	PEK	P-O12-C04	-2.81	105.45	121.50
19	P	1268	PGV	C02-O01-C1	-2.80	111.18	117.89
17	A	516	HEA	CAA-C2A-C1A	-2.79	123.98	127.01
25	T	1264	PEK	C2-C3-C4	-2.78	107.75	113.30
19	N	1524	PGV	C3-C2-C1	-2.78	102.68	113.59
25	C	264	PEK	C3-C2-C1	-2.76	102.75	113.59
23	J	60	CHD	C19-C10-C9	-2.76	107.05	111.18
25	T	1264	PEK	P-O12-C04	-2.71	106.03	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C19-C10-C5	-2.71	105.47	110.25
18	O	1521	TGL	C12-C11-C10	-2.68	100.67	114.53
25	C	264	PEK	C23-C22-C21	-2.68	103.04	113.59
26	P	1270	CDL	CB4-OB6-CB5	-2.66	111.51	117.89
25	C	264	PEK	O03-C21-C22	-2.65	103.82	111.90
18	O	1521	TGL	CA8-CA7-CA6	-2.65	100.85	114.53
23	B	1086	CHD	C14-C8-C7	-2.63	108.10	111.74
18	O	1521	TGL	OG3-CC1-CC2	-2.61	103.95	111.90
25	T	1264	PEK	C3-C2-C1	-2.60	103.36	113.59
24	M	526	DMU	C8-C7-C5	-2.60	105.94	110.79
17	A	515	HEA	C21-C20-C19	-2.60	104.26	112.71
17	A	515	HEA	C12-C13-C14	-2.59	105.14	112.40
17	N	515	HEA	C21-C20-C19	-2.59	104.27	112.71
23	G	86	CHD	C14-C8-C9	-2.58	106.08	109.62
23	C	525	CHD	C19-C10-C9	-2.57	107.33	111.18
25	T	1264	PEK	O03-C01-C02	-2.57	101.78	108.69
17	N	515	HEA	C12-C13-C14	-2.56	105.22	112.40
22	O	1230	PSC	O03-C19-C20	-2.55	104.12	111.90
25	T	1264	PEK	O03-C21-C22	-2.54	104.15	111.90
25	C	264	PEK	C30-C29-C28	-2.54	101.44	114.53
18	A	521	TGL	C12-C11-C10	-2.52	101.52	114.53
25	T	1264	PEK	C30-C29-C28	-2.51	101.55	114.53
26	C	270	CDL	OB6-CB5-C51	-2.51	106.07	111.53
23	P	1525	CHD	C9-C10-C5	-2.46	105.04	108.67
23	J	60	CHD	C18-C13-C12	-2.44	106.71	109.09
19	P	1267	PGV	C9-C10-C11	-2.34	100.16	112.45
19	C	267	PGV	O01-C1-C2	-2.32	106.48	111.53
18	A	521	TGL	CA8-CA7-CA6	-2.31	102.62	114.53
26	T	1269	CDL	OB8-CB7-C71	-2.28	104.95	111.90
18	N	1523	TGL	CG3-CG2-CG1	-2.27	106.76	112.07
19	A	524	PGV	O01-C1-C2	-2.26	106.61	111.53
18	A	521	TGL	OG3-CC1-CC2	-2.26	105.01	111.90
19	N	1266	PGV	C01-O03-C19	-2.26	110.54	116.85
19	C	267	PGV	O12-P-O13	-2.25	100.86	109.62
18	A	521	TGL	CB7-CB6-CB5	-2.24	102.94	114.53
19	C	267	PGV	C9-C10-C11	-2.23	100.73	112.45
26	C	270	CDL	C52-C51-CB5	-2.21	104.91	113.59
23	C	525	CHD	C16-C17-C13	-2.20	101.41	103.60
17	N	516	HEA	CMC-C2C-C1C	-2.17	124.77	128.36
22	B	230	PSC	O01-C1-C2	-2.17	106.81	111.53
18	N	1523	TGL	OG3-CG3-CG2	-2.16	102.88	108.69
25	T	1264	PEK	C24-C23-C22	-2.16	105.38	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C14-C13-C12	-2.15	105.47	107.39
23	B	1086	CHD	O3-C3-C4	-2.14	105.61	109.86
24	Z	1526	DMU	C8-C7-C5	-2.14	106.80	110.79
18	A	523	TGL	CC3-CC2-CC1	-2.14	105.19	113.59
23	G	86	CHD	C18-C13-C17	-2.13	107.85	111.22
19	C	267	PGV	C02-O01-C1	-2.13	112.77	117.89
26	C	270	CDL	CB4-OB6-CB5	-2.13	112.77	117.89
17	A	515	HEA	OMA-CMA-C3A	-2.13	120.81	125.11
17	N	515	HEA	C3C-CAC-CBC	-2.12	121.99	126.32
22	O	1230	PSC	C07-N-C06	-2.11	103.56	108.98
23	B	1086	CHD	C18-C13-C17	-2.09	107.92	111.22
25	C	264	PEK	O03-C01-C02	-2.08	103.09	108.69
17	N	515	HEA	C17-C18-C19	-2.07	123.26	127.76
24	C	272	DMU	C2-C3-C4	-2.07	106.16	110.84
19	N	1524	PGV	O01-C1-C2	-2.05	107.06	111.53
18	O	1521	TGL	CB9-CB8-CB7	-2.05	103.94	114.53
22	B	230	PSC	O03-C19-C20	-2.05	105.66	111.90
18	L	522	TGL	C14-C13-C12	-2.04	104.00	114.53
23	G	86	CHD	C14-C8-C7	-2.03	108.92	111.74
18	A	523	TGL	CC4-CC3-CC2	-2.02	105.89	113.29
26	P	1270	CDL	C52-C51-CB5	-2.01	105.69	113.59
26	G	269	CDL	OA8-CA6-CA4	2.01	114.09	108.69
26	G	269	CDL	OB8-CB6-CB4	2.01	114.10	108.69
23	P	1271	CHD	C1-C2-C3	2.02	113.70	110.43
23	J	60	CHD	O7-C7-C6	2.02	115.00	110.06
23	B	1086	CHD	C4-C3-C2	2.03	113.11	110.52
25	T	263	PEK	C03-C02-C01	2.03	116.83	112.07
18	O	1521	TGL	CG3-OG3-CC1	2.04	122.54	116.85
18	O	1521	TGL	C33-C19-C18	2.04	125.06	114.53
25	C	264	PEK	O03-C21-O04	2.05	128.79	123.49
19	A	525	PGV	O01-C1-O02	2.05	129.18	123.67
17	A	516	HEA	C21-C20-C19	2.06	119.41	112.71
18	L	522	TGL	CC4-CC3-CC2	2.06	120.84	113.29
23	P	1271	CHD	O12-C12-C13	2.08	114.49	111.11
25	C	264	PEK	O13-P-O14	2.12	124.01	112.53
18	A	521	TGL	C33-C19-C18	2.13	125.52	114.53
23	C	271	CHD	C1-C2-C3	2.13	113.89	110.43
26	T	1269	CDL	C79-C78-C77	2.13	125.53	114.53
18	O	1521	TGL	OG2-CG2-CG3	2.14	115.89	108.36
26	T	1269	CDL	OB8-CB6-CB4	2.14	114.45	108.69
23	P	1271	CHD	O7-C7-C6	2.15	115.32	110.06
19	N	1524	PGV	C02-O01-C1	2.15	123.05	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1524	PGV	C04-C05-C06	2.16	119.82	111.08
23	G	86	CHD	C11-C9-C10	2.18	116.06	113.79
23	G	86	CHD	C15-C16-C17	2.18	109.51	105.12
26	G	269	CDL	C80-C79-C78	2.18	125.80	114.53
25	P	1265	PEK	P-O12-C04	2.19	133.98	121.50
19	C	267	PGV	C03-C02-C01	2.19	117.20	112.07
26	T	1269	CDL	C83-C82-C81	2.19	125.86	114.53
18	Y	1522	TGL	C10-CB9-CB8	2.20	125.88	114.53
24	P	1272	DMU	O55-C2-C3	2.20	115.08	109.87
26	P	1270	CDL	OB6-CB5-OB7	2.21	129.59	123.67
26	T	1269	CDL	C80-C79-C78	2.21	125.94	114.53
23	G	86	CHD	C2-C1-C10	2.22	116.81	112.84
26	C	270	CDL	C80-C79-C78	2.22	126.02	114.53
25	G	1263	PEK	C2-C3-C4	2.23	117.75	113.30
23	P	1271	CHD	C9-C11-C12	2.23	117.18	114.36
18	N	1523	TGL	OG1-CG1-CG2	2.24	114.73	108.69
26	G	269	CDL	C19-C18-C17	2.24	126.12	114.53
26	T	1269	CDL	C19-C18-C17	2.25	126.16	114.53
18	L	522	TGL	CC7-CC6-CC5	2.25	126.16	114.53
23	C	525	CHD	C6-C5-C10	2.26	115.15	112.66
23	P	1271	CHD	C2-C1-C10	2.28	116.91	112.84
25	P	1265	PEK	C2-C3-C4	2.28	117.84	113.30
23	J	60	CHD	C5-C4-C3	2.28	116.31	112.91
18	L	522	TGL	C20-CA9-CA8	2.29	126.34	114.53
24	P	1272	DMU	O55-C2-C1	2.30	115.51	110.34
18	N	1523	TGL	OG2-CG2-CG1	2.30	116.48	108.36
23	B	1086	CHD	C11-C9-C10	2.32	116.20	113.79
26	G	269	CDL	C79-C78-C77	2.32	126.50	114.53
25	T	263	PEK	O03-C21-C22	2.32	118.97	111.90
23	B	1086	CHD	C2-C1-C10	2.33	116.99	112.84
25	T	263	PEK	P-O12-C04	2.33	134.80	121.50
19	P	1268	PGV	O03-C01-C02	2.33	114.96	108.69
25	C	265	PEK	C2-C3-C4	2.33	117.95	113.30
23	J	60	CHD	C14-C8-C7	2.33	114.98	111.74
26	G	269	CDL	C83-C82-C81	2.34	126.63	114.53
23	C	271	CHD	C2-C1-C10	2.35	117.03	112.84
23	W	1060	CHD	C5-C4-C3	2.35	116.41	112.91
23	J	60	CHD	C9-C11-C12	2.36	117.34	114.36
23	W	1060	CHD	O7-C7-C6	2.36	115.84	110.06
17	N	515	HEA	C20-C19-C18	2.36	125.53	121.05
17	N	516	HEA	C4B-C3B-C11	2.37	129.58	127.01
23	P	1525	CHD	C4-C3-C2	2.37	113.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C15-C16-C17	2.37	109.90	105.12
24	C	272	DMU	O55-C2-C3	2.38	115.50	109.87
26	C	270	CDL	OA8-CA6-CA4	2.40	115.15	108.69
24	M	526	DMU	O7-C10-O1	2.41	116.78	110.68
25	T	263	PEK	C11-C10-C9	2.41	120.03	112.00
19	C	268	PGV	O03-C01-C02	2.42	115.20	108.69
22	O	1230	PSC	P-O12-C04	2.42	135.33	121.50
26	T	1269	CDL	C23-C22-C21	2.43	127.10	114.53
24	Z	1526	DMU	C6-C1-C2	2.45	114.80	109.97
26	G	269	CDL	OA6-CA4-CA6	2.45	117.01	108.36
23	W	1060	CHD	O12-C12-C13	2.46	115.11	111.11
18	A	521	TGL	OG2-CG2-CG3	2.47	117.06	108.36
25	G	1263	PEK	P-O12-C04	2.48	135.64	121.50
23	W	1060	CHD	C14-C8-C9	2.48	113.04	109.62
23	C	525	CHD	C4-C3-C2	2.50	113.71	110.52
25	G	1263	PEK	C03-C02-C01	2.52	117.96	112.07
23	B	1086	CHD	O12-C12-C11	2.52	114.22	109.06
26	G	269	CDL	C23-C22-C21	2.52	127.55	114.53
18	A	521	TGL	OG3-CG3-CG2	2.53	115.50	108.69
18	A	523	TGL	OG2-CG2-CG1	2.53	117.29	108.36
23	C	525	CHD	C1-C2-C3	2.54	114.55	110.43
25	C	265	PEK	P-O12-C04	2.56	136.10	121.50
23	P	1525	CHD	C9-C11-C12	2.59	117.63	114.36
23	P	1525	CHD	C17-C13-C12	2.59	119.97	117.68
18	L	522	TGL	C13-C12-C11	2.61	128.00	114.53
23	J	60	CHD	C14-C8-C9	2.63	113.25	109.62
23	G	86	CHD	O12-C12-C11	2.64	114.47	109.06
18	O	1521	TGL	CG3-CG2-CG1	2.65	118.28	112.07
23	W	1060	CHD	C14-C8-C7	2.67	115.44	111.74
25	T	263	PEK	C2-C3-C4	2.67	118.62	113.30
22	B	230	PSC	P-O12-C04	2.68	136.81	121.50
17	N	516	HEA	C27-C19-C20	2.68	119.51	115.41
26	P	1270	CDL	OA8-CA6-CA4	2.69	115.92	108.69
24	Z	1526	DMU	C10-O1-C9	2.69	118.97	113.75
25	C	265	PEK	C24-C23-C22	2.70	123.18	113.29
23	W	1060	CHD	C1-C2-C3	2.70	114.81	110.43
23	B	1086	CHD	C1-C2-C3	2.71	114.84	110.43
24	M	526	DMU	C6-C1-C2	2.72	115.34	109.97
25	G	1263	PEK	C11-C10-C9	2.72	121.06	112.00
19	A	524	PGV	C02-O01-C1	2.73	124.45	117.89
23	C	271	CHD	C15-C16-C17	2.74	110.64	105.12
24	P	1272	DMU	C10-O7-C3	2.74	125.17	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	521	TGL	CG3-CG2-CG1	2.75	118.50	112.07
24	C	272	DMU	O1-C10-C5	2.76	115.94	110.28
17	N	515	HEA	C20-C21-C22	2.77	118.95	111.69
23	P	1271	CHD	C16-C15-C14	2.78	110.72	105.12
24	Z	1526	DMU	C10-O7-C3	2.78	125.28	118.01
18	A	523	TGL	OG2-CG2-CG3	2.81	118.27	108.36
23	P	1271	CHD	C11-C12-C13	2.82	114.07	111.20
18	Y	1522	TGL	C13-C12-C11	2.85	129.26	114.53
25	P	1265	PEK	C24-C23-C22	2.87	123.80	113.29
23	P	1271	CHD	C15-C16-C17	2.87	110.91	105.12
23	B	1086	CHD	C1-C10-C5	2.87	112.53	107.81
23	C	525	CHD	C17-C13-C14	2.88	102.96	100.05
26	G	269	CDL	C22-C21-C20	2.90	129.49	114.53
23	G	86	CHD	C9-C11-C12	2.90	118.02	114.36
23	P	1525	CHD	O12-C12-C11	2.92	115.03	109.06
24	M	526	DMU	C10-O1-C9	2.93	119.42	113.75
23	C	271	CHD	C9-C11-C12	2.94	118.08	114.36
26	T	1269	CDL	C22-C21-C20	2.95	129.77	114.53
23	J	60	CHD	C1-C2-C3	2.96	115.23	110.43
23	P	1525	CHD	C1-C2-C3	2.96	115.24	110.43
23	G	86	CHD	C1-C10-C5	2.98	112.71	107.81
23	C	271	CHD	C16-C15-C14	2.98	111.13	105.12
23	C	271	CHD	C5-C4-C3	2.99	117.35	112.91
23	W	1060	CHD	C15-C16-C17	2.99	111.14	105.12
23	C	271	CHD	C11-C12-C13	3.01	114.25	111.20
23	J	60	CHD	C15-C16-C17	3.04	111.24	105.12
17	A	515	HEA	C20-C21-C22	3.05	119.67	111.69
18	A	523	TGL	OG1-CG1-CG2	3.06	116.92	108.69
23	G	86	CHD	C1-C2-C3	3.09	115.45	110.43
17	N	515	HEA	C16-C17-C18	3.09	119.79	111.69
23	C	525	CHD	C9-C11-C12	3.09	118.27	114.36
23	W	1060	CHD	C16-C15-C14	3.10	111.38	105.12
23	J	60	CHD	C16-C15-C14	3.10	111.38	105.12
18	A	523	TGL	CB3-CB2-CB1	3.11	125.80	113.59
18	N	1523	TGL	CB3-CB2-CB1	3.11	125.81	113.59
23	P	1525	CHD	C5-C6-C7	3.14	117.93	114.44
25	T	263	PEK	C14-C13-C12	3.14	122.46	112.00
24	M	526	DMU	O1-C10-C5	3.15	116.73	110.28
24	Z	1526	DMU	O1-C10-C5	3.15	116.74	110.28
23	P	1271	CHD	C5-C4-C3	3.15	117.60	112.91
24	P	1272	DMU	C7-C8-C9	3.17	115.73	110.20
23	C	525	CHD	C5-C6-C7	3.20	118.00	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	515	HEA	C27-C19-C20	3.20	120.30	115.41
24	M	526	DMU	C18-O16-C6	3.21	119.55	113.94
19	A	524	PGV	O01-C02-C03	3.30	119.99	108.36
18	N	1523	TGL	OG2-CG2-CG3	3.33	120.10	108.36
23	G	86	CHD	C5-C6-C7	3.34	118.16	114.44
18	Y	1522	TGL	CC3-CC2-CC1	3.35	126.75	113.59
24	P	1272	DMU	C10-O1-C9	3.35	120.25	113.75
24	Z	1526	DMU	O7-C10-O1	3.36	119.18	110.68
23	C	525	CHD	C1-C10-C5	3.36	113.33	107.81
23	P	1525	CHD	C1-C10-C5	3.40	113.40	107.81
23	P	1525	CHD	C6-C5-C10	3.41	116.41	112.66
18	Y	1522	TGL	C11-C10-CB9	3.44	132.32	114.53
18	Y	1522	TGL	CG2-OG2-CB1	3.46	126.20	117.89
23	W	1060	CHD	C9-C11-C12	3.48	118.76	114.36
17	A	516	HEA	C3C-C4C-NC	3.48	113.71	109.21
17	A	515	HEA	C26-C15-C16	3.50	120.75	115.41
23	B	1086	CHD	C10-C9-C8	3.51	115.73	111.88
19	N	1524	PGV	O01-C02-C03	3.51	120.72	108.36
17	A	516	HEA	C4B-C3B-C11	3.52	130.83	127.01
17	A	515	HEA	C27-C19-C20	3.53	120.80	115.41
23	J	60	CHD	C6-C5-C4	3.54	115.00	111.05
25	G	1263	PEK	C14-C13-C12	3.58	123.92	112.00
18	L	522	TGL	CC3-CC2-CC1	3.59	127.71	113.59
23	P	1271	CHD	C1-C10-C9	3.59	117.24	111.45
24	M	526	DMU	O16-C6-C1	3.60	112.59	108.04
23	W	1060	CHD	C2-C1-C10	3.64	119.34	112.84
18	L	522	TGL	C11-C10-CB9	3.65	133.40	114.53
23	B	1086	CHD	C9-C11-C12	3.66	118.98	114.36
23	P	1271	CHD	C4-C5-C10	3.66	116.69	112.66
23	J	60	CHD	C2-C1-C10	3.68	119.42	112.84
18	L	522	TGL	C16-C15-CC9	3.70	133.62	114.53
23	C	271	CHD	C1-C10-C9	3.71	117.43	111.45
23	C	271	CHD	C14-C13-C12	3.71	110.71	107.39
23	G	86	CHD	C5-C4-C3	3.72	118.44	112.91
24	C	272	DMU	O7-C10-O1	3.74	120.16	110.68
24	P	1272	DMU	C8-C7-C5	3.77	117.83	110.79
24	C	272	DMU	C10-O1-C9	3.82	121.15	113.75
18	Y	1522	TGL	C16-C15-CC9	3.83	134.31	114.53
24	M	526	DMU	C10-O7-C3	3.83	128.02	118.01
23	W	1060	CHD	C13-C14-C8	3.84	119.70	114.75
17	A	515	HEA	C16-C17-C18	3.84	121.74	111.69
23	B	1086	CHD	C5-C4-C3	3.85	118.64	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C13-C14-C8	3.89	119.77	114.75
18	Y	1522	TGL	C15-CC9-CC8	3.96	134.96	114.53
24	P	1272	DMU	O7-C10-C5	4.01	117.85	108.10
24	P	1272	DMU	O1-C10-C5	4.02	118.52	110.28
25	G	1263	PEK	C02-O01-C1	4.02	127.53	117.89
18	L	522	TGL	C15-CC9-CC8	4.03	135.33	114.53
24	Z	1526	DMU	O16-C6-C1	4.07	113.19	108.04
23	C	271	CHD	C5-C6-C7	4.08	118.98	114.44
23	P	1271	CHD	C14-C8-C7	4.11	117.45	111.74
24	Z	1526	DMU	C18-O16-C6	4.15	121.20	113.94
24	Z	1526	DMU	C1-C2-C3	4.15	118.72	109.60
24	Z	1526	DMU	O7-C10-C5	4.18	118.28	108.10
25	T	263	PEK	O03-C01-C02	4.20	120.01	108.69
25	G	1263	PEK	O03-C01-C02	4.22	120.04	108.69
24	M	526	DMU	C1-C2-C3	4.22	118.88	109.60
23	C	271	CHD	C4-C5-C10	4.23	117.32	112.66
18	L	522	TGL	CG2-OG2-CB1	4.23	128.04	117.89
17	N	516	HEA	C3C-C4C-NC	4.24	114.69	109.21
23	C	525	CHD	O12-C12-C11	4.26	117.78	109.06
23	P	1525	CHD	C2-C1-C10	4.27	120.46	112.84
25	T	263	PEK	C02-O01-C1	4.28	128.16	117.89
24	P	1272	DMU	O7-C10-O1	4.28	121.52	110.68
24	Z	1526	DMU	O1-C9-C8	4.29	117.73	109.68
23	W	1060	CHD	C6-C5-C4	4.34	115.89	111.05
23	C	271	CHD	C14-C8-C7	4.34	117.76	111.74
24	M	526	DMU	O1-C9-C8	4.37	117.88	109.68
25	P	1265	PEK	C11-C10-C9	4.42	126.69	112.00
17	N	515	HEA	C26-C15-C16	4.44	122.19	115.41
23	J	60	CHD	C1-C10-C5	4.45	115.12	107.81
25	C	265	PEK	C11-C10-C9	4.49	126.93	112.00
23	P	1271	CHD	C5-C6-C7	4.49	119.44	114.44
23	G	86	CHD	C10-C9-C8	4.49	116.81	111.88
23	W	1060	CHD	C1-C10-C5	4.57	115.31	107.81
23	C	525	CHD	C2-C1-C10	4.60	121.05	112.84
17	A	516	HEA	C20-C21-C22	4.61	123.75	111.69
24	Z	1526	DMU	C10-C5-C7	4.61	119.07	109.97
24	M	526	DMU	O7-C3-C4	4.65	121.54	109.32
24	P	1272	DMU	C18-O16-C6	4.65	122.07	113.94
24	C	272	DMU	C8-C7-C5	4.65	119.48	110.79
18	A	521	TGL	CG2-OG2-CB1	4.69	129.14	117.89
23	C	271	CHD	C4-C3-C2	4.76	116.59	110.52
18	N	1523	TGL	CG3-OG3-CC1	4.79	130.24	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C4-C3-C2	4.79	116.63	110.52
24	P	1272	DMU	O1-C9-C8	4.88	118.84	109.68
23	P	1271	CHD	C14-C13-C12	4.90	111.78	107.39
24	M	526	DMU	O7-C10-C5	4.94	120.11	108.10
24	Z	1526	DMU	O7-C3-C4	4.94	122.31	109.32
18	A	523	TGL	CG3-OG3-CC1	5.05	130.96	116.85
18	O	1521	TGL	CG2-OG2-CB1	5.08	130.07	117.89
17	N	516	HEA	C20-C21-C22	5.09	125.03	111.69
24	M	526	DMU	C10-C5-C7	5.11	120.05	109.97
24	P	1272	DMU	O7-C3-C2	5.14	120.42	107.17
24	C	272	DMU	O5-C4-C57	5.14	119.34	106.36
24	Z	1526	DMU	O7-C3-C2	5.16	120.48	107.17
23	W	1060	CHD	C9-C8-C7	5.30	118.18	111.92
24	M	526	DMU	O5-C6-C1	5.34	121.23	110.28
23	C	271	CHD	C6-C5-C10	5.41	118.61	112.66
23	C	271	CHD	C1-C10-C5	5.46	116.79	107.81
23	C	525	CHD	C13-C17-C20	5.48	126.18	119.50
23	J	60	CHD	C9-C8-C7	5.54	118.47	111.92
23	P	1271	CHD	C1-C10-C5	5.58	116.99	107.81
24	P	1272	DMU	O5-C6-C1	5.60	121.77	110.28
24	C	272	DMU	O1-C9-C8	5.69	120.36	109.68
24	Z	1526	DMU	O5-C6-C1	5.70	121.97	110.28
23	P	1271	CHD	C6-C5-C10	5.78	119.02	112.66
24	Z	1526	DMU	O5-C4-C57	5.88	121.23	106.36
24	C	272	DMU	O7-C10-C5	5.88	122.42	108.10
24	M	526	DMU	O7-C3-C2	5.93	122.47	107.17
24	P	1272	DMU	O5-C4-C57	5.95	121.40	106.36
24	Z	1526	DMU	C6-O5-C4	6.01	125.41	113.75
24	Z	1526	DMU	O5-C6-O16	6.05	124.63	110.05
23	J	60	CHD	C5-C6-C7	6.07	121.20	114.44
23	J	60	CHD	C4-C3-C2	6.07	118.26	110.52
24	P	1272	DMU	C1-C2-C3	6.08	122.96	109.60
23	W	1060	CHD	C4-C3-C2	6.15	118.36	110.52
24	C	272	DMU	O5-C6-C1	6.26	123.13	110.28
23	P	1525	CHD	C13-C17-C20	6.33	127.21	119.50
23	B	1086	CHD	C17-C13-C14	6.36	106.48	100.05
23	W	1060	CHD	C5-C6-C7	6.37	121.54	114.44
17	N	515	HEA	C4B-C3B-C11	6.44	134.00	127.01
24	C	272	DMU	O7-C3-C2	6.50	123.96	107.17
24	M	526	DMU	O5-C4-C57	6.52	122.83	106.36
24	M	526	DMU	O5-C6-O16	6.57	125.87	110.05
23	W	1060	CHD	C6-C5-C10	6.66	120.00	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C7-C8-C9	6.67	121.82	110.20
23	J	60	CHD	C6-C5-C10	6.71	120.05	112.66
24	M	526	DMU	C6-O5-C4	6.73	126.80	113.75
24	P	1272	DMU	C6-O5-C4	6.74	126.82	113.75
24	P	1272	DMU	O7-C3-C4	6.74	127.03	109.32
23	C	271	CHD	C9-C8-C7	6.81	119.96	111.92
24	M	526	DMU	C7-C8-C9	6.86	122.15	110.20
24	P	1272	DMU	O5-C4-C3	6.94	124.41	109.75
24	C	272	DMU	O7-C3-C4	6.96	127.61	109.32
24	M	526	DMU	O5-C4-C3	6.96	124.45	109.75
24	C	272	DMU	C18-O16-C6	6.97	126.12	113.94
24	C	272	DMU	C6-O5-C4	7.03	127.39	113.75
23	J	60	CHD	C10-C9-C8	7.07	119.64	111.88
23	G	86	CHD	C17-C13-C14	7.12	107.25	100.05
23	P	1271	CHD	C9-C8-C7	7.28	120.52	111.92
17	A	515	HEA	C4B-C3B-C11	7.31	134.94	127.01
24	C	272	DMU	O5-C4-C3	7.38	125.34	109.75
23	W	1060	CHD	C11-C12-C13	7.42	118.74	111.20
24	C	272	DMU	O1-C9-C11	7.54	125.40	106.36
23	W	1060	CHD	C10-C9-C8	7.56	120.18	111.88
24	Z	1526	DMU	O5-C4-C3	7.81	126.24	109.75
24	P	1272	DMU	O1-C9-C11	8.13	126.89	106.36
23	J	60	CHD	C11-C12-C13	8.23	119.56	111.20
23	W	1060	CHD	C17-C13-C14	8.50	108.65	100.05
24	M	526	DMU	O1-C9-C11	8.76	128.50	106.36
24	Z	1526	DMU	O1-C9-C11	8.80	128.59	106.36
23	P	1271	CHD	C17-C13-C14	9.03	109.18	100.05
23	W	1060	CHD	C13-C17-C20	9.03	130.50	119.50
24	C	272	DMU	C1-C2-C3	9.11	129.60	109.60
23	J	60	CHD	C17-C13-C14	9.19	109.34	100.05
23	C	271	CHD	C17-C13-C14	9.50	109.65	100.05
23	J	60	CHD	C13-C17-C20	9.82	131.46	119.50
23	C	271	CHD	C10-C9-C8	11.42	124.42	111.88
23	P	1271	CHD	C10-C9-C8	11.54	124.55	111.88
24	C	272	DMU	O16-C6-C1	11.69	122.80	108.04
24	P	1272	DMU	O16-C6-C1	13.99	125.71	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C12
23	P	1271	CHD	C8

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Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14
23	J	60	CHD	C12
23	J	60	CHD	C8
23	J	60	CHD	C9
23	J	60	CHD	C14
23	J	60	CHD	C17
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
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
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
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
23	C	271	CHD	C12
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C9
23	C	271	CHD	C14

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Mol	Chain	Res	Type	Atom
23	W	1060	CHD	C12
23	W	1060	CHD	C8
23	W	1060	CHD	C9
23	W	1060	CHD	C14
23	W	1060	CHD	C17
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C9
24	M	526	DMU	C5

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C02-O01-C1-C2
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	P-O11-C03-C02
19	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

41 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	12	0
17	A	516	HEA	3	0
18	A	521	TGL	8	0
18	A	523	TGL	3	0
19	A	524	PGV	5	0
19	A	525	PGV	4	0
23	B	1086	CHD	5	0
22	B	230	PSC	21	0
25	C	264	PEK	9	0
25	C	265	PEK	11	0
19	C	267	PGV	6	0
19	C	268	PGV	1	0
26	C	270	CDL	17	0
23	C	271	CHD	4	0
24	C	272	DMU	3	0
23	C	525	CHD	1	0
25	G	1263	PEK	10	0
26	G	269	CDL	23	0
23	G	86	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	60	CHD	4	0
18	L	522	TGL	20	0
24	M	526	DMU	1	0
19	N	1266	PGV	2	0
18	N	1523	TGL	8	0
19	N	1524	PGV	7	0
17	N	515	HEA	9	0
17	N	516	HEA	9	0
22	O	1230	PSC	20	0
18	O	1521	TGL	8	0
25	P	1265	PEK	10	0
19	P	1267	PGV	9	0
19	P	1268	PGV	2	0
26	P	1270	CDL	17	0
23	P	1271	CHD	5	0
24	P	1272	DMU	4	0
23	P	1525	CHD	1	0
25	T	1264	PEK	12	0
26	T	1269	CDL	32	0
25	T	263	PEK	11	0
23	W	1060	CHD	3	0
18	Y	1522	TGL	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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