



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 07:51 pm GMT

PDB ID : 1V55  
Title : Bovine heart cytochrome c oxidase at the fully reduced state  
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.  
Deposited on : 2003-11-21  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

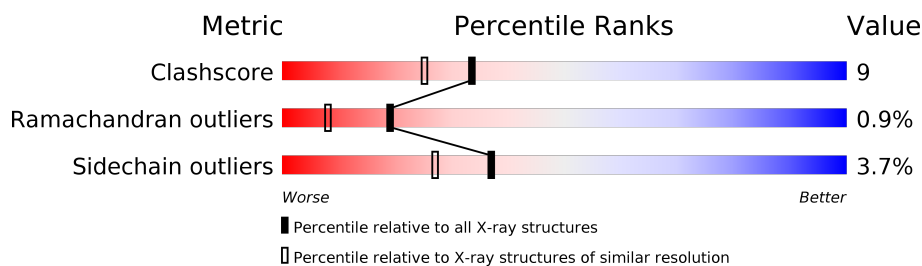
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	6112 (1.90-1.90)
Ramachandran outliers	120005	6045 (1.90-1.90)
Sidechain outliers	119972	6045 (1.90-1.90)















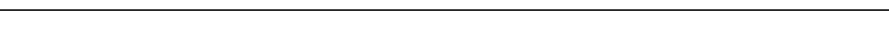




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria.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

Note EDS was not executed.

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
18	TGL	A	3522	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	TGL	N	4521	-	-	X	-
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	-
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	-
22	CDL	C	3270	-	-	X	-
27	DMU	M	3526	X	-	-	-
27	DMU	Z	4526	X	-	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32609 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 polypeptide I.

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 polypeptide II.

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 polypeptide III.

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 IV 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 polypeptide VIb.

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		

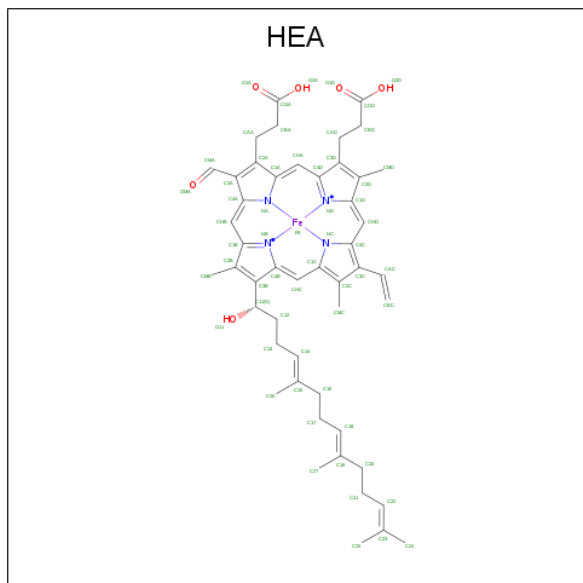
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

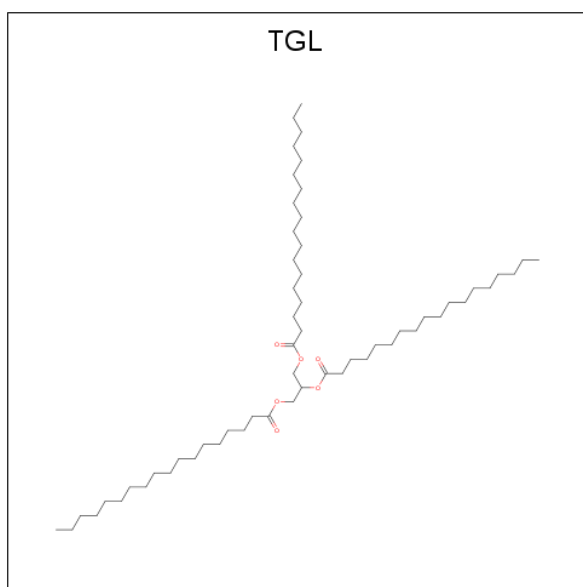
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



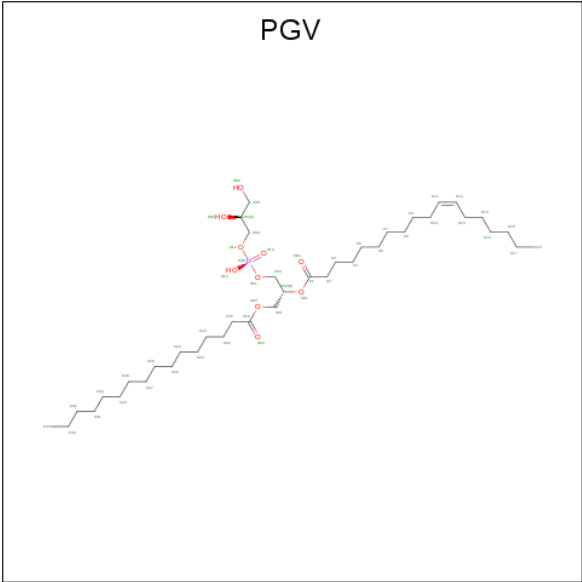
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



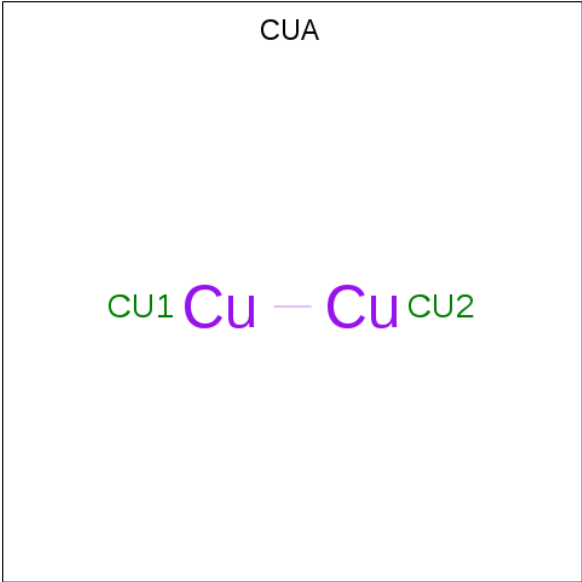
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- 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: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



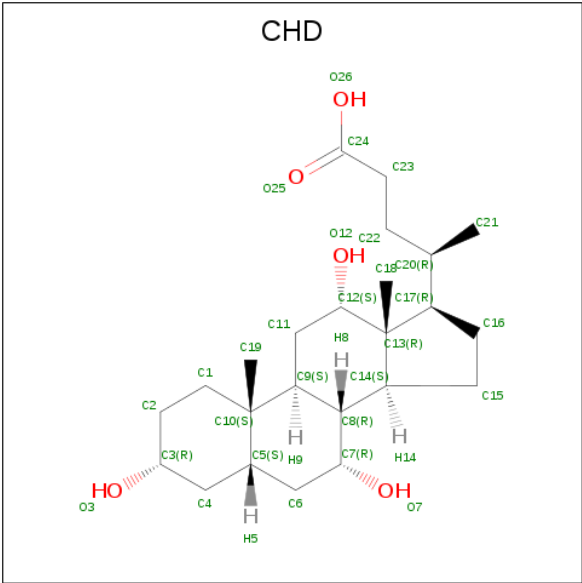
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



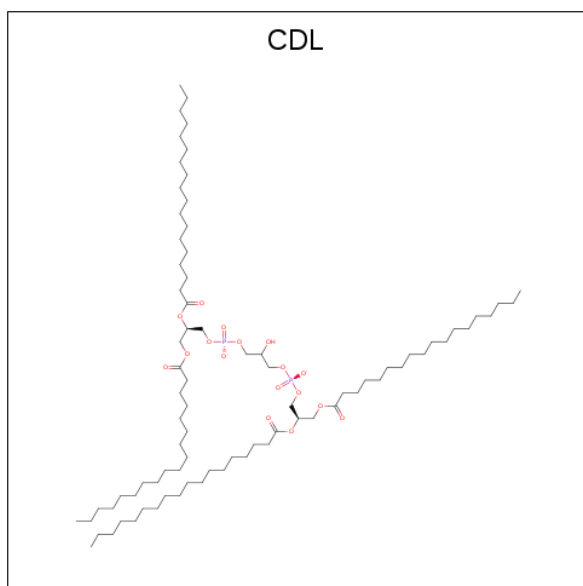
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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

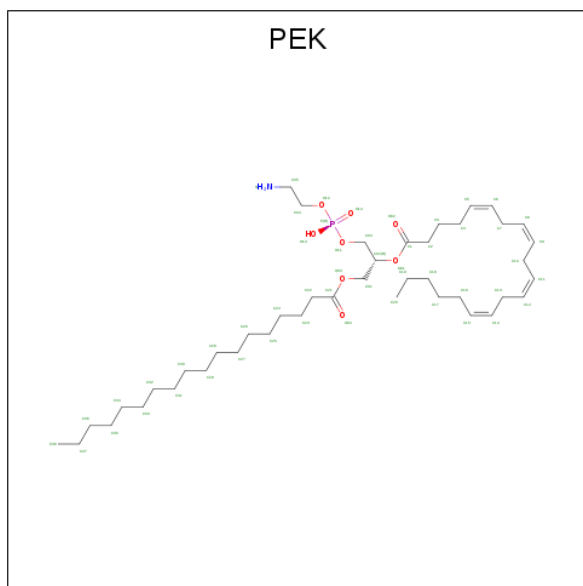
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

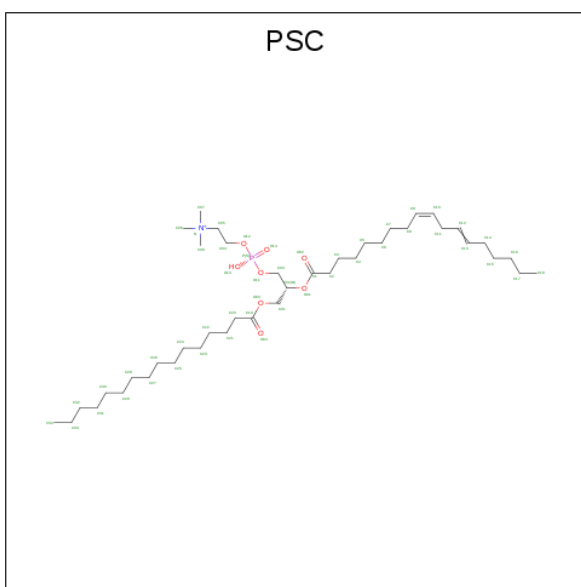


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	X	0	0
			1	1		
24	C	1	Total	X	0	0
			1	1		

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).

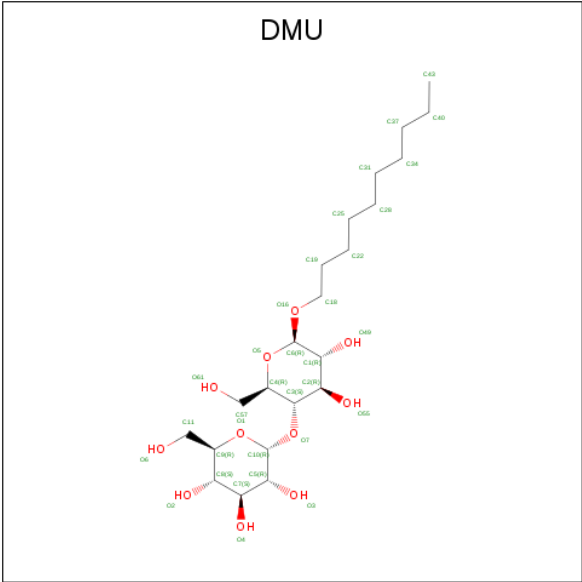


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	S	1	Total	Zn	0	0
			1	1		
26	F	1	Total	Zn	0	0
			1	1		

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	229	Total	O	0	0
			229	229		
28	B	167	Total	O	0	0
			167	167		
28	C	107	Total	O	0	0
			107	107		
28	D	112	Total	O	0	0
			112	112		
28	E	90	Total	O	0	0
			90	90		
28	F	109	Total	O	0	0
			109	109		
28	G	54	Total	O	0	0
			54	54		
28	H	61	Total	O	0	0
			61	61		
28	I	50	Total	O	0	0
			50	50		
28	J	34	Total	O	0	0
			34	34		

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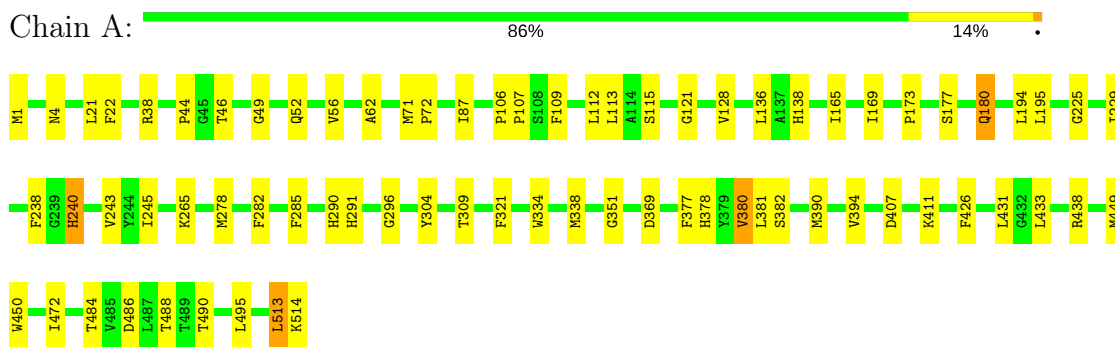
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	28	Total 28	O 28	0	0
28	L	21	Total 21	O 21	0	0
28	M	33	Total 33	O 33	0	0
28	N	214	Total 214	O 214	0	0
28	O	116	Total 116	O 116	0	0
28	P	112	Total 112	O 112	0	0
28	Q	72	Total 72	O 72	0	0
28	R	48	Total 48	O 48	0	0
28	S	77	Total 77	O 77	0	0
28	T	48	Total 48	O 48	0	0
28	U	54	Total 54	O 54	0	0
28	V	32	Total 32	O 32	0	0
28	W	20	Total 20	O 20	0	0
28	X	20	Total 20	O 20	0	0
28	Y	22	Total 22	O 22	0	0
28	Z	13	Total 13	O 13	0	0

### 3 Residue-property plots

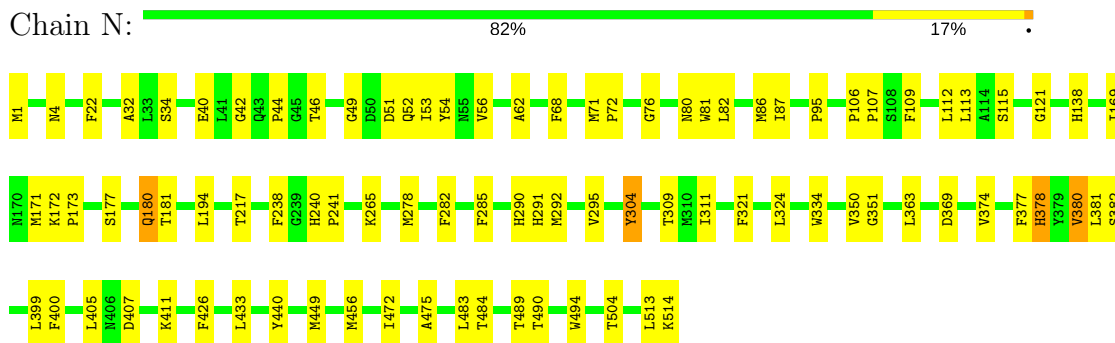
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

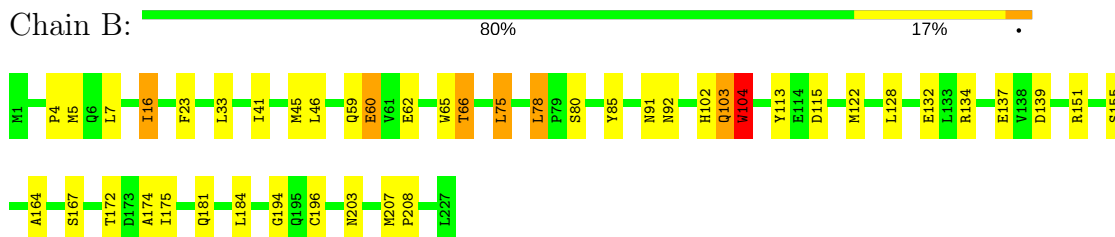
#### • Molecule 1: Cytochrome c oxidase polypeptide I



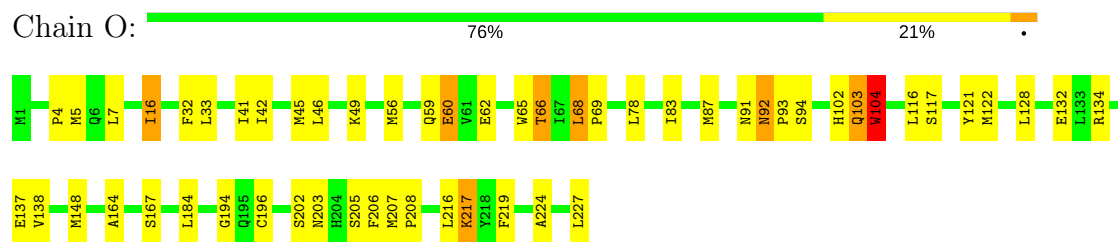
#### • Molecule 1: Cytochrome c oxidase polypeptide I



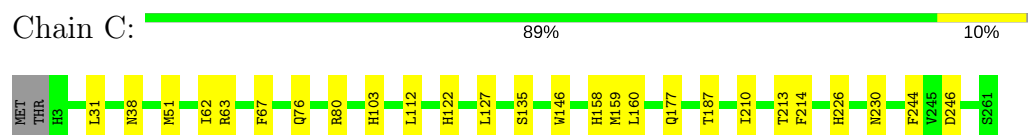
#### • Molecule 2: Cytochrome c oxidase polypeptide II



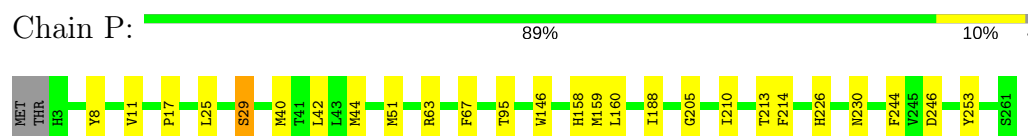
#### • Molecule 2: Cytochrome c oxidase polypeptide II



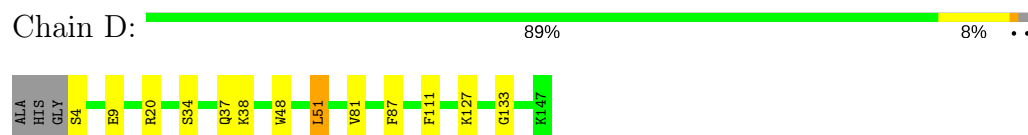
- Molecule 3: Cytochrome c oxidase polypeptide III



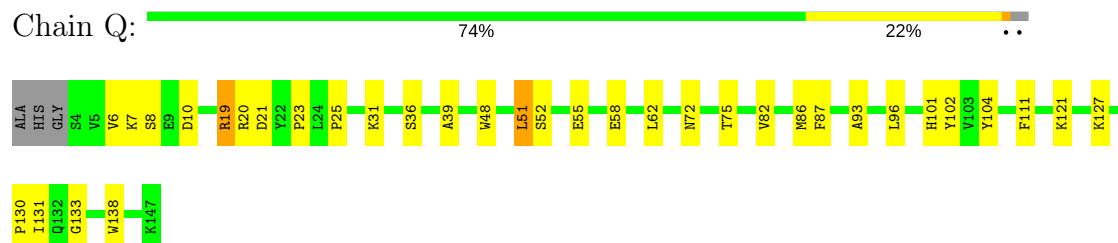
- Molecule 3: Cytochrome c oxidase polypeptide III



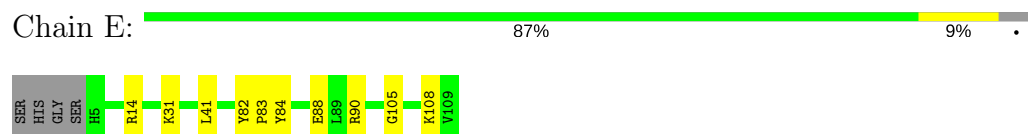
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1



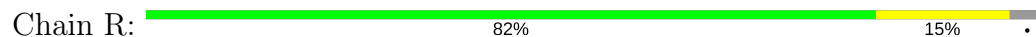
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1

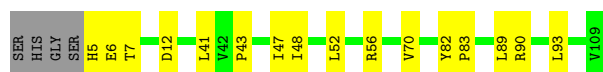


- Molecule 5: Cytochrome c oxidase polypeptide Va



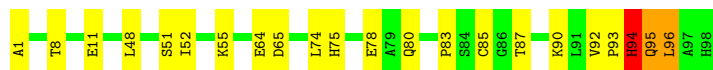
- Molecule 5: Cytochrome c oxidase polypeptide Va





- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 78% 19% ..



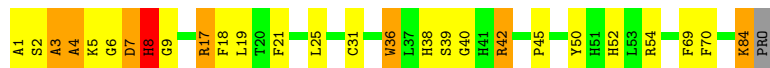
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S: 73% 22% ..



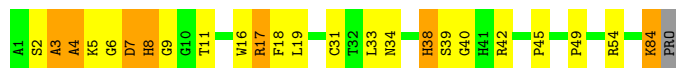
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G: 67% 22% 8% ..



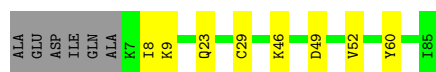
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T: 71% 20% 8% .



- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain H: 84% 9% 7%



- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain U: 76% 15% 7%

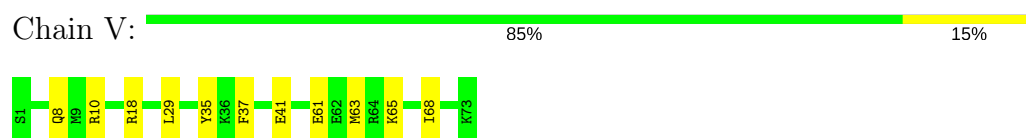


- Molecule 9: Cytochrome c oxidase polypeptide VIc

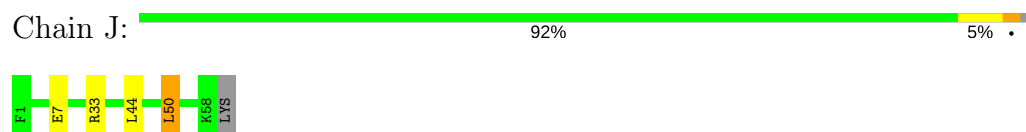
Chain I: 86% 12% .



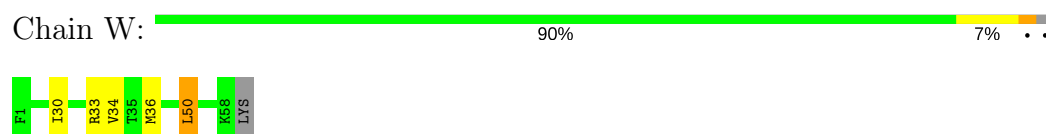
- Molecule 9: Cytochrome c oxidase polypeptide VIc



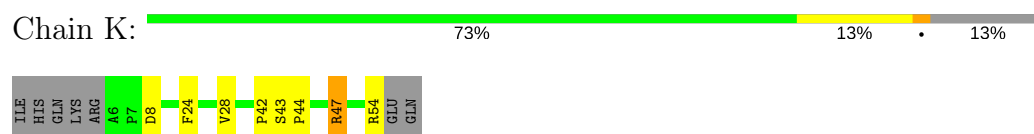
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



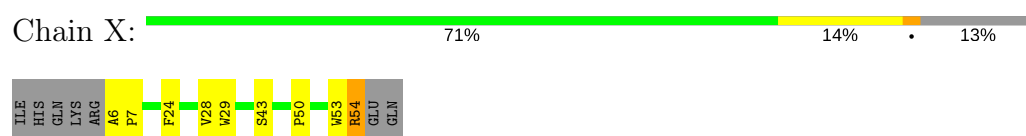
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



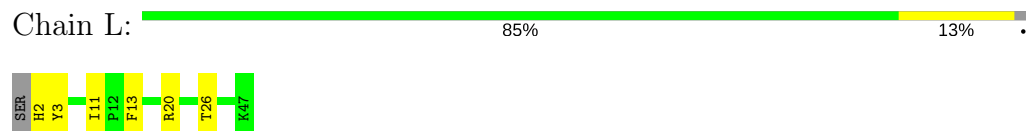
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



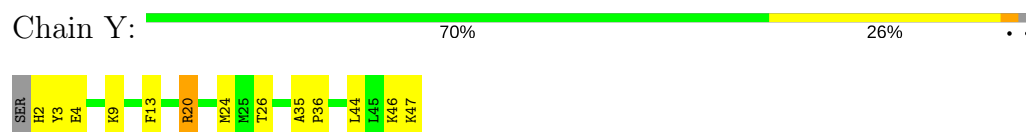
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

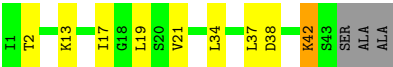


- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart





● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.203 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality [i](#)

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

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

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	0.53	0/4156	0.69	1/5678 (0.0%)
1	N	0.53	0/4156	0.68	1/5678 (0.0%)
2	B	0.52	0/1860	0.82	4/2534 (0.2%)
2	O	0.52	0/1860	0.82	3/2534 (0.1%)
3	C	0.53	0/2197	0.61	0/3005
3	P	0.52	0/2197	0.63	0/3005
4	D	0.50	0/1229	0.67	1/1658 (0.1%)
4	Q	0.51	0/1229	0.65	1/1658 (0.1%)
5	E	0.51	0/871	0.66	0/1182
5	R	0.51	0/871	0.67	0/1182
6	F	0.50	0/765	0.81	2/1038 (0.2%)
6	S	0.47	0/765	0.82	2/1038 (0.2%)
7	G	0.53	0/690	0.71	0/937
7	T	0.54	0/690	0.72	1/937 (0.1%)
8	H	0.48	0/682	0.67	0/921
8	U	0.51	0/682	0.69	0/921
9	I	0.52	0/605	0.64	0/802
9	V	0.53	0/605	0.61	0/802
10	J	0.47	0/471	0.63	0/636
10	W	0.49	0/471	0.66	0/636
11	K	0.54	0/398	0.68	0/546
11	X	0.56	0/398	0.68	0/546
12	L	0.54	0/393	0.55	0/526
12	Y	0.55	0/393	0.58	0/526
13	M	0.47	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.52	0/29324	0.69	16/39866 (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	1
1	N	0	2
2	B	0	2
2	O	0	1
8	U	0	1
All	All	0	7

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	GLN	CA-C-N	-6.93	101.94	117.20
6	S	94	HIS	N-CA-C	6.19	127.71	111.00
4	D	133	GLY	N-CA-C	6.09	128.33	113.10
2	O	103	GLN	CA-C-N	-6.04	103.91	117.20
6	F	94	HIS	N-CA-C	5.98	127.14	111.00
4	Q	133	GLY	N-CA-C	5.94	127.95	113.10
2	B	104	TRP	N-CA-C	5.87	126.85	111.00
7	T	33	LEU	CA-CB-CG	5.83	128.72	115.30
6	F	93	PRO	N-CA-C	5.77	127.10	112.10
1	N	378	HIS	CA-CB-CG	-5.58	104.11	113.60
2	O	104	TRP	N-CA-C	5.47	125.77	111.00
2	B	184	LEU	CA-CB-CG	5.46	127.86	115.30
2	O	184	LEU	CA-CB-CG	5.35	127.61	115.30
6	S	93	PRO	N-CA-C	5.32	125.92	112.10
1	A	438	ARG	CB-CA-C	-5.28	99.84	110.40
2	B	103	GLN	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
2	B	103	GLN	Mainchain
2	B	85	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
2	O	103	GLN	Mainchain
8	U	11	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	60	0
1	N	4027	0	4001	80	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	42	0
3	C	2110	0	2027	27	0
3	P	2110	0	2027	26	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	28	0
5	E	852	0	845	6	0
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	19	0
7	G	675	0	643	26	0
7	T	675	0	643	25	0
8	H	662	0	623	3	0
8	U	662	0	623	6	0
9	I	601	0	613	7	0
9	V	601	0	613	6	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	5	0
11	X	384	0	366	10	0
12	L	380	0	380	13	0
12	Y	380	0	380	11	0
13	M	335	0	352	6	0
13	Z	335	0	352	3	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	5	0
17	N	120	0	108	6	0
18	A	189	0	330	47	0
18	N	126	0	220	41	0
18	Q	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	102	0	152	7	0
19	C	102	0	152	9	0
19	N	102	0	152	6	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	4	0
21	J	29	0	39	3	0
21	O	29	0	39	0	0
21	P	58	0	78	2	0
21	W	29	0	39	3	0
22	C	100	0	156	23	0
22	G	100	0	156	17	0
22	P	100	0	156	20	0
22	T	100	0	156	20	0
23	C	106	0	154	13	0
23	G	53	0	77	6	0
23	P	106	0	154	8	0
23	T	53	0	77	8	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	12	0
25	O	52	0	80	11	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	37	0	0
27	Z	33	0	37	0	0
28	A	229	0	0	6	0
28	B	167	0	0	2	0
28	C	107	0	0	4	0
28	D	112	0	0	3	0
28	E	90	0	0	1	0
28	F	109	0	0	1	0
28	G	54	0	0	3	0
28	H	61	0	0	2	0
28	I	50	0	0	3	0
28	J	34	0	0	2	0
28	K	28	0	0	0	0
28	L	21	0	0	1	0
28	M	33	0	0	1	0
28	N	214	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	O	116	0	0	1	0
28	P	112	0	0	4	0
28	Q	72	0	0	3	0
28	R	48	0	0	0	0
28	S	77	0	0	3	0
28	T	48	0	0	2	0
28	U	54	0	0	1	0
28	V	32	0	0	2	0
28	W	20	0	0	0	0
28	X	20	0	0	1	0
28	Y	22	0	0	0	0
28	Z	13	0	0	1	0
All	All	32609	0	31222	568	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 9.

All (568) 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)
7:T:84:LYS:H	7:T:84:LYS:HD2	1.21	1.03
7:G:84:LYS:HD2	7:G:84:LYS:H	1.21	1.03
10:W:33:ARG:HG2	21:W:4060:CHD:H152	1.42	0.99
18:A:3522:TGL:HC32	12:L:20:ARG:HH22	1.29	0.98
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.92
10:J:33:ARG:HG2	21:J:3060:CHD:H152	1.51	0.92
22:C:3270:CDL:H242	22:C:3270:CDL:H661	1.54	0.89
22:P:4270:CDL:H242	22:P:4270:CDL:H661	1.54	0.89
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
25:O:4230:PSC:H21	25:O:4230:PSC:H222	1.55	0.88
18:A:3522:TGL:HC72	28:L:2344:HOH:O	1.73	0.88
18:A:3522:TGL:HC61	12:L:20:ARG:HH12	1.39	0.87
7:G:8:HIS:HD2	23:G:4263:PEK:H252	1.42	0.85
18:N:4522:TGL:HC31	12:Y:13:PHE:HA	1.59	0.85
25:E:3230:PSC:H21	25:E:3230:PSC:H222	1.59	0.84
18:A:3522:TGL:CC6	12:L:20:ARG:HH12	1.91	0.84
6:S:85:CYS:SG	6:S:87:THR:HG23	2.19	0.82
8:H:23:GLN:HG3	28:H:2104:HOH:O	1.79	0.81
2:O:41:ILE:HD13	25:O:4230:PSC:H342	1.62	0.81
3:C:67:PHE:HE1	22:C:3270:CDL:H1	1.44	0.80
3:C:63:ARG:HE	22:C:3270:CDL:HA22	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:HE1	22:P:4270:CDL:H1	1.47	0.80
1:N:1:FME:HCN	1:N:4:ASN:H	1.48	0.79
6:S:94:HIS:CG	6:S:95:GLN:H	2.02	0.78
3:P:63:ARG:HE	22:P:4270:CDL:HA22	1.47	0.78
1:N:112:LEU:HG	28:N:1379:HOH:O	1.85	0.76
18:A:3522:TGL:HC31	12:L:13:PHE:HA	1.66	0.76
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.68	0.76
23:P:4264:PEK:H161	23:P:4264:PEK:H102	1.68	0.76
18:A:3521:TGL:H241	18:A:3521:TGL:HA91	1.68	0.76
23:C:3264:PEK:H161	23:C:3264:PEK:H102	1.65	0.75
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.66	0.75
7:T:5:LYS:HD2	23:T:3263:PEK:H382	1.69	0.75
3:C:210:ILE:HG23	19:C:3267:PGV:H102	1.68	0.75
18:N:4522:TGL:HC22	18:N:4522:TGL:HC62	1.68	0.74
7:G:5:LYS:HB3	1:N:278:MET:SD	2.27	0.74
1:N:334:TRP:CZ3	18:Q:4523:TGL:HA42	2.23	0.74
6:F:85:CYS:SG	6:F:87:THR:HG23	2.28	0.73
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.50	0.73
18:A:3522:TGL:HC62	18:A:3522:TGL:HC22	1.69	0.73
3:C:160:LEU:HD13	21:C:3271:CHD:H181	1.69	0.73
19:A:3524:PGV:H321	19:A:3524:PGV:H162	1.71	0.72
19:N:4524:PGV:H321	19:N:4524:PGV:H162	1.70	0.72
3:P:210:ILE:HG23	19:P:4267:PGV:H102	1.72	0.72
18:N:4521:TGL:H241	18:N:4521:TGL:HA91	1.70	0.71
18:N:4521:TGL:HB91	2:O:32:PHE:CE2	2.25	0.71
3:P:160:LEU:HD13	21:P:4271:CHD:H181	1.73	0.70
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.74	0.70
23:G:4263:PEK:H9	3:P:244:PHE:HA	1.73	0.70
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.74	0.69
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.91	0.69
1:N:426:PHE:CE1	18:N:4521:TGL:H282	2.28	0.69
22:P:4270:CDL:H391	28:P:2645:HOH:O	1.91	0.69
6:S:75:HIS:H	6:S:80:GLN:HE22	1.41	0.68
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.74	0.68
7:T:31:CYS:SG	22:T:4269:CDL:H532	2.33	0.68
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.75	0.68
1:N:113:LEU:HB3	28:N:2240:HOH:O	1.93	0.68
19:A:3524:PGV:H032	28:A:3752:HOH:O	1.93	0.67
1:A:278:MET:SD	7:T:5:LYS:HB3	2.35	0.67
18:A:3522:TGL:HC61	12:L:20:ARG:NH1	2.09	0.67
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:89:LEU:O	5:R:93:LEU:HG	1.94	0.67
1:A:177:SER:H	1:A:180:GLN:HE21	1.43	0.67
19:C:3267:PGV:H12	19:C:3267:PGV:H161	1.78	0.66
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.78	0.66
7:T:84:LYS:N	7:T:84:LYS:HD2	2.03	0.66
4:D:34:SER:H	4:D:37:GLN:NE2	1.89	0.66
23:P:4265:PEK:H383	22:T:4269:CDL:H272	1.77	0.66
18:Q:4523:TGL:HG12	18:Q:4523:TGL:HC21	1.76	0.66
3:C:244:PHE:HA	23:T:3263:PEK:H9	1.77	0.66
2:O:56:MET:HA	25:O:4230:PSC:H202	1.78	0.65
18:A:3522:TGL:HC32	12:L:20:ARG:NH2	2.09	0.65
23:C:3264:PEK:H32	23:C:3264:PEK:H71	1.79	0.65
6:F:8:THR:OG1	6:F:11:GLU:HG3	1.99	0.63
7:G:36:TRP:HB3	28:G:628:HOH:O	1.97	0.63
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.63
18:A:3523:TGL:HC21	18:A:3523:TGL:HG12	1.79	0.63
7:G:84:LYS:H	7:G:84:LYS:CD	2.02	0.63
1:N:378:HIS:O	1:N:382:SER:HB2	1.99	0.63
1:N:53:ILE:HG12	28:N:1382:HOH:O	1.98	0.63
3:C:63:ARG:HE	22:C:3270:CDL:CA2	2.11	0.63
7:G:84:LYS:N	7:G:84:LYS:HD2	2.04	0.62
23:C:3265:PEK:H383	22:G:3269:CDL:H272	1.82	0.62
19:P:4267:PGV:H161	19:P:4267:PGV:H12	1.80	0.62
1:A:426:PHE:CE1	18:A:3521:TGL:H282	2.34	0.62
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.34	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.61
3:P:63:ARG:HE	22:P:4270:CDL:CA2	2.12	0.61
1:N:433:LEU:HD11	18:N:4521:TGL:OB1	2.00	0.61
25:O:4230:PSC:C07	9:V:10:ARG:HH21	2.13	0.61
1:A:472:ILE:HG21	18:A:3522:TGL:HA81	1.81	0.61
18:A:3523:TGL:H242	18:A:3523:TGL:HA81	1.80	0.61
3:P:67:PHE:CE1	22:P:4270:CDL:H1	2.32	0.61
22:C:3270:CDL:H312	22:C:3270:CDL:H151	1.81	0.61
1:A:449:MET:SD	2:B:5:MET:HG2	2.41	0.61
22:P:4270:CDL:H312	22:P:4270:CDL:H151	1.83	0.61
2:B:62:GLU:O	2:B:66:THR:HB	2.00	0.61
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.36	0.61
2:O:41:ILE:CD1	25:O:4230:PSC:H342	2.30	0.60
3:P:246:ASP:HB2	28:P:1272:HOH:O	2.01	0.60
1:N:472:ILE:HD13	18:N:4522:TGL:HA92	1.83	0.60
18:A:3523:TGL:HC31	28:A:3753:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.02	0.60
7:T:17:ARG:HD2	28:T:1509:HOH:O	2.02	0.60
18:A:3522:TGL:H271	12:L:11:ILE:HG22	1.82	0.60
19:A:3524:PGV:H311	13:M:19:LEU:HD23	1.83	0.60
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.37	0.60
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.36	0.60
18:Q:4523:TGL:HA81	18:Q:4523:TGL:H242	1.83	0.59
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.84	0.59
3:C:213:THR:HG23	22:C:3270:CDL:H762	1.82	0.59
8:U:49:ASP:O	8:U:52:VAL:HG22	2.03	0.59
1:A:484:THR:HB	13:M:2:THR:OG1	2.02	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.03	0.59
7:G:31:CYS:SG	22:G:3269:CDL:H532	2.43	0.59
11:K:24:PHE:O	11:K:28:VAL:HG12	2.02	0.59
1:A:1:FME:HCN	1:A:4:ASN:H	1.68	0.58
22:G:3269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.58
23:P:4264:PEK:H71	23:P:4264:PEK:H32	1.83	0.58
6:S:87:THR:HG21	28:S:1303:HOH:O	2.02	0.58
7:T:38:HIS:NE2	22:T:4269:CDL:H111	2.18	0.58
22:P:4270:CDL:H112	28:P:2598:HOH:O	2.03	0.58
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.03	0.58
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.86	0.58
6:F:92:VAL:O	6:F:92:VAL:HG23	2.03	0.58
1:A:177:SER:H	1:A:180:GLN:NE2	2.02	0.58
7:G:45:PRO:HD2	28:G:132:HOH:O	2.03	0.58
10:J:7:GLU:HG3	28:J:2487:HOH:O	2.03	0.58
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.86	0.58
1:A:113:LEU:HD12	18:A:3522:TGL:H292	1.85	0.57
7:T:45:PRO:HD2	28:T:1132:HOH:O	2.04	0.57
19:N:4524:PGV:H141	4:Q:87:PHE:CE2	2.39	0.57
19:A:3524:PGV:H141	4:D:87:PHE:CE2	2.39	0.57
3:P:51:MET:HB3	22:P:4270:CDL:H622	1.87	0.57
7:T:5:LYS:CD	23:T:3263:PEK:H382	2.33	0.57
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.33	0.57
1:N:350:VAL:HG11	18:N:4521:TGL:H281	1.87	0.57
1:N:113:LEU:CD1	18:N:4522:TGL:H292	2.35	0.56
18:N:4521:TGL:HB91	2:O:32:PHE:HE2	1.71	0.56
23:C:3265:PEK:H041	6:F:1:ALA:N	2.20	0.56
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.37	0.56
3:C:51:MET:HB3	22:C:3270:CDL:H622	1.87	0.56
6:S:22:LEU:HD12	28:S:2496:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
2:O:224:ALA:O	2:O:227:LEU:HG	2.06	0.56
1:N:113:LEU:HD12	18:N:4522:TGL:H292	1.88	0.56
2:O:49:LYS:NZ	18:Q:4523:TGL:HC71	2.21	0.56
3:C:246:ASP:HB2	28:C:3557:HOH:O	2.04	0.56
17:N:516:HEA:HMD1	17:N:516:HEA:HBD2	1.88	0.56
3:P:25:LEU:O	3:P:29:SER:HB2	2.06	0.56
3:P:226:HIS:CE1	22:P:4270:CDL:HB31	2.41	0.56
25:E:3230:PSC:H072	9:I:10:ARG:HH21	1.70	0.55
18:N:4521:TGL:H101	18:N:4521:TGL:H283	1.86	0.55
3:C:158:HIS:NE2	23:C:3265:PEK:H051	2.22	0.55
22:C:3270:CDL:H662	19:C:3267:PGV:H182	1.88	0.55
7:G:17:ARG:HD2	28:G:2008:HOH:O	2.06	0.55
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.88	0.55
1:A:136:LEU:HB2	28:A:3740:HOH:O	2.06	0.55
17:A:516:HEA:HMD1	17:A:516:HEA:HBD2	1.87	0.55
2:B:139:ASP:HB2	28:B:4220:HOH:O	2.07	0.55
18:N:4522:TGL:HG12	12:Y:13:PHE:HB3	1.88	0.55
1:A:377:PHE:O	1:A:381:LEU:HB3	2.07	0.55
3:C:67:PHE:CE1	22:C:3270:CDL:H1	2.34	0.55
2:O:83:ILE:O	2:O:87:MET:HG3	2.07	0.55
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.55
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.07	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.08	0.54
4:Q:86:MET:HE1	28:X:2287:HOH:O	2.06	0.54
1:A:113:LEU:CD1	18:A:3522:TGL:H292	2.37	0.54
18:A:3523:TGL:H122	18:A:3523:TGL:HB82	1.89	0.54
1:N:52:GLN:O	1:N:56:VAL:HG23	2.07	0.54
1:A:321:PHE:CD2	25:E:3230:PSC:H341	2.43	0.54
7:G:8:HIS:CD2	23:G:4263:PEK:H252	2.32	0.54
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.07	0.54
18:A:3521:TGL:H283	18:A:3521:TGL:H101	1.89	0.54
22:G:3269:CDL:H332	28:O:1358:HOH:O	2.08	0.54
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.90	0.54
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.90	0.53
22:P:4270:CDL:H121	28:P:2392:HOH:O	2.07	0.53
1:N:177:SER:H	1:N:180:GLN:NE2	2.06	0.53
18:N:4522:TGL:CC6	18:N:4522:TGL:HC22	2.37	0.53
2:O:62:GLU:O	2:O:66:THR:HB	2.08	0.53
7:T:38:HIS:CD2	22:T:4269:CDL:HA21	2.42	0.53
18:A:3522:TGL:HC62	12:L:20:ARG:HH12	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.72	0.53
2:B:102:HIS:O	2:B:104:TRP:N	2.41	0.53
3:P:213:THR:HG23	22:P:4270:CDL:H762	1.91	0.53
1:N:334:TRP:HZ3	18:Q:4523:TGL:HA62	1.72	0.53
9:I:8:GLN:HE22	9:I:10:ARG:H	1.57	0.53
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.89	0.53
4:D:20:ARG:HG3	28:D:168:HOH:O	2.09	0.53
1:A:514:LYS:HE3	28:A:3750:HOH:O	2.08	0.53
28:B:4144:HOH:O	22:T:4269:CDL:H332	2.09	0.53
18:N:4522:TGL:CG1	12:Y:13:PHE:HB3	2.39	0.53
18:N:4521:TGL:H101	18:N:4521:TGL:C28	2.39	0.52
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.92	0.52
18:Q:4523:TGL:H122	18:Q:4523:TGL:HB82	1.90	0.52
1:A:304:TYR:HD1	22:T:4269:CDL:HB32	1.75	0.52
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.74	0.52
2:B:164:ALA:O	2:B:194:GLY:HA3	2.09	0.52
1:A:21:LEU:HD23	18:A:3522:TGL:H211	1.92	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.39	0.52
6:F:64:GLU:O	6:F:65:ASP:HB2	2.10	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.44	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.52
8:U:7:LYS:O	8:U:8:ILE:HG22	2.09	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.92	0.52
23:P:4265:PEK:H041	6:S:1:ALA:N	2.24	0.52
1:N:472:ILE:HG21	18:N:4522:TGL:HA81	1.91	0.52
18:A:3522:TGL:CC6	18:A:3522:TGL:HC22	2.37	0.51
4:D:4:SER:N	28:D:257:HOH:O	2.44	0.51
22:G:3269:CDL:H612	22:G:3269:CDL:H751	1.92	0.51
6:S:92:VAL:HG23	6:S:92:VAL:O	2.11	0.51
2:O:116:LEU:HD12	2:O:117:SER:N	2.26	0.51
22:T:4269:CDL:H751	22:T:4269:CDL:H612	1.91	0.51
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.51
4:D:4:SER:HB2	28:D:257:HOH:O	2.09	0.51
5:E:84:TYR:O	5:E:88:GLU:HG2	2.11	0.51
6:F:75:HIS:H	6:F:80:GLN:HE22	1.58	0.51
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.93	0.51
1:A:472:ILE:HD13	18:A:3522:TGL:HA92	1.93	0.51
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.51
1:N:22:PHE:HA	18:N:4522:TGL:HB72	1.93	0.51
1:A:282:PHE:HA	7:T:4:ALA:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:4264:PEK:C16	23:P:4264:PEK:H102	2.40	0.51
1:A:1:FME:HCN	1:A:4:ASN:HB2	1.92	0.50
1:N:400:PHE:HB3	18:N:4522:TGL:H282	1.93	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.50
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.46	0.50
18:A:3521:TGL:HC52	2:B:7:LEU:HD12	1.94	0.50
6:S:51:SER:O	6:S:94:HIS:N	2.45	0.50
3:C:103:HIS:HA	19:C:3268:PGV:H012	1.94	0.50
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.50
18:N:4521:TGL:CB9	18:N:4521:TGL:H283	2.42	0.50
3:P:158:HIS:NE2	23:P:4265:PEK:H051	2.26	0.50
18:A:3521:TGL:OB1	18:A:3521:TGL:HB42	2.11	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.50
13:M:17:ILE:O	13:M:21:VAL:HG23	2.12	0.50
22:T:4269:CDL:HA62	22:T:4269:CDL:H322	1.94	0.50
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.42	0.50
7:T:34:ASN:ND2	22:T:4269:CDL:H151	2.26	0.50
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.93	0.50
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.94	0.50
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.50
22:C:3270:CDL:H372	22:C:3270:CDL:H192	1.94	0.50
18:A:3521:TGL:HC22	28:I:346:HOH:O	2.12	0.49
22:G:3269:CDL:HB32	1:N:304:TYR:CD1	2.47	0.49
9:I:22:VAL:O	9:I:26:MET:HG2	2.12	0.49
18:A:3521:TGL:C28	18:A:3521:TGL:H101	2.42	0.49
25:E:3230:PSC:C07	9:I:10:ARG:HH21	2.25	0.49
22:C:3270:CDL:H651	22:C:3270:CDL:H771	1.95	0.49
23:C:3264:PEK:C16	23:C:3264:PEK:H102	2.38	0.49
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.78	0.49
3:C:122:HIS:HD2	28:C:3562:HOH:O	1.95	0.49
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.93	0.49
2:O:102:HIS:O	2:O:104:TRP:N	2.45	0.49
1:A:52:GLN:O	1:A:56:VAL:HG23	2.12	0.49
5:E:41:LEU:HA	28:I:301:HOH:O	2.12	0.49
1:N:350:VAL:CG1	18:N:4521:TGL:H281	2.42	0.49
1:N:472:ILE:HG21	18:N:4522:TGL:CA8	2.42	0.49
7:T:2:SER:O	7:T:3:ALA:HB3	2.13	0.49
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.12	0.49
18:N:4521:TGL:HB92	18:N:4521:TGL:H283	1.94	0.49
18:N:4521:TGL:OB1	18:N:4521:TGL:HB42	2.12	0.49
22:P:4270:CDL:H641	22:P:4270:CDL:H231	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.12	0.49
2:B:172:THR:HG23	28:H:2574:HOH:O	2.12	0.49
3:C:226:HIS:CE1	22:C:3270:CDL:HB31	2.48	0.48
1:N:407:ASP:O	1:N:411:LYS:HG3	2.13	0.48
22:P:4270:CDL:H372	22:P:4270:CDL:H192	1.93	0.48
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.58	0.48
28:A:3691:HOH:O	19:C:3268:PGV:H12	2.13	0.48
6:F:92:VAL:O	6:F:92:VAL:CG2	2.61	0.48
18:A:3521:TGL:H283	18:A:3521:TGL:HB92	1.95	0.48
18:N:4522:TGL:HB52	18:N:4522:TGL:HB81	1.59	0.48
1:A:472:ILE:HG21	18:A:3522:TGL:CA8	2.44	0.48
1:N:87:ILE:O	1:N:173:PRO:HD3	2.13	0.48
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.48
1:N:377:PHE:O	1:N:381:LEU:HB3	2.14	0.48
18:N:4522:TGL:H181	18:N:4522:TGL:OA1	2.14	0.48
22:P:4270:CDL:H771	22:P:4270:CDL:H651	1.95	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.14	0.48
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.14	0.48
10:W:30:ILE:O	10:W:34:VAL:HG23	2.13	0.48
18:A:3521:TGL:H241	18:A:3521:TGL:CA9	2.43	0.48
23:C:3265:PEK:H301	2:O:66:THR:CG2	2.44	0.47
2:O:68:LEU:HD22	25:O:4230:PSC:H171	1.95	0.47
18:A:3521:TGL:CB9	18:A:3521:TGL:H283	2.44	0.47
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.14	0.47
18:A:3522:TGL:CG1	12:L:13:PHE:HB3	2.44	0.47
7:G:5:LYS:HD2	23:G:4263:PEK:H382	1.95	0.47
9:I:35:TYR:C	9:I:37:PHE:H	2.18	0.47
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.44	0.47
3:P:253:TYR:CE2	22:T:4269:CDL:H641	2.49	0.47
22:G:3269:CDL:H511	22:G:3269:CDL:H172	1.97	0.47
22:G:3269:CDL:HA62	22:G:3269:CDL:H322	1.95	0.47
2:B:59:GLN:O	2:B:59:GLN:HG3	2.14	0.47
5:E:14:ARG:HD2	28:E:3271:HOH:O	2.14	0.47
6:F:90:LYS:HD2	28:F:187:HOH:O	2.14	0.47
9:V:35:TYR:C	9:V:37:PHE:H	2.18	0.47
22:G:3269:CDL:H212	1:N:311:ILE:HD12	1.97	0.47
2:O:203:ASN:HD22	2:O:203:ASN:N	2.12	0.47
6:S:22:LEU:O	6:S:25:ARG:HB3	2.15	0.47
1:A:378:HIS:O	1:A:382:SER:HB2	2.15	0.47
1:N:115:SER:O	1:N:121:GLY:HA2	2.15	0.47
19:N:4524:PGV:H211	28:Z:2192:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.80	0.47
18:N:4521:TGL:HB91	2:O:32:PHE:CD2	2.49	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.14	0.47
22:G:3269:CDL:H252	22:G:3269:CDL:H222	1.73	0.47
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.47
1:A:1:FME:HA	1:A:1:FME:CE	2.45	0.47
25:O:4230:PSC:C14	25:O:4230:PSC:H343	2.45	0.47
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.33	0.47
23:C:3265:PEK:H232	7:G:21:PHE:CD2	2.49	0.46
8:H:49:ASP:O	8:H:52:VAL:HG22	2.15	0.46
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.46
7:T:8:HIS:CD2	23:T:3263:PEK:H231	2.50	0.46
2:B:41:ILE:HD13	25:E:3230:PSC:H342	1.97	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.63	0.46
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.29	0.46
1:A:390:MET:O	1:A:394:VAL:HG13	2.15	0.46
1:A:433:LEU:HD11	18:A:3521:TGL:OB1	2.15	0.46
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.80	0.46
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.50	0.46
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.46
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.80	0.46
25:E:3230:PSC:C14	25:E:3230:PSC:H343	2.46	0.46
1:N:95:PRO:HG2	3:P:11:VAL:CG2	2.46	0.46
4:Q:75:THR:HG22	28:Q:1438:HOH:O	2.14	0.46
23:C:3265:PEK:H131	23:C:3265:PEK:H102	1.76	0.46
22:C:3270:CDL:H621	22:C:3270:CDL:H652	1.59	0.46
1:N:426:PHE:CD1	18:N:4521:TGL:H282	2.50	0.46
18:N:4521:TGL:H101	18:N:4521:TGL:C27	2.46	0.46
13:Z:4:LYS:HB2	13:Z:5:PRO:CD	2.46	0.46
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.97	0.46
2:B:4:PRO:HB2	11:K:43:SER:HA	1.98	0.46
22:T:4269:CDL:H511	22:T:4269:CDL:H172	1.96	0.46
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.46	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.15	0.46
1:A:426:PHE:CD1	18:A:3521:TGL:H282	2.51	0.46
17:A:515:HEA:HBC1	17:A:515:HEA:HMC1	1.97	0.46
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.04	0.46
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	1.98	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.34	0.46
7:G:84:LYS:N	7:G:84:LYS:CD	2.74	0.45
7:T:31:CYS:SG	22:T:4269:CDL:C53	3.03	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:THR:HG22	23:C:3264:PEK:H052	1.97	0.45
4:D:127:LYS:HD2	28:I:353:HOH:O	2.17	0.45
7:G:7:ASP:O	1:N:169:ILE:HD12	2.15	0.45
1:N:426:PHE:HE1	18:N:4521:TGL:H282	1.78	0.45
22:P:4270:CDL:CB3	22:P:4270:CDL:HB21	2.47	0.45
7:G:69:PHE:HD1	7:G:70:PHE:CE1	2.35	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.48	0.45
8:U:23:GLN:HG3	28:U:1462:HOH:O	2.17	0.45
9:V:18:ARG:HD3	28:V:1387:HOH:O	2.16	0.45
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.52	0.45
3:C:63:ARG:NE	22:C:3270:CDL:HA22	2.23	0.45
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.52	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
1:N:82:LEU:O	1:N:86:MET:HG3	2.17	0.45
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.29	0.45
1:A:22:PHE:HA	18:A:3522:TGL:HB72	1.99	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.17	0.45
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.78	0.45
23:C:3265:PEK:H041	6:F:1:ALA:H1	1.79	0.45
3:C:210:ILE:HD13	19:C:3267:PGV:H301	1.99	0.45
22:C:3270:CDL:H632	22:C:3270:CDL:H602	1.64	0.45
18:A:3522:TGL:HG12	12:L:13:PHE:HB3	1.98	0.45
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.45
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.98	0.45
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.45
18:N:4521:TGL:H222	18:N:4521:TGL:HA91	1.57	0.45
1:A:165:ILE:O	1:A:169:ILE:HG12	2.15	0.45
3:P:67:PHE:HE1	22:P:4270:CDL:C1	2.23	0.45
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.99	0.44
1:A:1:FME:HE2	1:A:1:FME:HA	1.98	0.44
1:A:1:FME:HE2	12:L:3:TYR:HE1	1.81	0.44
21:J:3060:CHD:H3	28:J:2631:HOH:O	2.17	0.44
13:M:42:LYS:CE	13:M:42:LYS:HA	2.41	0.44
18:N:4521:TGL:H101	18:N:4521:TGL:H271	1.98	0.44
19:C:3268:PGV:H202	19:C:3268:PGV:H231	1.80	0.44
2:O:4:PRO:HB2	11:X:43:SER:HA	1.99	0.44
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.52	0.44
18:A:3522:TGL:HB52	18:A:3522:TGL:HB81	1.60	0.44
19:A:3524:PGV:H211	28:M:2318:HOH:O	2.17	0.44
22:G:3269:CDL:H152	22:G:3269:CDL:H181	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.44
3:C:158:HIS:CE1	23:C:3265:PEK:H051	2.53	0.44
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.44
1:N:378:HIS:CD2	1:N:382:SER:OG	2.71	0.44
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.53	0.44
1:A:513:LEU:HA	1:A:513:LEU:HD22	1.75	0.44
9:I:5:ALA:O	9:I:7:PRO:HD3	2.18	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.89	0.44
7:G:42:ARG:O	7:G:42:ARG:HD3	2.18	0.44
5:R:5:HIS:HB3	5:R:6:GLU:H	1.63	0.44
22:G:3269:CDL:H571	22:G:3269:CDL:H601	1.80	0.44
19:P:4268:PGV:H231	19:P:4268:PGV:H202	1.82	0.44
19:A:3524:PGV:H141	4:D:87:PHE:CD2	2.52	0.44
22:T:4269:CDL:H252	22:T:4269:CDL:H222	1.73	0.44
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.83	0.43
22:C:3270:CDL:HB21	22:C:3270:CDL:CB3	2.48	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.43
22:P:4270:CDL:H662	19:P:4267:PGV:H182	2.00	0.43
1:A:407:ASP:O	1:A:411:LYS:HG3	2.19	0.43
22:P:4270:CDL:H621	22:P:4270:CDL:H652	1.62	0.43
18:A:3522:TGL:H271	12:L:11:ILE:CG2	2.49	0.43
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.19	0.43
5:R:12:ASP:HA	5:R:47:ILE:HD11	2.01	0.43
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.00	0.43
18:A:3521:TGL:HG11	2:B:7:LEU:HB3	2.00	0.43
25:E:3230:PSC:H252	25:E:3230:PSC:H221	1.79	0.43
18:N:4522:TGL:H232	18:N:4522:TGL:H272	1.99	0.43
1:N:440:TYR:CZ	2:O:205:SER:HA	2.53	0.43
1:A:309:THR:HG22	17:A:516:HEA:HMB2	2.01	0.43
18:A:3522:TGL:OA1	18:A:3522:TGL:H181	2.19	0.43
22:C:3270:CDL:H231	22:C:3270:CDL:H641	2.00	0.43
25:E:3230:PSC:H232	25:E:3230:PSC:H201	1.84	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.88	0.43
6:S:94:HIS:CG	6:S:95:GLN:N	2.78	0.43
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.33	0.43
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.54	0.43
7:G:7:ASP:O	7:G:9:GLY:N	2.47	0.43
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.87	0.43
19:N:4524:PGV:H141	4:Q:87:PHE:CD2	2.53	0.43
10:W:50:LEU:HD22	10:W:50:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.43
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.43
5:R:48:ILE:O	5:R:52:LEU:HG	2.19	0.43
21:C:3271:CHD:H161	28:C:3628:HOH:O	2.18	0.43
21:C:3271:CHD:H222	21:C:3271:CHD:H162	1.72	0.43
7:G:1:ALA:HB2	19:P:4268:PGV:H321	2.00	0.43
22:G:3269:CDL:H202	22:G:3269:CDL:H522	2.01	0.43
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	2.01	0.43
1:A:115:SER:O	1:A:121:GLY:HA2	2.19	0.43
1:A:240:HIS:O	1:A:243:VAL:HG22	2.19	0.43
22:C:3270:CDL:H532	22:C:3270:CDL:H561	1.84	0.43
4:D:48:TRP:HA	4:D:51:LEU:HD22	2.00	0.43
18:N:4521:TGL:H283	18:N:4521:TGL:C10	2.49	0.43
25:O:4230:PSC:H241	25:O:4230:PSC:H62	2.00	0.43
7:T:5:LYS:HG3	23:T:3263:PEK:H382	2.01	0.43
19:A:3524:PGV:H012	19:A:3524:PGV:C4	2.50	0.42
25:E:3230:PSC:H62	25:E:3230:PSC:H241	2.01	0.42
21:J:3060:CHD:H212	21:J:3060:CHD:H161	1.70	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.54	0.42
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.42
25:O:4230:PSC:H42	25:O:4230:PSC:H231	2.01	0.42
4:D:9:GLU:H	4:D:9:GLU:CD	2.23	0.42
3:C:135:SER:HB3	22:G:3269:CDL:H581	2.01	0.42
28:A:3743:HOH:O	11:K:8:ASP:HB2	2.19	0.42
18:N:4521:TGL:HG11	2:O:7:LEU:HB3	2.00	0.42
7:T:8:HIS:ND1	23:T:3263:PEK:H311	2.34	0.42
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.42
5:E:31:LYS:HE3	6:F:83:PRO:O	2.19	0.42
1:N:426:PHE:CE1	18:N:4521:TGL:C28	3.01	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
22:P:4270:CDL:OB9	22:P:4270:CDL:H522	2.19	0.42
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.20	0.42
6:S:64:GLU:O	6:S:65:ASP:HB2	2.19	0.42
1:A:282:PHE:HZ	22:T:4269:CDL:H761	1.84	0.42
18:A:3521:TGL:H222	18:A:3521:TGL:HA91	1.60	0.42
22:C:3270:CDL:HB22	22:C:3270:CDL:PA1	2.60	0.42
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.54	0.42
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.85	0.42
1:N:292:MET:O	1:N:295:VAL:HG22	2.20	0.42
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.55	0.42
1:N:81:TRP:HZ2	18:N:4522:TGL:C28	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:3521:TGL:C27	18:A:3521:TGL:H101	2.49	0.42
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.72	0.42
10:W:36:MET:HB3	21:W:4060:CHD:H181	2.01	0.42
21:C:3271:CHD:H222	28:C:3628:HOH:O	2.19	0.42
25:E:3230:PSC:H062	25:E:3230:PSC:H042	1.75	0.42
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.93	0.42
1:N:351:GLY:C	1:N:380:VAL:HG13	2.40	0.42
8:U:36:PHE:CE1	8:U:57:ARG:HB2	2.54	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.42
2:O:217:LYS:HE2	2:O:217:LYS:CA	2.49	0.42
7:T:5:LYS:CG	23:T:3263:PEK:H382	2.50	0.42
1:N:53:ILE:HD12	12:Y:44:LEU:HD23	2.01	0.42
1:A:128:VAL:O	1:A:128:VAL:HG12	2.20	0.42
22:C:3270:CDL:H812	19:C:3267:PGV:H181	2.02	0.42
6:F:51:SER:O	6:F:94:HIS:N	2.53	0.42
1:N:46:THR:OG1	1:N:49:GLY:HA2	2.20	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.42
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.34	0.42
7:T:19:LEU:HD21	23:T:3263:PEK:H362	2.02	0.42
22:T:4269:CDL:H432	22:T:4269:CDL:H402	1.78	0.42
3:P:253:TYR:HE2	22:T:4269:CDL:H641	1.83	0.42
22:T:4269:CDL:H631	22:T:4269:CDL:H662	1.88	0.42
8:U:43:MET:HE1	8:U:52:VAL:HG21	2.02	0.42
21:W:4060:CHD:H161	21:W:4060:CHD:H212	1.71	0.42
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.01	0.41
18:A:3522:TGL:H232	18:A:3522:TGL:H272	2.02	0.41
1:A:46:THR:OG1	1:A:49:GLY:HA2	2.20	0.41
4:D:34:SER:O	4:D:38:LYS:HG3	2.20	0.41
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.41
2:O:104:TRP:HA	2:O:207:MET:SD	2.60	0.41
1:N:217:THR:HG22	3:P:188:ILE:HG12	2.01	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.56	0.41
25:E:3230:PSC:H141	25:E:3230:PSC:H343	2.02	0.41
11:K:43:SER:HA	11:K:44:PRO:HD3	1.96	0.41
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.91	0.41
3:C:31:LEU:HA	3:C:31:LEU:HD23	1.92	0.41
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.01	0.41
19:N:4524:PGV:H311	13:Z:19:LEU:HD23	2.02	0.41
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.55	0.41
1:N:95:PRO:HG2	3:P:11:VAL:HG23	2.01	0.41
6:S:13:ALA:O	6:S:18:ARG:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:3270:CDL:OB9	22:C:3270:CDL:H522	2.21	0.41
18:N:4521:TGL:H281	18:N:4521:TGL:HB81	2.03	0.41
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.02	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.20	0.41
18:A:3521:TGL:H101	18:A:3521:TGL:H271	2.01	0.41
22:G:3269:CDL:H331	22:G:3269:CDL:OA7	2.20	0.41
10:J:44:LEU:HD23	10:J:44:LEU:HA	1.96	0.41
18:N:4521:TGL:CA9	18:N:4521:TGL:H241	2.44	0.41
21:P:4271:CHD:H162	21:P:4271:CHD:H222	1.71	0.41
4:Q:93:ALA:HB2	11:X:29:TRP:CE2	2.55	0.41
22:G:3269:CDL:H402	22:G:3269:CDL:H432	1.76	0.41
7:G:2:SER:OG	23:G:4263:PEK:H291	2.21	0.41
17:N:516:HEA:HHa	17:N:516:HEA:HAD2	1.88	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.21	0.41
22:T:4269:CDL:H582	22:T:4269:CDL:H551	1.77	0.41
3:C:62:ILE:HG13	19:C:3267:PGV:H21	2.02	0.41
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.27	0.41
2:O:121:TYR:O	2:O:138:VAL:HA	2.20	0.41
1:N:321:PHE:CD2	25:O:4230:PSC:H341	2.56	0.41
2:O:42:ILE:O	2:O:46:LEU:HG	2.20	0.41
1:A:334:TRP:CZ3	18:A:3523:TGL:HA62	2.55	0.41
2:B:75:LEU:HD12	2:B:75:LEU:HA	1.79	0.41
18:N:4521:TGL:HC22	28:Q:1346:HOH:O	2.21	0.41
19:N:4524:PGV:C4	19:N:4524:PGV:H012	2.50	0.41
3:P:205:GLY:HA3	23:P:4264:PEK:H181	2.02	0.41
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.56	0.41
23:P:4265:PEK:H041	6:S:1:ALA:H1	1.84	0.41
5:R:41:LEU:HA	28:V:1301:HOH:O	2.21	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.41
22:T:4269:CDL:H611	22:T:4269:CDL:H561	2.02	0.41
3:C:67:PHE:HE1	22:C:3270:CDL:C1	2.25	0.41
6:F:52:ILE:HA	6:F:94:HIS:HA	2.02	0.41
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.51	0.41
25:O:4230:PSC:H141	25:O:4230:PSC:H343	2.03	0.41
8:U:8:ILE:HA	8:U:8:ILE:HD12	1.98	0.41
2:B:155:SER:O	2:B:174:ALA:HB1	2.21	0.40
21:B:4085:CHD:H12	21:B:4085:CHD:H212	2.03	0.40
18:A:3522:TGL:H122	18:A:3522:TGL:H291	1.90	0.40
18:A:3523:TGL:HB51	4:D:81:VAL:HG11	2.03	0.40
22:C:3270:CDL:HB22	22:C:3270:CDL:OA5	2.22	0.40
7:G:19:LEU:HD21	23:G:4263:PEK:H362	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2:HIS:CG	12:L:3:TYR:H	2.39	0.40
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.02	0.40
1:A:488:THR:HB	1:A:495:LEU:HD13	2.03	0.40
22:T:4269:CDL:H601	22:T:4269:CDL:H571	1.76	0.40
9:V:37:PHE:HA	9:V:41:GLU:HB2	2.03	0.40
3:C:76:GLN:O	3:C:80:ARG:HG3	2.21	0.40
1:N:514:LYS:HE2	28:S:1303:HOH:O	2.22	0.40
4:Q:31:LYS:HB3	28:Q:2391:HOH:O	2.21	0.40
23:C:3265:PEK:H383	22:G:3269:CDL:C27	2.50	0.40
5:E:105:GLY:O	5:E:108:LYS:HG2	2.22	0.40
25:E:3230:PSC:H231	25:E:3230:PSC:H42	2.03	0.40
1:N:400:PHE:O	18:N:4522:TGL:H283	2.22	0.40
1:N:309:THR:HG22	17:N:516:HEA:HMB2	2.04	0.40
3:P:95:THR:HG21	19:P:4268:PGV:H282	2.04	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%)	500 (98%)	12 (2%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	13	4
2	O	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	13	4
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	36	25
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	6	1
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3504/3614 (97%)	3360 (96%)	112 (3%)	32 (1%)	19	8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	104	TRP
6	F	94	HIS

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Mol	Chain	Res	Type
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
2	O	104	TRP
7	T	40	GLY
8	U	8	ILE
8	U	46	LYS
2	B	60	GLU
2	O	60	GLU
6	F	96	LEU
6	S	96	LEU
3	C	38	ASN
8	H	9	LYS
7	G	6	GLY
7	T	6	GLY
2	B	92	ASN
2	O	92	ASN

### 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%)	49	42
1	N	426/426 (100%)	416 (98%)	10 (2%)	53	47
2	B	210/210 (100%)	198 (94%)	12 (6%)	23	12
2	O	210/210 (100%)	198 (94%)	12 (6%)	23	12
3	C	224/226 (99%)	220 (98%)	4 (2%)	62	58
3	P	224/226 (99%)	219 (98%)	5 (2%)	55	49
4	D	128/129 (99%)	127 (99%)	1 (1%)	83	83
4	Q	128/129 (99%)	125 (98%)	3 (2%)	53	47
5	E	92/95 (97%)	91 (99%)	1 (1%)	76	75
5	R	92/95 (97%)	89 (97%)	3 (3%)	41	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	81/81 (100%)	77 (95%)	4 (5%)	27	17
6	S	81/81 (100%)	76 (94%)	5 (6%)	20	10
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	2
7	T	67/68 (98%)	60 (90%)	7 (10%)	8	3
8	H	71/75 (95%)	69 (97%)	2 (3%)	47	39
8	U	71/75 (95%)	67 (94%)	4 (6%)	23	12
9	I	57/57 (100%)	55 (96%)	2 (4%)	39	29
9	V	57/57 (100%)	54 (95%)	3 (5%)	25	14
10	J	49/50 (98%)	48 (98%)	1 (2%)	58	53
10	W	49/50 (98%)	48 (98%)	1 (2%)	58	53
11	K	39/46 (85%)	37 (95%)	2 (5%)	26	15
11	X	39/46 (85%)	38 (97%)	1 (3%)	49	42
12	L	39/40 (98%)	38 (97%)	1 (3%)	49	42
12	Y	39/40 (98%)	37 (95%)	2 (5%)	26	15
13	M	37/38 (97%)	33 (89%)	4 (11%)	7	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	2
All	All	3040/3082 (99%)	2927 (96%)	113 (4%)	37	27

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	486	ASP
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP

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Mol	Chain	Res	Type
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	104	TRP
2	B	113	TYR
2	B	115	ASP
2	B	167	SER
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
6	F	48	LEU
6	F	78	GLU
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	38	HIS
7	G	42	ARG
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE

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Mol	Chain	Res	Type
1	N	241	PRO
1	N	369	ASP
1	N	380	VAL
1	N	484	THR
1	N	504	THR
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	148	MET
2	O	167	SER
2	O	217	LYS
3	P	17	PRO
3	P	29	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
5	R	7	THR
5	R	70	VAL
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	42	ARG
7	T	49	PRO
7	T	54	ARG
7	T	84	LYS
8	U	21	PRO

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Mol	Chain	Res	Type
8	U	29	CYS
8	U	60	TYR
8	U	65	PRO
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
10	W	50	LEU
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	80	GLN
7	G	8	HIS
9	I	8	GLN
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN

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Mol	Chain	Res	Type
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	71	HIS
9	V	8	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	A	1	1	9,9,10	0.96	1 (11%)	7,9,11	1.34	2 (28%)
2	FME	B	1	2	9,9,10	0.88	0	7,9,11	1.48	1 (14%)
7	TPO	G	11	7	9,10,11	2.00	2 (22%)	11,14,16	1.03	0
9	SAC	I	1	9	8,8,9	2.45	3 (37%)	7,9,11	2.97	4 (57%)
1	FME	N	1	1	9,9,10	1.00	1 (11%)	7,9,11	1.91	2 (28%)
2	FME	O	1	2	9,9,10	0.81	0	7,9,11	1.70	1 (14%)
7	TPO	T	11	7	9,10,11	2.15	2 (22%)	11,14,16	1.01	0
9	SAC	V	1	9	8,8,9	2.82	3 (37%)	7,9,11	3.18	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	-	0/5/9/11	0/0/0/0
2	FME	B	1	2	-	0/5/9/11	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	-	0/5/9/11	0/0/0/0
2	FME	O	1	2	-	0/5/9/11	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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	FME	CA-C	2.09	1.53	1.50
1	A	1	FME	CA-C	2.16	1.53	1.50
7	G	11	TPO	CB-CA	2.71	1.58	1.53
9	I	1	SAC	CA-C	2.81	1.53	1.50
7	T	11	TPO	CB-CA	3.33	1.59	1.53
9	V	1	SAC	CA-C	3.52	1.54	1.50
9	I	1	SAC	CA-N	3.85	1.51	1.46
7	G	11	TPO	CA-C	4.47	1.56	1.50
9	V	1	SAC	CA-N	4.70	1.53	1.46
7	T	11	TPO	CA-C	4.75	1.56	1.50
9	I	1	SAC	OAC-C1A	4.81	1.34	1.23
9	V	1	SAC	OAC-C1A	5.00	1.34	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.71	111.00	123.24
9	I	1	SAC	CA-N-C1A	-6.40	111.58	123.24
1	N	1	FME	CA-N-CN	-4.22	116.33	122.82
2	O	1	FME	CA-N-CN	-3.93	116.77	122.82
2	B	1	FME	CA-N-CN	-2.74	118.61	122.82
1	N	1	FME	O-C-CA	-2.49	119.30	125.09
1	A	1	FME	CA-N-CN	-2.44	119.08	122.82
1	A	1	FME	O-C-CA	-2.28	119.77	125.09
9	V	1	SAC	OAC-C1A-C2A	-2.25	118.01	122.07
9	I	1	SAC	OAC-C1A-C2A	-2.20	118.10	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	C2A-C1A-N	2.10	119.78	116.10
9	V	1	SAC	C2A-C1A-N	2.83	121.05	116.10
9	V	1	SAC	CB-CA-N	2.91	117.27	110.61
9	I	1	SAC	CB-CA-N	3.02	117.50	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	5	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 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
19	PGV	A	3266	-	50,50,50	0.87	1 (2%)	53,56,56	0.75	1 (1%)
18	TGL	A	3521	-	62,62,62	1.09	4 (6%)	65,65,65	1.12	4 (6%)
18	TGL	A	3522	-	62,62,62	1.39	7 (11%)	65,65,65	1.25	5 (7%)
18	TGL	A	3523	-	62,62,62	1.07	3 (4%)	65,65,65	1.07	5 (7%)
19	PGV	A	3524	-	50,50,50	1.10	3 (6%)	53,56,56	1.06	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	HEA	A	515	1	43,67,67	1.17	4 (9%)	37,103,103	1.41	6 (16%)
17	HEA	A	516	1	43,67,67	1.25	5 (11%)	37,103,103	1.11	3 (8%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	B	4085	-	29,32,32	0.72	1 (3%)	47,51,51	1.86	15 (31%)
23	PEK	C	3264	-	52,52,52	1.48	5 (9%)	55,57,57	1.25	7 (12%)
23	PEK	C	3265	-	52,52,52	1.67	8 (15%)	55,57,57	1.13	6 (10%)
19	PGV	C	3267	-	50,50,50	0.81	1 (2%)	53,56,56	0.88	2 (3%)
19	PGV	C	3268	-	50,50,50	1.08	3 (6%)	53,56,56	0.71	1 (1%)
22	CDL	C	3270	-	99,99,99	0.74	2 (2%)	105,111,111	0.88	3 (2%)
21	CHD	C	3271	-	29,32,32	0.81	0	47,51,51	3.68	24 (51%)
21	CHD	C	3525	-	29,32,32	0.81	0	47,51,51	1.68	11 (23%)
25	PSC	E	3230	-	51,51,51	1.23	3 (5%)	57,59,59	1.14	4 (7%)
22	CDL	G	3269	-	99,99,99	0.98	6 (6%)	105,111,111	0.86	5 (4%)
23	PEK	G	4263	-	52,52,52	1.66	9 (17%)	55,57,57	1.06	3 (5%)
21	CHD	J	3060	-	29,32,32	1.09	2 (6%)	47,51,51	3.35	26 (55%)
27	DMU	M	3526	-	34,34,34	3.22	8 (23%)	45,45,45	4.04	20 (44%)
19	PGV	N	4266	-	50,50,50	0.92	2 (4%)	53,56,56	0.84	3 (5%)
18	TGL	N	4521	-	62,62,62	1.12	4 (6%)	65,65,65	1.09	2 (3%)
18	TGL	N	4522	-	62,62,62	1.45	8 (12%)	65,65,65	1.23	5 (7%)
19	PGV	N	4524	-	50,50,50	1.13	5 (10%)	53,56,56	1.03	3 (5%)
17	HEA	N	515	1	43,67,67	1.22	7 (16%)	37,103,103	1.36	7 (18%)
17	HEA	N	516	1	43,67,67	1.19	6 (13%)	37,103,103	1.11	4 (10%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	O	3085	-	29,32,32	0.80	1 (3%)	47,51,51	1.91	16 (34%)
25	PSC	O	4230	-	51,51,51	1.24	3 (5%)	57,59,59	1.13	4 (7%)
23	PEK	P	4264	-	52,52,52	1.48	6 (11%)	55,57,57	1.30	8 (14%)
23	PEK	P	4265	-	52,52,52	1.70	11 (21%)	55,57,57	1.12	6 (10%)
19	PGV	P	4267	-	50,50,50	0.85	1 (2%)	53,56,56	0.88	1 (1%)
19	PGV	P	4268	-	50,50,50	1.09	3 (6%)	53,56,56	0.72	0
22	CDL	P	4270	-	99,99,99	0.76	3 (3%)	105,111,111	0.87	3 (2%)
21	CHD	P	4271	-	29,32,32	0.75	0	47,51,51	3.66	24 (51%)
21	CHD	P	4525	-	29,32,32	0.72	1 (3%)	47,51,51	1.65	9 (19%)
18	TGL	Q	4523	-	62,62,62	1.10	3 (4%)	65,65,65	1.06	6 (9%)
23	PEK	T	3263	-	52,52,52	1.70	10 (19%)	55,57,57	1.04	3 (5%)
22	CDL	T	4269	-	99,99,99	0.97	5 (5%)	105,111,111	0.88	6 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CHD	W	4060	-	29,32,32	1.13	2 (6%)	47,51,51	3.39	26 (55%)
27	DMU	Z	4526	-	34,34,34	3.19	9 (26%)	45,45,45	4.02	20 (44%)

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
19	PGV	A	3266	-	-	0/55/55/55	0/0/0/0
18	TGL	A	3521	-	-	0/65/65/65	0/0/0/0
18	TGL	A	3522	-	-	0/65/65/65	0/0/0/0
18	TGL	A	3523	-	-	1/65/65/65	0/0/0/0
19	PGV	A	3524	-	-	1/55/55/55	0/0/0/0
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
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	CHD	B	4085	-	-	0/7/74/74	0/4/4/4
23	PEK	C	3264	-	-	0/56/56/56	0/0/0/0
23	PEK	C	3265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	3267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	3268	-	-	0/55/55/55	0/0/0/0
22	CDL	C	3270	-	-	0/110/110/110	0/0/0/0
21	CHD	C	3271	-	5/5/12/12	0/7/74/74	0/4/4/4
21	CHD	C	3525	-	-	0/7/74/74	0/4/4/4
25	PSC	E	3230	-	-	0/55/55/55	0/0/0/0
22	CDL	G	3269	-	-	0/110/110/110	0/0/0/0
23	PEK	G	4263	-	-	0/56/56/56	0/0/0/0
21	CHD	J	3060	-	5/5/12/12	0/7/74/74	0/4/4/4
27	DMU	M	3526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	4266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	4521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	4522	-	-	0/65/65/65	0/0/0/0
19	PGV	N	4524	-	-	1/55/55/55	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
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
21	CHD	O	3085	-	-	0/7/74/74	0/4/4/4
25	PSC	O	4230	-	-	0/55/55/55	0/0/0/0
23	PEK	P	4264	-	-	0/56/56/56	0/0/0/0
23	PEK	P	4265	-	-	0/56/56/56	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	P	4267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	4268	-	-	0/55/55/55	0/0/0/0
22	CDL	P	4270	-	-	0/110/110/110	0/0/0/0
21	CHD	P	4271	-	5/5/12/12	0/7/74/74	0/4/4/4
21	CHD	P	4525	-	-	0/7/74/74	0/4/4/4
18	TGL	Q	4523	-	-	1/65/65/65	0/0/0/0
23	PEK	T	3263	-	-	0/56/56/56	0/0/0/0
22	CDL	T	4269	-	-	0/110/110/110	0/0/0/0
21	CHD	W	4060	-	5/5/12/12	0/7/74/74	0/4/4/4
27	DMU	Z	4526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-7.97	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.77	1.26	1.40
27	M	3526	DMU	O16-C6	-7.61	1.26	1.40
27	Z	4526	DMU	O7-C3	-7.47	1.24	1.43
27	M	3526	DMU	O5-C4	-7.04	1.27	1.44
27	Z	4526	DMU	O16-C18	-6.94	1.24	1.43
27	M	3526	DMU	O16-C18	-6.89	1.24	1.43
27	Z	4526	DMU	O5-C4	-6.40	1.28	1.44
27	M	3526	DMU	O1-C9	-6.20	1.29	1.44
27	Z	4526	DMU	O1-C9	-6.07	1.29	1.44
27	Z	4526	DMU	O7-C10	-6.04	1.24	1.41
27	M	3526	DMU	O7-C10	-5.88	1.25	1.41
27	Z	4526	DMU	O1-C10	-5.40	1.27	1.41
27	M	3526	DMU	O1-C10	-5.31	1.28	1.41
27	M	3526	DMU	O5-C6	-4.98	1.29	1.41
27	Z	4526	DMU	O5-C6	-4.87	1.29	1.41
17	A	515	HEA	C3A-CMA	-3.03	1.39	1.46
17	N	516	HEA	C3A-CMA	-3.01	1.39	1.46
17	A	516	HEA	C3C-C2C	-2.68	1.36	1.40
17	A	516	HEA	C3A-C2A	-2.64	1.36	1.40
17	N	515	HEA	C3A-CMA	-2.57	1.40	1.46
17	A	516	HEA	C3A-CMA	-2.55	1.40	1.46
23	P	4264	PEK	O03-C01	-2.28	1.40	1.45
18	A	3521	TGL	OG1-CG1	-2.26	1.40	1.45
17	N	516	HEA	C3A-C2A	-2.21	1.37	1.40
17	N	515	HEA	C3A-C2A	-2.21	1.37	1.40
18	N	4521	TGL	OG1-CG1	-2.19	1.40	1.45
17	N	516	HEA	C3C-C2C	-2.17	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	4085	CHD	C13-C12	-2.15	1.51	1.54
23	C	3264	PEK	O03-C01	-2.07	1.40	1.45
17	N	515	HEA	C4D-ND	2.00	1.40	1.36
22	P	4270	CDL	CA6-CA4	2.02	1.56	1.50
22	C	3270	CDL	CA3-CA4	2.02	1.56	1.50
21	J	3060	CHD	C8-C7	2.04	1.57	1.53
22	P	4270	CDL	CA3-CA4	2.04	1.56	1.50
18	A	3522	TGL	CB2-CB1	2.04	1.56	1.50
21	O	3085	CHD	C8-C9	2.05	1.57	1.53
17	N	515	HEA	C1D-C2D	2.05	1.47	1.42
21	P	4525	CHD	C8-C9	2.07	1.57	1.53
23	P	4264	PEK	C2-C1	2.08	1.56	1.50
23	P	4265	PEK	O01-C1	2.09	1.40	1.34
17	N	516	HEA	C3C-CAC	2.09	1.52	1.47
23	T	3263	PEK	C2-C1	2.09	1.56	1.50
23	C	3265	PEK	P-O11	2.10	1.67	1.59
19	N	4524	PGV	C01-C02	2.12	1.56	1.50
23	T	3263	PEK	P-O11	2.12	1.67	1.59
18	N	4522	TGL	OG2-CG2	2.13	1.52	1.46
22	T	4269	CDL	CB2-C1	2.13	1.59	1.51
17	A	516	HEA	C4B-C3B	2.14	1.47	1.42
23	G	4263	PEK	P-O11	2.14	1.68	1.59
23	P	4265	PEK	P-O12	2.15	1.68	1.59
18	N	4522	TGL	CB2-CB1	2.15	1.56	1.50
23	P	4265	PEK	P-O11	2.18	1.68	1.59
17	N	516	HEA	C1B-NB	2.18	1.40	1.36
27	Z	4526	DMU	C8-C9	2.19	1.57	1.53
18	A	3522	TGL	CG3-CG2	2.19	1.57	1.50
22	G	3269	CDL	C71-CB7	2.19	1.56	1.50
23	P	4265	PEK	C22-C21	2.23	1.57	1.50
21	W	4060	CHD	C8-C7	2.23	1.57	1.53
19	N	4524	PGV	C03-C02	2.23	1.57	1.50
22	T	4269	CDL	C11-CA5	2.23	1.57	1.50
22	G	3269	CDL	C11-CA5	2.24	1.57	1.50
19	A	3524	PGV	P-O11	2.28	1.68	1.59
22	G	3269	CDL	OB6-CB5	2.32	1.41	1.34
18	N	4522	TGL	CC2-CC1	2.36	1.57	1.50
17	N	515	HEA	C1B-NB	2.37	1.41	1.36
19	C	3268	PGV	C2-C1	2.37	1.57	1.50
22	P	4270	CDL	C71-CB7	2.39	1.57	1.50
19	N	4524	PGV	P-O11	2.41	1.69	1.59
22	T	4269	CDL	OA6-CA5	2.44	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	515	HEA	C4C-NC	2.45	1.41	1.36
18	N	4522	TGL	CG3-CG2	2.46	1.57	1.50
23	C	3265	PEK	C01-C02	2.48	1.57	1.50
23	G	4263	PEK	C22-C21	2.49	1.57	1.50
18	A	3522	TGL	OG3-CG3	2.51	1.50	1.45
19	P	4268	PGV	C2-C1	2.52	1.57	1.50
18	A	3522	TGL	OG2-CG2	2.54	1.53	1.46
19	A	3524	PGV	C20-C19	2.58	1.58	1.50
23	G	4263	PEK	O03-C21	2.59	1.40	1.33
22	C	3270	CDL	C71-CB7	2.60	1.58	1.50
19	C	3268	PGV	O01-C1	2.63	1.41	1.34
19	P	4268	PGV	O01-C1	2.66	1.42	1.34
19	N	4266	PGV	C01-C02	2.66	1.58	1.50
25	E	3230	PSC	C2-C1	2.67	1.58	1.50
23	P	4265	PEK	C01-C02	2.68	1.58	1.50
19	N	4524	PGV	C20-C19	2.72	1.58	1.50
17	A	515	HEA	C4D-ND	2.72	1.41	1.36
17	A	515	HEA	C1C-NC	2.74	1.41	1.36
23	T	3263	PEK	C22-C21	2.79	1.58	1.50
17	N	516	HEA	C4D-ND	2.85	1.42	1.36
23	P	4265	PEK	C03-C02	2.86	1.58	1.50
17	N	515	HEA	C1C-NC	2.86	1.42	1.36
23	T	3263	PEK	O03-C21	2.86	1.41	1.33
22	G	3269	CDL	OA6-CA5	2.87	1.42	1.34
22	G	3269	CDL	CB3-CB4	2.92	1.59	1.50
23	C	3265	PEK	C03-C02	2.92	1.59	1.50
23	C	3265	PEK	O03-C21	2.94	1.41	1.33
22	T	4269	CDL	CB3-CB4	3.02	1.59	1.50
25	O	4230	PSC	C2-C1	3.03	1.59	1.50
23	P	4265	PEK	O03-C21	3.07	1.42	1.33
23	T	3263	PEK	C01-C02	3.08	1.59	1.50
23	G	4263	PEK	C01-C02	3.13	1.59	1.50
17	N	515	HEA	C4C-NC	3.13	1.42	1.36
19	C	3267	PGV	C12-C11	3.14	1.49	1.31
18	N	4522	TGL	OG3-CG3	3.17	1.52	1.45
19	P	4267	PGV	C12-C11	3.19	1.49	1.31
21	J	3060	CHD	C13-C17	3.36	1.61	1.55
22	G	3269	CDL	CB6-CB4	3.36	1.60	1.50
18	N	4521	TGL	OG3-CC1	3.37	1.43	1.33
18	A	3521	TGL	OG3-CC1	3.49	1.43	1.33
21	W	4060	CHD	C13-C17	3.56	1.61	1.55
18	A	3523	TGL	OG2-CB1	3.65	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	516	HEA	C4D-ND	3.66	1.43	1.36
23	T	3263	PEK	C03-C02	3.77	1.61	1.50
22	T	4269	CDL	CB6-CB4	3.77	1.61	1.50
18	Q	4523	TGL	OG3-CC1	3.81	1.44	1.33
18	N	4521	TGL	OG1-CA1	3.83	1.44	1.33
18	A	3521	TGL	OG1-CA1	3.84	1.44	1.33
23	G	4263	PEK	C03-C02	3.87	1.61	1.50
18	Q	4523	TGL	OG2-CB1	4.00	1.45	1.34
18	A	3523	TGL	OG3-CC1	4.03	1.45	1.33
19	A	3266	PGV	C12-C11	4.04	1.54	1.31
23	C	3264	PEK	C6-C5	4.05	1.54	1.31
23	P	4264	PEK	C6-C5	4.11	1.54	1.31
23	P	4264	PEK	C9-C8	4.11	1.54	1.31
18	A	3521	TGL	OG2-CB1	4.12	1.46	1.34
19	N	4266	PGV	C12-C11	4.12	1.54	1.31
18	A	3522	TGL	OG3-CC1	4.18	1.45	1.33
23	C	3264	PEK	C9-C8	4.18	1.55	1.31
23	T	3263	PEK	C15-C14	4.21	1.55	1.31
19	C	3268	PGV	C12-C11	4.22	1.55	1.31
23	G	4263	PEK	C6-C5	4.26	1.55	1.31
23	G	4263	PEK	C15-C14	4.26	1.55	1.31
25	E	3230	PSC	C13-C12	4.27	1.55	1.31
25	E	3230	PSC	C10-C9	4.27	1.55	1.31
23	C	3265	PEK	C9-C8	4.31	1.55	1.31
23	P	4265	PEK	C9-C8	4.31	1.55	1.31
25	O	4230	PSC	C13-C12	4.31	1.55	1.31
19	P	4268	PGV	C12-C11	4.31	1.55	1.31
23	G	4263	PEK	C9-C8	4.32	1.55	1.31
19	A	3524	PGV	C12-C11	4.33	1.55	1.31
19	N	4524	PGV	C12-C11	4.33	1.55	1.31
18	Q	4523	TGL	OG1-CA1	4.34	1.45	1.33
23	C	3265	PEK	C6-C5	4.34	1.55	1.31
23	T	3263	PEK	C6-C5	4.34	1.55	1.31
23	P	4265	PEK	C15-C14	4.36	1.56	1.31
23	P	4265	PEK	C6-C5	4.39	1.56	1.31
25	O	4230	PSC	C10-C9	4.42	1.56	1.31
23	P	4265	PEK	C12-C11	4.44	1.56	1.31
23	C	3265	PEK	C12-C11	4.44	1.56	1.31
18	A	3523	TGL	OG1-CA1	4.44	1.46	1.33
23	C	3265	PEK	C15-C14	4.44	1.56	1.31
23	T	3263	PEK	C9-C8	4.45	1.56	1.31
18	N	4522	TGL	OG3-CC1	4.57	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	3522	TGL	OG1-CA1	4.60	1.46	1.33
23	T	3263	PEK	C12-C11	4.70	1.57	1.31
23	C	3264	PEK	C12-C11	4.71	1.57	1.31
18	N	4521	TGL	OG2-CB1	4.73	1.48	1.34
23	P	4264	PEK	C12-C11	4.83	1.58	1.31
23	P	4264	PEK	C15-C14	4.84	1.58	1.31
23	G	4263	PEK	C12-C11	4.86	1.58	1.31
23	C	3264	PEK	C15-C14	4.88	1.58	1.31
18	N	4522	TGL	OG1-CA1	4.96	1.47	1.33
18	N	4522	TGL	OG2-CB1	5.43	1.50	1.34
18	A	3522	TGL	OG2-CB1	5.71	1.50	1.34

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	4271	CHD	C17-C13-C12	-8.54	109.78	117.67
21	C	3271	CHD	C17-C13-C12	-8.22	110.08	117.67
27	Z	4526	DMU	C8-C7-C5	-7.99	96.81	110.83
27	M	3526	DMU	C8-C7-C5	-7.79	97.16	110.83
21	C	3271	CHD	C19-C10-C9	-7.78	100.16	111.17
21	P	4271	CHD	C19-C10-C9	-7.56	100.46	111.17
21	C	3271	CHD	C19-C10-C1	-5.88	98.69	108.25
21	W	4060	CHD	C18-C13-C14	-5.63	102.36	111.23
21	P	4271	CHD	C19-C10-C1	-5.62	99.10	108.25
21	J	3060	CHD	C15-C14-C8	-5.36	110.76	118.33
21	W	4060	CHD	C15-C14-C8	-5.35	110.79	118.33
21	J	3060	CHD	C18-C13-C14	-5.21	103.02	111.23
21	P	4271	CHD	C15-C14-C8	-4.98	111.30	118.33
21	C	3271	CHD	C15-C14-C8	-4.95	111.35	118.33
21	B	4085	CHD	C15-C14-C8	-3.86	112.88	118.33
21	O	3085	CHD	C16-C17-C13	-3.78	99.79	103.57
21	O	3085	CHD	C15-C14-C13	-3.74	99.83	103.57
21	B	4085	CHD	C15-C14-C13	-3.74	99.83	103.57
23	C	3264	PEK	O03-C21-C22	-3.73	101.14	111.92
25	O	4230	PSC	C01-O03-C19	-3.72	106.01	117.13
25	E	3230	PSC	C01-O03-C19	-3.69	106.11	117.13
21	C	3525	CHD	C15-C14-C8	-3.65	113.17	118.33
17	A	515	HEA	CMC-C2C-C1C	-3.65	122.86	128.46
23	P	4264	PEK	O03-C21-C22	-3.64	101.37	111.92
21	C	3271	CHD	C18-C13-C12	-3.60	105.35	109.07
21	O	3085	CHD	C15-C14-C8	-3.56	113.30	118.33
21	P	4525	CHD	C15-C14-C8	-3.53	113.35	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	4270	CDL	CB6-OB8-CB7	-3.40	106.97	117.13
21	B	4085	CHD	C16-C17-C13	-3.34	100.23	103.57
21	O	3085	CHD	C19-C10-C9	-3.27	106.54	111.17
22	C	3270	CDL	CB6-OB8-CB7	-3.26	107.38	117.13
21	P	4271	CHD	C18-C13-C12	-3.20	105.76	109.07
21	B	4085	CHD	C14-C8-C9	-3.18	105.31	109.64
21	B	4085	CHD	C18-C13-C12	-3.14	105.82	109.07
21	W	4060	CHD	C17-C13-C12	-3.12	114.79	117.67
21	W	4060	CHD	C18-C13-C12	-3.11	105.86	109.07
17	N	515	HEA	CMB-C2B-C1B	-2.90	124.01	128.46
19	A	3524	PGV	C3-C2-C1	-2.85	103.31	113.60
21	P	4525	CHD	C14-C8-C9	-2.85	105.77	109.64
18	A	3521	TGL	OG3-CC1-OC1	-2.81	116.72	123.58
21	J	3060	CHD	C18-C13-C12	-2.81	106.17	109.07
21	C	3525	CHD	C16-C17-C13	-2.79	100.78	103.57
21	J	3060	CHD	C17-C13-C12	-2.78	115.10	117.67
22	C	3270	CDL	OB6-CB5-C51	-2.77	105.71	111.55
21	B	4085	CHD	O3-C3-C4	-2.75	104.36	109.86
21	C	3271	CHD	C18-C13-C14	-2.73	106.92	111.23
21	C	3525	CHD	C14-C8-C9	-2.73	105.92	109.64
23	P	4264	PEK	C3-C2-C1	-2.71	103.81	113.60
21	C	3525	CHD	C14-C13-C12	-2.70	104.81	107.39
21	P	4271	CHD	C18-C13-C14	-2.68	107.01	111.23
19	N	4266	PGV	C01-O03-C19	-2.66	109.18	117.13
18	N	4521	TGL	OG3-CC1-OC1	-2.64	117.14	123.58
19	C	3267	PGV	C9-C10-C11	-2.62	98.25	112.48
21	C	3271	CHD	C13-C17-C20	-2.62	116.31	119.50
21	O	3085	CHD	C14-C13-C12	-2.58	104.93	107.39
23	C	3264	PEK	C3-C2-C1	-2.58	104.29	113.60
19	P	4267	PGV	C9-C10-C11	-2.55	98.62	112.48
19	N	4524	PGV	C3-C2-C1	-2.51	104.55	113.60
21	J	3060	CHD	C19-C10-C9	-2.50	107.63	111.17
21	O	3085	CHD	C14-C8-C9	-2.48	106.26	109.64
18	Q	4523	TGL	CG3-OG3-CC1	-2.48	109.71	117.13
21	P	4271	CHD	C13-C17-C20	-2.48	116.48	119.50
18	A	3522	TGL	OG3-CC1-OC1	-2.47	117.54	123.58
21	O	3085	CHD	C18-C13-C12	-2.44	106.55	109.07
17	A	515	HEA	CMB-C2B-C1B	-2.42	124.74	128.46
18	N	4522	TGL	OG3-CC1-OC1	-2.39	117.75	123.58
18	A	3523	TGL	CG3-OG3-CC1	-2.38	110.02	117.13
21	O	3085	CHD	O3-C3-C4	-2.38	105.11	109.86
22	P	4270	CDL	OB6-CB5-C51	-2.31	106.69	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	E	3230	PSC	C14-C13-C12	-2.30	108.11	124.90
23	P	4264	PEK	C24-C23-C22	-2.23	105.11	113.23
23	C	3264	PEK	C30-C29-C28	-2.22	102.37	114.41
23	C	3264	PEK	C23-C22-C21	-2.21	105.62	113.60
17	A	515	HEA	C26-C15-C14	-2.21	117.89	123.70
19	N	4266	PGV	O01-C1-C2	-2.21	106.90	111.55
23	P	4264	PEK	C30-C29-C28	-2.20	102.45	114.41
25	O	4230	PSC	C14-C13-C12	-2.17	109.05	124.90
17	N	516	HEA	C20-C19-C18	-2.16	116.70	121.10
23	C	3264	PEK	C24-C23-C22	-2.15	105.43	113.23
21	P	4525	CHD	C19-C10-C9	-2.14	108.13	111.17
17	N	515	HEA	CMC-C2C-C1C	-2.14	125.18	128.46
21	C	3525	CHD	C15-C14-C13	-2.14	101.43	103.57
21	C	3525	CHD	C19-C10-C9	-2.13	108.15	111.17
22	T	4269	CDL	OB8-CB7-C71	-2.13	105.76	111.92
19	C	3267	PGV	O01-C1-C2	-2.12	107.08	111.55
21	W	4060	CHD	C19-C10-C9	-2.11	108.17	111.17
19	C	3268	PGV	C21-C20-C19	-2.11	105.99	113.60
23	C	3264	PEK	C02-O01-C1	-2.10	112.92	117.88
23	P	4264	PEK	C32-C31-C30	-2.09	103.07	114.41
17	A	516	HEA	C20-C19-C18	-2.09	116.85	121.10
21	B	4085	CHD	C19-C10-C9	-2.08	108.22	111.17
19	A	3266	PGV	O01-C1-C2	-2.06	107.21	111.55
18	Q	4523	TGL	OG3-CC1-OC1	-2.03	118.62	123.58
17	A	516	HEA	CMC-C2C-C1C	-2.03	125.35	128.46
17	N	516	HEA	CMC-C2C-C1C	-2.01	125.38	128.46
22	C	3270	CDL	C52-C51-CB5	-2.01	106.37	113.60
22	G	3269	CDL	OB8-CB7-C71	-2.00	106.12	111.92
18	Q	4523	TGL	OG3-CC1-CC2	2.00	117.70	111.92
23	P	4264	PEK	C2-C3-C4	2.00	116.82	113.28
18	A	3523	TGL	OG3-CC1-CC2	2.00	117.71	111.92
18	A	3521	TGL	CB5-CB4-CB3	2.00	125.29	114.41
22	T	4269	CDL	C83-C82-C81	2.00	125.29	114.41
17	N	515	HEA	C26-C15-C16	2.04	118.80	115.29
19	A	3524	PGV	O01-C02-C03	2.04	115.82	108.43
19	A	3524	PGV	P-O12-C04	2.04	133.66	121.68
21	P	4525	CHD	C10-C9-C8	2.04	114.07	111.87
21	P	4271	CHD	C9-C10-C5	2.06	111.58	108.61
23	P	4264	PEK	C11-C10-C9	2.07	118.88	111.84
19	A	3524	PGV	C02-O01-C1	2.07	122.76	117.88
18	A	3521	TGL	CB6-CB5-CB4	2.08	125.69	114.41
22	P	4270	CDL	OB6-CB5-OB7	2.08	128.82	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	4269	CDL	C19-C18-C17	2.08	125.70	114.41
17	N	515	HEA	C3C-C4C-NC	2.08	111.90	109.21
22	G	3269	CDL	C19-C18-C17	2.08	125.72	114.41
21	O	3085	CHD	C2-C1-C10	2.09	116.41	112.79
21	B	4085	CHD	C5-C4-C3	2.10	115.93	112.83
22	G	3269	CDL	C23-C22-C21	2.10	125.82	114.41
17	A	516	HEA	C27-C19-C20	2.12	118.94	115.29
21	C	3525	CHD	C9-C11-C12	2.12	117.13	114.33
22	T	4269	CDL	C23-C22-C21	2.13	125.98	114.41
22	G	3269	CDL	C22-C21-C20	2.14	126.01	114.41
18	N	4522	TGL	OG1-CG1-CG2	2.14	113.98	108.64
22	T	4269	CDL	C22-C21-C20	2.15	126.06	114.41
17	N	516	HEA	C17-C18-C19	2.17	133.04	127.66
18	Q	4523	TGL	OG1-CA1-CA2	2.18	118.23	111.92
21	W	4060	CHD	C4-C5-C10	2.19	115.03	112.66
18	A	3522	TGL	OG1-CG1-CG2	2.20	114.13	108.64
18	A	3523	TGL	CB6-CB5-CB4	2.22	126.47	114.41
21	B	4085	CHD	C18-C13-C14	2.22	114.74	111.23
21	W	4060	CHD	O7-C7-C6	2.23	115.53	109.95
21	C	3271	CHD	C9-C10-C5	2.23	111.82	108.61
21	O	3085	CHD	C1-C10-C5	2.26	111.23	107.77
18	A	3523	TGL	OG1-CA1-CA2	2.28	118.50	111.92
18	Q	4523	TGL	CB6-CB5-CB4	2.29	126.84	114.41
23	C	3265	PEK	P-O12-C04	2.29	132.87	121.59
21	C	3271	CHD	C9-C11-C12	2.30	117.36	114.33
21	J	3060	CHD	O7-C7-C6	2.37	115.88	109.95
17	A	515	HEA	C26-C15-C16	2.39	119.41	115.29
21	J	3060	CHD	C4-C5-C10	2.41	115.27	112.66
19	A	3524	PGV	C03-C02-C01	2.42	117.32	111.86
21	B	4085	CHD	C5-C6-C7	2.42	117.12	114.44
23	C	3265	PEK	C14-C13-C12	2.43	120.09	111.84
21	J	3060	CHD	C14-C13-C12	2.43	109.70	107.39
21	P	4271	CHD	C9-C11-C12	2.46	117.59	114.33
21	P	4271	CHD	C16-C15-C14	2.49	110.08	105.13
23	P	4265	PEK	P-O12-C04	2.49	133.83	121.59
21	C	3525	CHD	C1-C10-C5	2.50	111.61	107.77
22	G	3269	CDL	OB8-CB6-CB4	2.50	114.88	108.64
21	C	3271	CHD	C16-C15-C14	2.53	110.18	105.13
23	P	4265	PEK	O03-C01-C02	2.54	114.96	108.64
17	N	515	HEA	CMB-C2B-C3B	2.56	129.83	124.92
18	N	4522	TGL	OG1-CA1-CA2	2.56	119.32	111.92
23	C	3265	PEK	C8-C7-C6	2.56	120.56	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	4060	CHD	C14-C8-C9	2.57	113.13	109.64
23	P	4265	PEK	C14-C13-C12	2.57	120.59	111.84
21	O	3085	CHD	C17-C13-C14	2.60	102.74	100.08
21	O	3085	CHD	C5-C4-C3	2.61	116.69	112.83
19	N	4266	PGV	O03-C01-C02	2.61	115.15	108.64
21	W	4060	CHD	C15-C16-C17	2.61	110.34	105.13
23	P	4265	PEK	C8-C7-C6	2.62	120.74	111.84
21	J	3060	CHD	C14-C8-C9	2.64	113.23	109.64
18	A	3522	TGL	OG1-CA1-CA2	2.64	119.56	111.92
22	T	4269	CDL	OB8-CB6-CB4	2.65	115.24	108.64
21	O	3085	CHD	C1-C2-C3	2.66	113.84	110.45
17	N	516	HEA	C27-C19-C20	2.68	119.91	115.29
21	P	4525	CHD	C9-C11-C12	2.69	117.88	114.33
21	C	3271	CHD	C15-C16-C17	2.69	110.49	105.13
21	P	4271	CHD	C1-C2-C3	2.69	113.88	110.45
23	C	3265	PEK	O03-C01-C02	2.70	115.36	108.64
21	P	4271	CHD	C15-C16-C17	2.72	110.55	105.13
21	J	3060	CHD	C15-C16-C17	2.72	110.55	105.13
23	C	3264	PEK	O03-C21-O04	2.72	130.22	123.58
21	B	4085	CHD	C17-C13-C14	2.73	102.88	100.08
25	E	3230	PSC	C15-C14-C13	2.74	127.35	112.48
17	N	515	HEA	CMC-C2C-C3C	2.77	129.92	124.88
21	O	3085	CHD	C9-C11-C12	2.77	117.99	114.33
25	O	4230	PSC	C15-C14-C13	2.82	127.75	112.48
21	J	3060	CHD	C16-C15-C14	2.85	110.81	105.13
21	C	3271	CHD	C1-C2-C3	2.85	114.08	110.45
21	C	3525	CHD	C10-C9-C8	2.85	114.94	111.87
21	B	4085	CHD	C9-C11-C12	2.86	118.11	114.33
23	P	4265	PEK	P-O11-C03	2.86	138.46	121.68
23	P	4264	PEK	O03-C21-O04	2.87	130.57	123.58
17	A	515	HEA	CMD-C2D-C3D	2.88	130.38	124.94
21	P	4525	CHD	C1-C2-C3	2.89	114.13	110.45
27	Z	4526	DMU	O7-C10-C5	2.89	115.74	108.08
27	M	3526	DMU	C1-C2-C3	2.89	116.33	109.68
23	C	3265	PEK	P-O11-C03	2.89	138.65	121.68
19	N	4524	PGV	C03-C02-C01	2.91	118.42	111.86
23	T	3263	PEK	O03-C01-C02	2.91	115.90	108.64
21	W	4060	CHD	C16-C15-C14	2.95	111.02	105.13
27	Z	4526	DMU	C1-C2-C3	3.01	116.60	109.68
21	P	4525	CHD	C1-C10-C5	3.04	112.43	107.77
21	W	4060	CHD	C14-C13-C12	3.09	110.32	107.39
21	B	4085	CHD	C1-C10-C5	3.09	112.51	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	4085	CHD	C1-C2-C3	3.09	114.40	110.45
27	M	3526	DMU	O7-C10-C5	3.10	116.31	108.08
23	G	4263	PEK	O03-C01-C02	3.11	116.38	108.64
21	C	3271	CHD	C6-C5-C10	3.11	116.02	112.66
21	C	3271	CHD	C14-C8-C7	3.11	116.00	111.80
21	P	4271	CHD	C5-C6-C7	3.11	117.88	114.44
21	C	3271	CHD	C5-C4-C3	3.13	117.45	112.83
23	P	4265	PEK	C11-C10-C9	3.15	122.55	111.84
21	J	3060	CHD	C5-C4-C3	3.16	117.50	112.83
23	G	4263	PEK	P-O11-C03	3.16	140.24	121.68
17	N	515	HEA	CMD-C2D-C3D	3.17	130.91	124.94
27	Z	4526	DMU	C10-O1-C9	3.19	119.99	113.71
23	T	3263	PEK	P-O11-C03	3.19	140.38	121.68
27	M	3526	DMU	O7-C3-C4	3.21	118.32	109.42
21	P	4271	CHD	C5-C4-C3	3.22	117.59	112.83
23	C	3265	PEK	C11-C10-C9	3.24	122.87	111.84
21	P	4271	CHD	C14-C8-C7	3.26	116.21	111.80
21	C	3525	CHD	C5-C6-C7	3.26	118.05	114.44
19	N	4524	PGV	P-O11-C03	3.28	140.93	121.68
21	J	3060	CHD	C9-C11-C12	3.29	118.68	114.33
21	B	4085	CHD	C10-C9-C8	3.31	115.42	111.87
21	O	3085	CHD	C5-C6-C7	3.32	118.11	114.44
21	P	4271	CHD	C6-C5-C10	3.34	116.27	112.66
21	C	3271	CHD	C5-C6-C7	3.44	118.25	114.44
25	O	4230	PSC	C16-C15-C14	3.47	127.01	113.70
21	W	4060	CHD	C1-C2-C3	3.48	114.89	110.45
21	C	3271	CHD	C1-C10-C9	3.49	116.91	111.36
23	G	4263	PEK	C03-C02-C01	3.51	119.77	111.86
19	A	3524	PGV	P-O11-C03	3.51	142.25	121.68
21	P	4271	CHD	C1-C10-C9	3.52	116.96	111.36
21	J	3060	CHD	C1-C2-C3	3.52	114.94	110.45
27	M	3526	DMU	C10-O1-C9	3.52	120.65	113.71
27	M	3526	DMU	O7-C10-O1	3.54	120.69	110.66
21	W	4060	CHD	C9-C11-C12	3.54	119.01	114.33
27	Z	4526	DMU	O5-C6-C1	3.57	118.02	110.34
25	E	3230	PSC	C16-C15-C14	3.58	127.41	113.70
27	Z	4526	DMU	O7-C3-C4	3.58	119.34	109.42
27	M	3526	DMU	O5-C6-C1	3.62	118.11	110.34
21	W	4060	CHD	C5-C4-C3	3.63	118.19	112.83
21	P	4525	CHD	C5-C6-C7	3.67	118.50	114.44
17	A	515	HEA	CMC-C2C-C3C	3.69	131.59	124.88
27	Z	4526	DMU	O7-C10-O1	3.69	121.12	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	3263	PEK	C03-C02-C01	3.69	120.19	111.86
27	Z	4526	DMU	O16-C6-C1	3.72	114.26	108.24
21	W	4060	CHD	C13-C14-C8	3.90	119.78	114.77
21	J	3060	CHD	C13-C14-C8	3.92	119.80	114.77
21	W	4060	CHD	C1-C10-C5	3.92	113.79	107.77
18	A	3522	TGL	OG2-CB1-CB2	3.94	119.86	111.55
18	N	4522	TGL	OG2-CB1-CB2	3.96	119.89	111.55
27	Z	4526	DMU	C10-O7-C3	3.98	127.91	117.97
27	M	3526	DMU	C6-C1-C2	4.04	118.44	109.98
27	Z	4526	DMU	C6-C1-C2	4.07	118.50	109.98
21	J	3060	CHD	C1-C10-C5	4.11	114.07	107.77
21	P	4271	CHD	C4-C5-C10	4.14	117.13	112.66
18	Q	4523	TGL	OG2-CB1-CB2	4.15	120.30	111.55
21	O	3085	CHD	C10-C9-C8	4.19	116.38	111.87
27	M	3526	DMU	C10-O7-C3	4.20	128.47	117.97
21	W	4060	CHD	C9-C8-C7	4.22	116.87	111.92
21	J	3060	CHD	C2-C1-C10	4.25	120.16	112.79
27	M	3526	DMU	O16-C6-C1	4.32	115.23	108.24
21	C	3271	CHD	C4-C5-C10	4.36	117.37	112.66
21	C	3525	CHD	C13-C17-C20	4.36	124.79	119.50
21	J	3060	CHD	C9-C8-C7	4.40	117.08	111.92
18	A	3523	TGL	OG2-CB1-CB2	4.53	121.10	111.55
21	W	4060	CHD	C2-C1-C10	4.54	120.66	112.79
21	P	4525	CHD	C13-C17-C20	4.60	125.09	119.50
21	J	3060	CHD	C10-C9-C8	4.68	116.90	111.87
18	N	4521	TGL	OG2-CB1-CB2	4.78	121.64	111.55
18	A	3521	TGL	OG2-CB1-CB2	4.86	121.79	111.55
21	J	3060	CHD	C6-C5-C10	4.90	117.95	112.66
21	W	4060	CHD	C10-C9-C8	4.98	117.22	111.87
27	Z	4526	DMU	C18-O16-C6	5.05	122.48	113.85
21	W	4060	CHD	C11-C9-C10	5.06	119.08	113.74
21	C	3271	CHD	C4-C3-C2	5.11	116.80	110.56
18	A	3522	TGL	OG3-CG3-CG2	5.11	121.37	108.64
21	P	4271	CHD	C4-C3-C2	5.17	116.87	110.56
18	N	4522	TGL	OG3-CG3-CG2	5.19	121.58	108.64
21	W	4060	CHD	C6-C5-C10	5.21	118.29	112.66
21	W	4060	CHD	C11-C12-C13	5.36	116.79	111.23
21	J	3060	CHD	C11-C9-C10	5.41	119.45	113.74
21	J	3060	CHD	C5-C6-C7	5.49	120.51	114.44
21	W	4060	CHD	C4-C3-C2	5.53	117.31	110.56
21	W	4060	CHD	C5-C6-C7	5.55	120.58	114.44
21	P	4271	CHD	C1-C10-C5	5.60	116.35	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	3060	CHD	C11-C12-C13	5.61	117.04	111.23
27	M	3526	DMU	C18-O16-C6	5.62	123.44	113.85
21	C	3271	CHD	C1-C10-C5	5.64	116.41	107.77
21	J	3060	CHD	C4-C3-C2	5.88	117.75	110.56
21	P	4271	CHD	C14-C13-C12	5.93	113.02	107.39
21	C	3271	CHD	C9-C8-C7	6.00	118.95	111.92
21	P	4271	CHD	C9-C8-C7	6.07	119.04	111.92
27	Z	4526	DMU	O7-C3-C2	6.10	123.67	107.27
21	C	3271	CHD	C14-C13-C12	6.24	113.32	107.39
27	M	3526	DMU	O7-C3-C2	6.35	124.34	107.27
27	M	3526	DMU	O5-C4-C57	6.49	122.74	106.43
21	J	3060	CHD	C13-C17-C20	6.53	127.44	119.50
27	Z	4526	DMU	O5-C4-C57	6.68	123.23	106.43
21	W	4060	CHD	C13-C17-C20	6.81	127.77	119.50
27	Z	4526	DMU	C6-O5-C4	6.85	127.22	113.71
27	Z	4526	DMU	O1-C9-C8	6.86	122.29	109.69
27	M	3526	DMU	C6-O5-C4	6.88	127.27	113.71
27	M	3526	DMU	O5-C6-O16	7.03	126.60	109.96
27	M	3526	DMU	O1-C9-C8	7.09	122.71	109.69
27	Z	4526	DMU	O5-C4-C3	7.35	125.36	109.76
27	M	3526	DMU	O5-C4-C3	7.45	125.58	109.76
27	Z	4526	DMU	O5-C6-O16	7.51	127.72	109.96
27	M	3526	DMU	C7-C8-C9	7.66	123.94	110.24
27	Z	4526	DMU	O1-C9-C11	7.66	125.70	106.43
27	M	3526	DMU	O1-C9-C11	7.73	125.87	106.43
27	Z	4526	DMU	C7-C8-C9	7.88	124.34	110.24
21	W	4060	CHD	C17-C13-C14	8.66	108.95	100.08
21	J	3060	CHD	C17-C13-C14	8.74	109.03	100.08
21	C	3271	CHD	C10-C9-C8	8.83	121.36	111.87
21	P	4271	CHD	C10-C9-C8	8.85	121.38	111.87
21	C	3271	CHD	C17-C13-C14	9.57	109.88	100.08
21	P	4271	CHD	C17-C13-C14	9.76	110.08	100.08
27	Z	4526	DMU	C10-C5-C7	10.16	131.24	109.98
27	M	3526	DMU	C10-C5-C7	10.21	131.34	109.98

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C12
21	C	3271	CHD	C8
21	C	3271	CHD	C3
21	C	3271	CHD	C9

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Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C14
27	M	3526	DMU	C2
27	M	3526	DMU	C4
27	M	3526	DMU	C6
27	M	3526	DMU	C5
27	M	3526	DMU	C9
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
21	J	3060	CHD	C12
21	J	3060	CHD	C8
21	J	3060	CHD	C9
21	J	3060	CHD	C14
21	J	3060	CHD	C17
21	P	4271	CHD	C12
21	P	4271	CHD	C8
21	P	4271	CHD	C3
21	P	4271	CHD	C9
21	P	4271	CHD	C14
21	W	4060	CHD	C12
21	W	4060	CHD	C8
21	W	4060	CHD	C9
21	W	4060	CHD	C14
21	W	4060	CHD	C17
27	Z	4526	DMU	C2
27	Z	4526	DMU	C4
27	Z	4526	DMU	C6
27	Z	4526	DMU	C5
27	Z	4526	DMU	C9
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB

All (4) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
18	Q	4523	TGL	CG2-OG2-CB1-CB2
18	A	3523	TGL	CG2-OG2-CB1-CB2
19	N	4524	PGV	P-O11-C03-C02
19	A	3524	PGV	P-O11-C03-C02

There are no ring outliers.

33 monomers are involved in 278 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	3521	TGL	16	0
18	A	3522	TGL	25	0
18	A	3523	TGL	6	0
19	A	3524	PGV	7	0
17	A	515	HEA	2	0
17	A	516	HEA	3	0
21	B	4085	CHD	1	0
23	C	3264	PEK	4	0
23	C	3265	PEK	9	0
19	C	3267	PGV	6	0
19	C	3268	PGV	3	0
22	C	3270	CDL	23	0
21	C	3271	CHD	4	0
25	E	3230	PSC	12	0
22	G	3269	CDL	17	0
23	G	4263	PEK	6	0
21	J	3060	CHD	3	0
18	N	4521	TGL	24	0
18	N	4522	TGL	17	0
19	N	4524	PGV	6	0
17	N	515	HEA	3	0
17	N	516	HEA	3	0
25	O	4230	PSC	11	0
23	P	4264	PEK	4	0
23	P	4265	PEK	4	0
19	P	4267	PGV	3	0
19	P	4268	PGV	3	0
22	P	4270	CDL	20	0
21	P	4271	CHD	2	0
18	Q	4523	TGL	6	0
23	T	3263	PEK	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	T	4269	CDL	20	0
21	W	4060	CHD	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.