



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2017 – 06:57 PM EST

PDB ID : 5X1B  
Title : CO bound cytochrome c oxidase at 20 nsec after pump laser irradiation to release CO from O<sub>2</sub> reduction center  
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : unknown  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

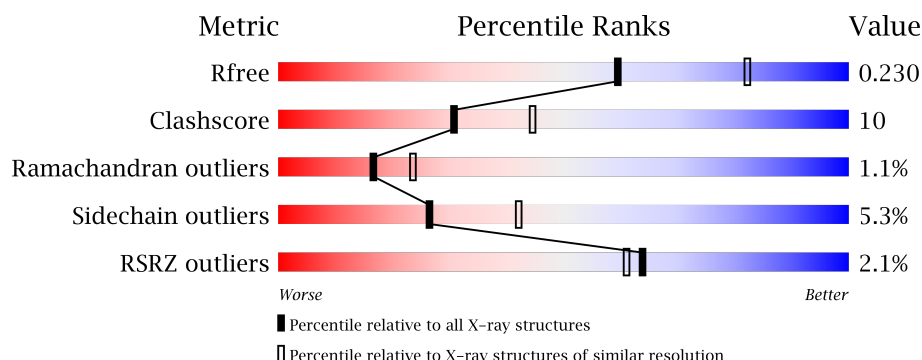
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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






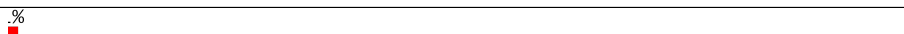
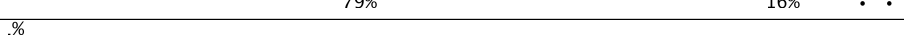




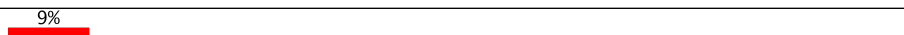
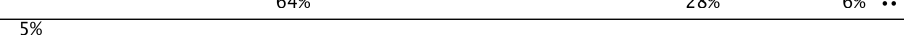




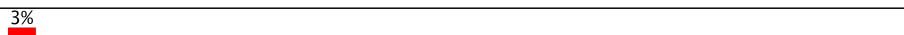
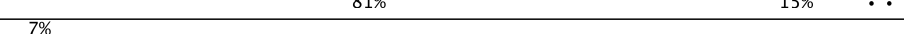




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	N	514	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	B	227	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	O	227	<div> <div>74%</div> <div>24%</div> <div>.</div> </div>
3	C	261	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
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
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
17	NA	A	605	-	-	-	X
18	CMO	N	606	-	-	-	X
19	TGL	A	607	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	N	610	-	-	-	X
19	TGL	N	611	-	-	-	X
20	PGV	A	609	-	-	-	X
20	PGV	N	607	-	-	-	X
21	EDO	A	612	-	-	-	X
21	EDO	A	613	-	-	-	X
21	EDO	A	614	-	-	X	X
21	EDO	B	305	-	-	-	X
21	EDO	F	102	-	-	-	X
21	EDO	G	104	-	-	-	X
21	EDO	T	104	-	-	-	X
23	CHD	J	101	-	-	-	X
23	CHD	W	101	-	-	-	X
24	PSC	B	303	-	-	-	X
24	PSC	R	201	-	-	-	X
26	CDL	C	303	-	-	-	X
26	CDL	C	307	-	-	-	X
26	CDL	P	304	-	-	-	X
26	CDL	T	103	-	-	-	X
27	PEK	G	102	-	-	-	X
27	PEK	T	101	-	-	-	X
27	PEK	T	102	-	-	-	X
29	DMU	Z	101	-	-	-	X

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 31717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	1	0
			4030	2694	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

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

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

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 subunit 5A, mitochondrial.

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 subunit 5B, mitochondrial.

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 subunit 6A2, mitochondrial.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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 subunit 6C.

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 subunit 7A1, mitochondrial.

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 subunit 7B, mitochondrial.

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			

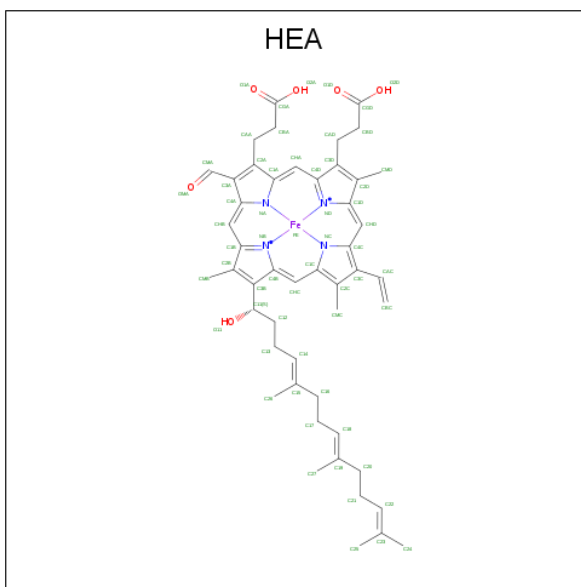
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 subunit 8B, mitochondrial.

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 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
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

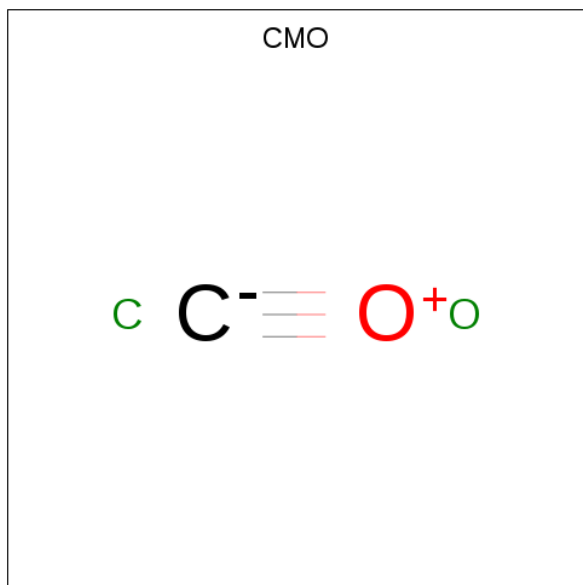
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).



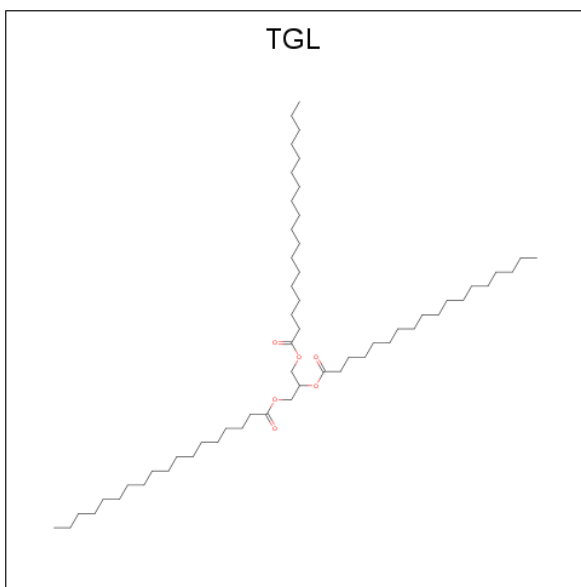
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



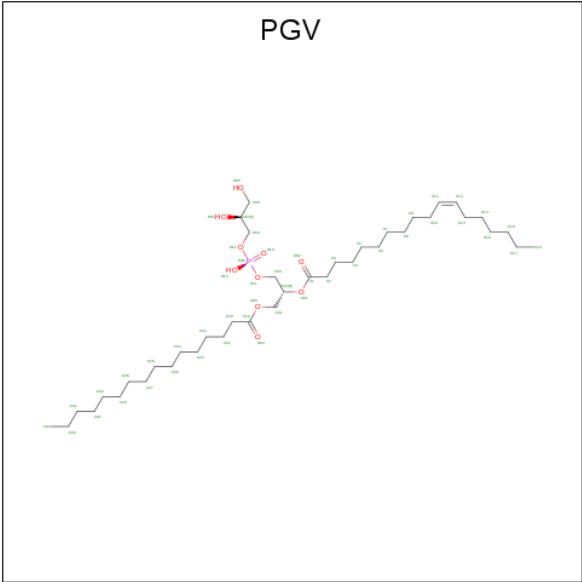
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

- Molecule 19 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
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 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
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



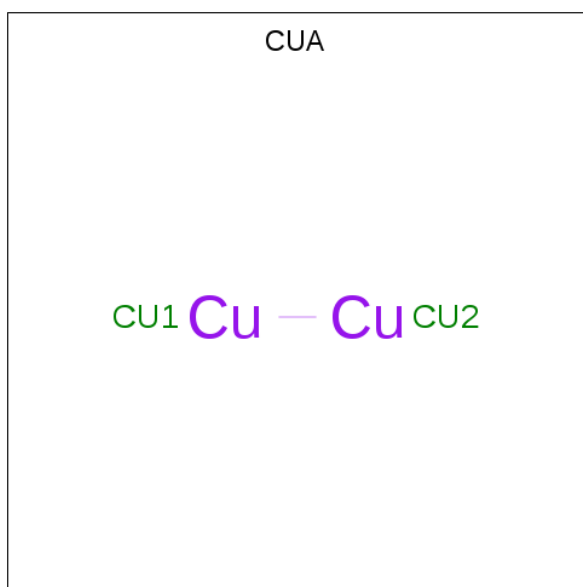
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	F	1	Total	C	O	0	0
			4	2	2		
21	G	1	Total	C	O	0	0
			4	2	2		
21	K	1	Total	C	O	0	0
			4	2	2		
21	K	1	Total	C	O	0	0
			4	2	2		

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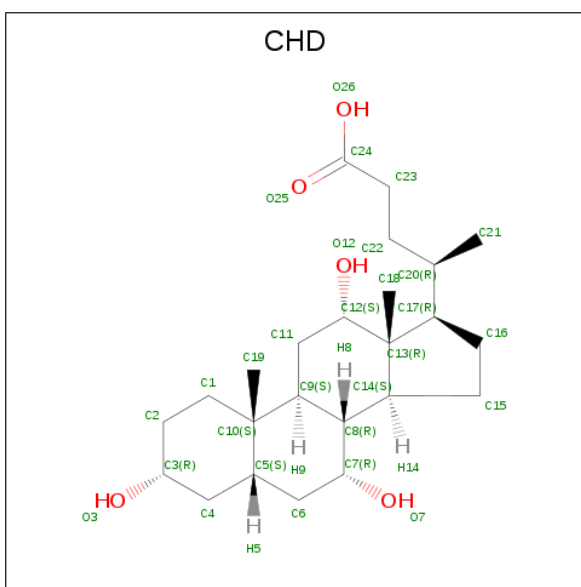
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C O 4 2 2	0	0
21	L	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



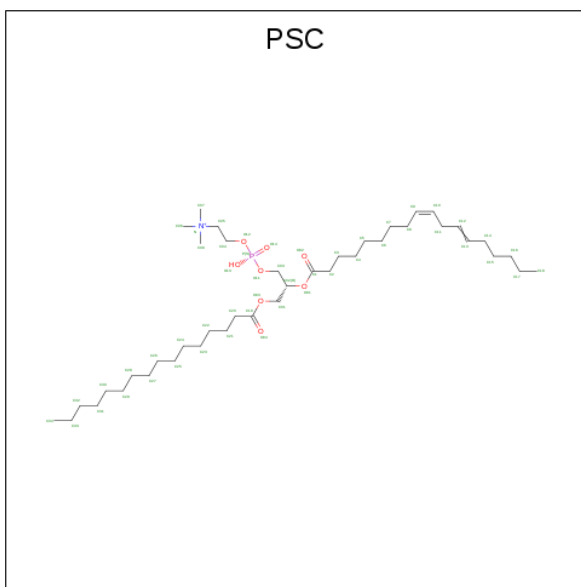
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 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
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	O	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0

- Molecule 24 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).

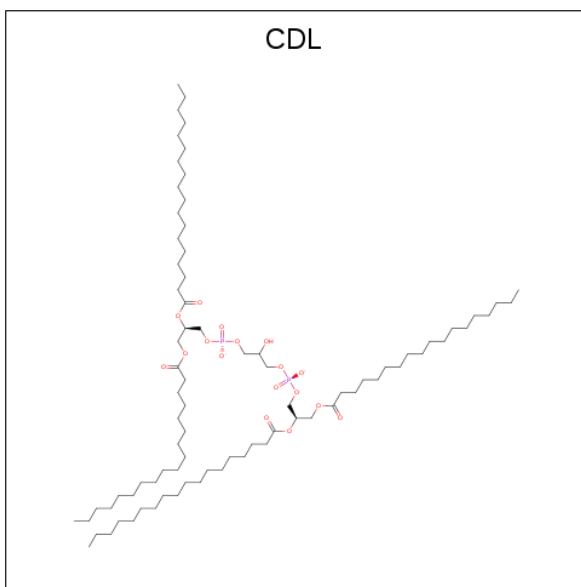


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

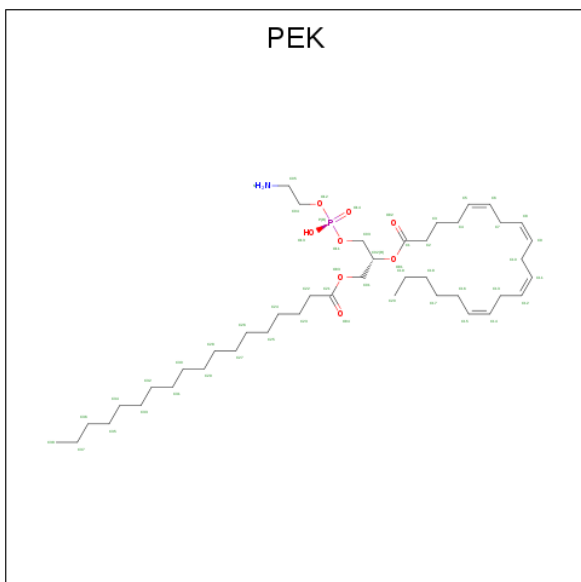
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	X	0	0
			1	1		
25	C	1	Total	X	0	0
			1	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 27 is (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).



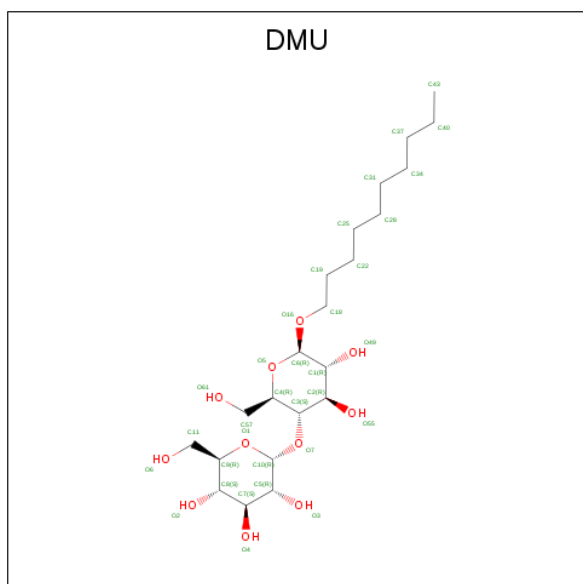


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 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
29	M	1	Total	C	O	0	0
			33	22	11		

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	125	Total	O	0	0
			125	125		
30	B	77	Total	O	0	1
			78	78		
30	C	70	Total	O	0	0
			70	70		
30	D	41	Total	O	0	0
			41	41		
30	E	24	Total	O	0	0
			24	24		
30	F	36	Total	O	0	0
			36	36		
30	G	31	Total	O	0	0
			31	31		
30	H	33	Total	O	0	0
			33	33		
30	I	12	Total	O	0	0
			12	12		
30	J	19	Total	O	0	0
			19	19		
30	K	19	Total	O	0	0
			19	19		
30	L	14	Total	O	0	0
			14	14		
30	M	15	Total	O	0	0
			15	15		
30	N	117	Total	O	0	0
			117	117		
30	O	76	Total	O	0	1
			77	77		
30	P	54	Total	O	0	0
			54	54		
30	Q	29	Total	O	0	0
			29	29		
30	R	29	Total	O	0	0
			29	29		

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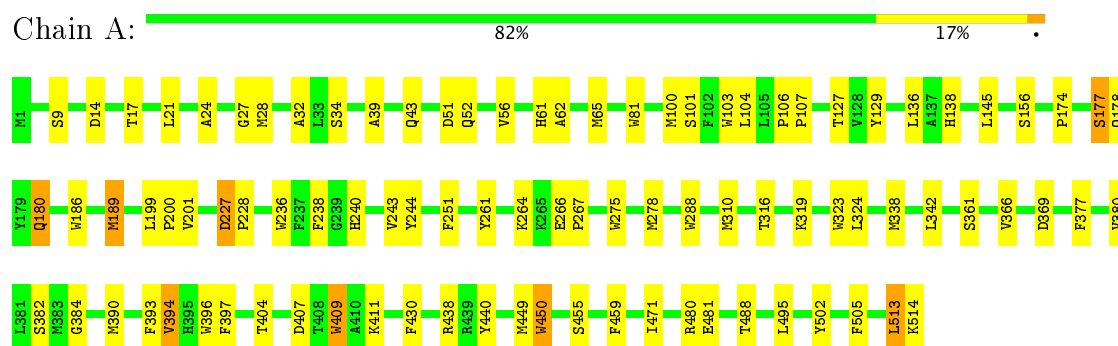
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	43	Total 43	O 43	0	0
30	T	20	Total 20	O 20	0	0
30	U	31	Total 31	O 31	0	0
30	V	19	Total 19	O 19	0	0
30	W	17	Total 17	O 17	0	0
30	X	9	Total 9	O 9	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	4	Total 4	O 4	0	0

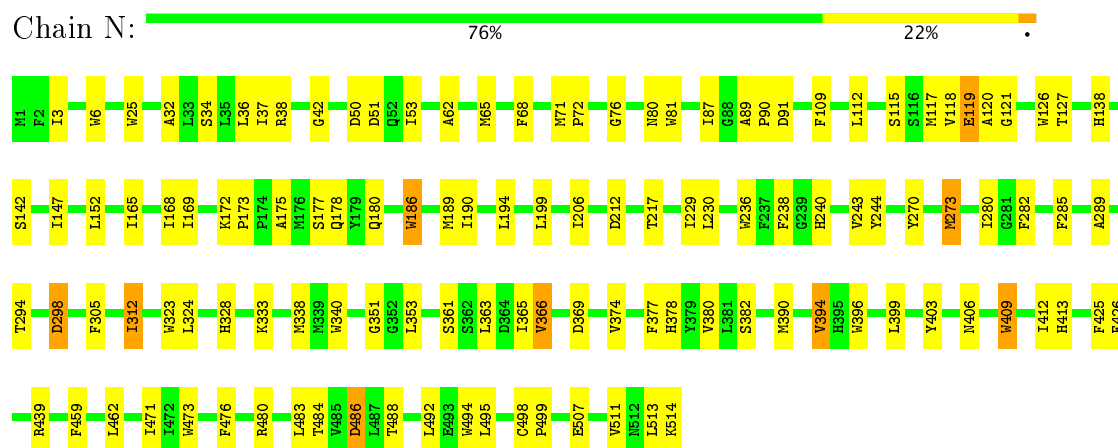
### 3 Residue-property plots [i](#)

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.

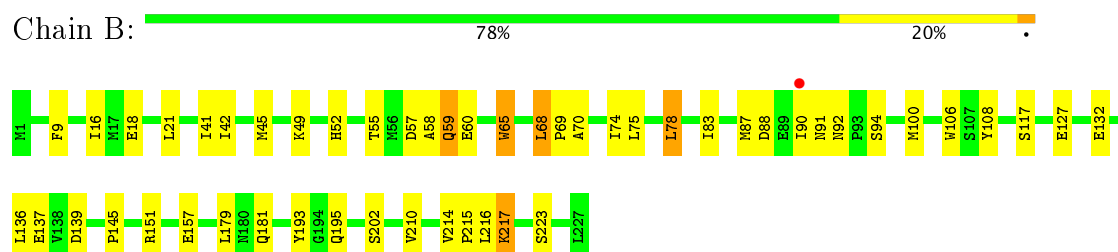
#### • Molecule 1: Cytochrome c oxidase subunit 1



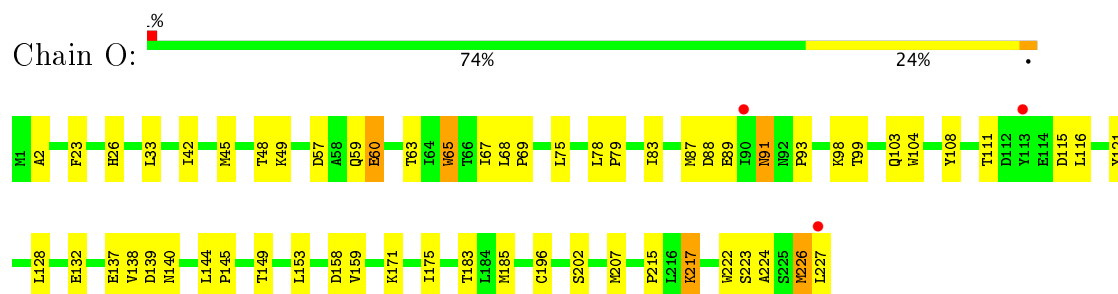
#### • Molecule 1: Cytochrome c oxidase subunit 1



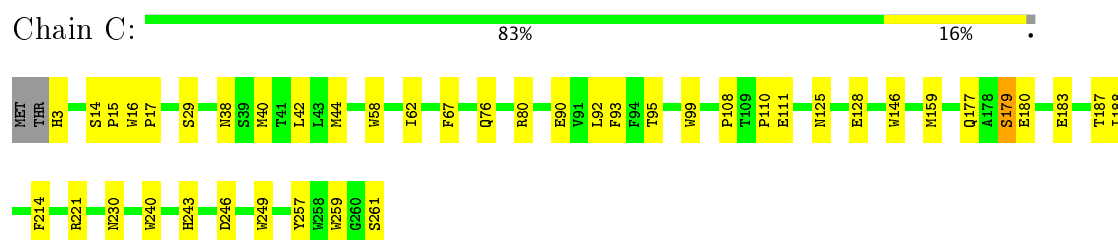
#### • Molecule 2: Cytochrome c oxidase subunit 2



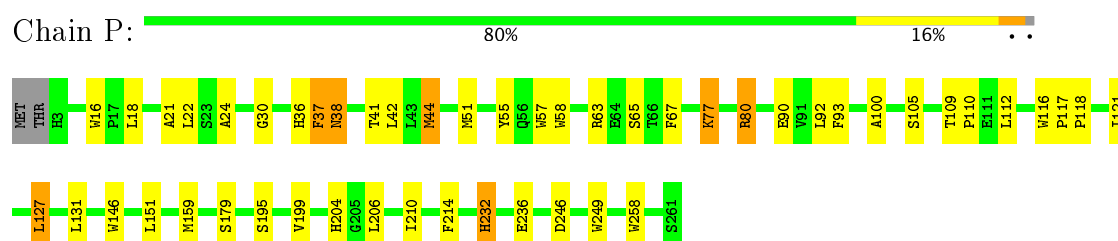
- Molecule 2: Cytochrome c oxidase subunit 2



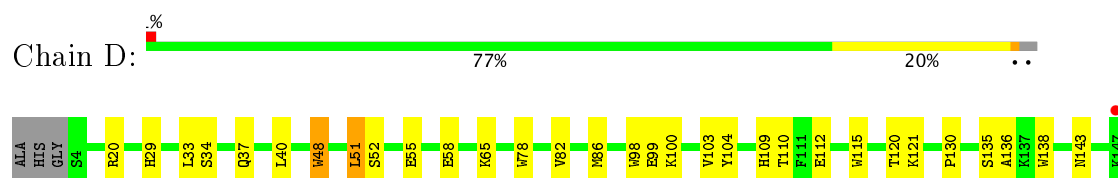
- Molecule 3: Cytochrome c oxidase subunit 3



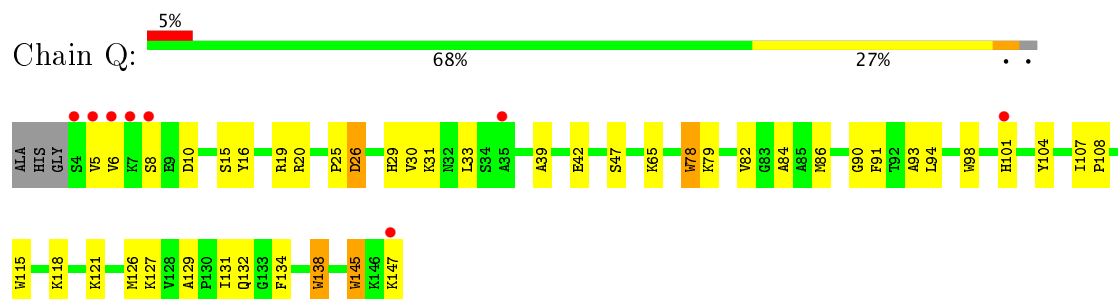
- Molecule 3: Cytochrome c oxidase subunit 3



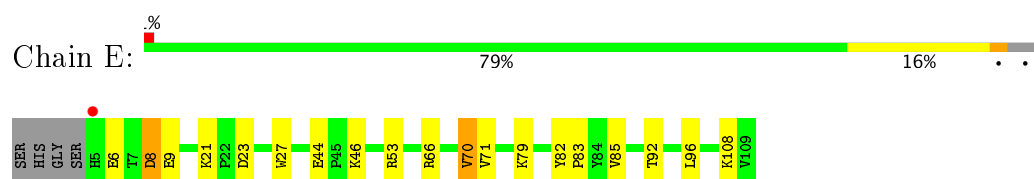
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



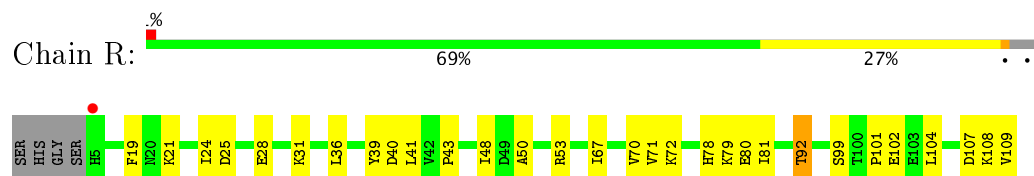
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



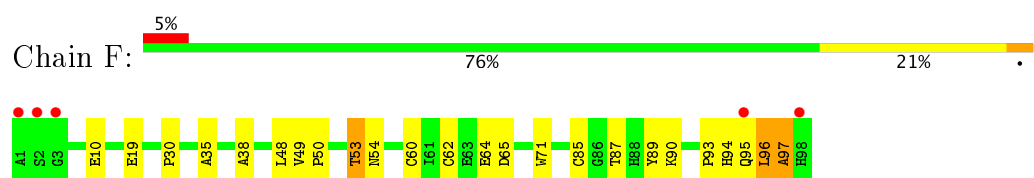
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



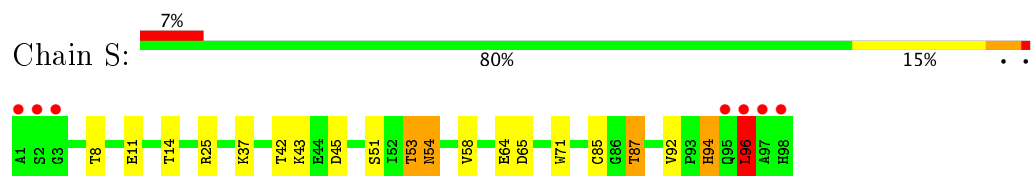
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



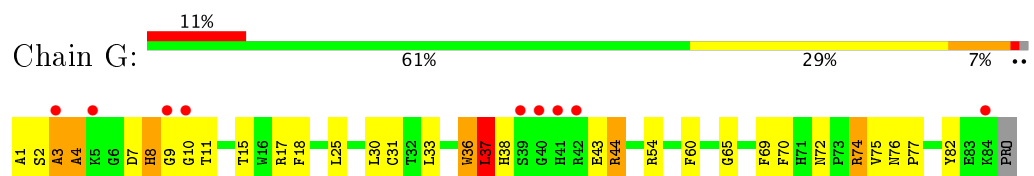
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



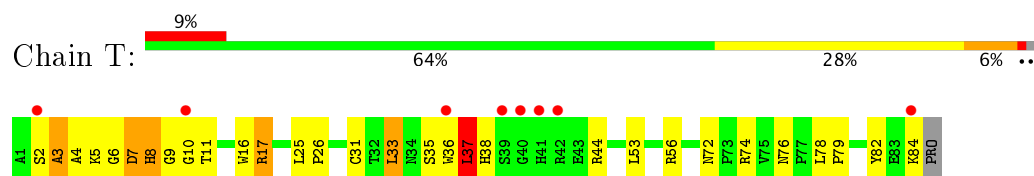
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



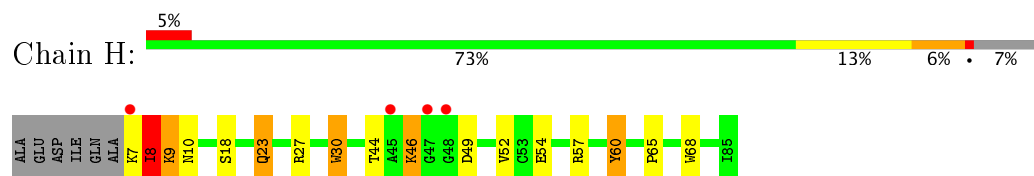
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



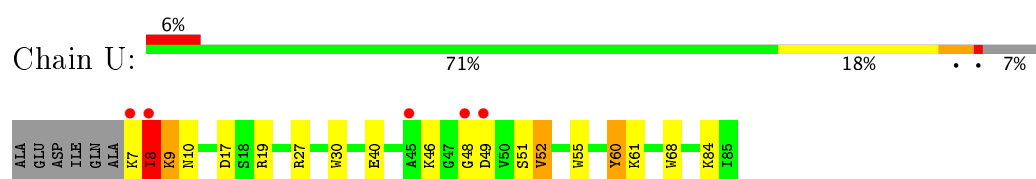
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



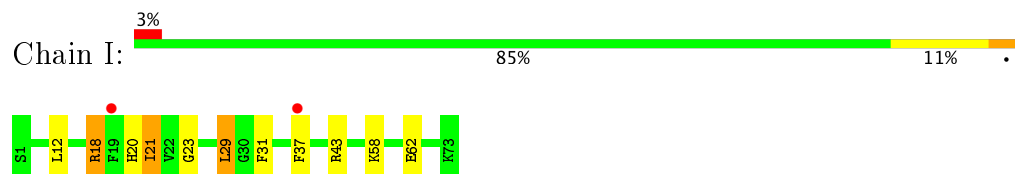
- Molecule 8: Cytochrome c oxidase subunit 6B1



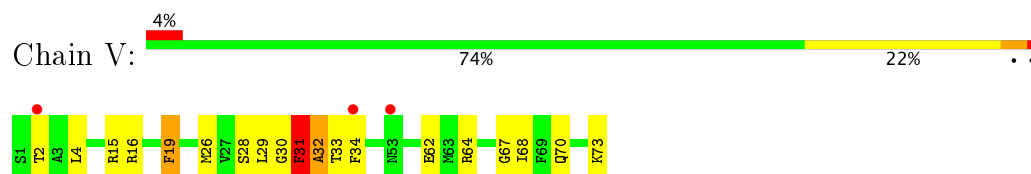
- Molecule 8: Cytochrome c oxidase subunit 6B1



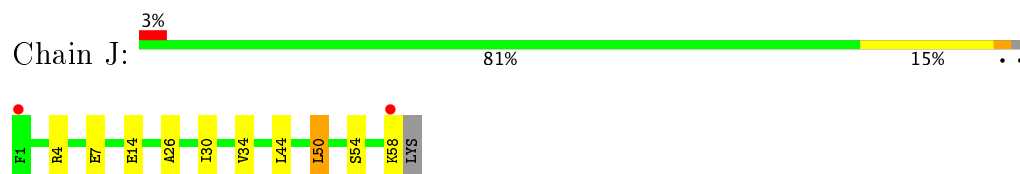
- Molecule 9: Cytochrome c oxidase subunit 6C



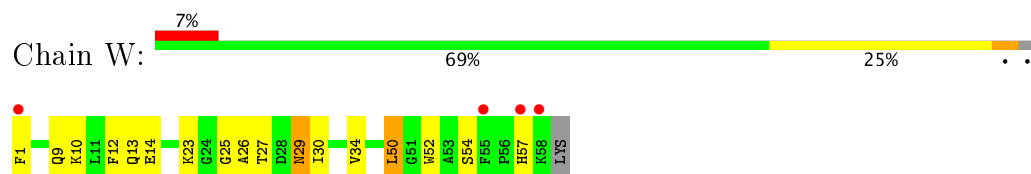
- Molecule 9: Cytochrome c oxidase subunit 6C



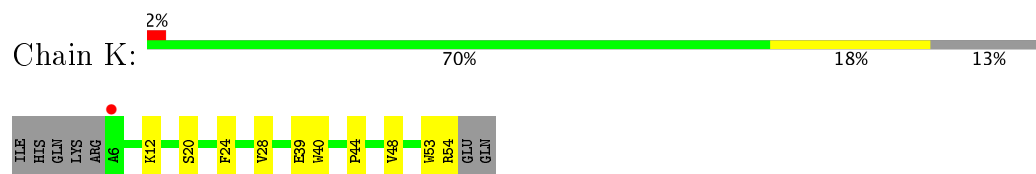
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



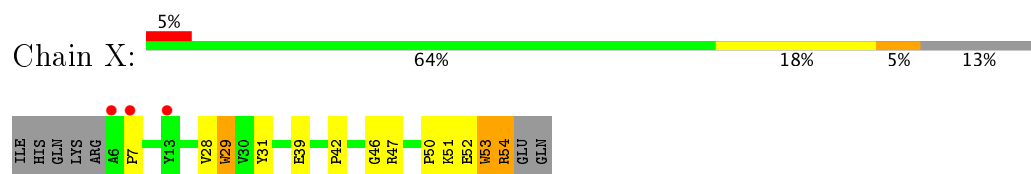
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



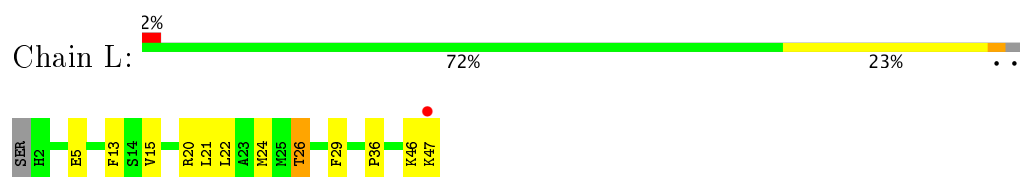
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



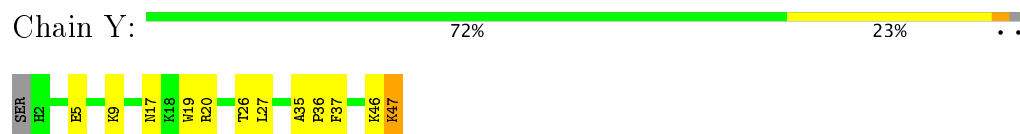
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



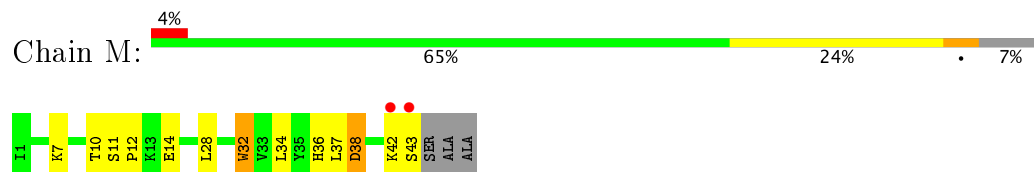
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



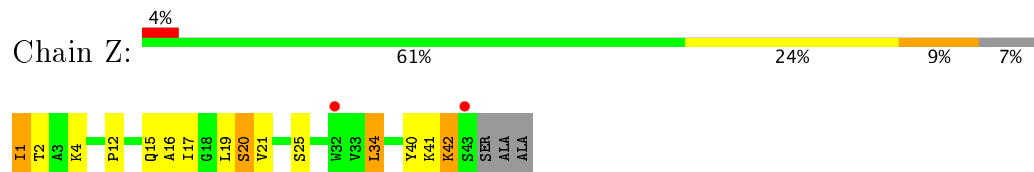
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.40) 98.2 (14.99-2.40)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.182 , 0.230 0.182 , 0.230	Depositor DCC
$R_{free}$ test set	13569 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 72.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, EDO, 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	0.91	10/4164 (0.2%)	0.89	4/5689 (0.1%)
1	N	0.86	11/4156 (0.3%)	0.82	0/5678
2	B	0.81	2/1860 (0.1%)	0.90	1/2534 (0.0%)
2	O	0.73	2/1860 (0.1%)	0.83	0/2534
3	C	0.92	7/2197 (0.3%)	0.81	0/3005
3	P	0.89	4/2197 (0.2%)	0.80	0/3005
4	D	0.82	4/1229 (0.3%)	0.79	0/1658
4	Q	0.76	4/1229 (0.3%)	0.74	0/1658
5	E	0.67	1/871 (0.1%)	0.80	0/1182
5	R	0.65	0/871	0.74	0/1182
6	F	0.74	1/765 (0.1%)	0.86	2/1038 (0.2%)
6	S	0.72	0/765	0.82	1/1038 (0.1%)
7	G	0.86	1/690 (0.1%)	0.87	1/937 (0.1%)
7	T	0.80	1/690 (0.1%)	0.83	1/937 (0.1%)
8	H	0.85	2/682 (0.3%)	0.86	0/921
8	U	0.79	3/682 (0.4%)	0.79	0/921
9	I	0.69	0/605	0.83	0/802
9	V	0.60	0/605	0.80	1/802 (0.1%)
10	J	0.72	0/471	0.75	0/636
10	W	0.66	1/471 (0.2%)	0.77	0/636
11	K	0.81	1/398 (0.3%)	0.76	0/546
11	X	0.80	2/398 (0.5%)	0.75	0/546
12	L	0.80	0/393	0.76	0/526
12	Y	0.75	1/393 (0.3%)	0.75	0/526
13	M	0.81	1/345 (0.3%)	0.78	0/470
13	Z	0.68	0/345	0.75	0/470
All	All	0.82	59/29332 (0.2%)	0.82	11/39877 (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
7	G	0	1
7	T	0	2
All	All	0	3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	TRP	CD2-CE2	7.46	1.50	1.41
1	N	126	TRP	CD2-CE2	7.33	1.50	1.41
1	A	396	TRP	CD2-CE2	6.55	1.49	1.41
2	B	106	TRP	CD2-CE2	6.42	1.49	1.41
1	N	340	TRP	CD2-CE2	6.38	1.49	1.41
2	O	65	TRP	CD2-CE2	6.36	1.49	1.41
6	F	71	TRP	CD2-CE2	6.27	1.48	1.41
1	A	275	TRP	CD2-CE2	6.22	1.48	1.41
7	G	36	TRP	CD2-CE2	6.13	1.48	1.41
1	A	409	TRP	CD2-CE2	6.12	1.48	1.41
1	N	186	TRP	CD2-CE2	6.12	1.48	1.41
3	C	58	TRP	CD2-CE2	6.08	1.48	1.41
2	B	65	TRP	CD2-CE2	6.02	1.48	1.41
3	C	240	TRP	CD2-CE2	6.01	1.48	1.41
4	Q	138	TRP	CD2-CE2	5.94	1.48	1.41
1	A	81	TRP	CD2-CE2	5.93	1.48	1.41
8	U	30	TRP	CD2-CE2	5.93	1.48	1.41
1	A	323	TRP	CD2-CE2	5.84	1.48	1.41
4	Q	145	TRP	CD2-CE2	5.74	1.48	1.41
1	N	473	TRP	CD2-CE2	5.73	1.48	1.41
11	X	53	TRP	CD2-CE2	5.69	1.48	1.41
1	N	6	TRP	CD2-CE2	5.68	1.48	1.41
11	X	29	TRP	CD2-CE2	5.63	1.48	1.41
1	N	323	TRP	CD2-CE2	5.60	1.48	1.41
3	C	249	TRP	CD2-CE2	5.59	1.48	1.41
4	Q	78	TRP	CD2-CE2	5.58	1.48	1.41
1	N	236	TRP	CD2-CE2	5.54	1.48	1.41
1	A	186	TRP	CD2-CE2	5.54	1.48	1.41
11	K	53	TRP	CD2-CE2	5.53	1.48	1.41
8	H	68	TRP	CD2-CE2	5.53	1.48	1.41
5	E	27	TRP	CD2-CE2	5.52	1.48	1.41
1	A	236	TRP	CD2-CE2	5.51	1.48	1.41
3	P	16	TRP	CD2-CE2	5.46	1.48	1.41
3	C	146	TRP	CD2-CE2	5.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CD2-CE2	5.38	1.47	1.41
2	O	222	TRP	CD2-CE2	5.38	1.47	1.41
1	A	103	TRP	CD2-CE2	5.37	1.47	1.41
13	M	32	TRP	CD2-CE2	5.30	1.47	1.41
8	U	68	TRP	CD2-CE2	5.29	1.47	1.41
4	D	98	TRP	CD2-CE2	5.28	1.47	1.41
12	Y	19	TRP	CD2-CE2	5.26	1.47	1.41
3	C	259	TRP	CD2-CE2	5.25	1.47	1.41
3	P	258	TRP	CD2-CE2	5.24	1.47	1.41
3	C	16	TRP	CD2-CE2	5.22	1.47	1.41
4	D	138	TRP	CD2-CE2	5.20	1.47	1.41
1	N	396	TRP	CD2-CE2	5.17	1.47	1.41
1	N	25	TRP	CD2-CE2	5.17	1.47	1.41
4	D	48	TRP	CD2-CE2	5.17	1.47	1.41
8	U	55	TRP	CD2-CE2	5.12	1.47	1.41
1	N	81	TRP	CD2-CE2	5.12	1.47	1.41
4	Q	115	TRP	CD2-CE2	5.12	1.47	1.41
4	D	78	TRP	CD2-CE2	5.11	1.47	1.41
3	P	57	TRP	CD2-CE2	5.09	1.47	1.41
3	C	99	TRP	CD2-CE2	5.06	1.47	1.41
8	H	30	TRP	CD2-CE2	5.06	1.47	1.41
1	A	450	TRP	CD2-CE2	5.01	1.47	1.41
10	W	52	TRP	CD2-CE2	5.01	1.47	1.41
1	A	288	TRP	CD2-CE2	5.01	1.47	1.41
1	N	409	TRP	CD2-CE2	5.00	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	438	ARG	NE-CZ-NH1	-6.50	117.05	120.30
6	S	96	LEU	CA-CB-CG	6.36	129.92	115.30
7	G	37	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	48	LEU	CB-CG-CD2	-6.00	100.81	111.00
2	B	139	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	100	MET	CG-SD-CE	5.53	109.05	100.20
9	V	31	PHE	N-CA-C	-5.52	96.10	111.00
6	F	96	LEU	CA-CB-CG	5.34	127.59	115.30
7	T	37	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	310	MET	CA-CB-CG	-5.08	104.66	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	Peptide

## 5.2 Too-close contacts [i](#)

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	4030	0	4009	73	0
1	N	4027	0	4002	99	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	38	0
3	C	2110	0	2027	31	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	8	0
5	R	852	0	845	21	0
6	F	748	0	728	13	0
6	S	748	0	728	18	0
7	G	675	0	643	29	0
7	T	675	0	643	23	0
8	H	662	0	623	13	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	23	0
10	J	460	0	459	8	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	12	0
12	L	380	0	380	12	0
12	Y	380	0	380	13	0
13	M	335	0	352	9	0
13	Z	335	0	352	15	0
14	A	120	0	108	12	0
14	N	120	0	108	13	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	11	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0
20	N	102	0	152	8	0
20	P	51	0	76	3	0
21	A	20	0	30	9	0
21	B	8	0	12	1	0
21	C	12	0	18	0	0
21	F	4	0	6	0	0
21	G	4	0	6	0	0
21	K	12	0	18	0	0
21	L	4	0	6	0	0
21	N	4	0	6	1	0
21	T	4	0	6	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	1	0
23	P	58	0	78	2	0
23	W	29	0	38	1	0
24	B	52	0	80	12	0
24	R	52	0	80	6	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	200	0	312	15	0
26	P	100	0	156	7	0
26	T	100	0	156	13	0
27	C	53	0	77	3	0
27	G	106	0	154	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	53	0	77	4	0
27	T	106	0	154	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	1	0
29	Z	33	0	42	1	0
30	A	125	0	0	22	0
30	B	78	0	0	6	0
30	C	70	0	0	18	0
30	D	41	0	0	2	0
30	E	24	0	0	2	0
30	F	36	0	0	2	0
30	G	31	0	0	2	0
30	H	33	0	0	2	0
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	645	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 10.

All (645) 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)
1:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28
5:R:50:ALA:HB3	30:R:303:HOH:O	1.43	1.18
6:S:85:CYS:SG	6:S:87:THR:CG2	2.30	1.18
9:V:26:MET:O	9:V:30:GLY:HA3	1.44	1.15
1:N:298:ASP:HB2	30:N:724:HOH:O	1.49	1.11
6:S:85:CYS:SG	6:S:87:THR:HG22	1.90	1.10
3:P:118:PRO:HD2	30:P:403:HOH:O	1.53	1.08
8:H:9:LYS:HD3	8:H:10:ASN:H	1.12	1.08
5:R:41:LEU:HD23	24:R:201:PSC:H082	1.31	1.08
26:C:307:CDL:H511	26:C:307:CDL:H221	1.12	1.05
1:A:240:HIS:CD2	1:A:244:TYR:CE2	2.33	1.03
1:N:50:ASP:HB3	1:N:53:ILE:HD12	1.39	1.02
2:O:223:SER:HA	30:O:414:HOH:O	1.61	1.01
6:F:19:GLU:HG2	30:F:231:HOH:O	1.60	1.01
24:R:201:PSC:H211	24:R:201:PSC:H031	1.44	0.99
9:V:15:ARG:HD3	30:V:113:HOH:O	1.62	0.98
1:A:104:LEU:HB2	30:A:788:HOH:O	1.64	0.97
1:N:353:LEU:HA	30:N:715:HOH:O	1.65	0.96
26:C:307:CDL:H221	26:C:307:CDL:C51	1.94	0.96
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.14	0.95
6:S:85:CYS:SG	6:S:87:THR:HG23	2.04	0.95
19:N:609:TGL:OC1	30:N:701:HOH:O	1.84	0.94
8:H:9:LYS:HD3	8:H:10:ASN:N	1.82	0.94
2:B:57:ASP:H	24:B:303:PSC:H241	1.33	0.94
12:L:47:LYS:HB2	13:M:43:SER:HB3	1.48	0.94
3:C:90:GLU:HA	30:C:413:HOH:O	1.67	0.92
1:N:240:HIS:CE1	1:N:244:TYR:HE2	1.86	0.92
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.52	0.92
1:N:439:ARG:NH2	30:N:702:HOH:O	2.01	0.92
6:S:54:ASN:H	6:S:54:ASN:HD22	1.18	0.91
30:A:799:HOH:O	12:L:36:PRO:HB2	1.72	0.89
1:N:240:HIS:CD2	1:N:244:TYR:HE2	1.88	0.89
19:N:609:TGL:CC1	30:N:701:HOH:O	2.19	0.89
2:B:90:ILE:HA	30:B:464:HOH:O	1.71	0.88
4:Q:107:ILE:HB	30:Q:202:HOH:O	1.73	0.88
11:K:24:PHE:O	11:K:28:VAL:HG12	1.74	0.87
11:X:42:PRO:HD2	30:X:101:HOH:O	1.72	0.87
9:V:32:ALA:O	30:V:101:HOH:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:607:TGL:H201	19:A:607:TGL:H361	1.55	0.86
7:G:10:GLY:HA3	1:N:177:SER:HB2	1.55	0.86
30:A:751:HOH:O	8:H:23:GLN:HG3	1.74	0.86
1:A:39:ALA:HA	21:A:614:EDO:H21	1.56	0.85
11:K:48:VAL:HB	30:K:207:HOH:O	1.77	0.84
4:Q:93:ALA:HB1	30:X:102:HOH:O	1.76	0.84
26:T:103:CDL:H531	26:T:103:CDL:H241	1.60	0.84
7:G:3:ALA:HB2	27:G:102:PEK:H292	1.60	0.84
1:A:243:VAL:HG21	18:A:606:CMO:C	2.08	0.83
1:N:240:HIS:CD2	1:N:244:TYR:CE2	2.63	0.83
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.44	0.82
19:N:611:TGL:HC42	19:N:611:TGL:OC1	1.80	0.81
19:N:611:TGL:H231	19:N:611:TGL:H282	1.62	0.81
9:V:30:GLY:C	9:V:32:ALA:N	2.28	0.81
20:N:607:PGV:H011	13:Z:15:GLN:HE22	1.43	0.81
2:O:226:MET:HB2	30:O:414:HOH:O	1.81	0.81
7:T:79:PRO:HD3	30:T:201:HOH:O	1.80	0.80
3:C:90:GLU:HG2	30:C:413:HOH:O	1.80	0.80
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.47	0.80
26:C:307:CDL:H542	26:C:307:CDL:H771	1.64	0.80
26:T:103:CDL:H222	26:T:103:CDL:H511	1.63	0.79
1:A:513:LEU:O	1:A:514:LYS:HB2	1.82	0.79
21:A:613:EDO:H11	11:K:39:GLU:H	1.45	0.79
9:V:26:MET:O	9:V:30:GLY:CA	2.30	0.79
24:B:303:PSC:H272	24:B:303:PSC:H202	1.64	0.78
1:A:61:HIS:CD2	30:A:754:HOH:O	2.36	0.78
2:B:210:VAL:HG13	30:B:415:HOH:O	1.84	0.78
3:C:62:ILE:HG12	30:C:404:HOH:O	1.84	0.77
12:Y:17:ASN:HB3	12:Y:20:ARG:NH1	2.00	0.77
6:S:54:ASN:ND2	6:S:54:ASN:H	1.82	0.76
9:V:29:LEU:O	9:V:32:ALA:HB2	1.85	0.75
6:F:64:GLU:O	6:F:65:ASP:HB2	1.84	0.75
7:T:17:ARG:HH22	27:T:102:PEK:H041	1.51	0.75
5:R:31:LYS:HE2	30:S:229:HOH:O	1.85	0.74
12:L:47:LYS:HB2	13:M:43:SER:CB	2.18	0.74
1:N:513:LEU:O	1:N:514:LYS:HB2	1.86	0.74
11:X:29:TRP:HA	30:X:102:HOH:O	1.88	0.73
1:N:406:ASN:HD21	20:N:607:PGV:C03	2.00	0.73
13:Z:1:ILE:O	13:Z:1:ILE:HG13	1.86	0.73
10:W:30:ILE:O	10:W:34:VAL:HG23	1.88	0.73
26:T:103:CDL:H381	26:T:103:CDL:H141	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:92:VAL:HG11	30:S:240:HOH:O	1.89	0.72
3:C:221:ARG:CZ	30:C:404:HOH:O	2.38	0.72
1:A:104:LEU:CB	30:A:788:HOH:O	2.29	0.72
26:C:307:CDL:C22	26:C:307:CDL:H511	2.06	0.72
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.72	0.71
1:N:406:ASN:HD21	20:N:607:PGV:H031	1.53	0.71
7:G:44:ARG:HG2	30:G:224:HOH:O	1.90	0.71
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.71	0.71
6:F:93:PRO:HA	30:F:225:HOH:O	1.90	0.71
14:A:602:HEA:HMC1	14:A:602:HEA:HBC1	1.73	0.71
26:C:307:CDL:H871	27:G:102:PEK:H322	1.72	0.71
1:N:240:HIS:CE1	1:N:244:TYR:CE2	2.69	0.71
2:O:57:ASP:HB2	24:R:201:PSC:H202	1.72	0.70
12:Y:17:ASN:HB3	12:Y:20:ARG:HH12	1.54	0.70
1:N:115:SER:O	1:N:121:GLY:HA2	1.92	0.70
2:O:139:ASP:OD1	2:O:140:ASN:N	2.23	0.70
2:O:217:LYS:NZ	2:O:217:LYS:H	1.89	0.70
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.74	0.70
1:N:50:ASP:HB3	1:N:53:ILE:CD1	2.21	0.69
1:A:62:ALA:HA	30:A:754:HOH:O	1.91	0.69
8:U:9:LYS:HB2	30:U:114:HOH:O	1.92	0.69
1:N:65:MET:HB3	14:N:601:HEA:CBC	2.23	0.69
1:N:406:ASN:ND2	20:N:607:PGV:H031	2.07	0.69
3:P:18:LEU:O	3:P:22:LEU:HD12	1.93	0.68
20:A:608:PGV:H332	30:C:413:HOH:O	1.93	0.68
27:P:302:PEK:H131	20:P:303:PGV:H181	1.75	0.68
12:Y:47:LYS:HB2	13:Z:42:LYS:CD	2.23	0.68
7:T:72:ASN:H	7:T:76:ASN:HD22	1.39	0.68
9:V:30:GLY:O	9:V:31:PHE:C	2.33	0.68
10:W:9:GLN:O	10:W:13:GLN:HG3	1.94	0.68
4:D:112:GLU:HB3	30:D:328:HOH:O	1.93	0.67
6:S:54:ASN:N	6:S:54:ASN:HD22	1.86	0.67
1:A:32:ALA:HB1	30:A:799:HOH:O	1.94	0.67
2:B:18:GLU:OE1	21:B:305:EDO:O1	2.11	0.67
14:A:601:HEA:H212	30:A:743:HOH:O	1.95	0.66
9:V:29:LEU:C	9:V:32:ALA:HB2	2.15	0.66
7:G:3:ALA:HA	27:G:102:PEK:H331	1.78	0.66
26:C:307:CDL:OA7	26:C:307:CDL:H351	1.96	0.66
1:N:165:ILE:HA	30:N:805:HOH:O	1.93	0.66
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.31	0.66
1:A:156:SER:HB2	30:A:788:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:307:CDL:OB4	26:C:307:CDL:H161	1.96	0.66
2:B:127:GLU:HG2	30:B:432:HOH:O	1.95	0.65
14:N:601:HEA:HMC1	14:N:601:HEA:CBC	2.26	0.65
1:A:505:PHE:HA	30:A:702:HOH:O	1.96	0.65
4:D:109:HIS:HD2	30:D:317:HOH:O	1.79	0.65
4:Q:121:LYS:HB2	11:X:50:PRO:HB3	1.78	0.65
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.61	0.65
3:C:257:TYR:O	3:C:261:SER:HB3	1.97	0.64
2:O:217:LYS:HZ3	2:O:217:LYS:H	1.42	0.64
7:G:72:ASN:H	7:G:76:ASN:HD22	1.45	0.64
1:N:312:ILE:O	1:N:312:ILE:HD13	1.97	0.64
27:C:306:PEK:H031	30:C:412:HOH:O	1.97	0.64
9:V:28:SER:C	9:V:30:GLY:H	1.98	0.64
3:P:36:HIS:O	3:P:38:ASN:N	2.27	0.64
1:N:147:ILE:HG23	1:N:206:ILE:HD12	1.78	0.63
2:O:207:MET:HG3	30:O:402:HOH:O	1.98	0.63
1:A:455:SER:HB3	21:A:614:EDO:H12	1.79	0.63
1:N:353:LEU:HD23	30:N:715:HOH:O	1.97	0.63
1:N:488:THR:HB	1:N:495:LEU:HD13	1.79	0.63
1:A:24:ALA:HB2	30:A:723:HOH:O	1.98	0.62
3:P:36:HIS:C	3:P:38:ASN:H	2.02	0.62
26:C:307:CDL:H541	26:C:307:CDL:H752	1.79	0.62
2:O:196:CYS:HB3	30:O:402:HOH:O	1.98	0.62
13:Z:17:ILE:O	13:Z:21:VAL:HG23	1.98	0.62
9:V:30:GLY:C	9:V:32:ALA:H	2.00	0.62
11:X:39:GLU:HB3	30:X:106:HOH:O	1.98	0.62
1:N:484:THR:HB	13:Z:2:THR:OG1	2.00	0.62
1:A:240:HIS:O	1:A:243:VAL:HG22	1.98	0.61
4:Q:108:PRO:HD2	30:Q:202:HOH:O	1.98	0.61
12:Y:47:LYS:HB2	13:Z:42:LYS:HD3	1.81	0.61
7:G:17:ARG:HD3	30:O:433:HOH:O	2.00	0.61
27:P:302:PEK:HN2	7:T:76:ASN:HD21	1.48	0.61
26:C:307:CDL:H241	26:C:307:CDL:H511	1.83	0.61
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.83	0.61
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.60
14:N:602:HEA:C26	30:N:715:HOH:O	2.49	0.60
26:T:103:CDL:C53	26:T:103:CDL:H241	2.31	0.60
1:N:175:ALA:HB3	1:N:511:VAL:HG12	1.83	0.60
7:G:10:GLY:HA3	1:N:177:SER:CB	2.31	0.60
4:Q:78:TRP:O	4:Q:82:VAL:HG23	2.00	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:26:ASP:OD1	4:Q:26:ASP:N	2.33	0.60
14:A:601:HEA:C1D	30:A:754:HOH:O	2.49	0.60
12:L:20:ARG:NH2	19:L:101:TGL:HC31	2.16	0.60
6:S:43:LYS:HG3	30:S:236:HOH:O	2.02	0.60
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.83	0.60
1:A:488:THR:HB	1:A:495:LEU:HD11	1.84	0.59
3:C:125:ASN:HB3	3:C:128:GLU:OE2	2.01	0.59
3:C:221:ARG:NH2	30:C:404:HOH:O	2.35	0.59
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.59
1:N:68:PHE:HE2	1:N:112:LEU:HD22	1.67	0.59
3:P:146:TRP:HB2	7:T:16:TRP:HB3	1.84	0.59
10:J:4:ARG:HD2	10:J:7:GLU:OE1	2.03	0.59
13:Z:16:ALA:O	13:Z:20:SER:OG	2.20	0.59
3:P:246:ASP:HB2	30:P:442:HOH:O	2.03	0.59
30:A:812:HOH:O	26:T:103:CDL:HB22	2.03	0.59
1:N:280:ILE:HG12	1:N:312:ILE:HD11	1.83	0.58
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.84	0.58
1:A:156:SER:CB	30:A:788:HOH:O	2.49	0.58
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.85	0.58
1:N:390:MET:O	1:N:394:VAL:HG13	2.03	0.58
7:T:31:CYS:SG	26:T:103:CDL:H532	2.42	0.58
30:B:404:HOH:O	9:I:23:GLY:HA3	2.04	0.58
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.84	0.58
5:R:80:GLU:CD	5:R:80:GLU:H	2.06	0.58
2:B:52:HIS:HE1	24:B:303:PSC:H201	1.69	0.58
5:E:8:ASP:HB2	30:E:219:HOH:O	2.04	0.58
3:C:188:ILE:HG22	27:G:101:PEK:O13	2.04	0.58
20:N:607:PGV:H202	13:Z:12:PRO:HG3	1.85	0.57
1:N:476:PHE:HZ	19:N:611:TGL:H251	1.70	0.57
1:N:37:ILE:CG2	14:N:601:HEA:HMA	2.34	0.57
1:A:27:GLY:HA3	30:A:743:HOH:O	2.02	0.57
1:A:488:THR:HB	1:A:495:LEU:CD1	2.35	0.57
8:H:7:LYS:C	8:H:8:ILE:HG13	2.26	0.56
6:S:64:GLU:HB2	30:S:230:HOH:O	2.05	0.56
10:W:9:GLN:O	10:W:13:GLN:CG	2.53	0.56
1:N:142:SER:HB2	30:N:785:HOH:O	2.03	0.56
12:Y:46:LYS:HA	30:Y:102:HOH:O	2.04	0.56
2:B:41:ILE:O	2:B:45:MET:HG2	2.06	0.56
1:A:251:PHE:CD2	1:A:319:LYS:HE2	2.41	0.56
1:A:43:GLN:HG2	4:D:104:TYR:CD1	2.40	0.56
3:P:206:LEU:HD22	27:P:302:PEK:H102	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:56:ARG:NH2	30:T:201:HOH:O	2.39	0.56
1:A:449:MET:HE2	11:K:40:TRP:HB3	1.87	0.56
9:V:31:PHE:C	9:V:31:PHE:CD1	2.78	0.56
4:Q:108:PRO:CD	30:Q:202:HOH:O	2.54	0.56
7:G:7:ASP:O	7:G:8:HIS:HB2	2.06	0.56
3:C:3:HIS:HB2	30:C:444:HOH:O	2.05	0.55
7:G:31:CYS:HA	30:G:207:HOH:O	2.05	0.55
4:Q:101:HIS:HB3	30:Q:218:HOH:O	2.06	0.55
4:Q:39:ALA:O	4:Q:42:GLU:HB2	2.05	0.55
3:P:116:TRP:HA	3:P:117:PRO:C	2.26	0.55
3:P:118:PRO:CD	30:P:403:HOH:O	2.27	0.55
7:G:8:HIS:HE1	27:G:102:PEK:H051	1.71	0.55
11:K:44:PRO:HB2	30:K:207:HOH:O	2.07	0.55
2:O:98:LYS:HG2	2:O:153:LEU:HB2	1.89	0.55
7:G:8:HIS:CE1	27:G:102:PEK:H051	2.41	0.55
19:N:609:TGL:HA71	19:N:609:TGL:H222	1.88	0.55
23:P:306:CHD:H212	23:P:306:CHD:H12	1.89	0.55
10:W:26:ALA:O	10:W:30:ILE:HD13	2.07	0.55
9:V:31:PHE:CD1	9:V:32:ALA:N	2.74	0.54
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.73	0.54
9:V:30:GLY:O	9:V:32:ALA:N	2.39	0.54
2:B:217:LYS:HG3	30:B:458:HOH:O	2.06	0.54
3:C:246:ASP:HB2	30:C:455:HOH:O	2.06	0.54
3:C:90:GLU:CA	30:C:413:HOH:O	2.37	0.54
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.90	0.54
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.90	0.54
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.89	0.54
1:A:240:HIS:CD2	1:A:244:TYR:CD2	2.94	0.54
2:B:9:PHE:HB2	2:B:21:LEU:HD21	1.90	0.54
8:U:40:GLU:HB2	30:U:105:HOH:O	2.08	0.54
9:V:64:ARG:NH1	9:V:73:LYS:O	2.40	0.54
3:P:65:SER:HB2	20:P:303:PGV:H041	1.90	0.53
26:C:307:CDL:H662	20:G:103:PGV:H172	1.90	0.53
1:N:483:LEU:HG	13:Z:4:LYS:HG2	1.90	0.53
12:Y:20:ARG:CZ	12:Y:20:ARG:HB3	2.38	0.53
1:N:127:THR:HG23	30:N:702:HOH:O	2.07	0.53
1:A:51:ASP:HB2	2:B:202:SER:O	2.09	0.53
2:O:91:ASN:HD22	2:O:93:PRO:HD3	1.72	0.53
9:V:19:PHE:CD1	9:V:19:PHE:C	2.82	0.53
3:C:67:PHE:HE2	26:C:303:CDL:H1	1.74	0.53
20:N:608:PGV:H51	20:N:608:PGV:H251	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:89:GLU:O	2:O:91:ASN:OD1	2.27	0.53
7:T:3:ALA:HB2	27:T:101:PEK:H351	1.89	0.53
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.44	0.53
1:N:486:ASP:N	1:N:486:ASP:OD1	2.38	0.53
1:A:502:TYR:OH	21:A:612:EDO:H22	2.09	0.53
7:G:72:ASN:N	7:G:76:ASN:HD22	2.07	0.53
7:G:37:LEU:O	7:G:38:HIS:ND1	2.42	0.52
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.43	0.52
26:P:304:CDL:H331	26:P:304:CDL:H432	1.90	0.52
10:W:29:ASN:HD22	10:W:29:ASN:H	1.57	0.52
1:A:177:SER:H	1:A:180:GLN:NE2	2.07	0.52
1:N:365:ILE:HB	30:N:704:HOH:O	2.09	0.52
14:N:601:HEA:HBC1	14:N:601:HEA:CMC	2.31	0.52
5:R:102:GLU:N	5:R:102:GLU:OE1	2.40	0.52
23:J:101:CHD:H183	23:J:101:CHD:H212	1.91	0.52
7:T:37:LEU:HD21	26:T:103:CDL:H401	1.91	0.52
5:R:99:SER:HB2	5:R:104:LEU:HD21	1.91	0.52
26:C:307:CDL:H712	26:C:307:CDL:H522	1.92	0.52
7:G:1:ALA:H1	20:G:103:PGV:H301	1.74	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.52
21:A:613:EDO:O2	4:D:100:LYS:HE2	2.10	0.52
4:D:99:GLU:O	4:D:103:VAL:HB	2.09	0.52
2:B:90:ILE:H	2:B:90:ILE:HD12	1.74	0.52
2:O:63:THR:O	2:O:67:ILE:HG12	2.09	0.52
3:P:18:LEU:HG	3:P:22:LEU:CD1	2.40	0.52
5:R:108:LYS:O	5:R:109:VAL:C	2.48	0.52
10:J:54:SER:O	12:L:46:LYS:HE3	2.10	0.52
1:N:459:PHE:O	1:N:462:LEU:HB3	2.09	0.52
7:G:4:ALA:HB1	1:N:282:PHE:HA	1.91	0.51
2:O:139:ASP:O	9:V:70:GLN:NE2	2.43	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.90	0.51
8:U:7:LYS:C	8:U:8:ILE:HG13	2.30	0.51
4:D:130:PRO:HA	4:D:135:SER:HB2	1.92	0.51
3:P:63:ARG:HE	26:P:304:CDL:HA22	1.75	0.51
2:B:108:TYR:O	2:B:117:SER:HA	2.11	0.51
7:T:8:HIS:CE1	27:T:101:PEK:H312	2.46	0.51
9:V:28:SER:C	9:V:30:GLY:N	2.64	0.51
11:X:42:PRO:O	11:X:47:ARG:NH2	2.43	0.51
1:A:177:SER:H	1:A:180:GLN:HE21	1.59	0.50
7:G:60:PHE:O	7:G:65:GLY:HA2	2.12	0.50
1:A:393:PHE:O	1:A:397:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:492:LEU:HD13	6:S:71:TRP:CD2	2.47	0.50
14:A:602:HEA:HMC1	14:A:602:HEA:CBC	2.40	0.50
4:D:34:SER:H	4:D:37:GLN:NE2	2.08	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.11	0.50
1:A:156:SER:CA	30:A:788:HOH:O	2.60	0.50
1:N:366:VAL:N	30:N:704:HOH:O	2.34	0.50
1:A:14:ASP:O	1:A:17:THR:HB	2.11	0.50
5:R:109:VAL:O	5:R:109:VAL:HG23	2.10	0.50
1:N:68:PHE:O	1:N:72:PRO:HG2	2.11	0.50
5:R:53:ARG:NH2	5:R:92:THR:HG23	2.27	0.50
1:A:201:VAL:HA	30:A:720:HOH:O	2.10	0.50
3:C:187:THR:HG22	27:G:101:PEK:H051	1.94	0.50
12:L:15:VAL:HG12	12:L:21:LEU:HD22	1.94	0.50
14:N:602:HEA:H263	30:N:715:HOH:O	2.12	0.50
1:N:76:GLY:O	1:N:80:ASN:HB2	2.11	0.50
8:H:10:ASN:HA	30:H:117:HOH:O	2.11	0.49
3:P:18:LEU:HG	3:P:22:LEU:HD12	1.94	0.49
5:E:21:LYS:HE2	5:E:23:ASP:OD1	2.12	0.49
13:M:28:LEU:HD23	29:M:101:DMU:H7	1.94	0.49
1:N:117:MET:HB3	10:W:54:SER:OG	2.12	0.49
1:N:168:ILE:HD12	30:N:805:HOH:O	2.13	0.49
1:N:186:TRP:O	1:N:190:ILE:HG13	2.12	0.49
3:P:112:LEU:HB3	3:P:118:PRO:HB3	1.93	0.49
6:S:42:THR:OG1	6:S:45:ASP:HB3	2.12	0.49
10:W:50:LEU:HD22	10:W:50:LEU:O	2.12	0.49
12:Y:26:THR:CG2	13:Z:25:SER:HB3	2.42	0.49
1:A:505:PHE:HD1	30:A:702:HOH:O	1.94	0.49
1:A:52:GLN:O	1:A:56:VAL:HG23	2.12	0.49
2:B:83:ILE:O	2:B:87:MET:HG3	2.12	0.49
1:N:37:ILE:HG22	14:N:601:HEA:HMA	1.93	0.49
4:Q:129:ALA:HB3	4:Q:134:PHE:HB3	1.94	0.49
6:F:64:GLU:O	6:F:65:ASP:CB	2.57	0.49
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.47	0.49
3:C:180:GLU:HG3	30:C:402:HOH:O	2.13	0.49
23:C:305:CHD:H212	23:C:305:CHD:H12	1.94	0.49
1:N:270:TYR:O	1:N:273:MET:HB2	2.12	0.49
10:W:12:PHE:O	10:W:23:LYS:HE2	2.12	0.49
1:A:199:LEU:N	1:A:200:PRO:CD	2.75	0.49
4:D:33:LEU:HA	4:D:37:GLN:HE21	1.77	0.49
3:P:127:LEU:HD12	3:P:131:LEU:HD22	1.95	0.49
24:R:201:PSC:H252	24:R:201:PSC:H21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:HIS:CB	30:C:444:HOH:O	2.60	0.49
3:P:67:PHE:HE2	26:P:304:CDL:H1	1.77	0.49
12:Y:5:GLU:O	12:Y:9:LYS:HG3	2.12	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
5:R:43:PRO:HG2	5:R:48:ILE:HD11	1.94	0.48
1:A:430:PHE:CE1	19:A:607:TGL:HB22	2.48	0.48
7:G:9:GLY:H	1:N:178:GLN:HE21	1.60	0.48
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.21	0.48
1:N:240:HIS:O	1:N:243:VAL:HG22	2.13	0.48
5:R:40:ASP:H	24:R:201:PSC:H071	1.79	0.48
1:A:380:VAL:O	1:A:384:GLY:HA3	2.14	0.48
3:C:17:PRO:HG2	30:C:445:HOH:O	2.13	0.48
26:T:103:CDL:H331	26:T:103:CDL:OA7	2.13	0.48
7:G:9:GLY:H	1:N:178:GLN:NE2	2.12	0.48
1:N:240:HIS:CD2	1:N:244:TYR:CD2	3.00	0.48
4:Q:131:ILE:HG22	4:Q:132:GLN:HG3	1.96	0.48
2:O:49:LYS:HE2	4:Q:20:ARG:CZ	2.44	0.48
10:W:25:GLY:HA2	30:W:203:HOH:O	2.13	0.48
1:A:189:MET:HG3	1:A:189:MET:O	2.10	0.48
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.48	0.48
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.26	0.48
21:A:614:EDO:H22	4:D:99:GLU:OE1	2.14	0.48
12:L:22:LEU:O	12:L:26:THR:HB	2.13	0.48
2:B:52:HIS:CE1	24:B:303:PSC:H201	2.49	0.48
7:T:78:LEU:HA	30:T:201:HOH:O	2.13	0.48
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.95	0.48
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.47	0.48
1:A:180:GLN:HB2	1:A:180:GLN:HE21	1.54	0.47
24:B:303:PSC:H011	24:B:303:PSC:H261	1.95	0.47
1:N:324:LEU:HD21	2:O:42:ILE:HG13	1.96	0.47
10:W:29:ASN:HD22	10:W:29:ASN:N	2.12	0.47
1:N:294:THR:HG22	1:N:365:ILE:HD13	1.96	0.47
5:R:72:LYS:NZ	5:R:102:GLU:OE2	2.39	0.47
1:A:21:LEU:HD23	19:L:101:TGL:H211	1.97	0.47
1:A:450:TRP:HA	1:A:450:TRP:CE3	2.50	0.47
26:C:307:CDL:H871	27:G:102:PEK:C32	2.42	0.47
1:N:328:HIS:HB2	2:O:45:MET:SD	2.54	0.47
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.61	0.47
1:N:507:GLU:OE1	6:S:51:SER:HA	2.14	0.47
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.44	0.47
3:C:38:ASN:ND2	30:C:406:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.96	0.47
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.50	0.47
23:W:101:CHD:H183	23:W:101:CHD:H222	1.97	0.47
23:C:304:CHD:H12	23:C:304:CHD:H212	1.95	0.47
6:F:96:LEU:O	6:F:97:ALA:HB2	2.14	0.47
1:N:378:HIS:O	1:N:382:SER:HB2	2.15	0.47
14:A:601:HEA:OMA	14:A:601:HEA:HHB	2.15	0.47
7:G:44:ARG:HD2	7:G:74:ARG:O	2.15	0.47
19:N:609:TGL:HC31	30:N:815:HOH:O	2.14	0.47
1:A:278:MET:HB3	21:T:104:EDO:H22	1.97	0.46
9:V:19:PHE:HD1	9:V:19:PHE:C	2.18	0.46
13:Z:34:LEU:HA	13:Z:34:LEU:HD12	1.77	0.46
5:E:53:ARG:NH2	5:E:92:THR:HG23	2.30	0.46
9:I:18:ARG:HB2	9:I:18:ARG:HH11	1.80	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.46	0.46
4:D:82:VAL:O	4:D:86:MET:HG3	2.14	0.46
6:F:53:THR:HB	6:F:54:ASN:H	1.56	0.46
21:N:612:EDO:C1	13:Z:1:ILE:HG21	2.46	0.46
4:Q:127:LYS:HE2	30:Q:225:HOH:O	2.15	0.46
24:B:303:PSC:C27	24:B:303:PSC:H202	2.39	0.46
20:N:608:PGV:H042	20:N:608:PGV:C03	2.45	0.46
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.16	0.46
5:R:25:ASP:HB2	30:R:307:HOH:O	2.14	0.46
5:R:39:TYR:HB3	24:R:201:PSC:H073	1.96	0.46
2:B:100:MET:HE2	2:B:157:GLU:HG3	1.97	0.46
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.46
10:J:50:LEU:HD22	10:J:50:LEU:O	2.15	0.46
13:M:38:ASP:HB3	30:M:210:HOH:O	2.15	0.46
1:N:37:ILE:HG21	14:N:601:HEA:HMA	1.97	0.46
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.16	0.46
8:H:44:THR:C	8:H:46:LYS:H	2.19	0.46
9:I:12:LEU:H	9:I:12:LEU:HD12	1.81	0.46
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.71	0.46
3:P:77:LYS:O	3:P:80:ARG:HB2	2.16	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.46
2:O:158:ASP:OD1	2:O:159:VAL:N	2.43	0.46
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.83	0.46
3:P:21:ALA:O	3:P:24:ALA:HB3	2.16	0.46
3:P:41:THR:O	3:P:44:MET:HB2	2.15	0.46
7:T:17:ARG:HD2	30:T:206:HOH:O	2.15	0.46
2:O:224:ALA:HA	30:O:466:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:302:PEK:H181	27:P:302:PEK:H101	1.97	0.45
19:A:607:TGL:HC61	19:A:607:TGL:H151	1.97	0.45
3:C:243:HIS:HD2	30:C:430:HOH:O	1.99	0.45
8:U:10:ASN:HA	30:U:115:HOH:O	2.16	0.45
1:A:316:THR:HG21	14:A:602:HEA:H14	1.98	0.45
1:A:43:GLN:HG2	4:D:104:TYR:CE1	2.52	0.45
9:I:29:LEU:HD13	9:I:29:LEU:HA	1.71	0.45
11:K:12:LYS:HB2	11:K:12:LYS:NZ	2.31	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.51	0.45
7:G:2:SER:O	7:G:3:ALA:HB2	2.16	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.90	0.45
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.99	0.45
4:Q:147:LYS:HA	30:Q:220:HOH:O	2.16	0.45
4:Q:29:HIS:CD2	4:Q:30:VAL:HG23	2.51	0.45
1:N:51:ASP:HB2	2:O:202:SER:O	2.16	0.45
27:C:306:PEK:H42	27:C:306:PEK:H221	1.99	0.45
2:B:145:PRO:HA	2:B:214:VAL:O	2.16	0.45
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	1.99	0.45
2:O:111:THR:HG22	2:O:115:ASP:HA	1.97	0.45
2:O:226:MET:HA	2:O:226:MET:CE	2.47	0.45
2:O:128:LEU:HD22	2:O:132:GLU:HB3	1.99	0.45
2:B:74:ILE:HG22	2:B:78:LEU:HD22	1.98	0.45
7:G:77:PRO:HD3	7:G:82:TYR:CE1	2.52	0.45
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.52	0.45
4:Q:118:LYS:HA	11:X:51:LYS:O	2.17	0.45
19:N:610:TGL:HG12	19:N:610:TGL:HC42	1.98	0.44
9:I:58:LYS:O	9:I:62:GLU:HG3	2.17	0.44
19:N:611:TGL:CC4	19:N:611:TGL:OC1	2.58	0.44
4:D:130:PRO:O	4:D:136:ALA:HB2	2.18	0.44
27:G:101:PEK:H331	27:G:101:PEK:H361	1.71	0.44
1:A:28:MET:HG3	12:L:29:PHE:HD1	1.82	0.44
2:O:68:LEU:HD12	2:O:68:LEU:HA	1.78	0.44
5:R:67:ILE:O	5:R:71:VAL:HG23	2.18	0.44
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.85	0.44
9:V:19:PHE:HB2	30:V:118:HOH:O	2.18	0.44
23:B:302:CHD:H12	23:B:302:CHD:H212	1.98	0.44
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.00	0.44
1:N:118:VAL:O	1:N:119:GLU:C	2.55	0.44
2:B:179:LEU:HD11	8:H:65:PRO:HD3	2.00	0.44
4:Q:8:SER:C	4:Q:10:ASP:H	2.20	0.44
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:230:LEU:HD21	3:P:100:ALA:HA	1.99	0.44
1:A:127:THR:HB	1:A:129:TYR:CE1	2.52	0.44
2:B:181:GLN:O	8:H:23:GLN:HG2	2.17	0.44
30:L:210:HOH:O	13:M:32:TRP:HH2	2.00	0.44
23:P:305:CHD:H41	23:P:305:CHD:O7	2.18	0.44
7:T:7:ASP:O	7:T:9:GLY:N	2.51	0.44
8:U:17:ASP:OD2	8:U:19:ARG:NH2	2.51	0.44
1:A:390:MET:O	1:A:394:VAL:HG13	2.18	0.43
24:B:303:PSC:H272	24:B:303:PSC:C20	2.40	0.43
1:A:156:SER:HA	30:A:788:HOH:O	2.17	0.43
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.48	0.43
3:P:121:ILE:HB	30:P:403:HOH:O	2.18	0.43
6:S:53:THR:HB	6:S:54:ASN:HD22	1.83	0.43
19:N:610:TGL:H351	9:V:16:ARG:HH21	1.84	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.00	0.43
14:A:601:HEA:H11	14:A:601:HEA:HH2	1.81	0.43
3:C:14:SER:HA	3:C:15:PRO:HD3	1.87	0.43
1:A:43:GLN:OE1	4:D:104:TYR:HB3	2.18	0.43
3:P:195:SER:O	3:P:199:VAL:HG23	2.18	0.43
5:R:102:GLU:HA	5:R:107:ASP:OD1	2.19	0.43
9:V:67:GLY:HA2	30:V:102:HOH:O	2.17	0.43
26:C:307:CDL:H131	26:C:307:CDL:H1	1.99	0.43
10:J:50:LEU:HB2	30:J:215:HOH:O	2.18	0.43
13:M:10:THR:HA	13:M:14:GLU:OE2	2.19	0.43
6:S:58:VAL:O	6:S:71:TRP:HA	2.18	0.43
3:P:30:GLY:HA2	3:P:42:LEU:HB3	2.00	0.43
6:S:53:THR:HB	6:S:54:ASN:H	1.44	0.43
24:B:303:PSC:H221	24:B:303:PSC:H012	2.00	0.43
2:B:49:LYS:O	4:D:20:ARG:NH2	2.41	0.43
2:O:215:PRO:HB2	2:O:217:LYS:HE2	2.01	0.43
4:Q:108:PRO:N	30:Q:202:HOH:O	2.52	0.43
1:N:412:ILE:HD13	4:Q:84:ALA:CB	2.49	0.43
30:A:779:HOH:O	3:C:111:GLU:HB3	2.18	0.43
12:L:21:LEU:O	12:L:24:MET:HB2	2.19	0.43
6:S:94:HIS:O	6:S:96:LEU:HD13	2.19	0.43
7:T:33:LEU:HD22	7:T:33:LEU:HA	1.75	0.43
1:A:106:PRO:N	1:A:107:PRO:HD2	2.33	0.43
1:A:316:THR:HG21	14:A:602:HEA:C14	2.49	0.43
1:A:459:PHE:CE1	21:A:614:EDO:H11	2.54	0.43
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.43
3:C:179:SER:O	3:C:183:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ILE:O	2:O:171:LYS:HD2	2.18	0.43
3:P:90:GLU:O	3:P:93:PHE:HB3	2.19	0.43
3:C:92:LEU:O	3:C:95:THR:HB	2.19	0.43
1:N:194:LEU:CD2	1:N:285:PHE:HE2	2.30	0.43
1:N:298:ASP:N	1:N:298:ASP:OD1	2.46	0.43
26:T:103:CDL:H762	26:T:103:CDL:H561	2.00	0.43
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.01	0.43
3:C:108:PRO:HA	30:C:446:HOH:O	2.18	0.43
4:D:120:THR:HG21	30:K:207:HOH:O	2.18	0.43
1:A:174:PRO:HB2	6:F:35:ALA:HB2	2.01	0.43
7:G:15:THR:O	7:G:18:PHE:HB3	2.18	0.43
1:N:199:LEU:HA	1:N:199:LEU:HD23	1.78	0.43
8:H:7:LYS:O	8:U:46:LYS:NZ	2.47	0.42
10:J:50:LEU:HD22	10:J:50:LEU:C	2.40	0.42
1:N:498:CYS:HA	1:N:499:PRO:HA	1.93	0.42
3:P:55:TYR:HA	26:P:304:CDL:H552	2.01	0.42
3:P:36:HIS:C	3:P:38:ASN:N	2.70	0.42
4:Q:145:TRP:CD1	11:X:46:GLY:HA2	2.54	0.42
7:G:74:ARG:HD2	7:G:75:VAL:HG13	2.01	0.42
3:P:63:ARG:HE	26:P:304:CDL:CA2	2.32	0.42
5:R:24:ILE:HG13	5:R:28:GLU:HB2	2.01	0.42
12:L:47:LYS:HA	30:L:212:HOH:O	2.18	0.42
19:N:609:TGL:H283	19:N:609:TGL:H102	2.01	0.42
8:U:49:ASP:O	8:U:52:VAL:HG23	2.19	0.42
13:Z:40:TYR:O	13:Z:42:LYS:N	2.52	0.42
1:A:407:ASP:O	1:A:411:LYS:HG3	2.19	0.42
1:N:89:ALA:HA	1:N:90:PRO:HD3	1.83	0.42
8:U:9:LYS:HA	8:U:9:LYS:HD3	1.82	0.42
1:A:227:ASP:HA	1:A:228:PRO:HD3	1.74	0.42
1:A:380:VAL:HG21	14:A:602:HEA:C4C	2.50	0.42
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.73	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.20	0.42
1:N:36:LEU:HD21	12:Y:37:PHE:CE1	2.54	0.42
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.01	0.42
3:P:92:LEU:HA	3:P:92:LEU:HD13	1.85	0.42
4:Q:90:GLY:O	4:Q:93:ALA:HB3	2.19	0.42
23:C:304:CHD:H12A	23:C:304:CHD:H112	1.86	0.42
7:G:30:LEU:HA	7:G:30:LEU:HD23	1.83	0.42
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.55	0.42
1:A:324:LEU:HD21	2:B:42:ILE:HG12	2.02	0.42
26:C:303:CDL:H112	26:C:303:CDL:HA4	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:30:ILE:O	10:J:34:VAL:HG23	2.19	0.42
1:N:366:VAL:HB	30:N:704:HOH:O	2.19	0.42
1:N:425:PHE:O	1:N:426:PHE:C	2.55	0.42
2:O:78:LEU:N	2:O:79:PRO:HD2	2.35	0.42
9:V:33:THR:O	9:V:34:PHE:C	2.57	0.42
20:A:609:PGV:O14	20:A:609:PGV:O02	2.37	0.42
1:A:9:SER:HA	21:A:612:EDO:H11	2.02	0.42
5:E:96:LEU:HA	5:E:96:LEU:HD23	1.77	0.42
2:O:103:GLN:HA	2:O:104:TRP:HA	1.81	0.42
2:O:144:LEU:HA	2:O:145:PRO:HD3	1.83	0.42
2:O:2:ALA:HB3	30:O:458:HOH:O	2.19	0.42
23:O:302:CHD:H161	23:O:302:CHD:H221	1.73	0.42
26:P:304:CDL:PA1	26:P:304:CDL:HB21	2.60	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.42
30:A:720:HOH:O	3:C:93:PHE:HA	2.20	0.42
6:F:60:CYS:SG	6:F:89:TYR:OH	2.73	0.42
6:S:8:THR:OG1	6:S:11:GLU:HG3	2.19	0.42
10:W:50:LEU:HD22	10:W:50:LEU:C	2.40	0.42
24:B:303:PSC:H242	24:B:303:PSC:H202	2.02	0.42
4:D:52:SER:OG	4:D:55:GLU:HG3	2.20	0.42
27:C:306:PEK:O14	7:G:17:ARG:NH2	2.52	0.42
2:O:68:LEU:HB3	2:O:69:PRO:HD3	2.01	0.42
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.01	0.41
12:L:13:PHE:HA	19:L:101:TGL:HC21	2.01	0.41
4:Q:129:ALA:HB3	4:Q:134:PHE:CB	2.50	0.41
5:R:80:GLU:CD	5:R:80:GLU:N	2.73	0.41
2:B:215:PRO:O	2:B:216:LEU:C	2.57	0.41
6:F:30:PRO:O	6:F:96:LEU:HD23	2.20	0.41
30:A:825:HOH:O	19:L:101:TGL:H101	2.19	0.41
2:O:23:PHE:O	2:O:26:HIS:HB3	2.20	0.41
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.20	0.41
5:R:78:HIS:HB2	5:R:81:ILE:HD12	2.01	0.41
7:G:69:PHE:HD2	7:G:70:PHE:CE1	2.37	0.41
1:N:280:ILE:HG12	1:N:312:ILE:CD1	2.48	0.41
3:P:116:TRP:CE3	3:P:118:PRO:HD3	2.55	0.41
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.20	0.41
27:T:101:PEK:H241	27:T:101:PEK:H271	1.83	0.41
3:C:177:GLN:HA	30:C:402:HOH:O	2.21	0.41
8:H:54:GLU:CD	8:H:57:ARG:HH21	2.24	0.41
7:T:53:LEU:HA	7:T:53:LEU:HD23	1.83	0.41
1:A:404:THR:OG1	1:A:480:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:59:GLN:C	2.58	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.65	0.41
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.56	0.41
4:Q:98:TRP:HE1	29:Z:101:DMU:H29	1.86	0.41
26:T:103:CDL:H111	26:T:103:CDL:H372	2.03	0.41
8:U:60:TYR:C	8:U:60:TYR:CD1	2.94	0.41
1:A:261:TYR:OH	21:A:610:EDO:H12	2.19	0.41
6:F:49:VAL:HA	6:F:50:PRO:HD2	1.87	0.41
2:B:100:MET:CE	2:B:157:GLU:HG3	2.50	0.41
1:N:68:PHE:C	1:N:72:PRO:HG2	2.41	0.41
3:P:51:MET:HG2	26:P:304:CDL:H602	2.02	0.41
7:T:44:ARG:HD3	7:T:74:ARG:O	2.19	0.41
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.55	0.41
4:D:29:HIS:CE1	4:D:65:LYS:HG3	2.56	0.41
1:N:119:GLU:HB2	1:N:120:ALA:H	1.71	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.55	0.41
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.56	0.41
9:V:31:PHE:CE1	9:V:32:ALA:O	2.74	0.41
24:B:303:PSC:H272	24:B:303:PSC:H242	1.82	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
1:N:3:ILE:N	1:N:3:ILE:HD12	2.35	0.41
1:N:390:MET:CE	1:N:413:HIS:HE1	2.34	0.41
1:N:65:MET:HG3	14:N:601:HEA:C2C	2.51	0.41
1:A:481:GLU:OE1	13:M:7:LYS:NZ	2.49	0.41
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.84	0.41
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
8:H:18:SER:HB2	30:H:115:HOH:O	2.21	0.41
1:N:212:ASP:HA	1:N:217:THR:OG1	2.21	0.41
1:N:406:ASN:HD21	20:N:607:PGV:H032	1.82	0.41
2:O:99:THR:HB	2:O:108:TYR:CE1	2.56	0.41
3:P:151:LEU:HD21	3:P:232:HIS:CG	2.56	0.41
5:R:31:LYS:HD2	5:R:31:LYS:HA	1.96	0.41
7:T:25:LEU:N	7:T:26:PRO:CD	2.83	0.41
3:P:210:ILE:HG23	20:P:303:PGV:H91	2.03	0.41
5:E:66:ARG:O	5:E:70:VAL:HG12	2.21	0.40
13:M:11:SER:HB2	13:M:12:PRO:HD2	2.01	0.40
13:M:36:HIS:O	13:M:37:LEU:C	2.60	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.21	0.40
2:O:149:THR:HG22	30:O:448:HOH:O	2.21	0.40
3:P:109:THR:HB	3:P:110:PRO:CD	2.52	0.40
3:P:37:PHE:O	3:P:38:ASN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:103:CDL:H161	26:T:103:CDL:H402	2.03	0.40
1:A:266:GLU:HB2	1:A:267:PRO:HD2	2.02	0.40
24:B:303:PSC:C24	24:B:303:PSC:H202	2.52	0.40
19:D:201:TGL:HG31	19:D:201:TGL:HC21	1.92	0.40
1:N:403:TYR:HA	1:N:480:ARG:O	2.21	0.40
3:P:109:THR:HB	3:P:110:PRO:HD2	2.02	0.40
3:P:121:ILE:HG13	30:P:403:HOH:O	2.20	0.40
5:R:19:PHE:HB2	30:R:303:HOH:O	2.21	0.40
6:S:64:GLU:O	6:S:65:ASP:HB2	2.22	0.40
1:N:377:PHE:CE1	1:N:378:HIS:CE1	3.09	0.40
11:X:28:VAL:O	11:X:31:TYR:HB3	2.22	0.40
20:A:609:PGV:H12	20:A:609:PGV:H271	2.03	0.40
24:B:303:PSC:H221	24:B:303:PSC:H251	1.88	0.40
3:C:40:MET:O	3:C:44:MET:HG2	2.22	0.40
10:J:26:ALA:N	30:J:201:HOH:O	2.54	0.40
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.94	0.40
1:N:71:MET:N	1:N:72:PRO:CD	2.85	0.40
1:A:240:HIS:HE2	1:A:244:TYR:HH	1.68	0.40
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.87	0.40
1:A:65:MET:HB3	14:A:601:HEA:CBC	2.52	0.40
3:C:187:THR:OG1	30:C:401:HOH:O	2.22	0.40
4:D:33:LEU:HA	4:D:37:GLN:NE2	2.37	0.40
5:E:44:GLU:HB3	30:E:202:HOH:O	2.22	0.40
30:B:404:HOH:O	9:I:20:HIS:HA	2.21	0.40
9:I:43:ARG:HH11	9:I:43:ARG:HD3	1.74	0.40
10:J:44:LEU:HA	10:J:44:LEU:HD23	1.85	0.40
26:T:103:CDL:H312	30:T:205:HOH:O	2.21	0.40
7:T:38:HIS:CE1	26:T:103:CDL:H142	2.56	0.40
7:T:79:PRO:CD	30:T:201:HOH:O	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	51	67
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	38	54
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	20	29
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	15	21
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	8	9
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	18	26
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	18	26
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	8	9
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	18	26
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	2	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	1	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	14	19
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	13	18
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	10	12
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	8	9
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	7	7
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	7	7
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	17	23

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	97	ALA
7	G	3	ALA
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	8	HIS
8	H	8	ILE
2	O	59	GLN
7	T	4	ALA
7	T	8	HIS
9	V	32	ALA
7	G	43	GLU
2	O	60	GLU
3	P	37	PHE
3	P	38	ASN
4	Q	5	VAL
4	Q	65	LYS
6	S	94	HIS
7	T	2	SER
7	T	37	LEU
13	Z	41	LYS
13	M	42	LYS
1	N	119	GLU
7	T	6	GLY
7	T	7	ASP
8	U	8	ILE
8	U	51	SER
2	B	59	GLN
5	E	8	ASP
6	F	94	HIS
3	P	232	HIS
4	Q	47	SER
5	R	101	PRO
8	U	48	GLY
10	W	57	HIS
11	X	7	PRO
7	T	3	ALA
7	T	5	LYS
8	U	9	LYS

### 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	427/426 (100%)	411 (96%)	16 (4%)	39	59
1	N	426/426 (100%)	408 (96%)	18 (4%)	34	53
2	B	210/210 (100%)	198 (94%)	12 (6%)	24	38
2	O	210/210 (100%)	198 (94%)	12 (6%)	24	38
3	C	224/226 (99%)	220 (98%)	4 (2%)	64	81
3	P	224/226 (99%)	216 (96%)	8 (4%)	40	60
4	D	128/129 (99%)	125 (98%)	3 (2%)	56	75
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	40
5	E	92/95 (97%)	86 (94%)	6 (6%)	20	31
5	R	92/95 (97%)	87 (95%)	5 (5%)	26	41
6	F	81/81 (100%)	77 (95%)	4 (5%)	29	46
6	S	81/81 (100%)	74 (91%)	7 (9%)	12	18
7	G	67/68 (98%)	61 (91%)	6 (9%)	11	16
7	T	67/68 (98%)	63 (94%)	4 (6%)	22	35
8	H	71/75 (95%)	63 (89%)	8 (11%)	7	9
8	U	71/75 (95%)	65 (92%)	6 (8%)	12	19
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	17
9	V	57/57 (100%)	51 (90%)	6 (10%)	8	11
10	J	49/50 (98%)	46 (94%)	3 (6%)	22	34
10	W	49/50 (98%)	43 (88%)	6 (12%)	6	7
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	44
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	44
12	L	39/40 (98%)	37 (95%)	2 (5%)	28	44
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	44
13	M	37/38 (97%)	35 (95%)	2 (5%)	26	41
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	5
All	All	3041/3082 (99%)	2880 (95%)	161 (5%)	26	42

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	A	136	LEU
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	177	SER
1	A	178	GLN
1	A	180	GLN
1	A	189	MET
1	A	238	PHE
1	A	264	LYS
1	A	338	MET
1	A	361	SER
1	A	366	VAL
1	A	369	ASP
1	A	382	SER
1	A	394	VAL
1	A	513	LEU
2	B	55	THR
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	88	ASP
2	B	91	ASN
2	B	92	ASN
2	B	94	SER
2	B	217	LYS
2	B	223	SER
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
4	D	121	LYS
4	D	143	ASN
5	E	6	GLU
5	E	9	GLU
5	E	46	LYS
5	E	70	VAL
5	E	79	LYS
5	E	108	LYS
6	F	10	GLU
6	F	53	THR
6	F	90	LYS
6	F	95	GLN

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Mol	Chain	Res	Type
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	44	ARG
7	G	54	ARG
7	G	74	ARG
8	H	8	ILE
8	H	9	LYS
8	H	23	GLN
8	H	27	ARG
8	H	46	LYS
8	H	49	ASP
8	H	52	VAL
8	H	60	TYR
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
9	I	31	PHE
9	I	37	PHE
10	J	14	GLU
10	J	50	LEU
10	J	58	LYS
11	K	20	SER
11	K	54	ARG
12	L	5	GLU
12	L	26	THR
13	M	34	LEU
13	M	38	ASP
1	N	38	ARG
1	N	91	ASP
1	N	109	PHE
1	N	138	HIS
1	N	152	LEU
1	N	180	GLN
1	N	189	MET
1	N	238	PHE
1	N	273	MET
1	N	298	ASP
1	N	312	ILE
1	N	333	LYS
1	N	338	MET
1	N	361	SER

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Mol	Chain	Res	Type
1	N	366	VAL
1	N	369	ASP
1	N	394	VAL
1	N	486	ASP
2	O	33	LEU
2	O	48	THR
2	O	60	GLU
2	O	65	TRP
2	O	75	LEU
2	O	88	ASP
2	O	91	ASN
2	O	183	THR
2	O	185	MET
2	O	217	LYS
2	O	226	MET
2	O	227	LEU
3	P	44	MET
3	P	77	LYS
3	P	80	ARG
3	P	105	SER
3	P	127	LEU
3	P	159	MET
3	P	179	SER
3	P	214	PHE
4	Q	6	VAL
4	Q	15	SER
4	Q	19	ARG
4	Q	26	ASP
4	Q	31	LYS
4	Q	33	LEU
4	Q	126	MET
5	R	21	LYS
5	R	36	LEU
5	R	70	VAL
5	R	79	LYS
5	R	92	THR
6	S	14	THR
6	S	25	ARG
6	S	37	LYS
6	S	53	THR
6	S	54	ASN
6	S	87	THR

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Mol	Chain	Res	Type
6	S	96	LEU
7	T	17	ARG
7	T	33	LEU
7	T	35	SER
7	T	84	LYS
8	U	8	ILE
8	U	27	ARG
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	2	THR
9	V	4	LEU
9	V	19	PHE
9	V	31	PHE
9	V	62	GLU
9	V	68	ILE
10	W	1	PHE
10	W	10	LYS
10	W	14	GLU
10	W	27	THR
10	W	29	ASN
10	W	50	LEU
11	X	52	GLU
11	X	54	ARG
12	Y	27	LEU
12	Y	47	LYS
13	Z	1	ILE
13	Z	19	LEU
13	Z	20	SER
13	Z	34	LEU
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	413	HIS
2	B	10	GLN
2	B	52	HIS

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Mol	Chain	Res	Type
2	B	181	GLN
3	C	68	GLN
3	C	149	HIS
4	D	29	HIS
4	D	37	GLN
5	E	78	HIS
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
8	H	12	GLN
8	H	23	GLN
8	H	37	HIS
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	291	HIS
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
3	P	68	GLN
3	P	70	HIS
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
7	T	8	HIS
7	T	34	ASN
7	T	76	ASN
8	U	23	GLN
8	U	37	HIS
10	W	29	ASN
13	Z	15	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	0.41	0	7,9,11	1.72	3 (42%)
2	FME	B	1	2	9,9,10	0.92	0	7,9,11	2.07	4 (57%)
7	TPO	G	11	7	9,10,11	1.48	2 (22%)	10,14,16	2.32	2 (20%)
9	SAC	I	1	9	8,8,9	1.23	1 (12%)	6,9,11	0.96	1 (16%)
1	FME	N	1	1	9,9,10	0.79	1 (11%)	7,9,11	1.44	1 (14%)
2	FME	O	1	2	9,9,10	0.95	0	7,9,11	1.65	1 (14%)
7	TPO	T	11	7	9,10,11	2.05	4 (44%)	10,14,16	1.86	2 (20%)
9	SAC	V	1	9	8,8,9	1.75	2 (25%)	6,9,11	1.23	1 (16%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	FME	CA-C	2.02	1.52	1.50
7	G	11	TPO	CA-C	2.08	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.10	1.57	1.53
7	T	11	TPO	P-OG1	2.37	1.63	1.59
9	V	1	SAC	CA-C	2.38	1.53	1.50
7	G	11	TPO	P-O1P	2.62	1.59	1.50
7	T	11	TPO	P-O1P	2.64	1.59	1.50
9	I	1	SAC	CA-N	3.10	1.50	1.46
7	T	11	TPO	CA-C	3.71	1.55	1.50
9	V	1	SAC	CA-N	4.12	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CB-CA-C	-3.75	105.48	111.65
1	N	1	FME	O-C-CA	-2.83	118.55	125.15
1	A	1	FME	O-C-CA	-2.56	119.19	125.15
2	B	1	FME	O-C-CA	-2.42	119.50	125.15
1	A	1	FME	CG-CB-CA	-2.39	106.06	112.97
9	V	1	SAC	O-C-CA	-2.29	119.81	125.15
7	G	11	TPO	CB-CA-N	-2.26	99.43	114.78
7	T	11	TPO	CB-CA-N	-2.21	99.75	114.78
9	I	1	SAC	O-C-CA	-2.21	120.00	125.15
2	B	1	FME	CG-CB-CA	-2.14	106.77	112.97
2	B	1	FME	CA-N-CN	2.01	125.92	122.82
1	A	1	FME	CE-SD-CG	2.50	109.33	100.35
2	O	1	FME	CA-N-CN	3.70	128.51	122.82
7	T	11	TPO	C-CA-N	4.92	119.78	109.86
7	G	11	TPO	C-CA-N	6.76	123.50	109.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
7	G	11	TPO	OG1-CB-CA-N
7	T	11	TPO	OG1-CB-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 62 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	$\# Z  > 2$
14	HEA	A	601	1	44,67,67	1.10	3 (6%)	37,103,103	1.81	8 (21%)
14	HEA	A	602	1	44,67,67	1.03	3 (6%)	37,103,103	1.70	7 (18%)
18	CMO	A	606	15	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	607	-	62,62,62	1.21	4 (6%)	65,65,65	1.45	11 (16%)
20	PGV	A	608	-	50,50,50	0.78	2 (4%)	51,56,56	1.51	5 (9%)
20	PGV	A	609	-	50,50,50	1.09	2 (4%)	51,56,56	1.14	5 (9%)
21	EDO	A	610	-	3,3,3	0.51	0	2,2,2	0.59	0
21	EDO	A	611	-	3,3,3	0.36	0	2,2,2	0.64	0
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	0.11	0
21	EDO	A	613	-	3,3,3	0.53	0	2,2,2	0.27	0
21	EDO	A	614	-	3,3,3	0.58	0	2,2,2	0.09	0
22	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	B	302	-	29,32,32	0.77	0	47,51,51	1.25	4 (8%)
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	56,59,59	1.15	4 (7%)
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.63	0
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.51	0
20	PGV	C	302	-	50,50,50	0.90	2 (4%)	51,56,56	0.97	4 (7%)
26	CDL	C	303	-	99,99,99	1.37	12 (12%)	101,111,111	1.26	8 (7%)
23	CHD	C	304	-	29,32,32	0.57	0	47,51,51	2.02	13 (27%)
23	CHD	C	305	-	29,32,32	0.92	1 (3%)	47,51,51	1.18	6 (12%)
27	PEK	C	306	-	52,52,52	1.02	2 (3%)	54,57,57	0.97	3 (5%)
26	CDL	C	307	-	99,99,99	1.41	13 (13%)	101,111,111	1.28	8 (7%)
20	PGV	C	308	-	50,50,50	1.19	2 (4%)	51,56,56	1.09	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	EDO	C	309	-	3,3,3	0.37	0	2,2,2	0.70	0
21	EDO	C	310	-	3,3,3	0.52	0	2,2,2	0.35	0
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.32	0
19	TGL	D	201	-	62,62,62	1.12	3 (4%)	65,65,65	1.05	7 (10%)
21	EDO	F	102	-	3,3,3	0.56	0	2,2,2	0.05	0
27	PEK	G	101	-	52,52,52	0.93	2 (3%)	54,57,57	1.30	5 (9%)
27	PEK	G	102	-	52,52,52	1.20	3 (5%)	54,57,57	1.16	5 (9%)
20	PGV	G	103	-	50,50,50	1.05	2 (4%)	51,56,56	1.01	2 (3%)
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.59	0
23	CHD	J	101	-	29,32,32	0.60	0	47,51,51	1.54	9 (19%)
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.36	0
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.29	0
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
19	TGL	L	101	-	62,62,62	1.18	3 (4%)	65,65,65	1.30	6 (9%)
21	EDO	L	102	-	3,3,3	0.45	0	2,2,2	0.42	0
29	DMU	M	101	-	34,34,34	0.54	0	45,45,45	1.19	5 (11%)
14	HEA	N	601	1	44,67,67	1.05	4 (9%)	37,103,103	1.72	8 (21%)
14	HEA	N	602	1	44,67,67	1.12	2 (4%)	37,103,103	1.92	11 (29%)
18	CMO	N	606	-	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	N	607	-	50,50,50	1.08	2 (4%)	51,56,56	1.14	5 (9%)
20	PGV	N	608	-	50,50,50	0.89	3 (6%)	51,56,56	1.22	5 (9%)
19	TGL	N	609	-	62,62,62	1.11	3 (4%)	65,65,65	1.34	8 (12%)
19	TGL	N	610	-	62,62,62	1.12	3 (4%)	65,65,65	1.18	7 (10%)
19	TGL	N	611	-	62,62,62	1.17	3 (4%)	65,65,65	1.29	8 (12%)
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.14	0
22	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	302	-	29,32,32	0.97	1 (3%)	47,51,51	1.46	6 (12%)
27	PEK	P	302	-	52,52,52	0.86	2 (3%)	54,57,57	1.42	5 (9%)
20	PGV	P	303	-	50,50,50	0.92	2 (4%)	51,56,56	1.13	5 (9%)
26	CDL	P	304	-	99,99,99	1.37	12 (12%)	101,111,111	1.20	7 (6%)
23	CHD	P	305	-	29,32,32	0.49	0	47,51,51	1.84	13 (27%)
23	CHD	P	306	-	29,32,32	0.71	1 (3%)	47,51,51	1.52	11 (23%)
24	PSC	R	201	-	51,51,51	1.21	3 (5%)	56,59,59	1.06	5 (8%)
27	PEK	T	101	-	52,52,52	1.16	3 (5%)	54,57,57	1.14	5 (9%)
27	PEK	T	102	-	52,52,52	1.18	2 (3%)	54,57,57	1.19	4 (7%)
26	CDL	T	103	-	99,99,99	1.35	12 (12%)	101,111,111	1.36	12 (11%)
21	EDO	T	104	-	3,3,3	0.44	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CHD	W	101	-	29,32,32	0.81	1 (3%)	47,51,51	2.09	15 (31%)
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.18	5 (11%)

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
14	HEA	A	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1	1/1/7/16	0/24/76/76	0/0/8/8
18	CMO	A	606	15	-	0/0/0/0	0/0/0/0
19	TGL	A	607	-	-	0/65/65/65	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	PGV	A	609	-	-	0/55/55/55	0/0/0/0
21	EDO	A	610	-	-	0/1/1/1	0/0/0/0
21	EDO	A	611	-	-	0/1/1/1	0/0/0/0
21	EDO	A	612	-	-	0/1/1/1	0/0/0/0
21	EDO	A	613	-	-	0/1/1/1	0/0/0/0
21	EDO	A	614	-	-	0/1/1/1	0/0/0/0
22	CUA	B	301	2	-	0/0/0/0	0/0/0/0
23	CHD	B	302	-	-	0/7/74/74	0/4/4/4
24	PSC	B	303	-	-	0/55/55/55	0/0/0/0
21	EDO	B	304	-	-	0/1/1/1	0/0/0/0
21	EDO	B	305	-	-	0/1/1/1	0/0/0/0
20	PGV	C	302	-	-	0/55/55/55	0/0/0/0
26	CDL	C	303	-	-	2/110/110/110	0/0/0/0
23	CHD	C	304	-	-	0/7/74/74	0/4/4/4
23	CHD	C	305	-	-	0/7/74/74	0/4/4/4
27	PEK	C	306	-	-	0/56/56/56	0/0/0/0
26	CDL	C	307	-	-	0/110/110/110	0/0/0/0
20	PGV	C	308	-	-	0/55/55/55	0/0/0/0
21	EDO	C	309	-	-	0/1/1/1	0/0/0/0
21	EDO	C	310	-	-	0/1/1/1	0/0/0/0
21	EDO	C	311	-	-	0/1/1/1	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
21	EDO	F	102	-	-	0/1/1/1	0/0/0/0
27	PEK	G	101	-	-	0/56/56/56	0/0/0/0
27	PEK	G	102	-	-	0/56/56/56	0/0/0/0
20	PGV	G	103	-	-	0/55/55/55	0/0/0/0
21	EDO	G	104	-	-	0/1/1/1	0/0/0/0
23	CHD	J	101	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	K	101	-	-	0/1/1/1	0/0/0/0
21	EDO	K	102	-	-	0/1/1/1	0/0/0/0
21	EDO	K	103	-	-	0/1/1/1	0/0/0/0
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
21	EDO	L	102	-	-	0/1/1/1	0/0/0/0
29	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1	-	0/24/76/76	0/0/8/8
18	CMO	N	606	-	-	0/0/0/0	0/0/0/0
20	PGV	N	607	-	-	0/55/55/55	0/0/0/0
20	PGV	N	608	-	-	0/55/55/55	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
19	TGL	N	610	-	-	1/65/65/65	0/0/0/0
19	TGL	N	611	-	-	2/65/65/65	0/0/0/0
21	EDO	N	612	-	-	0/1/1/1	0/0/0/0
22	CUA	O	301	2	-	0/0/0/0	0/0/0/0
23	CHD	O	302	-	-	0/7/74/74	0/4/4/4
27	PEK	P	302	-	-	0/56/56/56	0/0/0/0
20	PGV	P	303	-	-	0/55/55/55	0/0/0/0
26	CDL	P	304	-	-	1/110/110/110	0/0/0/0
23	CHD	P	305	-	-	0/7/74/74	0/4/4/4
23	CHD	P	306	-	-	0/7/74/74	0/4/4/4
24	PSC	R	201	-	-	0/55/55/55	0/0/0/0
27	PEK	T	101	-	-	0/56/56/56	0/0/0/0
27	PEK	T	102	-	-	0/56/56/56	0/0/0/0
26	CDL	T	103	-	-	0/110/110/110	0/0/0/0
21	EDO	T	104	-	-	0/1/1/1	0/0/0/0
23	CHD	W	101	-	-	0/7/74/74	0/4/4/4
29	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C4B-NB	-4.01	1.32	1.36
14	A	601	HEA	C1D-ND	-3.78	1.32	1.36
14	A	602	HEA	C4B-NB	-3.60	1.32	1.36
26	C	307	CDL	C19-C18	-3.12	1.33	1.51
26	T	103	CDL	C19-C18	-3.07	1.34	1.51
26	C	303	CDL	C59-C58	-3.07	1.34	1.51
26	C	307	CDL	C59-C58	-3.06	1.34	1.51
26	P	304	CDL	C22-C21	-3.04	1.34	1.51
26	T	103	CDL	C62-C61	-3.03	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	303	CDL	C79-C78	-3.02	1.34	1.51
26	C	303	CDL	C22-C21	-3.02	1.34	1.51
26	T	103	CDL	C42-C41	-3.01	1.34	1.51
26	C	303	CDL	C19-C18	-3.00	1.34	1.51
26	P	304	CDL	C79-C78	-3.00	1.34	1.51
26	P	304	CDL	C82-C81	-2.99	1.34	1.51
26	P	304	CDL	C39-C38	-2.99	1.34	1.51
26	T	103	CDL	C79-C78	-2.98	1.34	1.51
26	C	307	CDL	C39-C38	-2.97	1.34	1.51
26	T	103	CDL	C39-C38	-2.96	1.34	1.51
26	P	304	CDL	C59-C58	-2.96	1.34	1.51
26	P	304	CDL	C19-C18	-2.95	1.34	1.51
26	C	307	CDL	C79-C78	-2.95	1.34	1.51
26	T	103	CDL	C59-C58	-2.94	1.34	1.51
26	P	304	CDL	C42-C41	-2.94	1.34	1.51
26	C	303	CDL	C39-C38	-2.94	1.34	1.51
26	C	307	CDL	C42-C41	-2.91	1.35	1.51
26	C	303	CDL	C42-C41	-2.90	1.35	1.51
26	C	307	CDL	C62-C61	-2.88	1.35	1.51
26	C	303	CDL	C62-C61	-2.88	1.35	1.51
26	T	103	CDL	C22-C21	-2.87	1.35	1.51
26	P	304	CDL	C62-C61	-2.86	1.35	1.51
26	C	303	CDL	C82-C81	-2.85	1.35	1.51
26	T	103	CDL	C82-C81	-2.79	1.35	1.51
26	C	307	CDL	C22-C21	-2.79	1.35	1.51
26	C	307	CDL	C82-C81	-2.75	1.35	1.51
14	N	602	HEA	C1D-ND	-2.58	1.33	1.36
14	N	601	HEA	C1D-ND	-2.36	1.34	1.36
14	N	601	HEA	C4A-NA	-2.31	1.34	1.36
14	N	601	HEA	C1B-NB	-2.30	1.31	1.36
14	A	601	HEA	C4B-NB	-2.23	1.34	1.36
23	C	305	CHD	C19-C10	-2.12	1.50	1.54
20	N	608	PGV	O01-C02	-2.11	1.41	1.46
19	A	607	TGL	OC1-CC1	-2.08	1.16	1.22
23	P	306	CHD	C13-C14	-2.06	1.51	1.55
23	O	302	CHD	C13-C17	-2.02	1.52	1.55
14	A	602	HEA	C3A-CMA	2.01	1.51	1.46
27	T	101	PEK	C01-C02	2.04	1.56	1.50
23	W	101	CHD	C20-C17	2.05	1.58	1.54
27	G	102	PEK	C01-C02	2.12	1.56	1.50
14	N	601	HEA	C3A-CMA	2.26	1.51	1.46
26	C	307	CDL	CB3-CB4	2.39	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4C-CHD	2.39	1.46	1.40
14	A	601	HEA	O11-C11	2.48	1.48	1.42
20	A	608	PGV	O01-C1	2.83	1.42	1.34
19	A	607	TGL	OG3-CC1	3.15	1.42	1.33
20	C	302	PGV	O01-C1	3.26	1.43	1.34
20	N	608	PGV	O01-C1	3.31	1.43	1.34
20	P	303	PGV	O01-C1	3.51	1.44	1.34
27	P	302	PEK	O03-C21	3.66	1.44	1.33
27	P	302	PEK	O01-C1	3.79	1.45	1.34
24	R	201	PSC	C13-C12	3.85	1.53	1.31
20	A	608	PGV	O03-C19	3.87	1.44	1.33
27	G	101	PEK	O01-C1	3.88	1.45	1.34
19	N	609	TGL	OG3-CC1	3.92	1.44	1.33
24	B	303	PSC	C13-C12	3.97	1.54	1.31
20	N	608	PGV	O03-C19	4.00	1.45	1.33
27	G	101	PEK	O03-C21	4.07	1.45	1.33
26	T	103	CDL	OA8-CA7	4.11	1.45	1.33
20	C	302	PGV	O03-C19	4.15	1.45	1.33
19	D	201	TGL	OG2-CB1	4.25	1.46	1.34
19	L	101	TGL	OG1-CA1	4.31	1.46	1.33
19	N	611	TGL	OG1-CA1	4.37	1.46	1.33
19	N	610	TGL	OG1-CA1	4.41	1.46	1.33
26	P	304	CDL	OB6-CB5	4.44	1.47	1.34
20	P	303	PGV	O03-C19	4.49	1.46	1.33
27	C	306	PEK	O01-C1	4.50	1.47	1.34
27	C	306	PEK	O03-C21	4.51	1.46	1.33
19	D	201	TGL	OG3-CC1	4.52	1.46	1.33
26	T	103	CDL	OB6-CB5	4.52	1.47	1.34
24	R	201	PSC	O03-C19	4.52	1.46	1.33
26	C	307	CDL	OA6-CA5	4.53	1.47	1.34
20	A	609	PGV	O03-C19	4.53	1.46	1.33
26	T	103	CDL	OA6-CA5	4.55	1.47	1.34
19	N	610	TGL	OG3-CC1	4.60	1.46	1.33
19	N	609	TGL	OG1-CA1	4.60	1.46	1.33
26	C	303	CDL	OA8-CA7	4.63	1.47	1.33
26	C	307	CDL	OA8-CA7	4.70	1.47	1.33
20	G	103	PGV	O01-C1	4.70	1.47	1.34
20	G	103	PGV	O03-C19	4.70	1.47	1.33
26	C	303	CDL	OA6-CA5	4.72	1.48	1.34
24	R	201	PSC	O01-C1	4.73	1.48	1.34
20	N	607	PGV	O03-C19	4.74	1.47	1.33
26	C	307	CDL	OB6-CB5	4.77	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	304	CDL	OA6-CA5	4.79	1.48	1.34
24	B	303	PSC	O01-C1	4.82	1.48	1.34
19	N	610	TGL	OG2-CB1	4.84	1.48	1.34
20	N	607	PGV	O01-C1	4.84	1.48	1.34
19	D	201	TGL	OG1-CA1	4.86	1.47	1.33
27	T	102	PEK	O03-C21	4.87	1.47	1.33
27	T	101	PEK	O01-C1	4.87	1.48	1.34
26	P	304	CDL	OA8-CA7	4.89	1.47	1.33
26	C	303	CDL	OB6-CB5	4.95	1.48	1.34
27	T	101	PEK	O03-C21	4.96	1.47	1.33
20	A	609	PGV	O01-C1	4.96	1.48	1.34
20	C	308	PGV	O03-C19	5.02	1.48	1.33
26	P	304	CDL	OB8-CB7	5.02	1.48	1.33
19	L	101	TGL	OG3-CC1	5.06	1.48	1.33
26	C	303	CDL	OB8-CB7	5.08	1.48	1.33
26	T	103	CDL	OB8-CB7	5.09	1.48	1.33
24	B	303	PSC	O03-C19	5.10	1.48	1.33
19	N	611	TGL	OG2-CB1	5.14	1.49	1.34
19	N	611	TGL	OG3-CC1	5.15	1.48	1.33
27	G	102	PEK	O01-C1	5.17	1.49	1.34
19	N	609	TGL	OG2-CB1	5.20	1.49	1.34
26	C	307	CDL	OB8-CB7	5.21	1.48	1.33
27	G	102	PEK	O03-C21	5.23	1.48	1.33
20	C	308	PGV	O01-C1	5.28	1.49	1.34
19	A	607	TGL	OG2-CB1	5.29	1.49	1.34
27	T	102	PEK	O01-C1	5.34	1.49	1.34
19	L	101	TGL	OG2-CB1	5.43	1.50	1.34
19	A	607	TGL	OG1-CA1	5.53	1.49	1.33

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	TGL	CG3-CG2-CG1	-5.40	99.69	111.86
14	A	602	HEA	CAD-CBD-CGD	-4.96	104.18	112.66
23	P	305	CHD	C6-C5-C4	-4.87	105.60	111.13
23	C	304	CHD	C23-C22-C20	-4.50	108.66	114.72
20	A	608	PGV	O03-C19-O04	-4.30	112.86	123.55
14	N	602	HEA	CAD-CBD-CGD	-4.13	105.61	112.66
23	C	304	CHD	C6-C5-C4	-3.88	106.72	111.13
27	P	302	PEK	O03-C21-O04	-3.80	114.12	123.55
14	N	601	HEA	C13-C12-C11	-3.72	108.83	114.46
19	A	607	TGL	OG3-CC1-OC1	-3.57	114.69	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	CMB-C2B-C1B	-3.49	123.09	128.46
27	G	101	PEK	O03-C01-C02	-3.49	99.90	108.66
23	J	101	CHD	C21-C20-C22	-3.46	104.90	110.35
19	N	609	TGL	CG3-CG2-CG1	-3.36	104.27	111.86
14	A	602	HEA	C1B-C2B-C3B	-3.34	104.67	107.00
14	A	601	HEA	C13-C12-C11	-3.31	109.44	114.46
23	B	302	CHD	C13-C17-C20	-3.26	115.54	119.49
23	P	306	CHD	C13-C17-C20	-3.19	115.63	119.49
29	M	101	DMU	O2-C8-C7	-3.18	103.43	110.36
20	A	608	PGV	C02-O01-C1	-3.18	110.37	117.88
23	O	302	CHD	C14-C8-C9	-3.15	105.35	109.64
19	N	611	TGL	OG2-CB1-OB1	-3.12	115.89	123.68
27	P	302	PEK	O01-C1-O02	-3.12	115.89	123.68
27	G	101	PEK	O01-C1-O02	-3.06	116.05	123.68
14	N	602	HEA	CMC-C2C-C1C	-3.02	123.82	128.46
20	N	608	PGV	O03-C19-O04	-3.02	116.05	123.55
14	N	601	HEA	C4B-C3B-C2B	-3.02	104.76	106.87
20	A	608	PGV	O01-C1-O02	-3.01	116.16	123.68
23	W	101	CHD	C6-C5-C4	-3.01	107.71	111.13
19	N	610	TGL	OG2-CB1-OB1	-2.98	116.24	123.68
19	D	201	TGL	CG2-OG2-CB1	-2.96	110.87	117.88
23	C	304	CHD	C9-C11-C12	-2.88	110.52	114.32
23	P	306	CHD	O12-C12-C11	-2.88	103.19	109.11
20	P	303	PGV	O01-C1-O02	-2.82	116.65	123.68
14	N	602	HEA	CMB-C2B-C1B	-2.80	124.16	128.46
14	A	601	HEA	C27-C19-C18	-2.80	116.22	123.69
23	P	306	CHD	C16-C15-C14	-2.78	99.56	105.12
20	N	607	PGV	O03-C19-O04	-2.73	116.76	123.55
14	N	602	HEA	C20-C19-C18	-2.69	115.59	121.10
23	P	305	CHD	C19-C10-C1	-2.69	103.82	108.24
23	P	306	CHD	C18-C13-C14	-2.63	107.06	111.23
27	P	302	PEK	C03-C02-C01	-2.62	105.94	111.86
19	N	610	TGL	OG3-CC1-OC1	-2.61	117.07	123.55
23	B	302	CHD	C6-C5-C4	-2.58	108.20	111.13
23	P	306	CHD	C9-C11-C12	-2.54	110.98	114.32
19	N	609	TGL	OG1-CA1-OA1	-2.53	117.26	123.55
26	T	103	CDL	OB6-CB5-OB7	-2.53	117.36	123.68
26	T	103	CDL	CA6-CA4-CA3	-2.52	106.17	111.86
26	C	303	CDL	OA6-CA5-OA7	-2.52	117.39	123.68
19	L	101	TGL	OG3-CC1-OC1	-2.50	117.33	123.55
20	C	302	PGV	C03-C02-C01	-2.50	106.22	111.86
26	P	304	CDL	OB8-CB7-OB9	-2.50	117.35	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	302	CHD	C6-C5-C4	-2.50	108.29	111.13
14	N	602	HEA	C1B-C2B-C3B	-2.49	105.26	107.00
14	N	602	HEA	O11-C11-C3B	-2.48	104.70	111.83
14	A	602	HEA	C20-C19-C18	-2.46	116.06	121.10
14	A	601	HEA	C1B-C2B-C3B	-2.46	105.29	107.00
24	R	201	PSC	O03-C19-O04	-2.44	117.48	123.55
19	N	609	TGL	OG3-CC1-OC1	-2.43	117.52	123.55
19	D	201	TGL	OG3-CC1-OC1	-2.41	117.57	123.55
26	C	307	CDL	OB6-CB5-OB7	-2.40	117.70	123.68
23	C	305	CHD	C19-C10-C1	-2.37	104.35	108.24
23	W	101	CHD	C18-C13-C14	-2.36	107.49	111.23
29	M	101	DMU	C18-O16-C6	-2.35	109.83	113.87
20	A	609	PGV	O03-C19-O04	-2.34	117.75	123.55
23	O	302	CHD	C22-C20-C17	-2.33	105.38	110.26
26	T	103	CDL	OA6-CA5-OA7	-2.29	117.96	123.68
19	N	610	TGL	OG1-CA1-OA1	-2.28	117.89	123.55
23	W	101	CHD	C18-C13-C12	-2.28	106.76	109.08
23	C	305	CHD	C6-C5-C4	-2.28	108.54	111.13
20	P	303	PGV	O03-C19-O04	-2.27	117.92	123.55
24	R	201	PSC	C11-C12-C13	-2.25	111.57	124.90
29	Z	101	DMU	C6-O5-C4	-2.25	109.48	113.72
23	W	101	CHD	C19-C10-C9	-2.23	107.97	111.16
29	Z	101	DMU	C18-O16-C6	-2.23	110.04	113.87
27	T	102	PEK	O03-C21-O04	-2.22	118.03	123.55
20	P	303	PGV	C03-C02-C01	-2.21	106.87	111.86
23	P	305	CHD	C14-C8-C9	-2.21	106.63	109.64
23	C	304	CHD	C11-C9-C10	-2.21	111.41	113.74
23	C	304	CHD	C19-C10-C1	-2.20	104.62	108.24
26	C	303	CDL	CA6-CA4-CA3	-2.20	106.90	111.86
19	L	101	TGL	CG3-CG2-CG1	-2.18	106.95	111.86
27	G	101	PEK	C02-O01-C1	-2.18	112.74	117.88
19	A	607	TGL	OB1-CB1-CB2	-2.14	115.23	123.68
19	A	607	TGL	OG1-CA1-OA1	-2.12	118.29	123.55
19	N	609	TGL	OB1-CB1-CB2	-2.09	115.42	123.68
19	N	611	TGL	OG3-CC1-OC1	-2.08	118.39	123.55
23	P	305	CHD	C13-C17-C20	-2.08	116.98	119.49
29	M	101	DMU	O1-C10-C5	-2.07	106.30	110.30
26	T	103	CDL	OA8-CA7-OA9	-2.07	118.41	123.55
26	T	103	CDL	OB8-CB7-OB9	-2.06	118.42	123.55
26	C	303	CDL	OA8-CA7-OA9	-2.06	118.43	123.55
20	N	608	PGV	O01-C1-O02	-2.06	118.53	123.68
24	R	201	PSC	C08-N-C06	-2.04	103.81	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	101	CHD	C19-C10-C1	-2.04	104.89	108.24
14	A	601	HEA	C26-C15-C14	-2.02	118.29	123.69
23	P	306	CHD	C21-C20-C17	-2.02	109.79	112.95
20	C	302	PGV	O03-C19-O04	-2.02	118.54	123.55
26	C	307	CDL	OA6-CA5-OA7	-2.01	118.66	123.68
23	C	305	CHD	C18-C13-C14	-2.01	108.06	111.23
23	J	101	CHD	C13-C17-C20	2.03	121.95	119.49
23	C	305	CHD	C4-C3-C2	2.03	113.07	110.55
19	L	101	TGL	OG1-CA1-CA2	2.04	117.84	111.90
19	N	611	TGL	CG3-OG3-CC1	2.05	123.29	117.13
19	A	607	TGL	OG3-CG3-CG2	2.05	113.81	108.66
23	P	306	CHD	C11-C12-C13	2.07	113.37	111.22
23	W	101	CHD	C14-C8-C7	2.10	114.65	111.80
20	N	608	PGV	O03-C01-C02	2.11	113.96	108.66
23	P	305	CHD	C5-C4-C3	2.12	115.98	112.87
27	T	101	PEK	O01-C02-C01	2.12	116.15	108.44
26	T	103	CDL	OB8-CB6-CB4	2.12	113.99	108.66
23	B	302	CHD	C22-C20-C17	2.13	114.74	110.26
14	A	602	HEA	C26-C15-C16	2.13	118.99	115.29
26	T	103	CDL	C83-C82-C81	2.14	125.48	114.45
23	P	306	CHD	C6-C7-C8	2.17	113.81	111.50
19	N	610	TGL	CG1-OG1-CA1	2.18	123.68	117.13
20	C	308	PGV	O03-C01-C02	2.18	114.14	108.66
23	O	302	CHD	C21-C20-C22	2.19	113.81	110.35
19	D	201	TGL	CG1-OG1-CA1	2.20	123.74	117.13
19	D	201	TGL	CG3-OG3-CC1	2.20	123.75	117.13
27	G	101	PEK	C01-O03-C21	2.21	123.77	117.13
23	W	101	CHD	C16-C17-C20	2.21	115.67	112.14
23	C	304	CHD	C1-C2-C3	2.21	113.24	110.42
23	W	101	CHD	C4-C3-C2	2.22	113.30	110.55
23	C	304	CHD	C14-C13-C12	2.22	109.50	107.39
29	Z	101	DMU	O7-C10-O1	2.23	116.10	110.70
20	A	609	PGV	O03-C01-C02	2.23	114.27	108.66
27	C	306	PEK	O03-C21-C22	2.27	118.49	111.90
14	A	601	HEA	CMC-C2C-C3C	2.27	129.11	124.89
19	N	609	TGL	OG3-CG3-CG2	2.29	114.41	108.66
23	W	101	CHD	C4-C5-C10	2.29	115.16	112.66
23	J	101	CHD	C4-C3-C2	2.30	113.40	110.55
23	P	305	CHD	C15-C14-C8	2.34	121.64	118.32
19	A	607	TGL	CG2-OG2-CB1	2.34	123.41	117.88
19	A	607	TGL	OG1-CG1-CG2	2.34	114.55	108.66
26	C	303	CDL	CB6-OB8-CB7	2.34	124.19	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C3A-C4A-NA	2.35	115.38	110.94
23	P	306	CHD	C18-C13-C12	2.35	111.47	109.08
23	P	305	CHD	C1-C10-C5	2.36	111.44	107.79
23	J	101	CHD	C10-C9-C8	2.38	114.43	111.87
23	C	305	CHD	C9-C10-C5	2.41	112.11	108.63
23	P	306	CHD	O12-C12-C13	2.42	115.15	111.12
14	N	602	HEA	CAA-CBA-CGA	2.42	116.80	112.66
29	Z	101	DMU	O1-C9-C11	2.42	112.22	106.41
27	T	101	PEK	C01-O03-C21	2.43	124.44	117.13
26	P	304	CDL	CB6-OB8-CB7	2.44	124.46	117.13
20	C	302	PGV	O01-C1-C2	2.45	116.64	111.55
19	N	611	TGL	CG2-OG2-CB1	2.45	123.67	117.88
20	N	607	PGV	C01-O03-C19	2.45	124.51	117.13
23	J	101	CHD	C5-C4-C3	2.47	116.49	112.87
23	P	306	CHD	C14-C13-C12	2.49	109.75	107.39
26	P	304	CDL	CA6-OA8-CA7	2.53	124.75	117.13
19	A	607	TGL	CG1-OG1-CA1	2.55	124.81	117.13
24	B	303	PSC	O03-C01-C02	2.56	115.09	108.66
26	C	303	CDL	OA8-CA7-C31	2.59	119.43	111.90
23	J	101	CHD	C21-C20-C17	2.60	117.01	112.95
19	N	611	TGL	OG1-CA1-CA2	2.62	119.53	111.90
23	O	302	CHD	C1-C10-C5	2.63	111.87	107.79
24	B	303	PSC	C01-O03-C19	2.64	125.07	117.13
14	N	601	HEA	C3C-C4C-NC	2.65	112.64	109.21
20	N	607	PGV	O03-C01-C02	2.67	115.36	108.66
29	Z	101	DMU	C10-O1-C9	2.67	118.74	113.72
27	T	101	PEK	O03-C21-C22	2.67	119.67	111.90
29	M	101	DMU	O1-C9-C11	2.68	112.83	106.41
26	C	307	CDL	OA8-CA6-CA4	2.68	115.39	108.66
20	C	302	PGV	O03-C19-C20	2.69	119.74	111.90
23	P	305	CHD	C10-C9-C8	2.72	114.80	111.87
20	A	609	PGV	C02-O01-C1	2.73	124.32	117.88
23	C	304	CHD	C1-C10-C5	2.74	112.04	107.79
27	T	102	PEK	O03-C01-C02	2.77	115.62	108.66
27	G	102	PEK	C01-O03-C21	2.81	125.59	117.13
23	P	305	CHD	C11-C12-C13	2.83	114.15	111.22
27	C	306	PEK	C01-O03-C21	2.83	125.64	117.13
23	W	101	CHD	C1-C2-C3	2.86	114.06	110.42
26	T	103	CDL	OA8-CA7-C31	2.87	120.24	111.90
26	P	304	CDL	OA8-CA7-C31	2.87	120.25	111.90
23	P	305	CHD	C16-C17-C13	2.89	106.44	103.57
19	D	201	TGL	OG2-CB1-CB2	2.90	117.57	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	102	PEK	C02-O01-C1	2.91	124.76	117.88
14	N	602	HEA	CMB-C2B-C3B	2.95	130.58	124.92
26	C	307	CDL	OB8-CB7-C71	2.95	120.49	111.90
26	P	304	CDL	OB8-CB7-C71	2.98	120.58	111.90
23	J	101	CHD	C6-C7-C8	3.01	114.70	111.50
26	T	103	CDL	CB6-OB8-CB7	3.05	126.30	117.13
23	C	304	CHD	C15-C14-C13	3.06	106.62	103.57
19	L	101	TGL	OG3-CG3-CG2	3.07	116.38	108.66
19	D	201	TGL	OG1-CA1-CA2	3.09	120.89	111.90
26	C	307	CDL	CB6-OB8-CB7	3.10	126.45	117.13
14	A	602	HEA	C27-C19-C20	3.10	120.67	115.29
14	A	602	HEA	CBD-CAD-C3D	3.13	118.47	112.48
14	N	601	HEA	CMB-C2B-C3B	3.15	130.97	124.92
23	C	305	CHD	C6-C7-C8	3.19	114.89	111.50
19	D	201	TGL	OG3-CC1-CC2	3.20	121.21	111.90
23	C	304	CHD	C4-C5-C10	3.20	116.16	112.66
20	P	303	PGV	O03-C19-C20	3.21	121.24	111.90
19	N	611	TGL	OG3-CG3-CG2	3.24	116.79	108.66
19	N	609	TGL	OG3-CC1-CC2	3.24	121.34	111.90
26	T	103	CDL	OB8-CB7-C71	3.26	121.39	111.90
20	C	308	PGV	O01-C1-C2	3.29	118.39	111.55
19	N	610	TGL	OG1-CA1-CA2	3.31	121.52	111.90
23	W	101	CHD	C17-C13-C12	3.33	120.74	117.67
27	G	102	PEK	O03-C21-C22	3.38	121.75	111.90
19	N	610	TGL	OG3-CC1-CC2	3.40	121.80	111.90
20	A	609	PGV	O03-C19-C20	3.43	121.88	111.90
27	T	102	PEK	O03-C21-C22	3.43	121.89	111.90
19	A	607	TGL	OG1-CA1-CA2	3.47	121.99	111.90
24	R	201	PSC	O01-C1-C2	3.49	118.81	111.55
23	W	101	CHD	C10-C9-C8	3.50	115.64	111.87
14	N	601	HEA	C12-C11-C3B	3.50	121.20	112.65
14	N	602	HEA	C27-C19-C20	3.52	121.39	115.29
27	G	102	PEK	O01-C1-C2	3.53	118.88	111.55
20	C	308	PGV	C01-O03-C19	3.53	127.74	117.13
14	N	601	HEA	CBA-CAA-C2A	3.55	119.23	112.47
23	J	101	CHD	C1-C2-C3	3.55	114.94	110.42
23	P	305	CHD	C15-C14-C13	3.56	107.12	103.57
26	C	303	CDL	OB8-CB7-C71	3.62	122.43	111.90
26	C	307	CDL	OA8-CA7-C31	3.62	122.44	111.90
19	N	611	TGL	OG3-CC1-CC2	3.63	122.45	111.90
29	M	101	DMU	C6-O5-C4	3.64	120.57	113.72
23	P	305	CHD	C9-C10-C5	3.64	113.89	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	607	PGV	O01-C1-C2	3.65	119.14	111.55
20	C	308	PGV	O03-C19-C20	3.66	122.56	111.90
20	N	607	PGV	O03-C19-C20	3.68	122.61	111.90
14	A	602	HEA	CBA-CAA-C2A	3.72	119.56	112.47
14	N	602	HEA	CMC-C2C-C3C	3.73	131.81	124.89
24	R	201	PSC	O03-C19-C20	3.77	122.87	111.90
20	G	103	PGV	O03-C19-C20	3.79	122.92	111.90
27	T	101	PEK	O01-C1-C2	3.79	119.43	111.55
23	B	302	CHD	C1-C2-C3	3.81	115.27	110.42
20	G	103	PGV	O01-C1-C2	3.82	119.49	111.55
23	P	305	CHD	C4-C5-C10	3.83	116.85	112.66
27	G	102	PEK	O03-C01-C02	3.85	118.32	108.66
26	P	304	CDL	OB6-CB5-C51	3.88	119.61	111.55
20	N	608	PGV	O01-C1-C2	3.88	119.61	111.55
24	B	303	PSC	O03-C19-C20	3.92	123.30	111.90
27	T	101	PEK	O03-C01-C02	3.96	118.61	108.66
19	L	101	TGL	OG3-CC1-CC2	3.97	123.46	111.90
23	C	304	CHD	C16-C17-C20	3.99	118.53	112.14
20	A	609	PGV	O01-C1-C2	4.00	119.87	111.55
19	A	607	TGL	OG3-CC1-CC2	4.02	123.59	111.90
20	P	303	PGV	O01-C1-C2	4.07	120.01	111.55
19	N	609	TGL	OG1-CA1-CA2	4.08	123.77	111.90
23	C	304	CHD	C15-C14-C8	4.08	124.10	118.32
20	N	608	PGV	O03-C19-C20	4.10	123.83	111.90
24	B	303	PSC	O01-C1-C2	4.13	120.12	111.55
14	A	601	HEA	C3C-C4C-NC	4.22	114.66	109.21
14	A	601	HEA	C27-C19-C20	4.30	122.75	115.29
27	C	306	PEK	O01-C1-C2	4.31	120.50	111.55
20	A	608	PGV	O01-C1-C2	4.35	120.58	111.55
26	C	307	CDL	OA6-CA5-C11	4.40	120.68	111.55
23	W	101	CHD	C22-C20-C17	4.48	119.66	110.26
23	W	101	CHD	C6-C5-C10	4.48	117.55	112.66
26	C	303	CDL	OB6-CB5-C51	4.51	120.93	111.55
23	W	101	CHD	C9-C10-C5	4.53	115.17	108.63
14	A	601	HEA	C26-C15-C16	4.56	123.20	115.29
19	A	607	TGL	OG2-CB1-CB2	4.80	121.51	111.55
14	N	602	HEA	CBD-CAD-C3D	4.83	121.72	112.48
23	O	302	CHD	C15-C14-C13	4.95	108.50	103.57
27	P	302	PEK	O03-C21-C22	4.99	126.42	111.90
23	C	304	CHD	C10-C9-C8	5.01	117.27	111.87
26	P	304	CDL	OA6-CA5-C11	5.06	122.06	111.55
19	L	101	TGL	OG2-CB1-CB2	5.13	122.20	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	302	PEK	O01-C1-C2	5.14	122.22	111.55
27	T	102	PEK	O01-C1-C2	5.23	122.40	111.55
26	C	307	CDL	OB6-CB5-C51	5.26	122.48	111.55
19	N	610	TGL	OG2-CB1-CB2	5.29	122.54	111.55
26	T	103	CDL	OA6-CA5-C11	5.32	122.60	111.55
20	A	608	PGV	O03-C19-C20	5.37	127.51	111.90
27	G	101	PEK	O01-C1-C2	5.48	122.93	111.55
26	C	303	CDL	OA6-CA5-C11	5.62	123.22	111.55
26	T	103	CDL	OB6-CB5-C51	5.72	123.42	111.55
19	N	609	TGL	OG2-CB1-CB2	5.83	123.66	111.55
23	W	101	CHD	C13-C17-C20	5.88	126.63	119.49
19	N	611	TGL	OG2-CB1-CB2	6.00	124.01	111.55

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	602	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	P	304	CDL	CA4-OA6-CA5-C11
19	N	611	TGL	CG2-OG2-CB1-OB1
19	N	610	TGL	CG2-OG2-CB1-CB2
19	N	611	TGL	CG2-OG2-CB1-CB2
26	C	303	CDL	CA4-OA6-CA5-OA7
26	C	303	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

46 monomers are involved in 154 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	6	0
14	A	602	HEA	6	0
18	A	606	CMO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	607	TGL	3	0
20	A	608	PGV	1	0
20	A	609	PGV	2	0
21	A	610	EDO	1	0
21	A	612	EDO	2	0
21	A	613	EDO	2	0
21	A	614	EDO	4	0
23	B	302	CHD	1	0
24	B	303	PSC	12	0
21	B	305	EDO	1	0
26	C	303	CDL	2	0
23	C	304	CHD	2	0
23	C	305	CHD	1	0
27	C	306	PEK	3	0
26	C	307	CDL	13	0
19	D	201	TGL	1	0
27	G	101	PEK	4	0
27	G	102	PEK	6	0
20	G	103	PGV	2	0
23	J	101	CHD	1	0
19	L	101	TGL	4	0
29	M	101	DMU	1	0
14	N	601	HEA	10	0
14	N	602	HEA	3	0
20	N	607	PGV	6	0
20	N	608	PGV	2	0
19	N	609	TGL	5	0
19	N	610	TGL	2	0
19	N	611	TGL	4	0
21	N	612	EDO	1	0
23	O	302	CHD	1	0
27	P	302	PEK	4	0
20	P	303	PGV	3	0
26	P	304	CDL	7	0
23	P	305	CHD	1	0
23	P	306	CHD	1	0
24	R	201	PSC	6	0
27	T	101	PEK	3	0
27	T	102	PEK	1	0
26	T	103	CDL	13	0
21	T	104	EDO	1	0
23	W	101	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Z	101	DMU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-1.13	0 100 100	41, 53, 66, 101	0
1	N	513/514 (99%)	-1.08	0 100 100	43, 60, 76, 104	0
2	B	226/227 (99%)	-0.98	1 (0%) 92 91	46, 59, 91, 128	0
2	O	226/227 (99%)	-0.81	3 (1%) 77 75	54, 69, 104, 151	0
3	C	259/261 (99%)	-0.90	0 100 100	46, 57, 75, 115	0
3	P	259/261 (99%)	-0.91	0 100 100	46, 62, 81, 121	0
4	D	144/147 (97%)	-0.68	1 (0%) 87 86	52, 66, 89, 117	0
4	Q	144/147 (97%)	-0.22	8 (5%) 25 24	64, 83, 125, 160	0
5	E	105/109 (96%)	-0.86	1 (0%) 82 80	50, 65, 92, 147	0
5	R	105/109 (96%)	-0.76	1 (0%) 82 80	62, 79, 105, 154	0
6	F	98/98 (100%)	-0.35	5 (5%) 29 27	52, 66, 134, 154	0
6	S	98/98 (100%)	-0.20	7 (7%) 17 15	58, 74, 145, 162	0
7	G	83/85 (97%)	-0.27	9 (10%) 6 6	55, 66, 143, 159	0
7	T	83/85 (97%)	-0.20	8 (9%) 9 8	53, 73, 147, 158	0
8	H	79/85 (92%)	-0.48	4 (5%) 29 27	54, 69, 141, 156	0
8	U	79/85 (92%)	-0.30	5 (6%) 21 19	61, 80, 139, 153	0
9	I	72/73 (98%)	-0.55	2 (2%) 53 51	58, 73, 101, 114	0
9	V	72/73 (98%)	-0.30	3 (4%) 37 35	59, 84, 114, 142	0
10	J	58/59 (98%)	-0.52	2 (3%) 46 44	57, 70, 111, 144	0
10	W	58/59 (98%)	-0.27	4 (6%) 18 16	66, 82, 123, 158	0
11	K	49/56 (87%)	-0.34	1 (2%) 65 63	59, 72, 93, 119	0
11	X	49/56 (87%)	-0.11	3 (6%) 22 20	70, 84, 119, 127	0
12	L	46/47 (97%)	-0.77	1 (2%) 62 59	49, 60, 80, 122	0
12	Y	46/47 (97%)	-0.63	0 100 100	60, 75, 102, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.43	2 (4%)	32 30	50, 63, 99, 147	0
13	Z	43/46 (93%)	-0.01	2 (4%)	32 30	70, 79, 121, 164	0
All	All	3550/3614 (98%)	-0.75	73 (2%)	64 61	41, 64, 107, 164	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	10.8
2	O	90	ILE	9.4
6	F	1	ALA	9.2
7	G	40	GLY	6.8
6	S	2	SER	6.3
7	T	40	GLY	6.2
6	S	1	ALA	5.9
6	S	98	HIS	5.9
7	G	10	GLY	5.5
4	Q	8	SER	5.4
4	Q	6	VAL	5.3
4	Q	5	VAL	5.2
4	Q	7	LYS	5.0
4	Q	4	SER	4.9
8	U	8	ILE	4.9
7	T	39	SER	4.8
6	S	96	LEU	4.6
7	G	41	HIS	4.6
8	H	48	GLY	4.5
10	W	58	LYS	4.5
6	F	2	SER	4.4
6	S	97	ALA	4.4
4	Q	147	LYS	4.2
9	V	2	THR	3.9
11	K	6	ALA	3.9
8	U	45	ALA	3.8
8	U	7	LYS	3.8
10	J	58	LYS	3.7
2	O	113	TYR	3.7
7	T	42	ARG	3.7
10	J	1	PHE	3.7
8	H	45	ALA	3.7
6	F	98	HIS	3.6
5	R	5	HIS	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	M	42	LYS	3.5
5	E	5	HIS	3.5
7	G	39	SER	3.4
10	W	1	PHE	3.3
7	G	9	GLY	3.3
9	V	53	ASN	3.2
6	S	95	GLN	3.2
8	U	48	GLY	3.2
7	T	84	LYS	3.1
13	M	43	SER	3.1
7	T	41	HIS	3.0
10	W	57	HIS	3.0
6	F	3	GLY	2.9
9	I	19	PHE	2.9
7	G	5	LYS	2.9
11	X	7	PRO	2.8
8	H	47	GLY	2.7
7	G	84	LYS	2.7
4	Q	35	ALA	2.7
6	S	3	GLY	2.7
13	Z	32	TRP	2.7
11	X	6	ALA	2.5
7	T	36	TRP	2.5
4	Q	101	HIS	2.4
7	T	2	SER	2.4
10	W	55	PHE	2.4
6	F	95	GLN	2.4
8	H	7	LYS	2.4
7	T	10	GLY	2.2
7	G	42	ARG	2.2
9	V	34	PHE	2.2
7	G	3	ALA	2.1
4	D	147	LYS	2.1
11	X	13	TYR	2.1
2	B	90	ILE	2.1
9	I	37	PHE	2.0
12	L	47	LYS	2.0
2	O	227	LEU	2.0
8	U	49	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	FME	N	1	10/11	0.93	0.31	-	80,86,125,151	0
7	TPO	T	11	11/12	0.65	0.30	-	101,147,160,160	0
9	SAC	I	1	9/10	0.72	0.36	-	116,134,157,165	0
1	FME	A	1	10/11	0.94	0.29	-	74,86,128,147	0
2	FME	O	1	10/11	0.99	0.08	-	64,71,76,79	0
7	TPO	G	11	11/12	0.77	0.26	-	102,140,157,157	0
2	FME	B	1	10/11	0.98	0.07	-	58,65,72,72	0
9	SAC	V	1	9/10	0.43	0.50	-	138,151,167,167	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
21	EDO	A	614	4/4	0.85	0.57	20.38	133,137,141,148	0
21	EDO	A	612	4/4	0.75	0.50	18.36	88,115,122,127	0
23	CHD	W	101	29/29	0.69	0.40	11.78	107,145,150,150	0
21	EDO	B	305	4/4	0.94	0.19	8.32	105,110,115,123	0
19	TGL	N	611	63/63	0.73	0.25	6.55	90,126,148,150	0
23	CHD	J	101	29/29	0.81	0.35	6.00	123,142,150,150	0
20	PGV	N	607	51/51	0.63	0.32	6.00	99,137,150,150	0
26	CDL	P	304	100/100	0.71	0.25	5.53	71,140,150,150	0
26	CDL	C	307	100/100	0.70	0.30	4.68	89,138,150,150	0
26	CDL	C	303	100/100	0.82	0.23	4.63	66,123,153,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
21	EDO	A	613	4/4	0.93	0.19	4.63	112,112,121,122	0
21	EDO	T	104	4/4	0.94	0.32	4.27	124,129,131,132	0
19	TGL	L	101	63/63	0.79	0.22	4.21	67,113,143,150	0
26	CDL	T	103	100/100	0.77	0.26	4.20	76,140,150,150	0
21	EDO	G	104	4/4	0.86	0.21	4.17	97,101,102,105	0
27	PEK	T	101	53/53	0.66	0.36	4.09	79,136,150,150	0
27	PEK	T	102	53/53	0.67	0.31	3.79	78,133,150,150	0
17	NA	A	605	1/1	0.99	0.16	3.69	59,59,59,59	0
19	TGL	N	609	63/63	0.85	0.18	3.60	60,120,149,150	0
18	CMO	N	606	2/2	0.99	0.14	3.50	77,77,77,80	0
21	EDO	F	102	4/4	0.87	0.27	3.45	80,88,96,96	0
24	PSC	B	303	52/52	0.53	0.35	3.15	75,147,150,150	0
20	PGV	A	609	51/51	0.65	0.26	3.09	69,115,159,161	0
19	TGL	N	610	63/63	0.64	0.29	2.98	90,134,149,150	0
19	TGL	A	607	63/63	0.84	0.18	2.76	54,97,122,132	0
24	PSC	R	201	52/52	0.67	0.29	2.61	76,137,150,150	0
19	TGL	D	201	63/63	0.75	0.24	2.51	87,126,147,150	0
29	DMU	Z	101	33/33	0.68	0.30	2.45	80,128,149,150	0
27	PEK	G	102	53/53	0.58	0.32	2.06	100,135,150,150	0
20	PGV	N	608	51/51	0.98	0.11	1.54	47,76,117,142	0
20	PGV	C	308	51/51	0.77	0.22	1.53	75,125,150,150	0
23	CHD	C	304	29/29	0.87	0.26	1.33	93,117,125,127	0
20	PGV	G	103	51/51	0.80	0.20	1.23	96,127,150,150	0
27	PEK	C	306	53/53	0.79	0.26	0.94	71,132,149,150	0
27	PEK	P	302	53/53	0.94	0.13	0.79	59,91,150,150	0
20	PGV	A	608	51/51	0.98	0.10	0.78	51,66,79,86	0
29	DMU	M	101	33/33	0.90	0.16	0.70	70,102,129,136	0
17	NA	N	605	1/1	0.98	0.11	0.60	70,70,70,70	0
27	PEK	G	101	53/53	0.94	0.12	0.56	57,72,126,136	0
20	PGV	P	303	51/51	0.98	0.10	0.48	51,72,132,148	0
23	CHD	P	305	29/29	0.91	0.19	0.40	120,135,145,147	0
21	EDO	B	304	4/4	0.98	0.09	0.28	71,75,75,75	0
21	EDO	N	612	4/4	0.95	0.10	0.16	79,80,82,84	0
21	EDO	A	610	4/4	0.97	0.10	-0.04	75,75,78,81	0
23	CHD	B	302	29/29	0.96	0.10	-0.06	48,64,74,77	0
23	CHD	O	302	29/29	0.97	0.09	-0.09	50,57,67,72	0
23	CHD	P	306	29/29	0.98	0.09	-0.10	57,65,72,73	0
14	HEA	N	601	60/60	0.99	0.09	-0.29	47,56,78,84	0
22	CUA	B	301	2/2	0.99	0.07	-0.41	54,54,54,58	0
23	CHD	C	305	29/29	0.96	0.09	-0.50	47,61,71,81	0
28	ZN	S	101	1/1	1.00	0.07	-0.52	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	HEA	N	602	60/60	0.99	0.08	-0.67	47,57,69,75	0
14	HEA	A	601	60/60	0.99	0.07	-0.74	34,46,65,70	0
20	PGV	C	302	51/51	0.98	0.08	-0.78	49,58,90,99	0
16	MG	A	604	1/1	0.99	0.06	-1.00	51,51,51,51	0
16	MG	N	604	1/1	0.98	0.07	-1.21	57,57,57,57	0
14	HEA	A	602	60/60	0.99	0.06	-1.34	45,51,60,62	0
28	ZN	F	101	1/1	1.00	0.04	-1.81	64,64,64,64	0
22	CUA	O	301	2/2	0.99	0.06	-2.07	66,66,66,67	0
25	UNX	C	301	1/1	0.94	0.37	-	26,26,26,26	1
18	CMO	A	606	2/2	1.00	0.06	-	55,55,55,55	0
21	EDO	K	103	4/4	0.85	0.23	-	90,92,99,101	0
25	UNX	P	301	1/1	0.84	0.40	-	15,15,15,15	1
21	EDO	L	102	4/4	0.97	0.06	-	83,84,84,90	0
21	EDO	K	101	4/4	0.76	0.18	-	86,107,118,131	0
15	CU	N	603	1/1	1.00	0.03	-	55,55,55,55	0
21	EDO	C	311	4/4	0.83	0.27	-	80,95,109,118	0
21	EDO	C	310	4/4	0.72	0.24	-	94,105,106,112	0
21	EDO	C	309	4/4	0.97	0.16	-	76,86,100,122	0
21	EDO	A	611	4/4	0.93	0.14	-	86,94,107,113	0
15	CU	A	603	1/1	1.00	0.01	-	55,55,55,55	0
21	EDO	K	102	4/4	0.88	0.21	-	101,108,112,116	0

## 6.5 Other polymers

There are no such residues in this entry.