



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:54 AM GMT

PDB ID : 2EIK  
Title : Cadmium ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state  
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-O, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2007-03-13  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

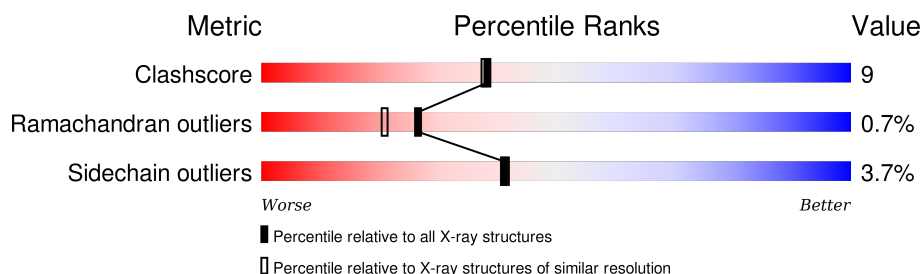
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)









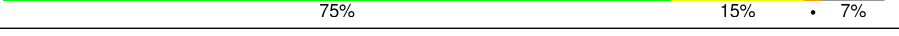


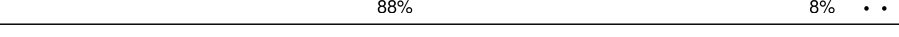

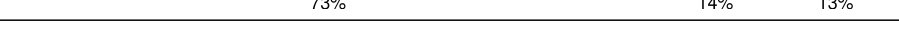


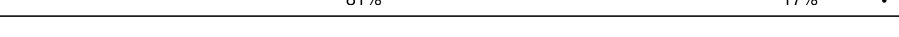

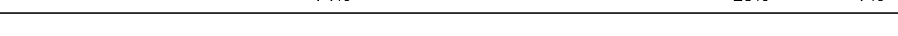
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>87%</div> <div>12% .</div> </div>
1	N	514	<div> <div>82%</div> <div>17% .</div> </div>
2	B	227	<div> <div>81%</div> <div>18% .</div> </div>
2	O	227	<div> <div>75%</div> <div>23% .</div> </div>
3	C	261	<div> <div>86%</div> <div>13% .</div> </div>
3	P	261	<div> <div>84%</div> <div>15% ..</div> </div>
4	D	147	<div> <div>85%</div> <div>12% ..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	L	522	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

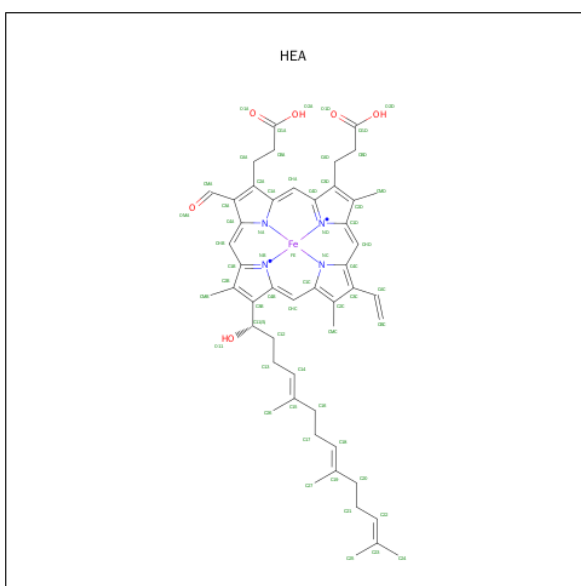
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	2	Total	Cd	0	0
			2	2		
17	A	1	Total	Cd	0	0
			1	1		
17	C	1	Total	Cd	0	0
			1	1		
17	N	1	Total	Cd	0	0
			1	1		
17	E	1	Total	Cd	0	0
			1	1		

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



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

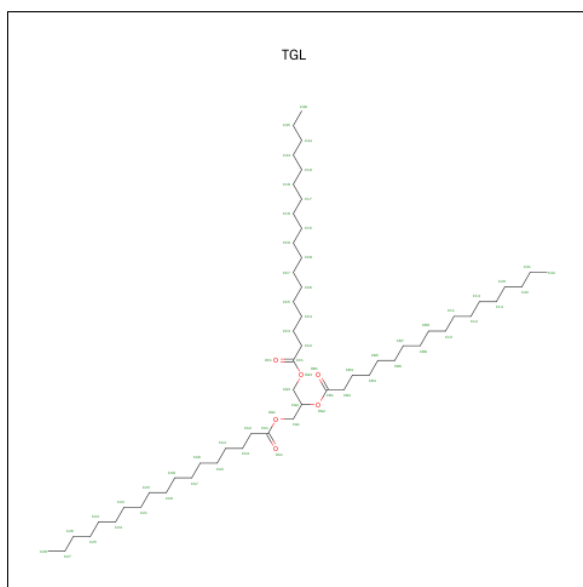
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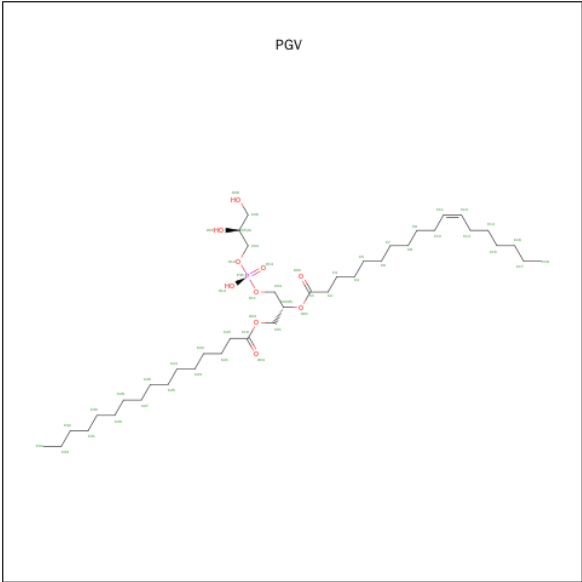
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



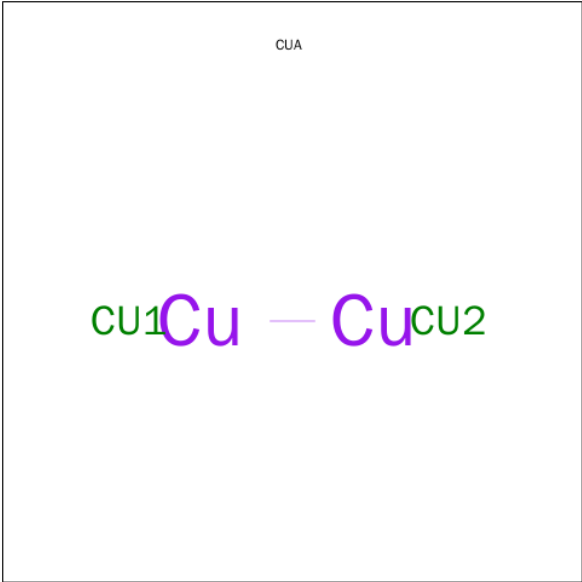
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O		
			63	57	6		
19	A	1	Total	C	O		
			63	57	6		
19	L	1	Total	C	O		
			63	57	6		
19	N	1	Total	C	O		
			63	57	6		
19	Q	1	Total	C	O		
			63	57	6		
19	Y	1	Total	C	O		
			63	57	6		

- 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:  $C_{40}H_{77}O_{10}P$ ).



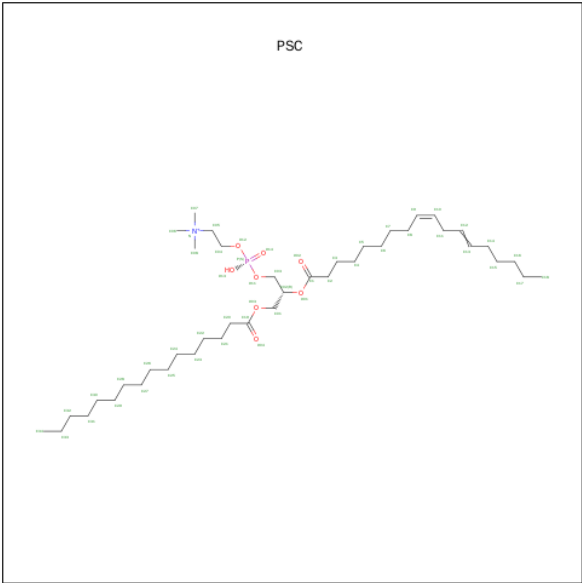
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is (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).



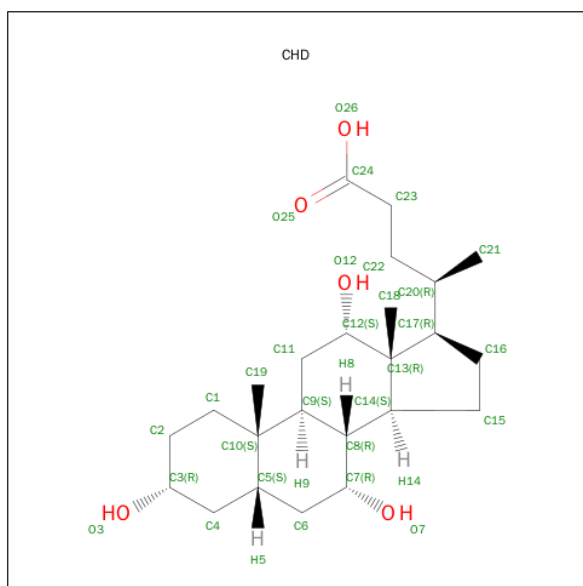
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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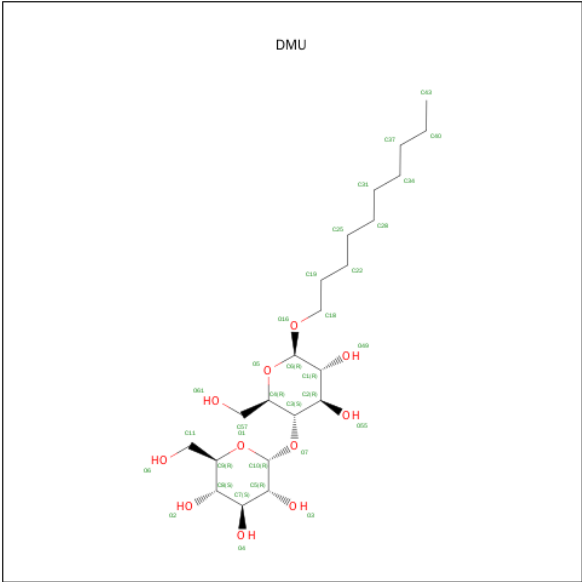
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



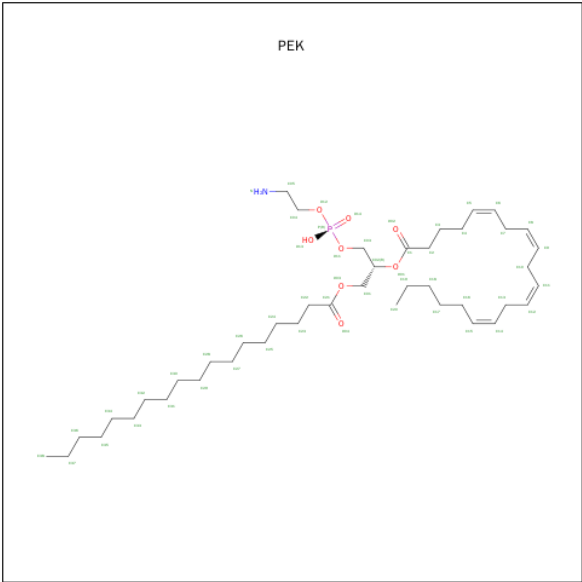
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

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



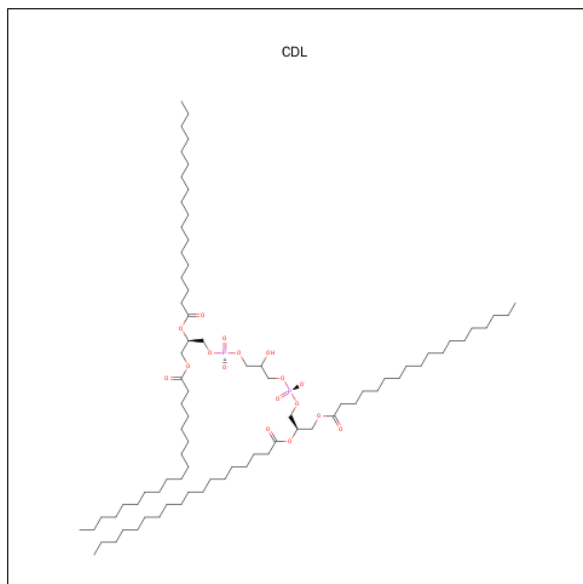
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

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



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

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



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

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	223	Total 223	O 223	0	0
28	B	146	Total 146	O 146	0	0
28	C	102	Total 102	O 102	0	0
28	D	98	Total 98	O 98	0	0
28	E	60	Total 60	O 60	0	0
28	F	85	Total 85	O 85	0	0
28	G	41	Total 41	O 41	0	0
28	H	49	Total 49	O 49	0	0
28	I	44	Total 44	O 44	0	0
28	J	26	Total 26	O 26	0	0
28	K	25	Total 25	O 25	0	0
28	L	23	Total 23	O 23	0	0
28	M	22	Total 22	O 22	0	0
28	N	213	Total 213	O 213	0	0
28	O	116	Total 116	O 116	0	0
28	P	103	Total 103	O 103	0	0
28	Q	52	Total 52	O 52	0	0
28	R	41	Total 41	O 41	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	S	69	Total 69	O 69	0	0
28	T	47	Total 47	O 47	0	0
28	U	43	Total 43	O 43	0	0
28	V	25	Total 25	O 25	0	0
28	W	15	Total 15	O 15	0	0
28	X	17	Total 17	O 17	0	0
28	Y	15	Total 15	O 15	0	0
28	Z	14	Total 14	O 14	0	0

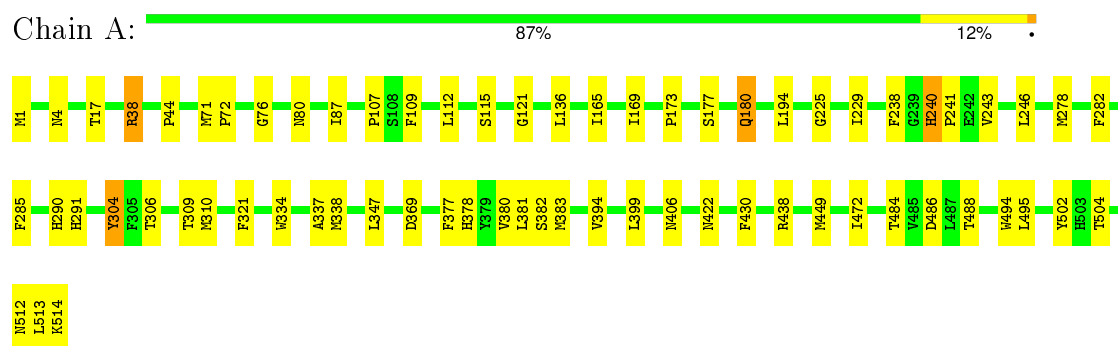


### 3 Residue-property plots

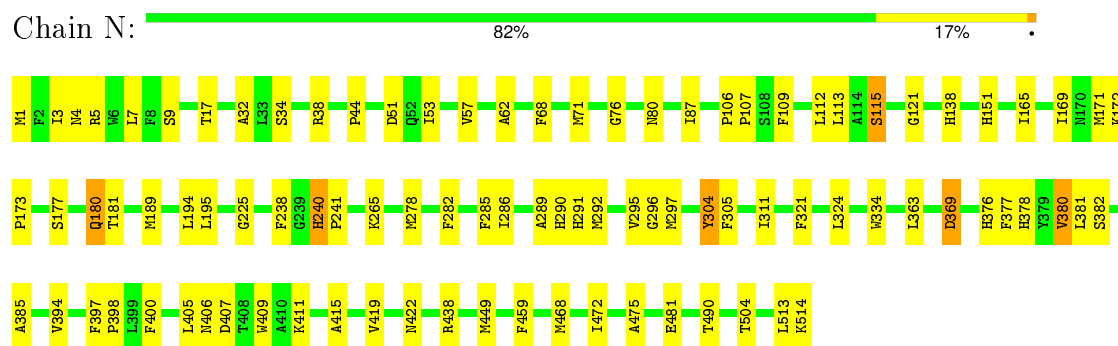
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

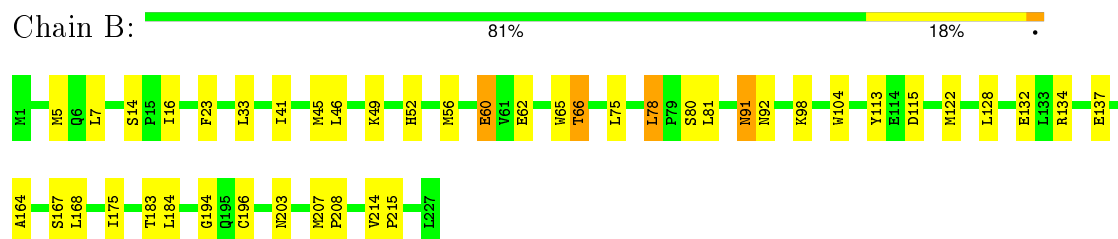
- Molecule 1: Cytochrome c oxidase subunit 1



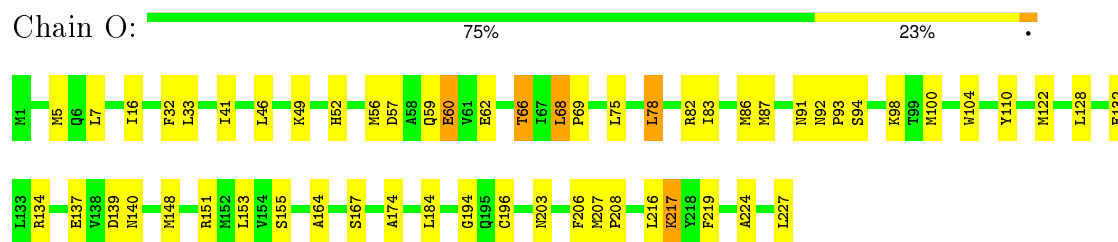
- Molecule 1: Cytochrome c oxidase subunit 1



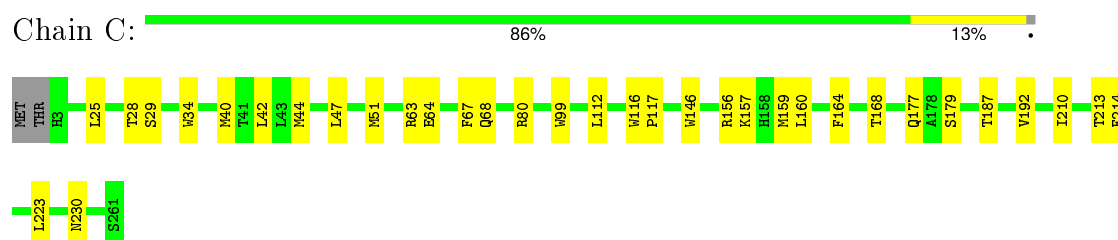
- Molecule 2: Cytochrome c oxidase subunit 2



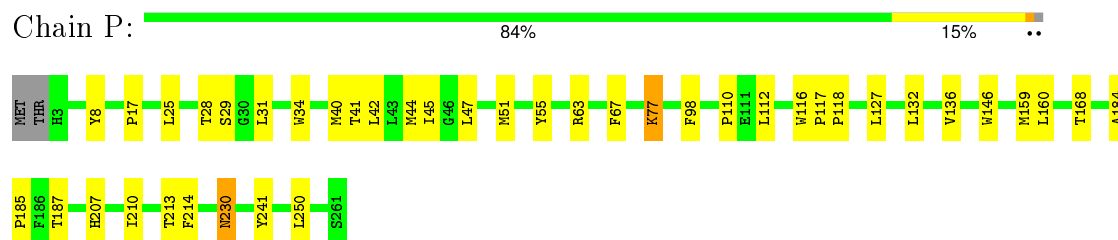
- Molecule 2: Cytochrome c oxidase subunit 2



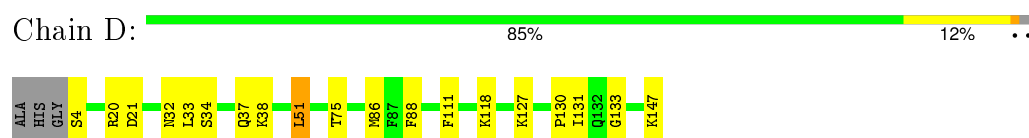
- Molecule 3: Cytochrome c oxidase subunit 3



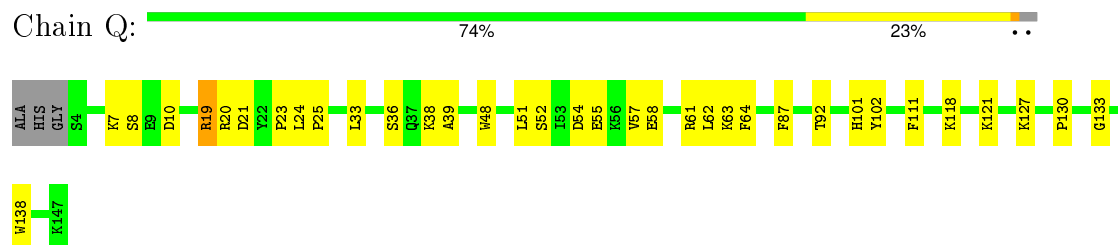
- Molecule 3: Cytochrome c oxidase subunit 3



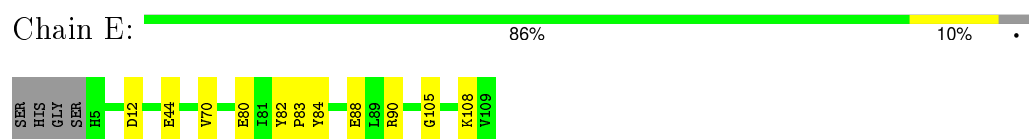
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



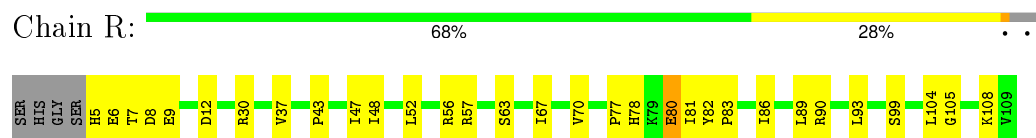
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



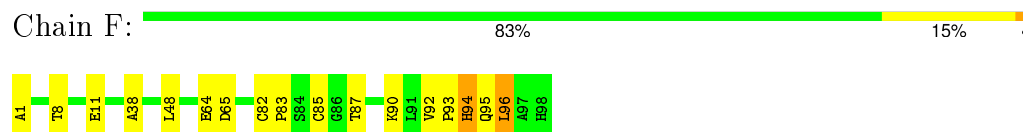
- Molecule 5: Cytochrome c oxidase polypeptide Va



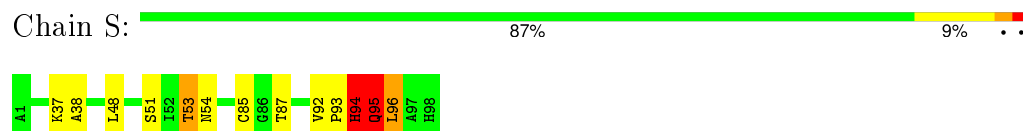
- Molecule 5: Cytochrome c oxidase polypeptide Va



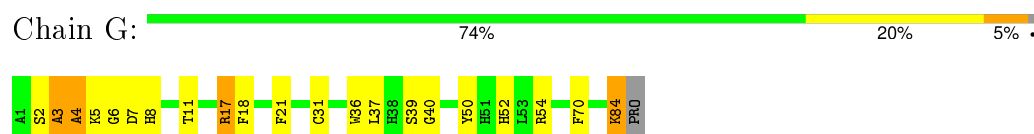
- Molecule 6: Cytochrome c oxidase polypeptide Vb



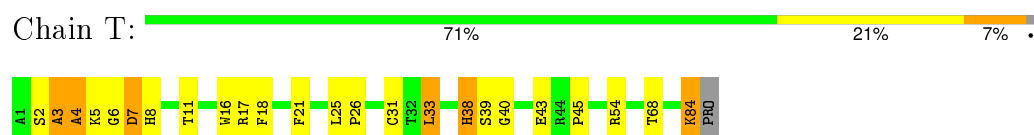
- Molecule 6: Cytochrome c oxidase polypeptide Vb



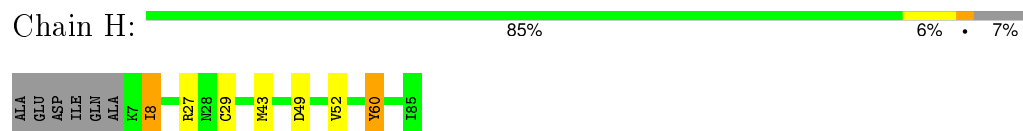
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



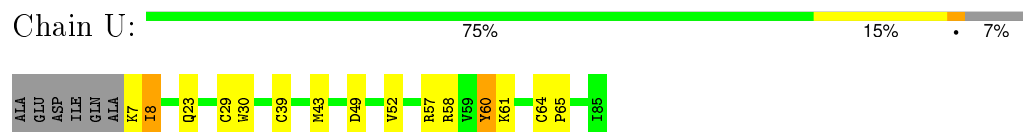
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



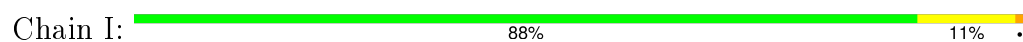
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

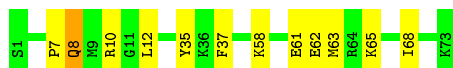
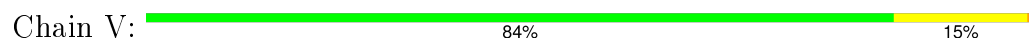


- Molecule 9: Cytochrome c oxidase polypeptide VIc

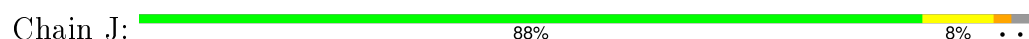




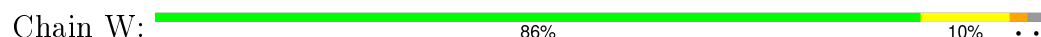
- Molecule 9: Cytochrome c oxidase polypeptide VIc



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



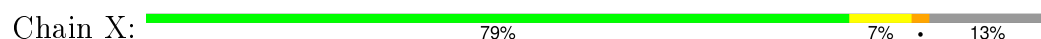
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



- Molecule 11: Cytochrome c oxidase polypeptide VIIb



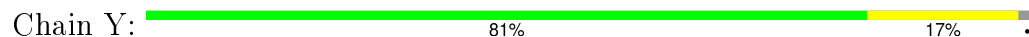
- Molecule 11: Cytochrome c oxidase polypeptide VIIb




- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  76% 15% 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  74% 20% 7%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.32Å 206.53Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.199 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.52	0/4156	0.68	1/5678 (0.0%)
1	N	0.52	0/4156	0.67	0/5678
2	B	0.52	0/1860	0.77	0/2534
2	O	0.53	0/1860	0.78	1/2534 (0.0%)
3	C	0.52	0/2197	0.61	0/3005
3	P	0.50	0/2197	0.62	0/3005
4	D	0.52	0/1229	0.68	2/1658 (0.1%)
4	Q	0.56	0/1229	0.67	1/1658 (0.1%)
5	E	0.52	0/871	0.68	0/1182
5	R	0.56	1/871 (0.1%)	0.73	0/1182
6	F	0.49	0/765	0.81	2/1038 (0.2%)
6	S	0.50	0/765	0.80	2/1038 (0.2%)
7	G	0.53	0/690	0.70	0/937
7	T	0.55	0/690	0.71	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.47	0/682	0.65	0/921
9	I	0.53	0/605	0.64	0/802
9	V	0.51	0/605	0.63	0/802
10	J	0.49	0/471	0.64	0/636
10	W	0.50	0/471	0.66	0/636
11	K	0.57	0/398	0.69	0/546
11	X	0.53	0/398	0.68	0/546
12	L	0.54	0/393	0.60	0/526
12	Y	0.57	0/393	0.63	0/526
13	M	0.48	0/345	0.63	0/470
13	Z	0.50	0/345	0.64	0/470
All	All	0.52	1/29324 (0.0%)	0.69	10/39866 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CD-OE2	5.15	1.31	1.25

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.57	128.74	111.00
6	F	94	HIS	N-CA-C	6.02	127.25	111.00
4	D	133	GLY	N-CA-C	5.85	127.72	113.10
4	Q	133	GLY	N-CA-C	5.48	126.80	113.10
6	F	93	PRO	N-CA-C	5.47	126.33	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	59	0
1	N	4027	0	4001	76	0
2	B	1824	0	1833	31	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	42	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	4	0
5	R	852	0	845	20	0
6	F	748	0	728	9	0
6	S	748	0	728	9	0
7	G	675	0	644	25	0
7	T	675	0	644	25	0
8	H	662	0	623	5	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	12	0
10	J	460	0	459	6	0
10	W	460	0	459	6	0
11	K	384	0	366	5	0
11	X	384	0	366	4	0
12	L	380	0	380	17	0
12	Y	380	0	380	8	0
13	M	335	0	352	8	0
13	Z	335	0	352	5	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	E	1	0	0	0	0
17	N	1	0	0	0	0
17	P	2	0	0	0	0
18	A	120	0	108	5	0
18	N	120	0	108	4	0
19	A	126	0	220	16	0
19	L	63	0	110	23	0
19	N	63	0	110	8	0
19	Q	63	0	110	7	0
19	Y	63	0	110	17	0
20	A	102	0	152	9	0
20	C	102	0	152	7	0
20	N	102	0	152	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	14	0
22	O	52	0	80	15	0
23	B	29	0	39	1	0
23	C	58	0	78	7	0
23	J	29	0	39	3	0
23	O	29	0	39	1	0
23	P	58	0	78	1	0
23	W	29	0	39	5	0
24	C	33	0	36	2	0
24	M	33	0	38	0	0
24	P	33	0	36	8	0
24	Z	33	0	38	0	0
25	C	106	0	154	11	0
25	G	53	0	77	9	0
25	P	106	0	154	12	0
25	T	53	0	77	9	0
26	C	100	0	156	16	0
26	G	100	0	156	22	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	223	0	0	2	0
28	B	146	0	0	4	0
28	C	102	0	0	2	0
28	D	98	0	0	4	0
28	E	60	0	0	1	0
28	F	85	0	0	1	0
28	G	41	0	0	1	0
28	H	49	0	0	2	0
28	I	44	0	0	3	0
28	J	26	0	0	2	0
28	K	25	0	0	1	0
28	L	23	0	0	0	0
28	M	22	0	0	1	0
28	N	213	0	0	3	0
28	O	116	0	0	1	0
28	P	103	0	0	2	0
28	Q	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	R	41	0	0	0	0
28	S	69	0	0	3	0
28	T	47	0	0	4	0
28	U	43	0	0	1	0
28	V	25	0	0	1	0
28	W	15	0	0	2	0
28	X	17	0	0	0	0
28	Y	15	0	0	1	0
28	Z	14	0	0	1	0
All	All	32450	0	31298	566	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 566 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.31	1.11
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.39	1.02
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.42	1.00
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.40	0.99
22:B:230:PSC:H343	22:B:230:PSC:H142	1.40	0.99

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	21	15
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	39	37
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	1
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	9
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	9
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3354 (96%)	125 (4%)	25 (1%)	26	21

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	414 (97%)	12 (3%)	51	55
1	N	426/426 (100%)	415 (97%)	11 (3%)	54	58
2	B	210/210 (100%)	200 (95%)	10 (5%)	31	29
2	O	210/210 (100%)	198 (94%)	12 (6%)	25	22
3	C	224/226 (99%)	219 (98%)	5 (2%)	60	64
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	56
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	76
4	Q	128/129 (99%)	123 (96%)	5 (4%)	39	39
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	47
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	47
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	59
6	S	81/81 (100%)	74 (91%)	7 (9%)	13	9
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	13
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	8
8	H	71/75 (95%)	69 (97%)	2 (3%)	51	55
8	U	71/75 (95%)	69 (97%)	2 (3%)	51	55
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	25
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	44
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	68
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	68
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	58
11	X	39/46 (85%)	38 (97%)	1 (3%)	54	58
12	L	39/40 (98%)	37 (95%)	2 (5%)	29	26
12	Y	39/40 (98%)	39 (100%)	0	100	100
13	M	37/38 (97%)	34 (92%)	3 (8%)	15	10
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	41	41

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	42	LYS
2	O	33	LEU
8	U	60	TYR
1	N	38	ARG
1	N	238	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
1	N	180	GLN
6	S	80	GLN
11	K	41	ASN
1	N	512	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.57	0	6,9,11	1.24	1 (16%)
2	FME	B	1	2	8,9,10	0.64	0	6,9,11	1.37	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TPO	G	11	7	8,10,11	1.63	1 (12%)	7,14,16	1.01	0
9	SAC	I	1	9	7,8,9	2.89	2 (28%)	7,9,11	2.03	3 (42%)
1	FME	N	1	1	8,9,10	0.69	0	6,9,11	1.74	2 (33%)
2	FME	O	1	2	8,9,10	0.62	0	6,9,11	1.74	1 (16%)
7	TPO	T	11	7	8,10,11	1.36	1 (12%)	7,14,16	0.93	0
9	SAC	V	1	9	7,8,9	2.87	2 (28%)	7,9,11	2.20	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	1/6/8/10	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.52	1.58	1.54
7	G	11	TPO	CB-CA	3.67	1.60	1.54
9	V	1	SAC	OAC-C1A	4.79	1.34	1.23
9	I	1	SAC	CA-N	5.16	1.53	1.46
9	V	1	SAC	CA-N	5.39	1.54	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-3.98	116.71	122.82
1	N	1	FME	CA-N-CN	-3.51	117.42	122.82
9	V	1	SAC	CA-N-C1A	-2.94	111.38	121.37
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	I	1	SAC	CA-N-C1A	-2.45	113.05	121.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	OAC-C1A-N-CA
1	N	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
7	G	11	TPO	1	0
9	I	1	SAC	1	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 58 ligands modelled in this entry, 14 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
18	HEA	A	515	1	40,67,67	1.10	6 (15%)	41,103,103	1.72	10 (24%)
18	HEA	A	516	1	40,67,67	1.48	5 (12%)	41,103,103	1.61	9 (21%)
19	TGL	A	521	-	62,62,62	0.70	1 (1%)	65,65,65	1.52	9 (13%)
19	TGL	A	523	-	62,62,62	0.75	1 (1%)	65,65,65	1.36	8 (12%)
20	PGV	A	524	-	50,50,50	1.05	4 (8%)	51,56,56	0.92	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	A	604	-	50,50,50	0.86	1 (2%)	51,56,56	0.77	2 (3%)
23	CHD	B	1086	-	29,32,32	0.65	0	48,51,51	1.75	12 (25%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.22	4 (7%)	55,59,59	0.97	1 (1%)
25	PEK	C	264	-	51,52,52	1.41	5 (9%)	52,57,57	1.25	5 (9%)
25	PEK	C	265	-	51,52,52	1.64	9 (17%)	52,57,57	1.16	6 (11%)
20	PGV	C	267	-	50,50,50	0.82	1 (2%)	51,56,56	0.97	2 (3%)
20	PGV	C	268	-	50,50,50	1.15	2 (4%)	51,56,56	0.78	0
26	CDL	C	270	-	99,99,99	0.84	3 (3%)	101,111,111	0.98	5 (4%)
23	CHD	C	271	-	29,32,32	0.93	1 (3%)	48,51,51	3.71	25 (52%)
24	DMU	C	272	-	34,34,34	2.77	11 (32%)	45,45,45	4.36	20 (44%)
23	CHD	C	525	-	29,32,32	0.84	1 (3%)	48,51,51	1.88	12 (25%)
25	PEK	G	1263	-	51,52,52	1.80	10 (19%)	52,57,57	1.12	5 (9%)
26	CDL	G	269	-	99,99,99	0.99	7 (7%)	101,111,111	0.94	6 (5%)
23	CHD	J	60	-	29,32,32	1.31	3 (10%)	48,51,51	3.56	27 (56%)
19	TGL	L	522	-	62,62,62	1.10	5 (8%)	65,65,65	1.69	13 (20%)
24	DMU	M	526	-	34,34,34	3.28	8 (23%)	45,45,45	4.09	20 (44%)
20	PGV	N	1266	-	50,50,50	0.90	2 (4%)	51,56,56	0.87	3 (5%)
19	TGL	N	1521	-	62,62,62	0.71	1 (1%)	65,65,65	1.50	9 (13%)
20	PGV	N	1524	-	50,50,50	1.05	4 (8%)	51,56,56	0.91	3 (5%)
18	HEA	N	515	1	40,67,67	1.35	5 (12%)	41,103,103	1.82	11 (26%)
18	HEA	N	516	1	40,67,67	1.34	5 (12%)	41,103,103	1.58	10 (24%)
22	PSC	O	1230	-	51,51,51	1.22	3 (5%)	55,59,59	0.99	1 (1%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	0.63	0	48,51,51	1.72	12 (25%)
25	PEK	P	1264	-	51,52,52	1.49	5 (9%)	52,57,57	1.24	8 (15%)
25	PEK	P	1265	-	51,52,52	1.65	9 (17%)	52,57,57	1.16	6 (11%)
20	PGV	P	1267	-	50,50,50	0.81	1 (2%)	51,56,56	0.89	1 (1%)
20	PGV	P	1268	-	50,50,50	1.13	2 (4%)	51,56,56	0.82	1 (1%)
26	CDL	P	1270	-	99,99,99	0.88	4 (4%)	101,111,111	0.97	5 (4%)
23	CHD	P	1271	-	29,32,32	0.87	1 (3%)	48,51,51	3.63	26 (54%)
24	DMU	P	1272	-	34,34,34	2.81	11 (32%)	45,45,45	4.18	19 (42%)
23	CHD	P	1525	-	29,32,32	0.82	1 (3%)	48,51,51	1.78	12 (25%)
19	TGL	Q	1523	-	62,62,62	0.79	1 (1%)	65,65,65	1.34	6 (9%)
26	CDL	T	1269	-	99,99,99	0.97	7 (7%)	101,111,111	0.95	6 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PEK	T	263	-	51,52,52	1.83	9 (17%)	52,57,57	1.11	5 (9%)
23	CHD	W	1060	-	29,32,32	1.37	3 (10%)	48,51,51	3.59	26 (54%)
19	TGL	Y	1522	-	62,62,62	1.14	5 (8%)	65,65,65	1.67	13 (20%)
24	DMU	Z	1526	-	34,34,34	3.19	9 (26%)	45,45,45	4.02	20 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	2/55/55/55	0/0/0/0
20	PGV	A	604	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	230	-	-	0/55/55/55	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
19	TGL	Y	1522	-	-	0/65/65/65	0/0/0/0
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.67	1.22	1.43
24	Z	1526	DMU	O7-C3	-8.21	1.23	1.43
24	M	526	DMU	O16-C6	-7.25	1.27	1.40
24	Z	1526	DMU	O16-C6	-7.09	1.27	1.40
24	M	526	DMU	O5-C4	-6.63	1.27	1.44

The worst 5 of 403 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C17-C13-C12	-8.42	110.22	117.68
23	C	271	CHD	C17-C13-C12	-8.16	110.44	117.68
23	C	271	CHD	C19-C10-C9	-8.13	98.99	111.18
23	P	1271	CHD	C19-C10-C9	-7.47	99.98	111.18
24	M	526	DMU	C8-C7-C5	-7.32	97.13	110.79

5 of 54 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB

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Mol	Chain	Res	Type	Atom
18	A	516	HEA	ND
18	A	516	HEA	NA

All (4) torsion outliers are listed below:

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

There are no ring outliers.

38 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	3	0
18	A	516	HEA	2	0
19	A	521	TGL	10	0
19	A	523	TGL	6	0
20	A	524	PGV	8	0
20	A	604	PGV	1	0
23	B	1086	CHD	1	0
22	B	230	PSC	14	0
25	C	264	PEK	4	0
25	C	265	PEK	7	0
20	C	267	PGV	5	0
20	C	268	PGV	2	0
26	C	270	CDL	16	0
23	C	271	CHD	7	0
24	C	272	DMU	2	0
25	G	1263	PEK	9	0
26	G	269	CDL	22	0
23	J	60	CHD	3	0
19	L	522	TGL	23	0
20	N	1266	PGV	1	0
19	N	1521	TGL	8	0
20	N	1524	PGV	9	0
18	N	515	HEA	3	0
18	N	516	HEA	1	0
22	O	1230	PSC	15	0
23	O	229	CHD	1	0
25	P	1264	PEK	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	1265	PEK	7	0
20	P	1267	PGV	4	0
20	P	1268	PGV	2	0
26	P	1270	CDL	18	0
23	P	1271	CHD	1	0
24	P	1272	DMU	8	0
19	Q	1523	TGL	7	0
26	T	1269	CDL	19	0
25	T	263	PEK	9	0
23	W	1060	CHD	5	0
19	Y	1522	TGL	17	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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