



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:30 am GMT

PDB ID : 3ABM
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (200-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-12-16
Resolution : 1.95 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

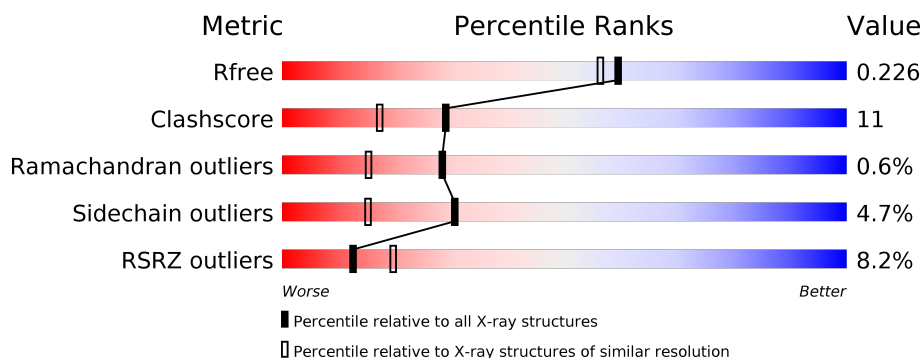
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
2	O	227	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>
3	C	261	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
3	P	261	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>...</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
17	NA	N	1519	-	-	-	X
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	O	1521	-	-	-	X
19	TGL	O	1523	-	-	-	X
19	TGL	Y	1522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	H	268	-	-	-	X
20	PGV	N	1268	-	-	-	X
20	PGV	N	1524	-	-	-	X
22	CHD	B	1086	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	X
24	PEK	T	263	-	-	X	-
25	CDL	C	270	-	-	-	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	X	X
26	PSC	E	230	-	-	X	X
26	PSC	R	1230	-	-	-	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32113 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 subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

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.

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			

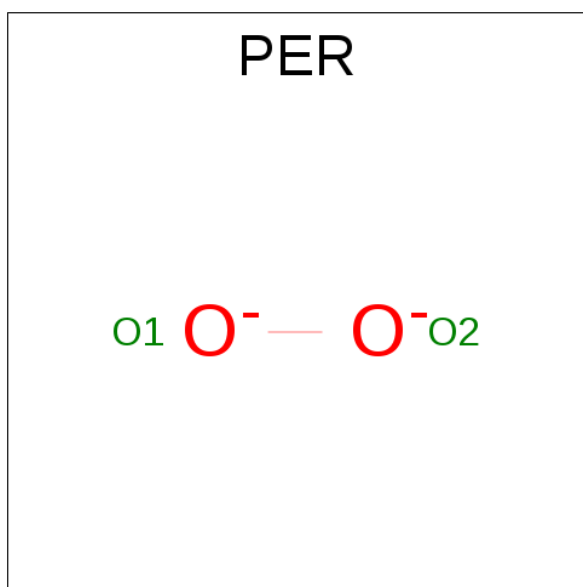
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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 PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

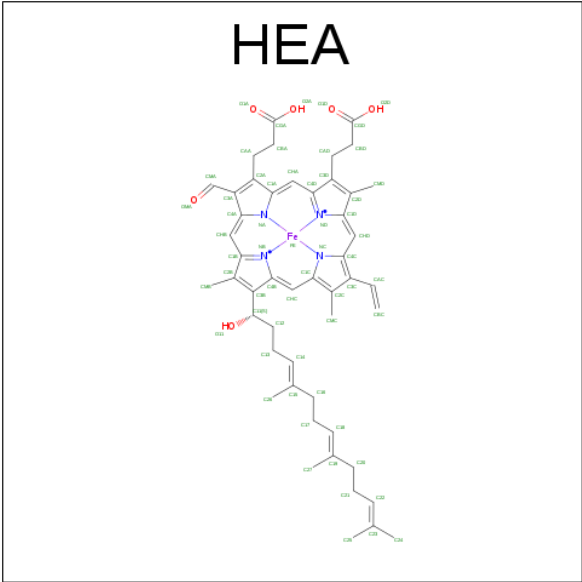
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

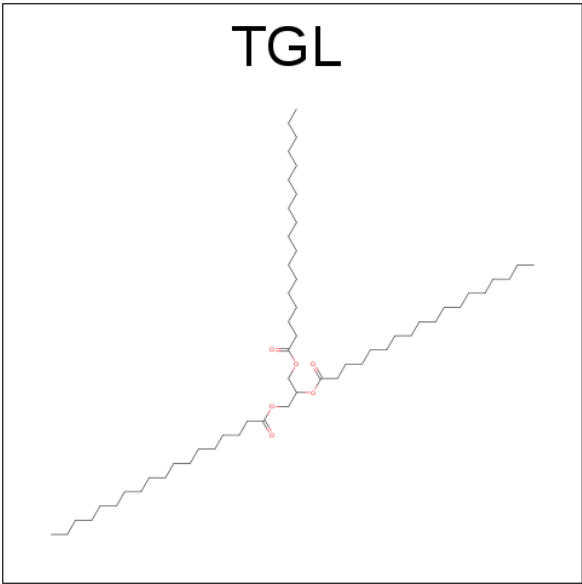
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



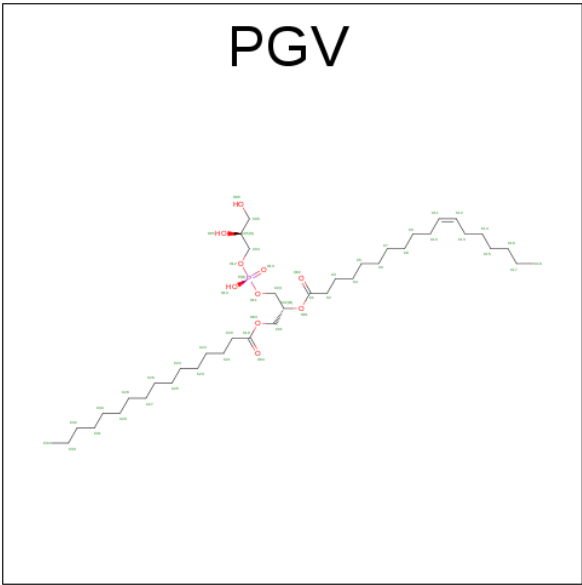
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



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	O	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Y	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: C₄₀H₇₇O₁₀P).



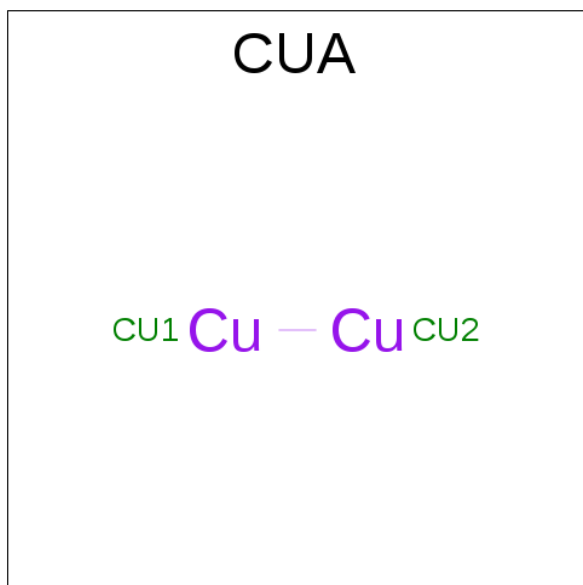
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	H	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

Continued on next page...

Continued from previous page...

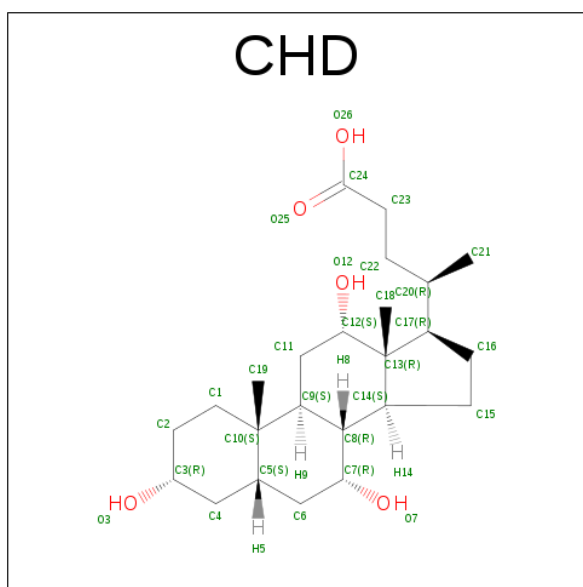
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total 51	C 40	O 10	P 1	0	0
20	N	1	Total 51	C 40	O 10	P 1	0	0
20	P	1	Total 51	C 40	O 10	P 1	0	0

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



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

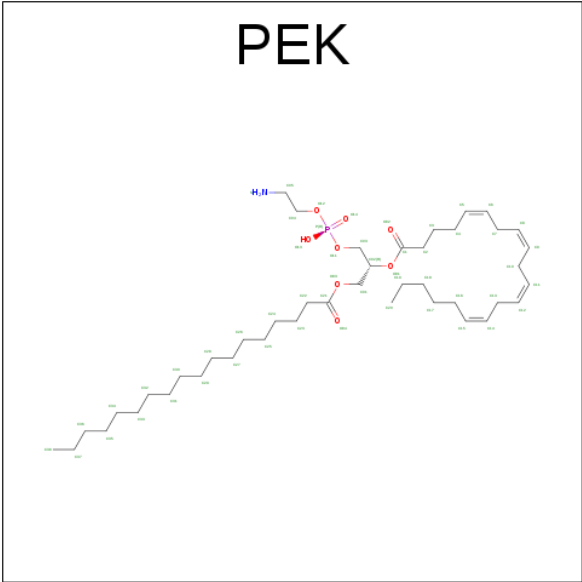


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

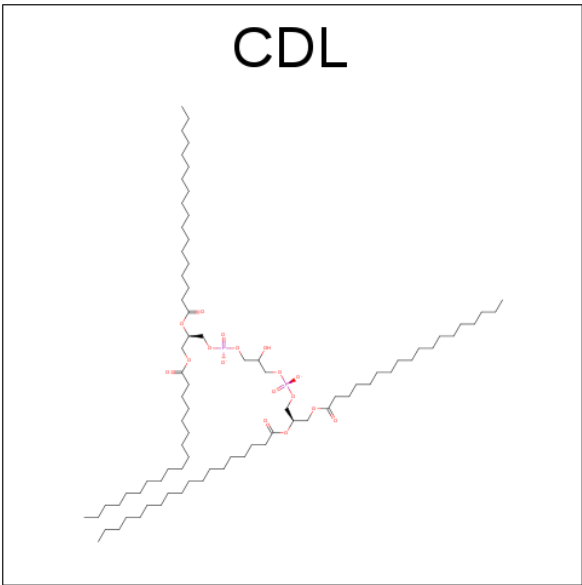
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total	X	0	0
			1	1		
23	C	1	Total	X	0	0
			1	1		

- Molecule 24 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: C₄₃H₇₈NO₈P).



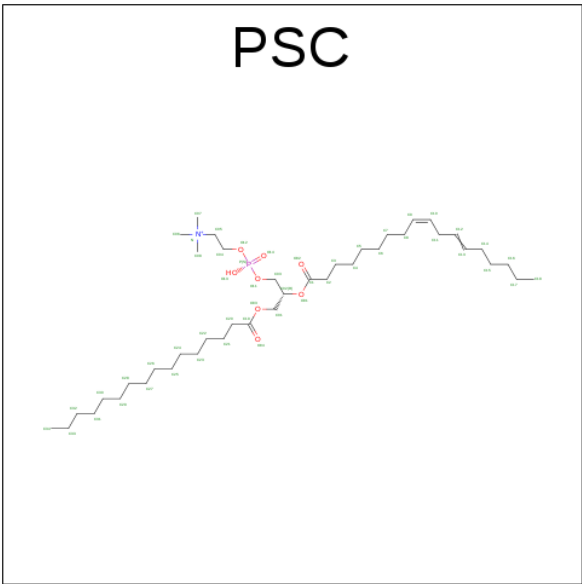
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).

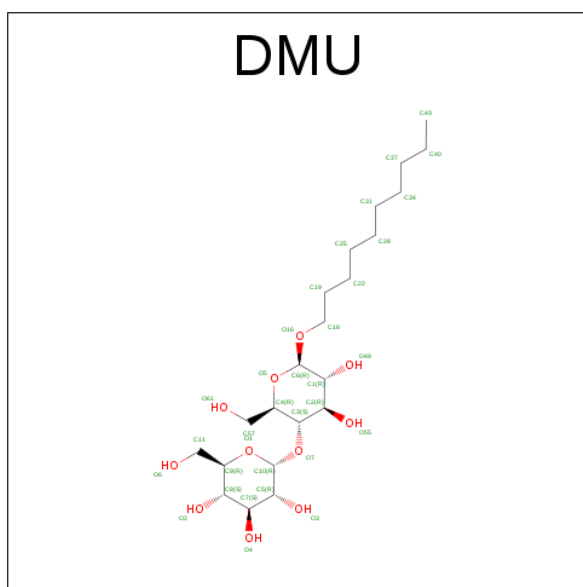


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	203	Total O 203 203	0	0
29	B	131	Total O 131 131	0	0
29	C	90	Total O 90 90	0	0
29	D	96	Total O 96 96	0	0
29	E	62	Total O 62 62	0	0
29	F	70	Total O 70 70	0	0
29	G	41	Total O 41 41	0	0
29	H	46	Total O 46 46	0	0
29	I	44	Total O 44 44	0	0
29	J	17	Total O 17 17	0	0
29	K	22	Total O 22 22	0	0
29	L	23	Total O 23 23	0	0
29	M	19	Total O 19 19	0	0
29	N	196	Total O 196 196	0	0
29	O	106	Total O 106 106	0	0
29	P	89	Total O 89 89	0	0
29	Q	54	Total O 54 54	0	0
29	R	52	Total O 52 52	0	0
29	S	62	Total O 62 62	0	0
29	T	39	Total O 39 39	0	0
29	U	39	Total O 39 39	0	0
29	V	16	Total O 16 16	0	0

Continued on next page...

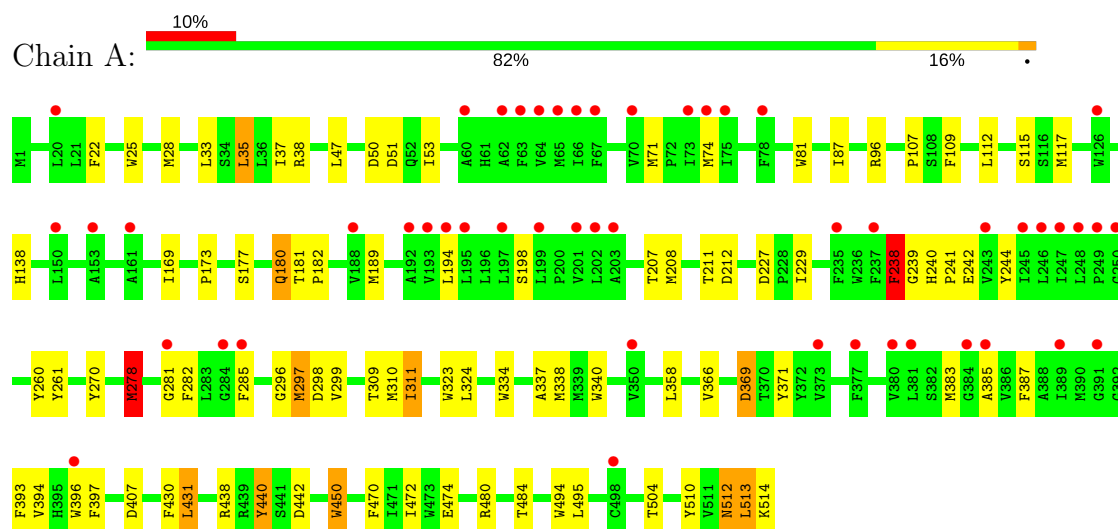
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	15	Total 15	O 15	0	0
29	X	16	Total 16	O 16	0	0
29	Y	19	Total 19	O 19	0	0
29	Z	10	Total 10	O 10	0	0

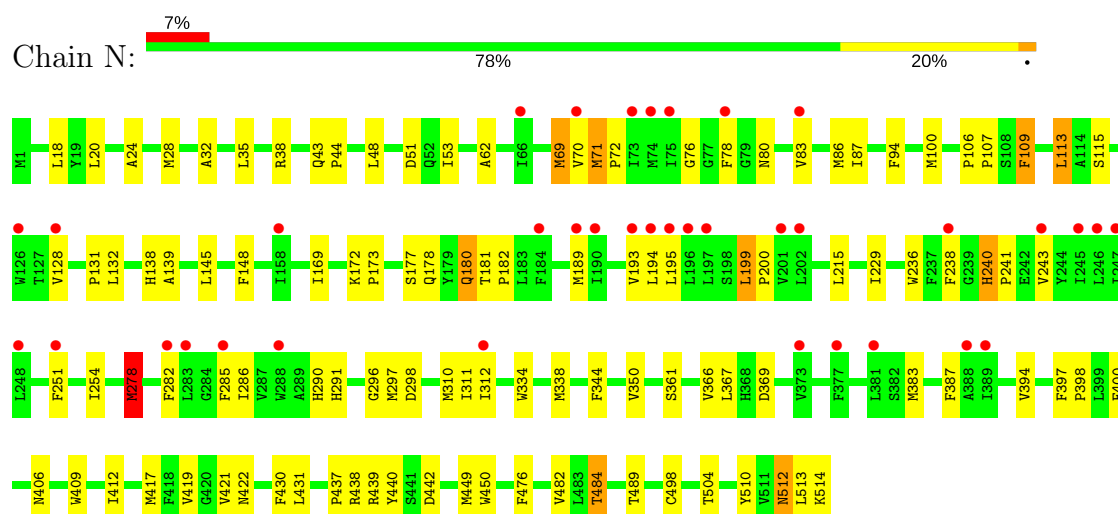
3 Residue-property plots [i](#)

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

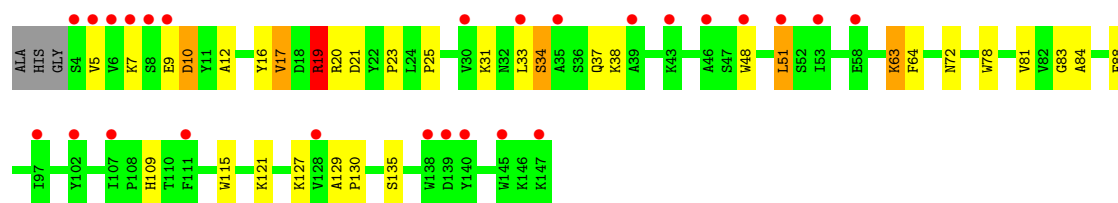


• Molecule 1: Cytochrome c oxidase subunit 1

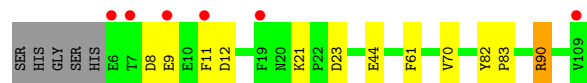
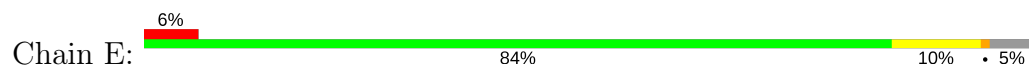


• Molecule 2: Cytochrome c oxidase subunit 2

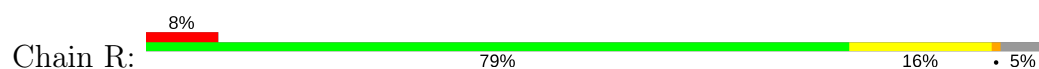




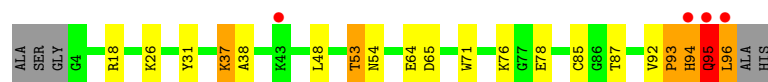
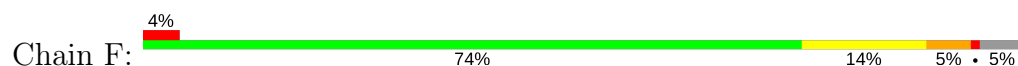
• Molecule 5: Cytochrome c oxidase subunit 5A



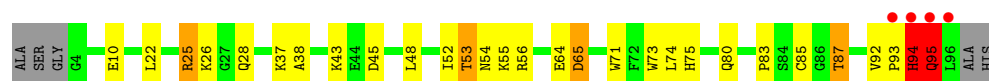
• Molecule 5: Cytochrome c oxidase subunit 5A



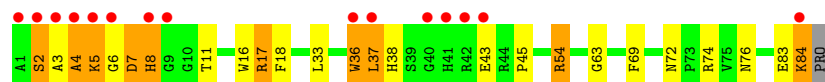
• Molecule 6: Cytochrome c oxidase subunit 5B



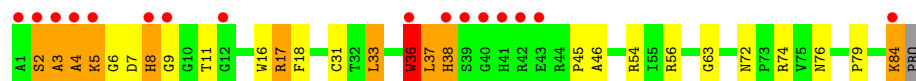
• Molecule 6: Cytochrome c oxidase subunit 5B



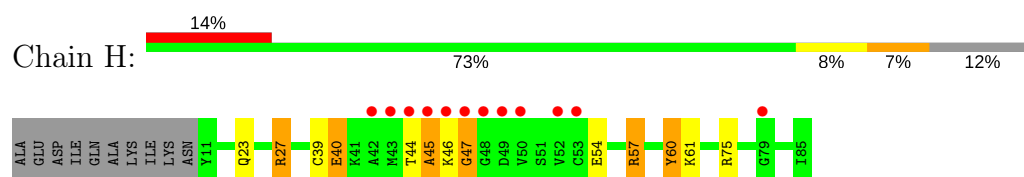
• Molecule 7: Cytochrome c oxidase subunit 6A2



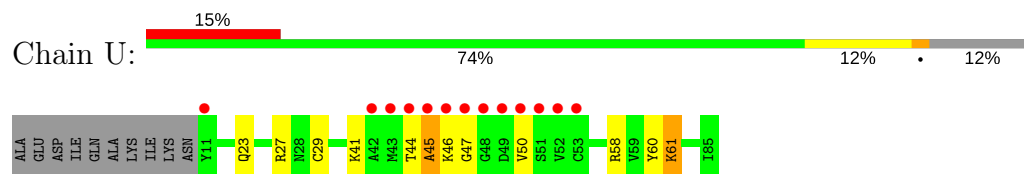
• Molecule 7: Cytochrome c oxidase subunit 6A2



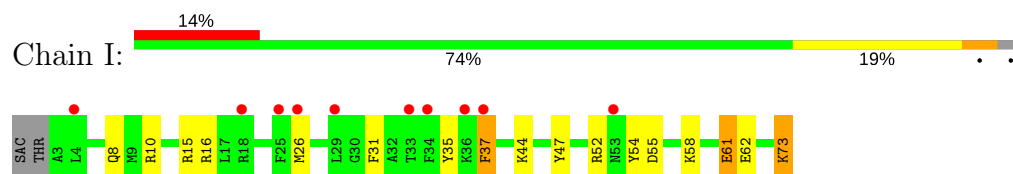
• Molecule 8: Cytochrome c oxidase subunit 6B1



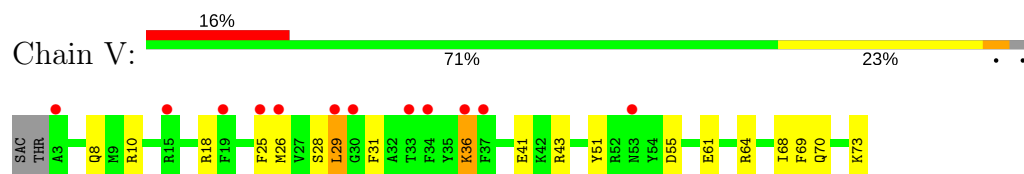
• Molecule 8: Cytochrome c oxidase subunit 6B1



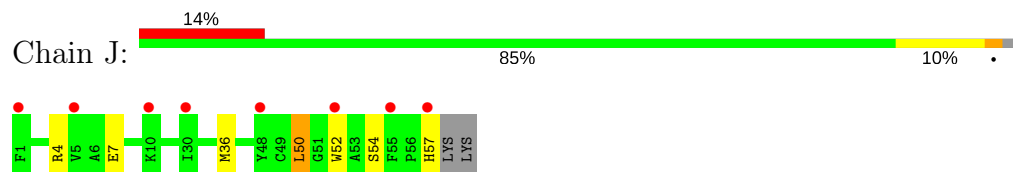
• Molecule 9: Cytochrome c oxidase subunit 6C



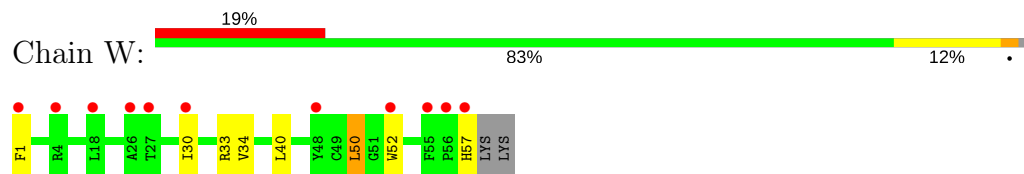
• Molecule 9: Cytochrome c oxidase subunit 6C



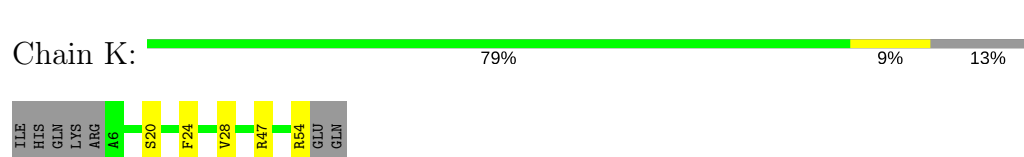
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



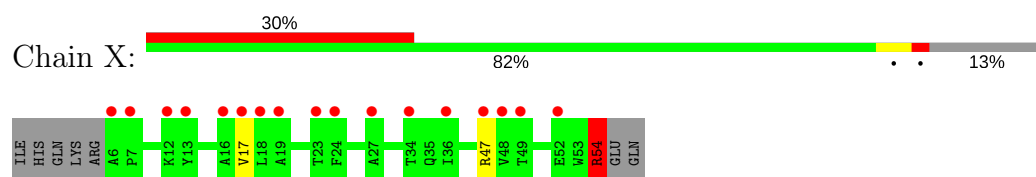
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



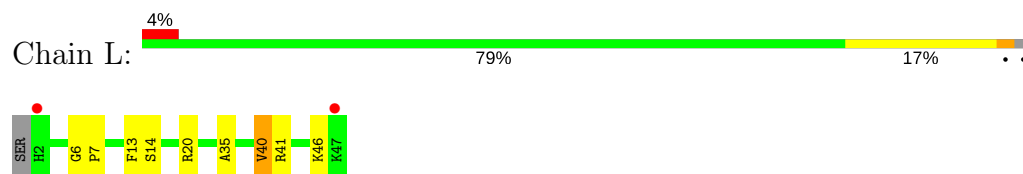
• Molecule 11: Cytochrome c oxidase subunit 7B



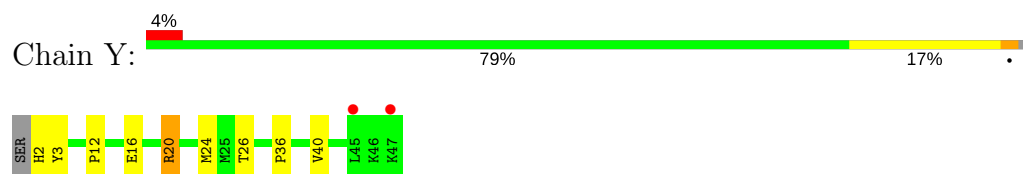
• Molecule 11: Cytochrome c oxidase subunit 7B



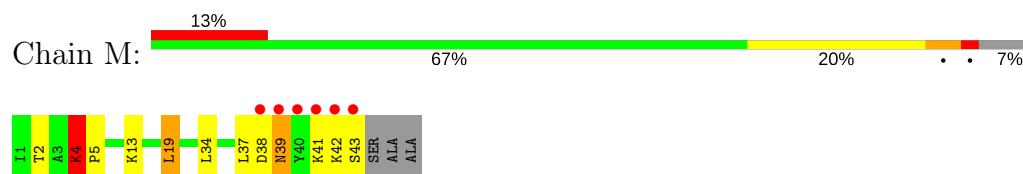
- Molecule 12: Cytochrome c oxidase subunit 7C



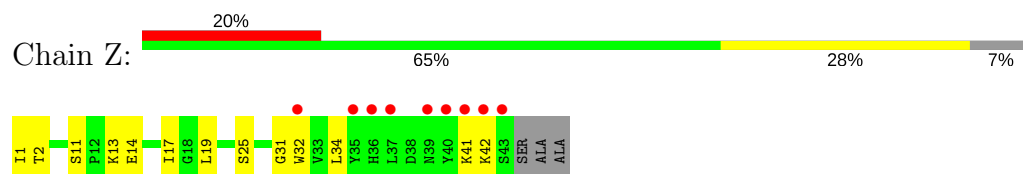
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 64.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.95) 96.4 (64.10-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.181 , 0.214 0.196 , 0.226	Depositor DCC
R_{free} test set	16433 reflections (3.61%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32113	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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, PER, PGV, UNX, 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	1.48	26/4156 (0.6%)	1.30	34/5678 (0.6%)
1	N	1.34	13/4156 (0.3%)	1.18	22/5678 (0.4%)
2	B	1.37	10/1860 (0.5%)	1.29	12/2534 (0.5%)
2	O	1.19	9/1860 (0.5%)	1.16	11/2534 (0.4%)
3	C	1.31	8/2197 (0.4%)	1.19	12/3005 (0.4%)
3	P	1.34	13/2197 (0.6%)	1.11	10/3005 (0.3%)
4	D	1.37	5/1229 (0.4%)	1.32	10/1658 (0.6%)
4	Q	1.07	3/1229 (0.2%)	1.08	4/1658 (0.2%)
5	E	1.20	3/860 (0.3%)	1.13	4/1167 (0.3%)
5	R	1.06	0/860	0.99	2/1167 (0.2%)
6	F	1.30	2/733 (0.3%)	1.16	2/996 (0.2%)
6	S	1.28	2/733 (0.3%)	1.29	7/996 (0.7%)
7	G	1.27	2/690 (0.3%)	1.10	3/937 (0.3%)
7	T	1.29	3/690 (0.4%)	1.22	4/937 (0.4%)
8	H	1.27	0/648	1.13	3/877 (0.3%)
8	U	1.03	0/648	0.99	0/877
9	I	1.23	3/598 (0.5%)	1.12	2/792 (0.3%)
9	V	1.09	1/598 (0.2%)	1.00	1/792 (0.1%)
10	J	1.10	0/462	1.04	1/625 (0.2%)
10	W	1.01	0/462	0.94	1/625 (0.2%)
11	K	1.30	1/398 (0.3%)	1.09	0/546
11	X	0.93	0/398	0.97	1/546 (0.2%)
12	L	1.41	2/393 (0.5%)	1.13	1/526 (0.2%)
12	Y	1.19	0/393	0.98	0/526
13	M	1.32	1/345 (0.3%)	1.15	1/470 (0.2%)
13	Z	0.92	0/345	0.95	0/470
All	All	1.29	107/29138 (0.4%)	1.17	148/39622 (0.4%)

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
6	S	0	2

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	54	ASN	CB-CG	-10.95	1.25	1.51
1	A	270	TYR	CD1-CE1	9.75	1.53	1.39
4	D	17	VAL	CB-CG1	-9.37	1.33	1.52
1	A	396	TRP	CE3-CZ3	9.08	1.53	1.38
1	A	371	TYR	CD1-CE1	8.87	1.52	1.39

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	ARG	NE-CZ-NH2	-17.04	111.78	120.30
4	D	20	ARG	NE-CZ-NH2	-16.31	112.14	120.30
4	Q	20	ARG	NE-CZ-NH1	14.03	127.31	120.30
4	D	20	ARG	NE-CZ-NH1	13.62	127.11	120.30
4	D	19	ARG	NE-CZ-NH1	-13.50	113.55	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide

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	47	0
1	N	4027	0	4001	75	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2110	0	2027	37	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	27	0
5	E	842	0	838	5	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	28	0
7	G	675	0	643	38	0
7	T	675	0	643	45	0
8	H	628	0	580	9	0
8	U	628	0	580	8	0
9	I	585	0	597	13	0
9	V	585	0	597	15	0
10	J	451	0	446	5	0
10	W	451	0	446	6	0
11	K	384	0	366	1	0
11	X	384	0	366	5	0
12	L	380	0	380	11	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	1	0
17	N	1	0	0	0	0
18	A	120	0	108	11	0
18	N	120	0	108	14	0
19	A	63	0	110	13	0
19	D	63	0	110	9	0
19	L	63	0	110	15	0
19	O	126	0	220	23	0
19	Y	63	0	110	18	0
20	A	102	0	152	8	0
20	C	51	0	76	4	0
20	H	51	0	76	3	0
20	N	153	0	228	12	0
20	P	51	0	76	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	2	0
22	C	58	0	70	5	0
22	J	29	0	36	1	0
22	O	29	0	36	0	0
22	P	58	0	71	1	0
22	W	29	0	36	4	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	7	0
24	G	106	0	154	31	0
24	P	53	0	77	7	0
24	T	106	0	154	30	0
25	C	100	0	156	19	0
25	G	100	0	156	27	0
25	P	100	0	156	24	0
25	T	100	0	156	19	0
26	E	52	0	80	22	0
26	R	52	0	80	15	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	5	0
28	M	33	0	39	0	0
28	P	33	0	40	1	0
28	Z	33	0	38	3	0
29	A	203	0	0	3	0
29	B	131	0	0	2	0
29	C	90	0	0	4	0
29	D	96	0	0	8	0
29	E	62	0	0	0	0
29	F	70	0	0	1	0
29	G	41	0	0	6	0
29	H	46	0	0	2	0
29	I	44	0	0	3	0
29	J	17	0	0	1	0
29	K	22	0	0	2	0
29	L	23	0	0	1	0
29	M	19	0	0	0	0
29	N	196	0	0	3	0
29	O	106	0	0	3	0
29	P	89	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	54	0	0	4	0
29	R	52	0	0	0	0
29	S	62	0	0	6	0
29	T	39	0	0	7	0
29	U	39	0	0	2	0
29	V	16	0	0	3	0
29	W	15	0	0	1	0
29	X	16	0	0	0	0
29	Y	19	0	0	1	0
29	Z	10	0	0	1	0
All	All	32113	0	31062	673	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 11.

The worst 5 of 673 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)
24:G:265:PEK:C8	24:G:265:PEK:C7	1.75	1.56
24:G:265:PEK:C9	24:G:265:PEK:C8	1.77	1.55
24:G:265:PEK:C10	24:G:265:PEK:C9	1.81	1.50
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.48
24:G:265:PEK:H383	25:G:269:CDL:C27	1.46	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	490 (96%)	22 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	38	25
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	25
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	25	13
5	E	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
5	R	102/109 (94%)	102 (100%)	0	0	100	100
6	F	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	8	1
6	S	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	17	6
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	2	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	0
8	U	73/85 (86%)	66 (90%)	5 (7%)	2 (3%)	6	1
9	I	69/73 (94%)	66 (96%)	3 (4%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	7	1
All	All	3478/3614 (96%)	3328 (96%)	128 (4%)	22 (1%)	28	15

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	51	40
1	N	426/426 (100%)	413 (97%)	13 (3%)	45	32
2	B	210/210 (100%)	198 (94%)	12 (6%)	24	10
2	O	210/210 (100%)	197 (94%)	13 (6%)	21	8
3	C	224/226 (99%)	217 (97%)	7 (3%)	45	32
3	P	224/226 (99%)	215 (96%)	9 (4%)	36	21
4	D	128/129 (99%)	127 (99%)	1 (1%)	85	83
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	11
5	E	91/95 (96%)	90 (99%)	1 (1%)	78	75
5	R	91/95 (96%)	88 (97%)	3 (3%)	43	30
6	F	79/81 (98%)	73 (92%)	6 (8%)	15	5
6	S	79/81 (98%)	73 (92%)	6 (8%)	15	5
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	1
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	1
8	H	67/75 (89%)	64 (96%)	3 (4%)	32	17
8	U	67/75 (89%)	62 (92%)	5 (8%)	16	5
9	I	56/57 (98%)	51 (91%)	5 (9%)	11	3
9	V	56/57 (98%)	52 (93%)	4 (7%)	17	6
10	J	48/50 (96%)	47 (98%)	1 (2%)	59	50
10	W	48/50 (96%)	47 (98%)	1 (2%)	59	50
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	13
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	13
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	40
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	13
13	M	37/38 (97%)	31 (84%)	6 (16%)	3	0
13	Z	37/38 (97%)	34 (92%)	3 (8%)	14	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3022/3082 (98%)	2880 (95%)	142 (5%)	30	15

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	42	LYS
2	O	60	GLU
9	V	26	MET
1	N	109	PHE
1	N	338	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
1	N	413	HIS
6	S	95	GLN
10	J	57	HIS
1	N	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	1.35	2 (22%)	7,9,11	5.07	4 (57%)
2	FME	B	1	2	9,9,10	1.80	3 (33%)	7,9,11	6.73	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	G	11	7	9,10,11	2.20	4 (44%)	10,14,16	2.47	5 (50%)
1	FME	N	1	1	9,9,10	1.08	1 (11%)	7,9,11	6.33	5 (71%)
2	FME	O	1	2	9,9,10	0.85	1 (11%)	7,9,11	5.59	4 (57%)
7	TPO	T	11	7	9,10,11	1.96	5 (55%)	10,14,16	2.07	2 (20%)

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
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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.54	1.11	1.22
2	B	1	FME	CG-SD	-2.22	1.69	1.81
1	A	1	FME	O1-CN	-2.20	1.15	1.22
2	O	1	FME	O1-CN	-2.03	1.16	1.22
7	T	11	TPO	P-O3P	2.05	1.63	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.38	97.64	122.82
1	N	1	FME	CA-N-CN	-15.33	99.25	122.82
2	O	1	FME	CA-N-CN	-13.71	101.73	122.82
1	A	1	FME	CA-N-CN	-12.21	104.05	122.82
2	B	1	FME	CB-CG-SD	-4.13	93.50	113.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	HEA	A	515	1	44,67,67	1.40	7 (15%)	37,103,103	2.45	18 (48%)
18	HEA	A	516	1,15	44,67,67	1.78	8 (18%)	37,103,103	2.17	10 (27%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.21	7 (11%)	65,65,65	2.07	12 (18%)
20	PGV	A	522	-	50,50,50	1.07	3 (6%)	51,56,56	1.57	7 (13%)
20	PGV	A	524	-	50,50,50	1.22	3 (6%)	51,56,56	1.68	10 (19%)
22	CHD	B	1086	-	29,32,32	1.27	4 (13%)	47,51,51	5.80	34 (72%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	C	264	-	52,52,52	0.99	3 (5%)	54,57,57	1.56	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	267	-	50,50,50	0.95	2 (4%)	51,56,56	1.31	6 (11%)
25	CDL	C	270	-	99,99,99	1.36	14 (14%)	101,111,111	1.63	16 (15%)
22	CHD	C	271	-	29,32,32	1.13	2 (6%)	47,51,51	5.41	33 (70%)
22	CHD	C	525	-	29,32,32	1.66	6 (20%)	47,51,51	5.59	38 (80%)
19	TGL	D	523	-	62,62,62	1.58	7 (11%)	65,65,65	1.70	16 (24%)
26	PSC	E	230	-	51,51,51	1.32	3 (5%)	56,59,59	1.21	5 (8%)
24	PEK	G	1263	-	52,52,52	1.17	2 (3%)	54,57,57	1.40	5 (9%)
24	PEK	G	265	-	52,52,52	1.93	5 (9%)	54,57,57	1.58	6 (11%)
25	CDL	G	269	-	99,99,99	1.46	13 (13%)	101,111,111	1.58	17 (16%)
28	DMU	G	272	-	34,34,34	1.32	5 (14%)	45,45,45	3.59	24 (53%)
20	PGV	H	268	-	50,50,50	1.32	2 (4%)	51,56,56	1.55	9 (17%)
22	CHD	J	60	-	29,32,32	0.76	0	47,51,51	5.03	37 (78%)
19	TGL	L	522	-	62,62,62	1.58	7 (11%)	65,65,65	2.00	18 (27%)
28	DMU	M	526	-	34,34,34	0.96	1 (2%)	45,45,45	3.38	28 (62%)
20	PGV	N	1266	-	50,50,50	0.89	2 (4%)	51,56,56	1.66	7 (13%)
20	PGV	N	1268	-	50,50,50	1.20	2 (4%)	51,56,56	1.53	6 (11%)
20	PGV	N	1524	-	50,50,50	1.06	2 (4%)	51,56,56	1.60	5 (9%)
18	HEA	N	515	1	44,67,67	1.40	6 (13%)	37,103,103	2.26	10 (27%)
18	HEA	N	516	1,15	44,67,67	1.30	6 (13%)	37,103,103	2.48	13 (35%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	O	1521	-	62,62,62	1.31	6 (9%)	65,65,65	1.65	12 (18%)
19	TGL	O	1523	-	62,62,62	1.39	6 (9%)	65,65,65	1.50	10 (15%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	1.37	5 (17%)	47,51,51	5.66	36 (76%)
24	PEK	P	1264	-	52,52,52	1.03	4 (7%)	54,57,57	1.84	10 (18%)
20	PGV	P	1267	-	50,50,50	0.89	2 (4%)	51,56,56	1.51	9 (17%)
25	CDL	P	1270	-	99,99,99	1.40	13 (13%)	101,111,111	1.51	16 (15%)
22	CHD	P	1271	-	29,32,32	0.84	0	47,51,51	5.42	30 (63%)
28	DMU	P	1272	-	34,34,34	1.32	4 (11%)	45,45,45	3.21	23 (51%)
22	CHD	P	1525	-	29,32,32	1.37	2 (6%)	47,51,51	5.72	37 (78%)
26	PSC	R	1230	-	51,51,51	1.20	3 (5%)	56,59,59	1.24	4 (7%)
24	PEK	T	1265	-	52,52,52	1.21	2 (3%)	54,57,57	1.43	6 (11%)
25	CDL	T	1269	-	99,99,99	1.37	12 (12%)	101,111,111	1.46	18 (17%)
24	PEK	T	263	-	52,52,52	1.20	3 (5%)	54,57,57	1.53	8 (14%)
22	CHD	W	1060	-	29,32,32	0.69	0	47,51,51	5.19	35 (74%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	Y	1522	-	62,62,62	1.53	6 (9%)	65,65,65	1.67	17 (26%)
28	DMU	Z	1526	-	34,34,34	1.11	3 (8%)	45,45,45	3.48	23 (51%)

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	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	A	520	18,14	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
20	PGV	A	524	-	-	0/55/55/55	0/0/0/0
22	CHD	B	1086	-	1/1/12/12	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PSC	E	230	-	-	0/55/55/55	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
24	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
28	DMU	G	272	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	H	268	-	-	0/55/55/55	0/0/0/0
22	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
28	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
20	PGV	N	1268	-	-	0/55/55/55	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	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	N	520	18,14	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	O	1523	-	-	0/65/65/65	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
24	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	4/4/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	PSC	R	1230	-	-	0/55/55/55	0/0/0/0
24	PEK	T	1265	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1060	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	Y	1522	-	-	0/65/65/65	0/0/0/0
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	1525	CHD	C13-C14	-4.28	1.48	1.55
24	P	1264	PEK	O03-C01	-4.15	1.35	1.45
22	C	525	CHD	C13-C12	-4.13	1.48	1.54
28	Z	1526	DMU	C3-C4	-3.94	1.42	1.52
19	L	522	TGL	C20-CA9	-3.79	1.30	1.51

The worst 5 of 698 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C12	-15.17	93.65	109.08
22	P	1271	CHD	C18-C13-C12	-11.94	96.93	109.08
22	P	1525	CHD	C18-C13-C12	-11.78	97.09	109.08
22	C	525	CHD	C18-C13-C12	-11.37	97.51	109.08
22	O	229	CHD	C19-C10-C9	-10.01	96.84	111.16

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C2
28	P	1272	DMU	C4
28	P	1272	DMU	C9
28	P	1272	DMU	C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	A	515	HEA	ND

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

40 monomers are involved in 344 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	9	0
18	A	516	HEA	2	0
15	A	520	PER	1	0
19	A	521	TGL	13	0
20	A	522	PGV	2	0
20	A	524	PGV	6	0
22	B	1086	CHD	2	0
24	C	264	PEK	7	0
20	C	267	PGV	4	0
25	C	270	CDL	19	0
22	C	271	CHD	2	0
22	C	525	CHD	3	0
19	D	523	TGL	9	0
26	E	230	PSC	22	0
24	G	1263	PEK	15	0
24	G	265	PEK	16	0
25	G	269	CDL	27	0
28	G	272	DMU	5	0
20	H	268	PGV	3	0
22	J	60	CHD	1	0
19	L	522	TGL	15	0
20	N	1268	PGV	1	0
20	N	1524	PGV	11	0
18	N	515	HEA	12	0
18	N	516	HEA	2	0
15	N	520	PER	1	0
19	O	1521	TGL	14	0
19	O	1523	TGL	9	0
24	P	1264	PEK	7	0
20	P	1267	PGV	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	1270	CDL	24	0
22	P	1271	CHD	1	0
28	P	1272	DMU	1	0
26	R	1230	PSC	15	0
24	T	1265	PEK	8	0
25	T	1269	CDL	19	0
24	T	263	PEK	22	0
22	W	1060	CHD	4	0
19	Y	1522	TGL	18	0
28	Z	1526	DMU	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	513/514 (99%)	0.70	50 (9%) 8 14	23, 29, 37, 63	0
1	N	513/514 (99%)	0.49	37 (7%) 16 25	27, 34, 43, 64	0
2	B	226/227 (99%)	-0.12	2 (0%) 84 89	24, 34, 56, 82	0
2	O	226/227 (99%)	-0.00	7 (3%) 49 60	30, 40, 63, 82	0
3	C	259/261 (99%)	-0.18	3 (1%) 79 85	25, 32, 44, 61	0
3	P	259/261 (99%)	-0.05	7 (2%) 55 65	28, 35, 47, 64	0
4	D	144/147 (97%)	-0.28	2 (1%) 75 83	29, 35, 50, 65	0
4	Q	144/147 (97%)	1.15	26 (18%) 1 2	36, 50, 70, 109	0
5	E	104/109 (95%)	0.17	6 (5%) 24 33	29, 35, 54, 70	0
5	R	104/109 (95%)	0.72	9 (8%) 11 17	32, 41, 57, 75	0
6	F	93/98 (94%)	0.24	4 (4%) 36 47	29, 38, 56, 93	0
6	S	93/98 (94%)	0.24	4 (4%) 36 47	32, 40, 62, 87	0
7	G	83/85 (97%)	0.87	15 (18%) 1 2	29, 38, 93, 99	0
7	T	83/85 (97%)	1.11	16 (19%) 1 1	30, 42, 90, 104	0
8	H	75/85 (88%)	0.60	12 (16%) 2 3	30, 41, 77, 83	0
8	U	75/85 (88%)	0.80	13 (17%) 2 2	36, 46, 80, 86	0
9	I	71/73 (97%)	0.66	10 (14%) 3 5	31, 41, 65, 71	0
9	V	71/73 (97%)	1.19	12 (16%) 2 2	36, 51, 66, 75	0
10	J	57/59 (96%)	0.45	8 (14%) 3 5	32, 41, 58, 73	0
10	W	57/59 (96%)	0.81	11 (19%) 1 1	36, 45, 62, 78	0
11	K	49/56 (87%)	-0.03	0 100 100	32, 38, 49, 58	0
11	X	49/56 (87%)	1.55	17 (34%) 0 0	42, 47, 62, 69	0
12	L	46/47 (97%)	-0.07	2 (4%) 36 47	30, 35, 54, 79	0
12	Y	46/47 (97%)	0.01	2 (4%) 36 47	34, 42, 62, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.46	6 (13%) 3 5	29, 35, 87, 107	0
13	Z	43/46 (93%)	0.98	9 (20%) 1 1	37, 44, 96, 112	0
All	All	3526/3614 (97%)	0.39	290 (8%) 12 20	23, 36, 61, 112	0

The worst 5 of 290 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	19.4
4	Q	4	SER	12.5
4	Q	5	VAL	12.2
6	F	96	LEU	12.2
13	Z	43	SER	10.0

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

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, 95th 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 ²)	Q<0.9
2	FME	O	1	10/11	0.96	0.11	-	39,40,48,52	0
1	FME	N	1	10/11	0.94	0.16	-	47,49,70,71	0
2	FME	B	1	10/11	0.96	0.12	-	32,33,40,58	0
7	TPO	G	11	11/12	0.61	0.26	-	71,78,96,97	0
1	FME	A	1	10/11	0.93	0.12	-	48,51,72,78	0
7	TPO	T	11	11/12	0.55	0.25	-	71,78,95,96	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
28	DMU	P	1272	33/33	0.54	0.36	10.33	80,103,111,112	0
28	DMU	G	272	33/33	0.48	0.34	9.97	65,94,105,105	0
20	PGV	A	524	51/51	0.81	0.26	9.28	33,74,105,108	0
22	CHD	W	1060	29/29	0.72	0.37	9.20	87,91,96,97	0
19	TGL	Y	1522	63/63	0.67	0.29	5.41	45,72,86,88	0
17	NA	N	1519	1/1	0.92	0.21	5.30	45,45,45,45	0
22	CHD	J	60	29/29	0.79	0.30	5.17	77,83,93,94	0
26	PSC	R	1230	52/52	0.65	0.31	5.05	43,96,122,124	0
25	CDL	P	1270	100/100	0.75	0.30	4.96	41,85,115,120	0
25	CDL	C	270	100/100	0.82	0.31	4.80	41,84,118,119	0
20	PGV	N	1524	51/51	0.80	0.29	4.18	41,75,113,114	0
26	PSC	E	230	52/52	0.64	0.36	4.10	58,99,125,127	0
19	TGL	D	523	63/63	0.80	0.19	3.45	44,63,81,82	0
19	TGL	L	522	63/63	0.79	0.25	3.42	38,59,77,79	0
19	TGL	O	1521	63/63	0.82	0.21	2.97	53,77,88,89	0
25	CDL	G	269	100/100	0.61	0.30	2.75	64,87,115,118	0
19	TGL	O	1523	63/63	0.77	0.20	2.60	54,76,89,94	0
20	PGV	H	268	51/51	0.70	0.34	2.47	59,84,110,112	0
20	PGV	N	1268	51/51	0.72	0.33	2.04	67,91,112,114	0
25	CDL	T	1269	100/100	0.69	0.26	1.93	61,84,108,111	0
24	PEK	T	263	53/53	0.59	0.37	1.92	55,95,117,119	0
19	TGL	A	521	63/63	0.87	0.18	1.72	48,69,84,89	0
24	PEK	G	265	53/53	0.62	0.28	1.67	45,82,114,116	0
24	PEK	T	1265	53/53	0.67	0.29	1.63	44,79,110,112	0
24	PEK	G	1263	53/53	0.59	0.34	1.48	60,95,118,119	0
28	DMU	Z	1526	33/33	0.85	0.22	1.34	39,54,67,69	0
20	PGV	P	1267	51/51	0.96	0.12	1.06	28,40,72,79	0
20	PGV	C	267	51/51	0.96	0.12	1.01	25,36,67,70	0
28	DMU	M	526	33/33	0.90	0.13	0.88	39,47,65,67	0
22	CHD	C	525	29/29	0.96	0.15	0.80	28,33,40,45	0
16	MG	A	518	1/1	0.98	0.15	0.77	27,27,27,27	0
27	ZN	S	99	1/1	0.99	0.09	0.75	38,38,38,38	0
20	PGV	A	522	51/51	0.97	0.14	0.61	25,39,65,66	0
18	HEA	N	516	60/60	0.98	0.18	0.55	26,32,39,41	0
22	CHD	P	1525	29/29	0.96	0.16	0.47	29,36,42,44	0
21	CUA	B	228	2/2	0.99	0.13	0.39	27,27,27,30	0
24	PEK	P	1264	53/53	0.95	0.13	0.37	29,48,75,78	0
22	CHD	C	271	29/29	0.94	0.14	0.33	46,51,53,55	0
20	PGV	N	1266	51/51	0.97	0.12	0.33	31,42,67,71	0
18	HEA	N	515	60/60	0.98	0.16	0.30	23,32,51,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	PEK	C	264	53/53	0.96	0.12	0.30	29,47,73,75	0
16	MG	N	1518	1/1	0.97	0.12	0.11	34,34,34,34	0
21	CUA	O	228	2/2	0.97	0.11	0.08	36,36,36,37	0
27	ZN	F	99	1/1	1.00	0.09	-0.04	34,34,34,34	0
18	HEA	A	515	60/60	0.99	0.17	-0.10	19,26,50,53	0
22	CHD	P	1271	29/29	0.94	0.15	-0.12	48,53,56,58	0
15	PER	A	520	2/2	0.97	0.17	-0.24	25,25,25,32	0
18	HEA	A	516	60/60	0.99	0.15	-0.33	20,26,33,36	0
22	CHD	O	229	29/29	0.96	0.09	-0.38	23,31,37,37	0
22	CHD	B	1086	29/29	0.97	0.08	-0.53	26,30,37,47	0
17	NA	A	519	1/1	0.92	0.11	-0.77	42,42,42,42	0
15	PER	N	520	2/2	0.97	0.16	-0.99	31,31,31,34	0
23	UNX	P	1262	1/1	0.87	0.47	-	22,22,22,22	0
14	CU	N	517	1/1	0.99	0.16	-	32,32,32,32	0
14	CU	A	517	1/1	1.00	0.15	-	29,29,29,29	0
23	UNX	C	262	1/1	0.71	0.47	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.